



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:36 pm BST

PDB ID : 6PGK  
Title : Membrane Protein Megahertz Crystallography at the European XFEL, Photosystem I XFEL at 2.9 Å  
Authors : Fromme, R.; Gisriel, C.; Fromme, P.  
Deposited on : 2019-06-24  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

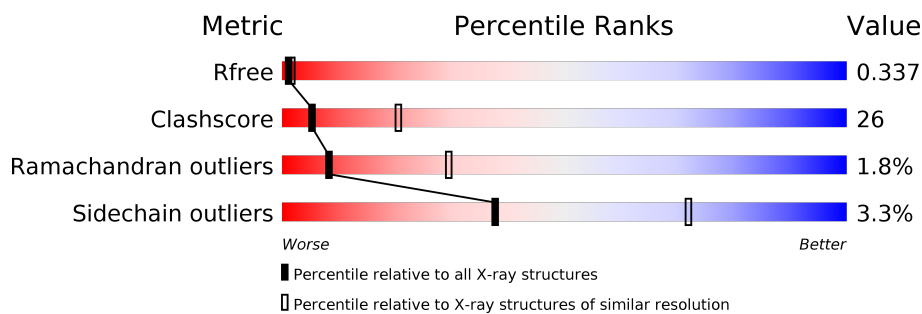
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1957 (2.90-2.90)                                      |
| Clashscore            | 141614                      | 2172 (2.90-2.90)                                      |
| Ramachandran outliers | 138981                      | 2115 (2.90-2.90)                                      |
| Sidechain outliers    | 138945                      | 2117 (2.90-2.90)                                      |


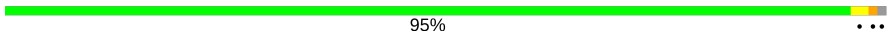









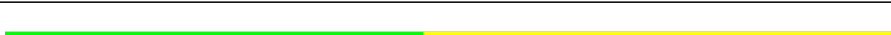


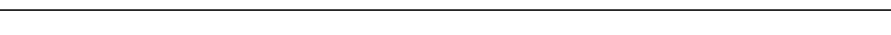
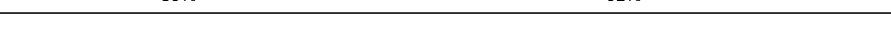

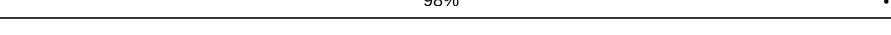


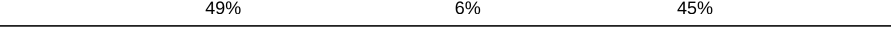




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 755    | 55% 42% ..       |
| 1   | G     | 755    | 52% 45% ..       |
| 1   | Y     | 755    | 50% 46% ..       |
| 2   | B     | 741    | 53% 44% .        |
| 2   | H     | 741    | 54% 43% .        |
| 2   | Z     | 741    | 54% 44% .        |
| 3   | C     | 81     | 56% 40% ...      |

*Continued on next page...*

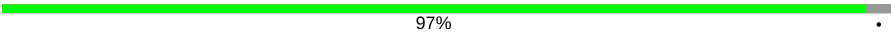
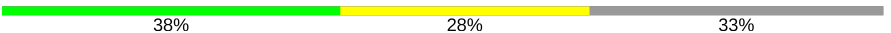




*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | N     | 81     |    |
| 3   | a     | 81     |    |
| 4   | D     | 139    |    |
| 4   | O     | 139    |    |
| 4   | b     | 139    |    |
| 5   | E     | 76     |    |
| 5   | P     | 76     |    |
| 5   | c     | 76     |    |
| 6   | F     | 164    |    |
| 6   | Q     | 164    |    |
| 6   | d     | 164    |    |
| 7   | I     | 38     |    |
| 7   | R     | 38     |  |
| 7   | e     | 38     |  |
| 8   | J     | 41     |  |
| 8   | S     | 41     |  |
| 8   | f     | 41     |  |
| 9   | K     | 83     |  |
| 9   | T     | 83     |  |
| 9   | g     | 83     |  |
| 10  | L     | 155    |  |
| 10  | U     | 155    |  |
| 10  | h     | 155    |  |
| 11  | M     | 31     |  |
| 11  | V     | 31     |  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 11  | i     | 31     |  97%         |
| 12  | W     | 39     |  38% 28% 33% |
| 12  | X     | 39     |  49% 15% 33% |
| 12  | j     | 39     |  64% 33%     |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | CL0  | A     | 801 | X         | -        | -       | -                |
| 13  | CL0  | G     | 801 | X         | -        | -       | -                |
| 13  | CL0  | Y     | 801 | X         | -        | -       | -                |
| 14  | CLA  | A     | 802 | X         | -        | -       | -                |
| 14  | CLA  | A     | 803 | X         | -        | -       | -                |
| 14  | CLA  | A     | 804 | X         | -        | -       | -                |
| 14  | CLA  | A     | 805 | X         | -        | -       | -                |
| 14  | CLA  | A     | 806 | X         | -        | -       | -                |
| 14  | CLA  | A     | 807 | X         | -        | -       | -                |
| 14  | CLA  | A     | 808 | X         | -        | -       | -                |
| 14  | CLA  | A     | 809 | X         | -        | -       | -                |
| 14  | CLA  | A     | 810 | X         | -        | -       | -                |
| 14  | CLA  | A     | 811 | X         | -        | -       | -                |
| 14  | CLA  | A     | 812 | X         | -        | -       | -                |
| 14  | CLA  | A     | 813 | X         | -        | -       | -                |
| 14  | CLA  | A     | 814 | X         | -        | -       | -                |
| 14  | CLA  | A     | 815 | X         | -        | -       | -                |
| 14  | CLA  | A     | 816 | X         | -        | -       | -                |
| 14  | CLA  | A     | 817 | X         | -        | -       | -                |
| 14  | CLA  | A     | 818 | X         | -        | -       | -                |
| 14  | CLA  | A     | 819 | X         | -        | -       | -                |
| 14  | CLA  | A     | 820 | X         | -        | -       | -                |
| 14  | CLA  | A     | 821 | X         | -        | -       | -                |
| 14  | CLA  | A     | 822 | X         | -        | -       | -                |
| 14  | CLA  | A     | 823 | X         | -        | -       | -                |
| 14  | CLA  | A     | 824 | X         | -        | -       | -                |
| 14  | CLA  | A     | 825 | X         | -        | -       | -                |
| 14  | CLA  | A     | 826 | X         | -        | -       | -                |
| 14  | CLA  | A     | 827 | X         | -        | -       | -                |
| 14  | CLA  | A     | 828 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | A     | 829 | X         | -        | -       | -                |
| 14  | CLA  | A     | 830 | X         | -        | -       | -                |
| 14  | CLA  | A     | 831 | X         | -        | -       | -                |
| 14  | CLA  | A     | 832 | X         | -        | -       | -                |
| 14  | CLA  | A     | 833 | X         | -        | -       | -                |
| 14  | CLA  | A     | 834 | X         | -        | -       | -                |
| 14  | CLA  | A     | 835 | X         | -        | -       | -                |
| 14  | CLA  | A     | 836 | X         | -        | -       | -                |
| 14  | CLA  | A     | 837 | X         | -        | -       | -                |
| 14  | CLA  | A     | 838 | X         | -        | -       | -                |
| 14  | CLA  | A     | 839 | X         | -        | -       | -                |
| 14  | CLA  | A     | 840 | X         | -        | -       | -                |
| 14  | CLA  | A     | 841 | X         | -        | -       | -                |
| 14  | CLA  | A     | 842 | X         | -        | -       | -                |
| 14  | CLA  | A     | 852 | X         | -        | -       | -                |
| 14  | CLA  | B     | 801 | X         | -        | -       | -                |
| 14  | CLA  | B     | 802 | X         | -        | -       | -                |
| 14  | CLA  | B     | 803 | X         | -        | -       | -                |
| 14  | CLA  | B     | 804 | X         | -        | -       | -                |
| 14  | CLA  | B     | 805 | X         | -        | -       | -                |
| 14  | CLA  | B     | 806 | X         | -        | -       | -                |
| 14  | CLA  | B     | 807 | X         | -        | -       | -                |
| 14  | CLA  | B     | 808 | X         | -        | -       | -                |
| 14  | CLA  | B     | 809 | X         | -        | -       | -                |
| 14  | CLA  | B     | 810 | X         | -        | -       | -                |
| 14  | CLA  | B     | 811 | X         | -        | -       | -                |
| 14  | CLA  | B     | 812 | X         | -        | -       | -                |
| 14  | CLA  | B     | 813 | X         | -        | -       | -                |
| 14  | CLA  | B     | 814 | X         | -        | -       | -                |
| 14  | CLA  | B     | 815 | X         | -        | -       | -                |
| 14  | CLA  | B     | 816 | X         | -        | -       | -                |
| 14  | CLA  | B     | 817 | X         | -        | -       | -                |
| 14  | CLA  | B     | 818 | X         | -        | -       | -                |
| 14  | CLA  | B     | 819 | X         | -        | -       | -                |
| 14  | CLA  | B     | 820 | X         | -        | -       | -                |
| 14  | CLA  | B     | 821 | X         | -        | -       | -                |
| 14  | CLA  | B     | 822 | X         | -        | -       | -                |
| 14  | CLA  | B     | 823 | X         | -        | -       | -                |
| 14  | CLA  | B     | 824 | X         | -        | -       | -                |
| 14  | CLA  | B     | 825 | X         | -        | -       | -                |
| 14  | CLA  | B     | 826 | X         | -        | -       | -                |
| 14  | CLA  | B     | 827 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | B     | 828 | X         | -        | -       | -                |
| 14  | CLA  | B     | 829 | X         | -        | -       | -                |
| 14  | CLA  | B     | 830 | X         | -        | -       | -                |
| 14  | CLA  | B     | 831 | X         | -        | -       | -                |
| 14  | CLA  | B     | 832 | X         | -        | -       | -                |
| 14  | CLA  | B     | 833 | X         | -        | -       | -                |
| 14  | CLA  | B     | 834 | X         | -        | -       | -                |
| 14  | CLA  | B     | 835 | X         | -        | -       | -                |
| 14  | CLA  | B     | 836 | X         | -        | -       | -                |
| 14  | CLA  | B     | 837 | X         | -        | -       | -                |
| 14  | CLA  | B     | 838 | X         | -        | -       | -                |
| 14  | CLA  | B     | 839 | X         | -        | -       | -                |
| 14  | CLA  | B     | 840 | X         | -        | -       | -                |
| 14  | CLA  | B     | 841 | X         | -        | -       | -                |
| 14  | CLA  | F     | 202 | X         | -        | -       | -                |
| 14  | CLA  | G     | 802 | X         | -        | -       | -                |
| 14  | CLA  | G     | 803 | X         | -        | -       | -                |
| 14  | CLA  | G     | 804 | X         | -        | -       | -                |
| 14  | CLA  | G     | 805 | X         | -        | -       | -                |
| 14  | CLA  | G     | 806 | X         | -        | -       | -                |
| 14  | CLA  | G     | 807 | X         | -        | -       | -                |
| 14  | CLA  | G     | 808 | X         | -        | -       | -                |
| 14  | CLA  | G     | 809 | X         | -        | -       | -                |
| 14  | CLA  | G     | 810 | X         | -        | -       | -                |
| 14  | CLA  | G     | 811 | X         | -        | -       | -                |
| 14  | CLA  | G     | 812 | X         | -        | -       | -                |
| 14  | CLA  | G     | 813 | X         | -        | -       | -                |
| 14  | CLA  | G     | 814 | X         | -        | -       | -                |
| 14  | CLA  | G     | 815 | X         | -        | -       | -                |
| 14  | CLA  | G     | 816 | X         | -        | -       | -                |
| 14  | CLA  | G     | 817 | X         | -        | -       | -                |
| 14  | CLA  | G     | 818 | X         | -        | -       | -                |
| 14  | CLA  | G     | 819 | X         | -        | -       | -                |
| 14  | CLA  | G     | 820 | X         | -        | -       | -                |
| 14  | CLA  | G     | 821 | X         | -        | -       | -                |
| 14  | CLA  | G     | 822 | X         | -        | -       | -                |
| 14  | CLA  | G     | 823 | X         | -        | -       | -                |
| 14  | CLA  | G     | 824 | X         | -        | -       | -                |
| 14  | CLA  | G     | 825 | X         | -        | -       | -                |
| 14  | CLA  | G     | 826 | X         | -        | -       | -                |
| 14  | CLA  | G     | 827 | X         | -        | -       | -                |
| 14  | CLA  | G     | 828 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | G     | 829 | X         | -        | -       | -                |
| 14  | CLA  | G     | 830 | X         | -        | -       | -                |
| 14  | CLA  | G     | 831 | X         | -        | -       | -                |
| 14  | CLA  | G     | 832 | X         | -        | -       | -                |
| 14  | CLA  | G     | 833 | X         | -        | -       | -                |
| 14  | CLA  | G     | 834 | X         | -        | -       | -                |
| 14  | CLA  | G     | 835 | X         | -        | -       | -                |
| 14  | CLA  | G     | 836 | X         | -        | -       | -                |
| 14  | CLA  | G     | 837 | X         | -        | -       | -                |
| 14  | CLA  | G     | 838 | X         | -        | -       | -                |
| 14  | CLA  | G     | 839 | X         | -        | -       | -                |
| 14  | CLA  | G     | 840 | X         | -        | -       | -                |
| 14  | CLA  | G     | 841 | X         | -        | -       | -                |
| 14  | CLA  | G     | 842 | X         | -        | -       | -                |
| 14  | CLA  | G     | 843 | X         | -        | -       | -                |
| 14  | CLA  | G     | 853 | X         | -        | -       | -                |
| 14  | CLA  | H     | 801 | X         | -        | X       | -                |
| 14  | CLA  | H     | 802 | X         | -        | -       | -                |
| 14  | CLA  | H     | 803 | X         | -        | -       | -                |
| 14  | CLA  | H     | 804 | X         | -        | -       | -                |
| 14  | CLA  | H     | 805 | X         | -        | -       | -                |
| 14  | CLA  | H     | 806 | X         | -        | -       | -                |
| 14  | CLA  | H     | 807 | X         | -        | -       | -                |
| 14  | CLA  | H     | 808 | X         | -        | -       | -                |
| 14  | CLA  | H     | 809 | X         | -        | -       | -                |
| 14  | CLA  | H     | 810 | X         | -        | -       | -                |
| 14  | CLA  | H     | 811 | X         | -        | -       | -                |
| 14  | CLA  | H     | 812 | X         | -        | -       | -                |
| 14  | CLA  | H     | 813 | X         | -        | -       | -                |
| 14  | CLA  | H     | 814 | X         | -        | -       | -                |
| 14  | CLA  | H     | 815 | X         | -        | -       | -                |
| 14  | CLA  | H     | 816 | X         | -        | -       | -                |
| 14  | CLA  | H     | 817 | X         | -        | -       | -                |
| 14  | CLA  | H     | 818 | X         | -        | -       | -                |
| 14  | CLA  | H     | 819 | X         | -        | -       | -                |
| 14  | CLA  | H     | 820 | X         | -        | -       | -                |
| 14  | CLA  | H     | 821 | X         | -        | -       | -                |
| 14  | CLA  | H     | 822 | X         | -        | -       | -                |
| 14  | CLA  | H     | 823 | X         | -        | -       | -                |
| 14  | CLA  | H     | 824 | X         | -        | -       | -                |
| 14  | CLA  | H     | 825 | X         | -        | -       | -                |
| 14  | CLA  | H     | 826 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | H     | 827  | X         | -        | -       | -                |
| 14  | CLA  | H     | 828  | X         | -        | -       | -                |
| 14  | CLA  | H     | 829  | X         | -        | -       | -                |
| 14  | CLA  | H     | 830  | X         | -        | -       | -                |
| 14  | CLA  | H     | 831  | X         | -        | -       | -                |
| 14  | CLA  | H     | 832  | X         | -        | -       | -                |
| 14  | CLA  | H     | 833  | X         | -        | -       | -                |
| 14  | CLA  | H     | 834  | X         | -        | -       | -                |
| 14  | CLA  | H     | 835  | X         | -        | -       | -                |
| 14  | CLA  | H     | 836  | X         | -        | -       | -                |
| 14  | CLA  | H     | 837  | X         | -        | -       | -                |
| 14  | CLA  | H     | 838  | X         | -        | -       | -                |
| 14  | CLA  | J     | 101  | X         | -        | -       | -                |
| 14  | CLA  | J     | 102  | X         | -        | -       | -                |
| 14  | CLA  | K     | 101  | X         | -        | -       | -                |
| 14  | CLA  | K     | 103  | X         | -        | -       | -                |
| 14  | CLA  | L     | 201  | X         | -        | -       | -                |
| 14  | CLA  | L     | 202  | X         | -        | -       | -                |
| 14  | CLA  | L     | 205  | X         | -        | -       | -                |
| 14  | CLA  | L     | 206  | X         | -        | -       | -                |
| 14  | CLA  | L     | 207  | X         | -        | -       | -                |
| 14  | CLA  | Q     | 201  | X         | -        | -       | -                |
| 14  | CLA  | Q     | 203  | X         | -        | -       | -                |
| 14  | CLA  | S     | 1101 | X         | -        | -       | -                |
| 14  | CLA  | S     | 1102 | X         | -        | -       | -                |
| 14  | CLA  | S     | 1103 | X         | -        | -       | -                |
| 14  | CLA  | T     | 101  | X         | -        | -       | -                |
| 14  | CLA  | T     | 103  | X         | -        | -       | -                |
| 14  | CLA  | U     | 1002 | X         | -        | -       | -                |
| 14  | CLA  | U     | 1003 | X         | -        | -       | -                |
| 14  | CLA  | U     | 1004 | X         | -        | -       | -                |
| 14  | CLA  | U     | 1006 | X         | -        | -       | -                |
| 14  | CLA  | V     | 1201 | X         | -        | -       | -                |
| 14  | CLA  | W     | 1701 | X         | -        | -       | -                |
| 14  | CLA  | X     | 1701 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 802  | X         | -        | -       | -                |
| 14  | CLA  | Y     | 803  | X         | -        | -       | -                |
| 14  | CLA  | Y     | 804  | X         | -        | -       | -                |
| 14  | CLA  | Y     | 805  | X         | -        | -       | -                |
| 14  | CLA  | Y     | 806  | X         | -        | -       | -                |
| 14  | CLA  | Y     | 807  | X         | -        | -       | -                |
| 14  | CLA  | Y     | 808  | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | Y     | 809 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 810 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 811 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 812 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 813 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 814 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 815 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 816 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 817 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 818 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 819 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 820 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 821 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 822 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 823 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 824 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 825 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 826 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 827 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 828 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 829 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 830 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 831 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 832 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 833 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 834 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 835 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 836 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 837 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 838 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 839 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 840 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 841 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 842 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 843 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 854 | X         | -        | -       | -                |
| 14  | CLA  | Y     | 855 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 801 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 802 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 803 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 804 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 805 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | Z     | 806 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 807 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 808 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 809 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 810 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 811 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 812 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 813 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 814 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 815 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 816 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 817 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 818 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 819 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 820 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 821 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 822 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 823 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 824 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 825 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 826 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 827 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 828 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 829 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 830 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 831 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 832 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 833 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 834 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 835 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 836 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 837 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 838 | X         | -        | -       | -                |
| 14  | CLA  | Z     | 839 | X         | -        | -       | -                |
| 14  | CLA  | d     | 201 | X         | -        | -       | -                |
| 14  | CLA  | d     | 202 | X         | -        | -       | -                |
| 14  | CLA  | f     | 101 | X         | -        | -       | -                |
| 14  | CLA  | f     | 102 | X         | -        | -       | -                |
| 14  | CLA  | g     | 101 | X         | -        | -       | -                |
| 14  | CLA  | g     | 102 | X         | -        | -       | -                |
| 14  | CLA  | h     | 201 | X         | -        | -       | -                |
| 14  | CLA  | h     | 205 | X         | -        | -       | -                |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | h     | 206 | X         | -        | -       | -                |
| 14  | CLA  | h     | 207 | X         | -        | -       | -                |
| 14  | CLA  | j     | 102 | X         | -        | -       | -                |
| 16  | SF4  | C     | 101 | -         | -        | X       | -                |
| 16  | SF4  | C     | 102 | -         | -        | X       | -                |
| 16  | SF4  | N     | 102 | -         | -        | X       | -                |

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 72532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 741      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5791  | 3799 | 989 | 977 | 26 |         |         |       |
| 1   | G     | 741      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5791  | 3799 | 989 | 977 | 26 |         |         |       |
| 1   | Y     | 741      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5791  | 3799 | 989 | 977 | 26 |         |         |       |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 2   | B     | 739      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5889  | 3876 | 987 | 1005 | 21 |         |         |       |
| 2   | H     | 739      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5889  | 3876 | 987 | 1005 | 21 |         |         |       |
| 2   | Z     | 739      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5889  | 3876 | 987 | 1005 | 21 |         |         |       |

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |         |       |
| 3   | N     | 80       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |         |       |
| 3   | a     | 80       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1075  | 682 | 186 | 204 | 3 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | O     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1075  | 682 | 186 | 204 | 3 |         |         |       |
| 4   | b     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1075  | 682 | 186 | 204 | 3 |         |         |       |

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | Atoms |     |    |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|--|---------|---------|-------|
| 5   | E     | 69       | Total | C   | N  | O   |  | 0       | 0       | 0     |
|     |       |          | 539   | 342 | 93 | 104 |  |         |         |       |
| 5   | P     | 69       | Total | C   | N  | O   |  | 0       | 0       | 0     |
|     |       |          | 539   | 342 | 93 | 104 |  |         |         |       |
| 5   | c     | 69       | Total | C   | N  | O   |  | 0       | 0       | 0     |
|     |       |          | 539   | 342 | 93 | 104 |  |         |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1065  | 680 | 184 | 197 | 4 |         |         |       |
| 6   | Q     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1065  | 680 | 184 | 197 | 4 |         |         |       |
| 6   | d     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1065  | 680 | 184 | 197 | 4 |         |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | I     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 301   | 208 | 40 | 48 | 5 |         |         |       |
| 7   | R     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 301   | 208 | 40 | 48 | 5 |         |         |       |
| 7   | e     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 301   | 208 | 40 | 48 | 5 |         |         |       |

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | J     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 338   | 231 | 51 | 54 | 2 |         |         |       |
| 8   | S     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 338   | 231 | 51 | 54 | 2 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | f     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 338   | 231 | 51 | 54 | 2 |         |         |       |

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | K     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 328   | 214 | 57 | 56 | 1 |         |         |       |
| 9   | T     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 328   | 214 | 57 | 56 | 1 |         |         |       |
| 9   | g     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 328   | 214 | 57 | 56 | 1 |         |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | L     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 735 | 179 | 201 | 4 |         |         |       |
| 10  | U     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 735 | 179 | 201 | 4 |         |         |       |
| 10  | h     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 735 | 179 | 201 | 4 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 143     | LEU      | SER    | conflict | UNP Q8DGB4 |
| U     | 143     | LEU      | SER    | conflict | UNP Q8DGB4 |
| h     | 143     | LEU      | SER    | conflict | UNP Q8DGB4 |

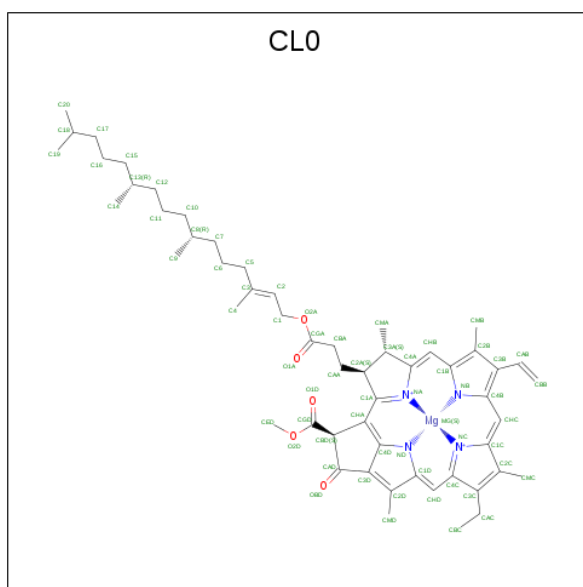
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 11  | M     | 30       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 233   | 156 | 35 | 42 |         |         |       |
| 11  | V     | 30       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 233   | 156 | 35 | 42 |         |         |       |
| 11  | i     | 30       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 233   | 156 | 35 | 42 |         |         |       |

- Molecule 12 is a protein called Photosystem I 4.8K protein.

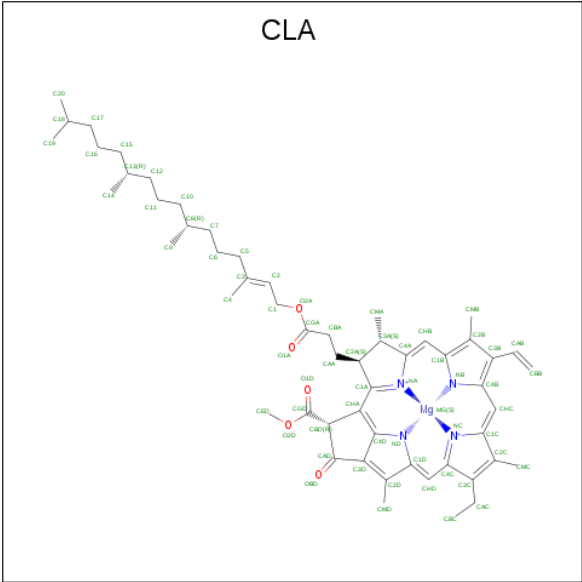
| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 12  | W     | 26       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 219   | 157 | 31 | 31 |         |         |       |
| 12  | X     | 26       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 219   | 157 | 31 | 31 |         |         |       |
| 12  | j     | 26       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 219   | 157 | 31 | 31 |         |         |       |

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by author).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 13  | A     | 1        | Total | C  | Mg | N | O       |         |
|     |       |          | 65    | 55 | 1  | 4 | 5       | 0       |
| 13  | G     | 1        | Total | C  | Mg | N | O       |         |
|     |       |          | 65    | 55 | 1  | 4 | 5       | 0       |
| 13  | Y     | 1        | Total | C  | Mg | N | O       |         |
|     |       |          | 65    | 55 | 1  | 4 | 5       | 0       |

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by author).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | H     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | J     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | J     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | K     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       | 0       |
| 14  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Q     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Q     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | S     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | S     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | T     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       | 0       |
| 14  | T     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | V     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | W     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | X     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 14  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

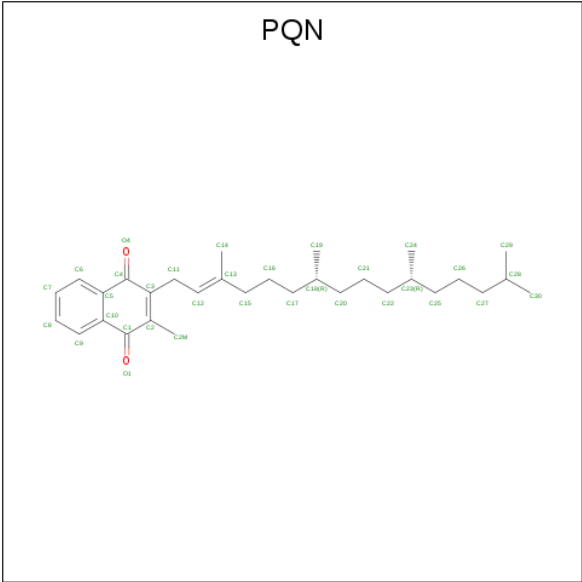
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | Z     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 14  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | f     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | f     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 14  | g     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 14  | g     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 14  | h     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | h     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | h     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | h     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 14  | j     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



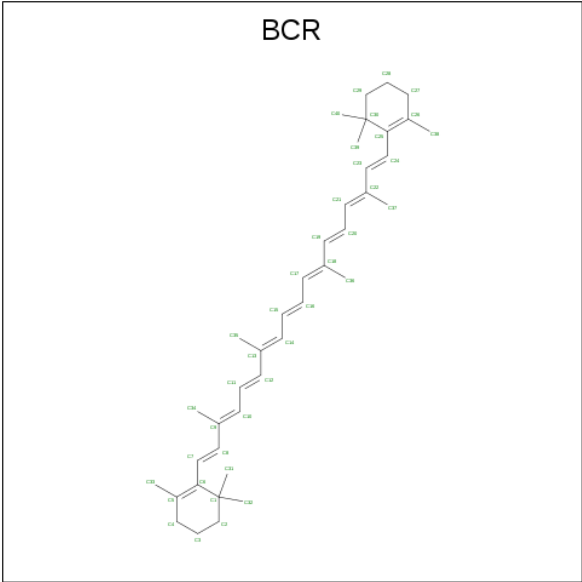
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 15  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |
| 15  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |
| 15  | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |
| 15  | H     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |
| 15  | Y     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |
| 15  | Z     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by author).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16  | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | G     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | Y     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | a     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 16  | a     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by author).



| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 17  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | B     | 1        | Total C<br>30 30 | 0       | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | B     | 1        | Total C<br>25 25 | 0       | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | F     | 1        | Total C<br>40 40 | 0       | 0       |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 17  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | H     | 1        | Total C<br>25 25 | 0       | 0       |
| 17  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | I     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | M     | 1        | Total C<br>40 40 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 17  | Q     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Q     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | R     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | R     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | S     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | U     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | U     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | U     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | V     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Z     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Z     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Z     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Z     | 1        | Total C<br>25 25 | 0       | 0       |

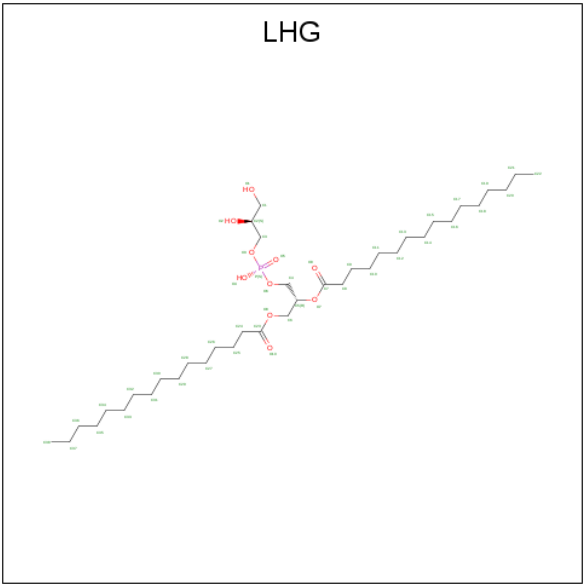
*Continued on next page...*



Continued from previous page...

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 17  | Z     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | Z     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | e     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | f     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | f     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | f     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | h     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | h     | 1        | Total C<br>40 40 | 0       | 0       |
| 17  | i     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



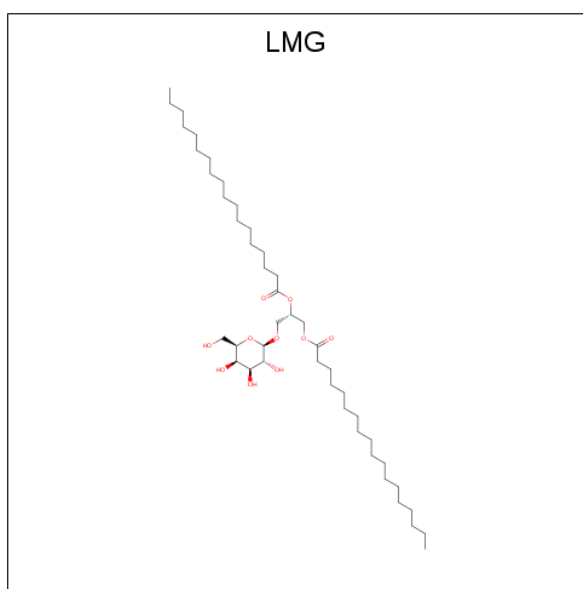
| Mol | Chain | Residues | Atoms                     | ZeroOcc | AltConf |
|-----|-------|----------|---------------------------|---------|---------|
| 18  | A     | 1        | Total C O P<br>49 38 10 1 | 0       | 0       |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |         |
| 18  | B     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 18  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 18  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |         |
| 18  | H     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |
| 18  | Y     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 18  | Y     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 25    | 14 | 10 | 1 |         |         |
| 18  | j     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 28    | 17 | 10 | 1 |         |         |

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 19  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 42 | 10 |         |         |
| 19  | H     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 19  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 20  | h     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 20  | L     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 20  | U     | 1        | Total Ca<br>1 1 | 0       | 0       |

- Molecule 21 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 21  | A     | 9        | Total O<br>9 9 | 0       | 0       |
| 21  | B     | 9        | Total O<br>9 9 | 0       | 0       |
| 21  | C     | 1        | Total O<br>1 1 | 0       | 0       |
| 21  | D     | 2        | Total O<br>2 2 | 0       | 0       |
| 21  | E     | 1        | Total O<br>1 1 | 0       | 0       |
| 21  | G     | 8        | Total O<br>8 8 | 0       | 0       |
| 21  | H     | 3        | Total O<br>3 3 | 0       | 0       |
| 21  | J     | 1        | Total O<br>1 1 | 0       | 0       |
| 21  | K     | 1        | Total O<br>1 1 | 0       | 0       |
| 21  | L     | 5        | Total O<br>5 5 | 0       | 0       |
| 21  | N     | 1        | Total O<br>1 1 | 0       | 0       |
| 21  | O     | 2        | Total O<br>2 2 | 0       | 0       |
| 21  | Q     | 2        | Total O<br>2 2 | 0       | 0       |
| 21  | T     | 1        | Total O<br>1 1 | 0       | 0       |
| 21  | U     | 4        | Total O<br>4 4 | 0       | 0       |
| 21  | W     | 1        | Total O<br>1 1 | 0       | 0       |

*Continued on next page...*

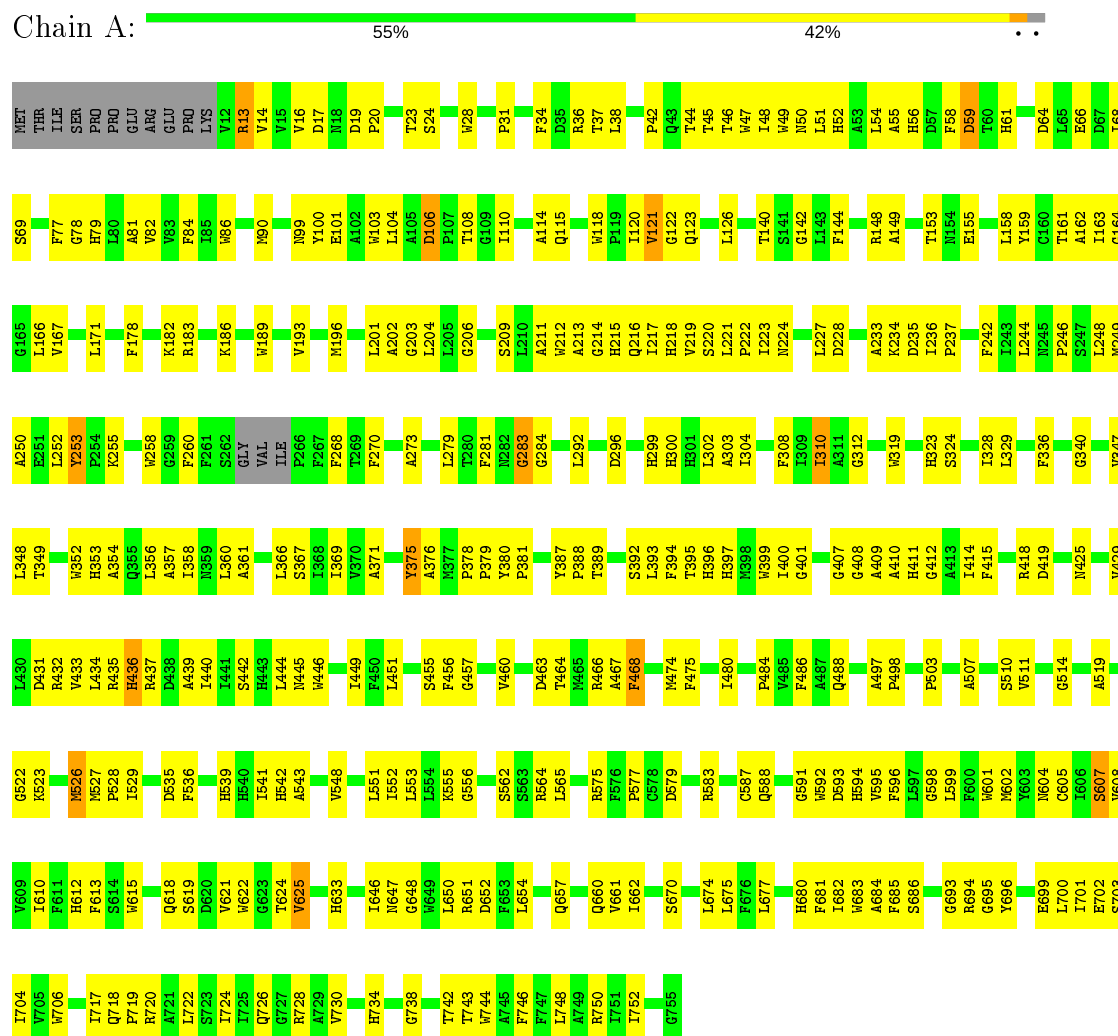
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 21  | Y     | 8        | Total<br>8 | O<br>8 | 0       | 0       |
| 21  | Z     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 21  | b     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 21  | c     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 21  | d     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 21  | f     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 21  | h     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 21  | j     | 1        | Total<br>1 | O<br>1 | 0       | 0       |

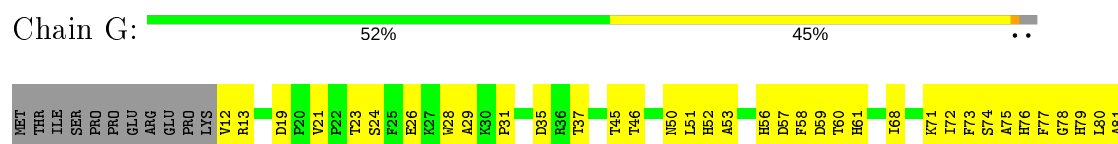
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

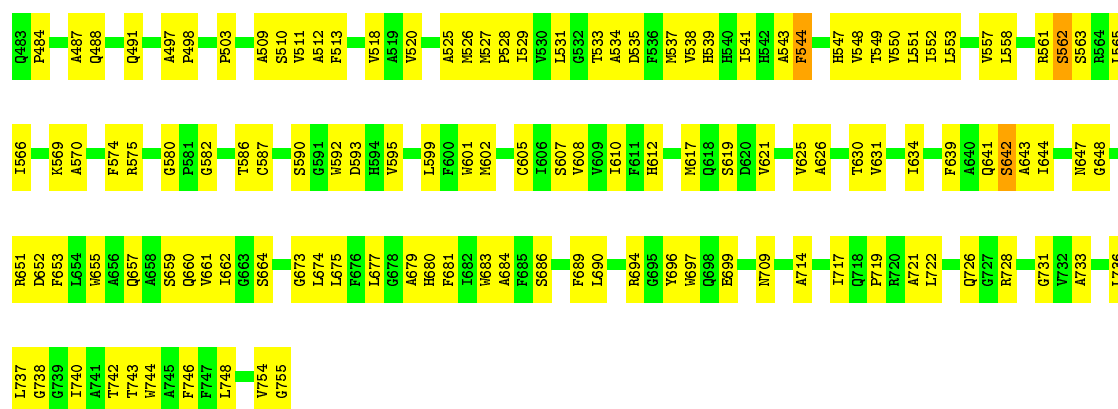
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

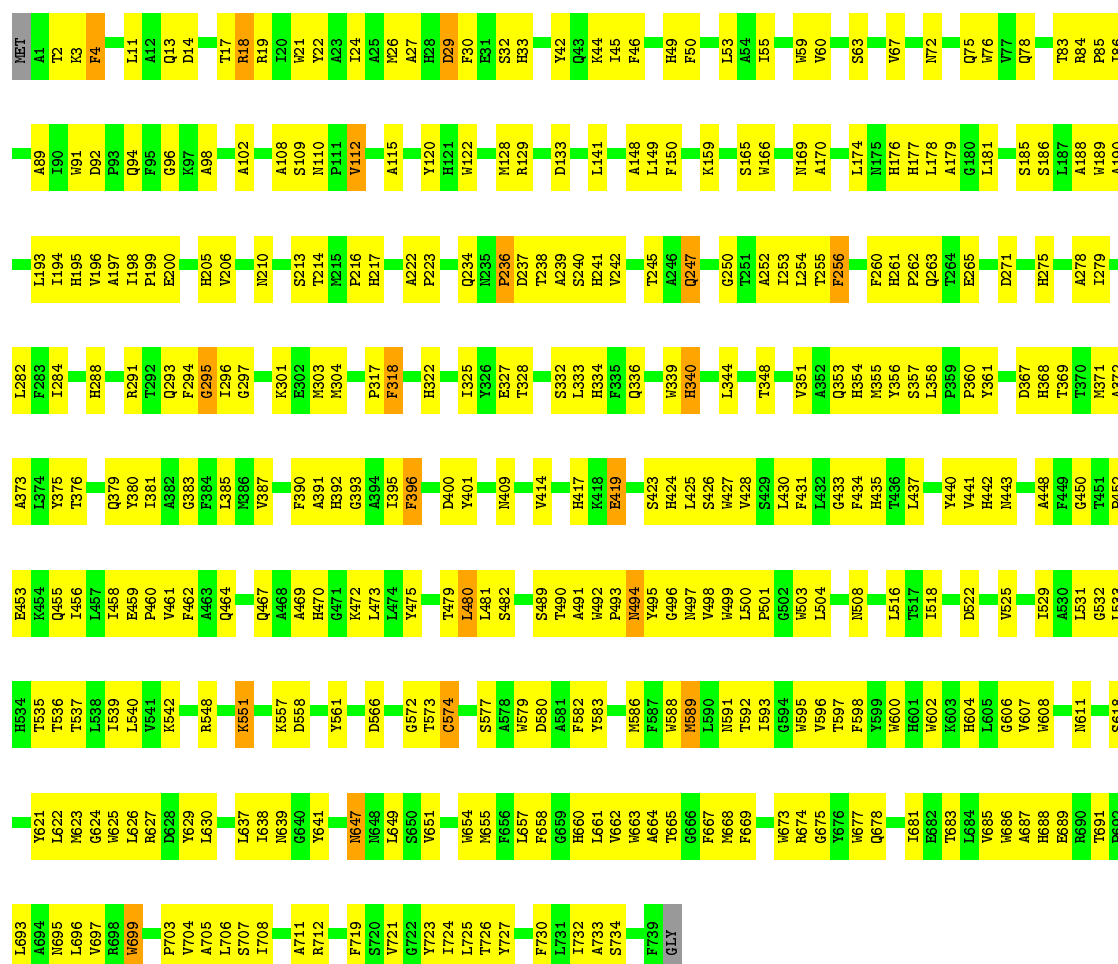






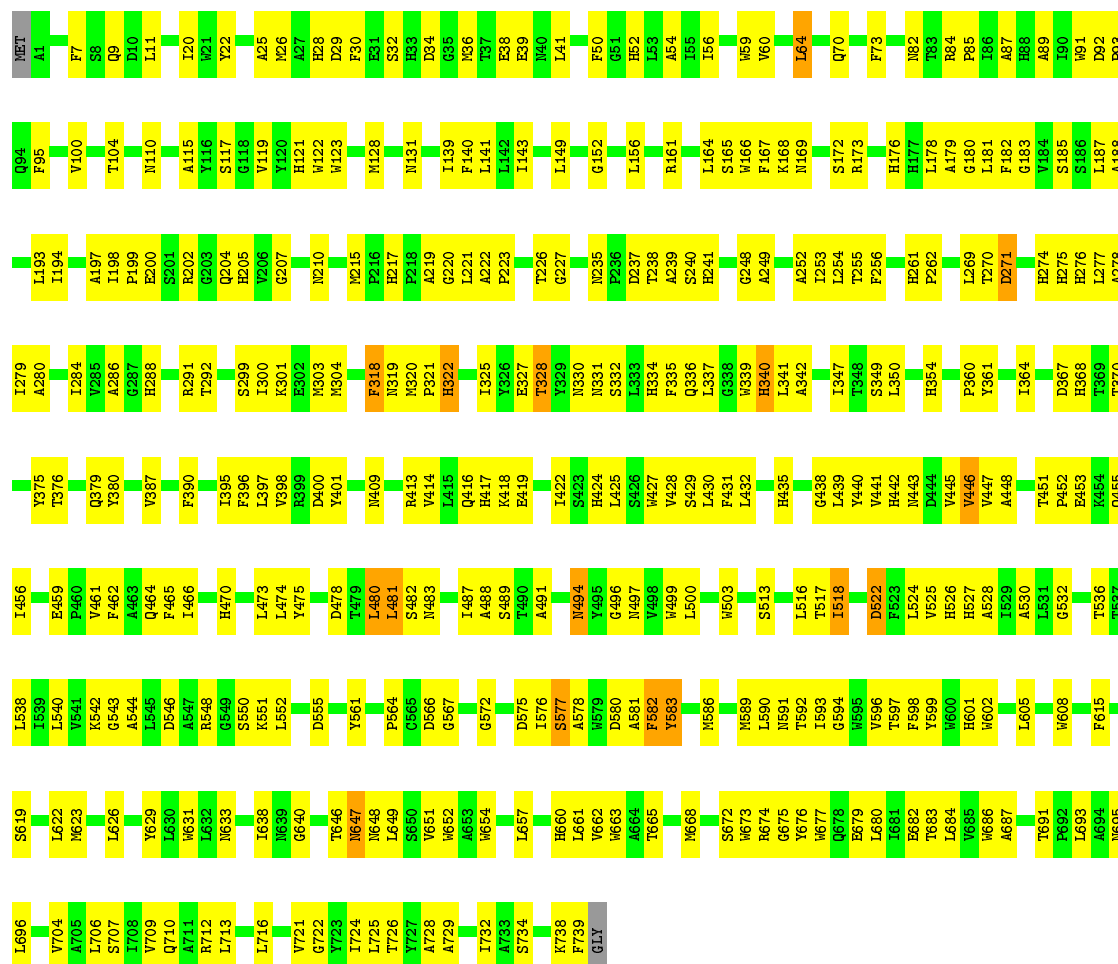
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 53% 44%

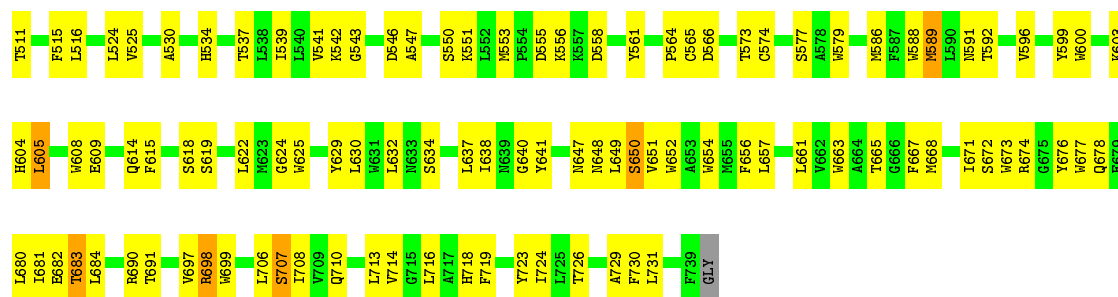


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 54% 43%







• Molecule 3: Photosystem I iron-sulfur center



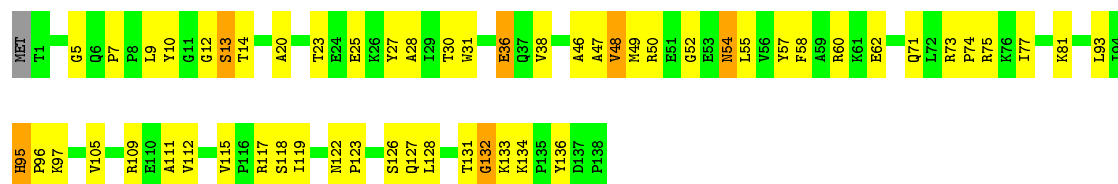
• Molecule 3: Photosystem I iron-sulfur center



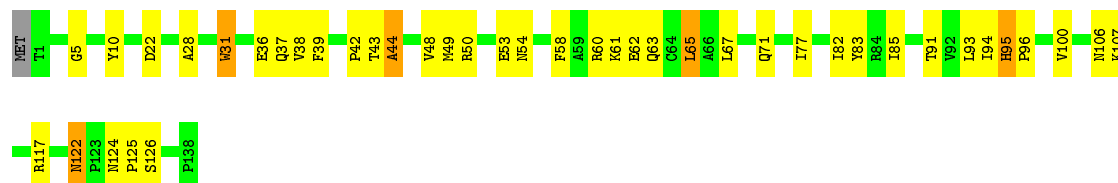
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II

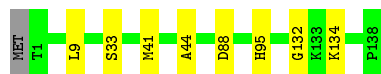


• Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II

Chain b:  94% 6%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  62% 25% 9%




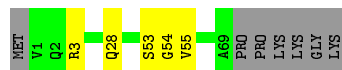
- Molecule 5: Photosystem I reaction center subunit IV

Chain P:  61% 28% 9%



- Molecule 5: Photosystem I reaction center subunit IV

Chain c:  84% 7% 9%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  54% 30% 14%




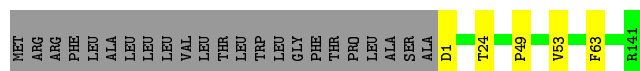
- Molecule 6: Photosystem I reaction center subunit III

Chain Q:  55% 28% 14%



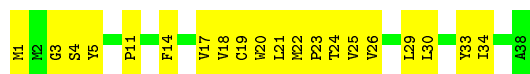
- Molecule 6: Photosystem I reaction center subunit III

Chain d:  83% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  47% 53%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain R:  63% 37%



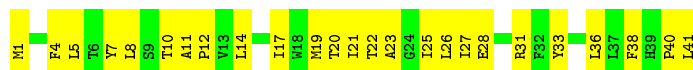
- Molecule 7: Photosystem I reaction center subunit VIII

Chain e:  95% 5%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  39% 61%



- Molecule 8: Photosystem I reaction center subunit IX

Chain S:  51% 46%



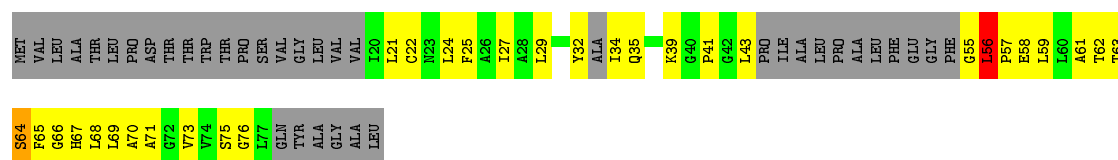
- Molecule 8: Photosystem I reaction center subunit IX

Chain f:  98%



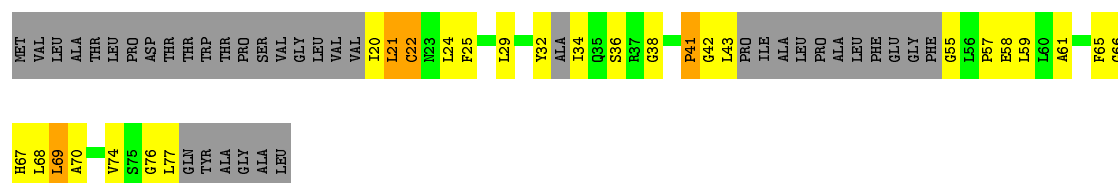
- Molecule 9: Photosystem I reaction center subunit Psak

Chain K: 



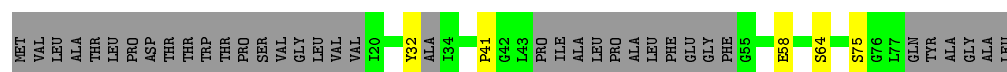
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain T: 



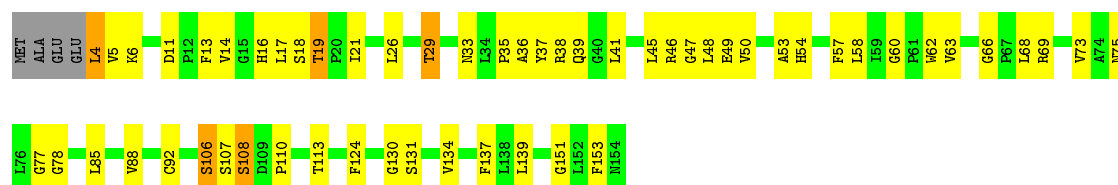
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain g: 



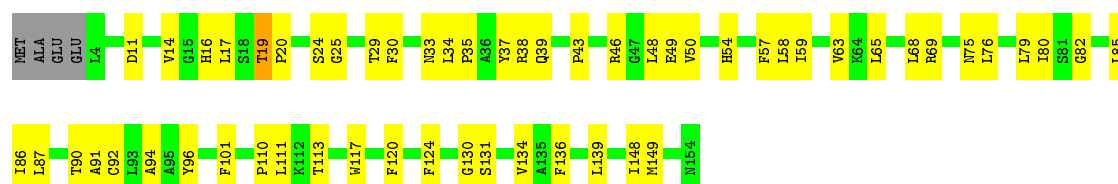
- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 




- Molecule 10: Photosystem I reaction center subunit XI

Chain U: 



- Molecule 10: Photosystem I reaction center subunit XI

Chain h: 



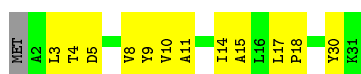
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 68% 29%



- Molecule 11: Photosystem I reaction center subunit XII

Chain V: 58% 39%



- Molecule 11: Photosystem I reaction center subunit XII

Chain i: 97%



- Molecule 12: Photosystem I 4.8K protein

Chain W: 38% 28% 33%



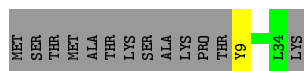
- Molecule 12: Photosystem I 4.8K protein

Chain X: 49% 15% 33%



- Molecule 12: Photosystem I 4.8K protein

Chain j: 64% 33%



## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 1 21 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 279.10Å 164.60Å 284.10Å<br>90.00° 119.25° 90.00°   | Depositor        |
| Resolution (Å)  | 39.88 – 2.90<br>64.24 – 2.90   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (39.88-2.90)<br>92.7 (64.24-2.90)   | Depositor<br>EDS |
| $R_{merge}$   | (Not available)  | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.04 (at 2.91Å)  | Xtriage          |
| Refinement program  | REFMAC 5.8.0238  | Depositor        |
| R, $R_{free}$   | 0.298 , 0.336<br>0.300 , 0.337   | Depositor<br>DCC |
| $R_{free}$ test set   | 24635 reflections (5.01%)  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.2   | Xtriage          |
| Anisotropy  | 0.073  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 65.1  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.27$ , $\langle L^2 \rangle = 0.11$  | Xtriage          |
| Estimated twinning fraction   | 0.268 for -h-l,k,h<br>0.268 for l,k,-h-l<br>0.347 for h,-k,-h-l<br>0.260 for -h-l,-k,l<br>0.259 for l,-k,h | Xtriage          |
| $F_o, F_c$ correlation  | 0.91   | EDS              |
| Total number of atoms   | 72532  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CA, CLA, PQN, CL0, SF4, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.66         | 0/5990  | 0.74        | 0/8168  |
| 1   | G     | 0.66         | 0/5990  | 0.75        | 0/8168  |
| 1   | Y     | 0.66         | 0/5990  | 0.75        | 0/8168  |
| 2   | B     | 0.64         | 0/6107  | 0.74        | 0/8345  |
| 2   | H     | 0.66         | 0/6107  | 0.75        | 0/8345  |
| 2   | Z     | 0.65         | 0/6107  | 0.73        | 0/8345  |
| 3   | C     | 0.69         | 0/608   | 0.84        | 0/824   |
| 3   | N     | 0.68         | 0/608   | 0.85        | 0/824   |
| 3   | a     | 0.69         | 0/608   | 0.82        | 0/824   |
| 4   | D     | 0.64         | 0/1101  | 0.78        | 0/1492  |
| 4   | O     | 0.63         | 0/1101  | 0.77        | 0/1492  |
| 4   | b     | 0.64         | 0/1101  | 0.79        | 0/1492  |
| 5   | E     | 0.68         | 0/551   | 0.78        | 0/750   |
| 5   | P     | 0.68         | 0/551   | 0.76        | 0/750   |
| 5   | c     | 0.67         | 0/551   | 0.77        | 0/750   |
| 6   | F     | 0.69         | 0/1087  | 0.78        | 0/1476  |
| 6   | Q     | 0.68         | 0/1087  | 0.76        | 0/1476  |
| 6   | d     | 0.68         | 0/1087  | 0.77        | 0/1476  |
| 7   | I     | 0.66         | 0/312   | 0.71        | 0/425   |
| 7   | R     | 0.66         | 0/312   | 0.69        | 0/425   |
| 7   | e     | 0.64         | 0/312   | 0.76        | 0/425   |
| 8   | J     | 0.64         | 0/350   | 0.72        | 0/477   |
| 8   | S     | 0.65         | 0/350   | 0.71        | 0/477   |
| 8   | f     | 0.64         | 0/350   | 0.71        | 0/477   |
| 9   | K     | 0.72         | 0/331   | 0.80        | 0/444   |
| 9   | T     | 0.72         | 0/331   | 0.86        | 0/444   |
| 9   | g     | 0.73         | 0/331   | 0.82        | 0/444   |
| 10  | L     | 0.68         | 0/1148  | 0.78        | 0/1558  |
| 10  | U     | 0.68         | 0/1148  | 0.75        | 0/1558  |
| 10  | h     | 0.68         | 0/1148  | 0.77        | 0/1558  |
| 11  | M     | 0.68         | 0/236   | 0.76        | 0/322   |
| 11  | V     | 0.69         | 0/236   | 0.75        | 0/322   |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 11  | i     | 0.70         | 0/236   | 0.74        | 0/322   |
| 12  | W     | 0.65         | 0/227   | 0.69        | 0/310   |
| 12  | X     | 0.66         | 0/227   | 0.70        | 0/310   |
| 12  | j     | 0.66         | 0/227   | 0.65        | 0/310   |
| All | All   | 0.66         | 0/54144 | 0.75        | 0/73773 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 9   | K     | 0                   | 1                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | K     | 56  | LEU  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5791  | 0        | 5648     | 334     | 0            |
| 1   | G     | 5791  | 0        | 5648     | 363     | 0            |
| 1   | Y     | 5791  | 0        | 5649     | 333     | 0            |
| 2   | B     | 5889  | 0        | 5651     | 350     | 0            |
| 2   | H     | 5889  | 0        | 5650     | 339     | 0            |
| 2   | Z     | 5889  | 0        | 5651     | 322     | 0            |
| 3   | C     | 598   | 0        | 582      | 33      | 0            |
| 3   | N     | 598   | 0        | 582      | 31      | 0            |
| 3   | a     | 598   | 0        | 582      | 0       | 0            |
| 4   | D     | 1075  | 0        | 1077     | 48      | 0            |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | O     | 1075  | 0        | 1077     | 36      | 0            |
| 4   | b     | 1075  | 0        | 1077     | 0       | 0            |
| 5   | E     | 539   | 0        | 528      | 16      | 0            |
| 5   | P     | 539   | 0        | 528      | 11      | 0            |
| 5   | c     | 539   | 0        | 528      | 0       | 1            |
| 6   | F     | 1065  | 0        | 1077     | 45      | 0            |
| 6   | Q     | 1065  | 0        | 1077     | 49      | 0            |
| 6   | d     | 1065  | 0        | 1077     | 0       | 1            |
| 7   | I     | 301   | 0        | 306      | 23      | 0            |
| 7   | R     | 301   | 0        | 306      | 15      | 0            |
| 7   | e     | 301   | 0        | 306      | 0       | 0            |
| 8   | J     | 338   | 0        | 347      | 28      | 0            |
| 8   | S     | 338   | 0        | 347      | 26      | 0            |
| 8   | f     | 338   | 0        | 347      | 0       | 0            |
| 9   | K     | 328   | 0        | 348      | 33      | 0            |
| 9   | T     | 328   | 0        | 348      | 22      | 0            |
| 9   | g     | 328   | 0        | 348      | 0       | 0            |
| 10  | L     | 1119  | 0        | 1125     | 50      | 0            |
| 10  | U     | 1119  | 0        | 1125     | 47      | 0            |
| 10  | h     | 1119  | 0        | 1125     | 0       | 0            |
| 11  | M     | 233   | 0        | 252      | 8       | 0            |
| 11  | V     | 233   | 0        | 252      | 8       | 0            |
| 11  | i     | 233   | 0        | 252      | 0       | 0            |
| 12  | W     | 219   | 0        | 221      | 9       | 0            |
| 12  | X     | 219   | 0        | 221      | 6       | 0            |
| 12  | j     | 219   | 0        | 221      | 0       | 0            |
| 13  | A     | 65    | 0        | 72       | 13      | 0            |
| 13  | G     | 65    | 0        | 72       | 16      | 0            |
| 13  | Y     | 65    | 0        | 72       | 11      | 0            |
| 14  | A     | 2489  | 0        | 2488     | 268     | 0            |
| 14  | B     | 2389  | 0        | 2373     | 250     | 0            |
| 14  | F     | 45    | 0        | 32       | 1       | 0            |
| 14  | G     | 2534  | 0        | 2522     | 287     | 0            |
| 14  | H     | 2220  | 0        | 2211     | 258     | 0            |
| 14  | J     | 100   | 0        | 81       | 4       | 0            |
| 14  | K     | 86    | 0        | 61       | 7       | 0            |
| 14  | L     | 325   | 0        | 360      | 34      | 0            |
| 14  | Q     | 110   | 0        | 104      | 9       | 0            |
| 14  | S     | 165   | 0        | 154      | 11      | 0            |
| 14  | T     | 86    | 0        | 62       | 6       | 0            |
| 14  | U     | 260   | 0        | 287      | 28      | 0            |
| 14  | V     | 54    | 0        | 48       | 6       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | W     | 45    | 0        | 33       | 4       | 0            |
| 14  | X     | 45    | 0        | 33       | 0       | 0            |
| 14  | Y     | 2640  | 0        | 2675     | 276     | 0            |
| 14  | Z     | 2254  | 0        | 2219     | 220     | 0            |
| 14  | d     | 95    | 0        | 70       | 0       | 0            |
| 14  | f     | 100   | 0        | 82       | 0       | 0            |
| 14  | g     | 86    | 0        | 62       | 0       | 0            |
| 14  | h     | 260   | 0        | 287      | 0       | 0            |
| 14  | j     | 45    | 0        | 33       | 0       | 0            |
| 15  | A     | 33    | 0        | 46       | 6       | 0            |
| 15  | B     | 33    | 0        | 46       | 11      | 0            |
| 15  | G     | 33    | 0        | 46       | 3       | 0            |
| 15  | H     | 33    | 0        | 46       | 7       | 0            |
| 15  | Y     | 33    | 0        | 46       | 2       | 0            |
| 15  | Z     | 33    | 0        | 46       | 4       | 0            |
| 16  | A     | 8     | 0        | 0        | 1       | 0            |
| 16  | C     | 16    | 0        | 0        | 5       | 0            |
| 16  | G     | 8     | 0        | 0        | 0       | 0            |
| 16  | N     | 16    | 0        | 0        | 3       | 0            |
| 16  | Y     | 8     | 0        | 0        | 0       | 0            |
| 16  | a     | 16    | 0        | 0        | 0       | 0            |
| 17  | A     | 200   | 0        | 243      | 33      | 0            |
| 17  | B     | 255   | 0        | 302      | 53      | 0            |
| 17  | F     | 80    | 0        | 98       | 8       | 0            |
| 17  | G     | 240   | 0        | 288      | 62      | 0            |
| 17  | H     | 265   | 0        | 320      | 47      | 0            |
| 17  | I     | 40    | 0        | 48       | 11      | 0            |
| 17  | J     | 80    | 0        | 96       | 21      | 0            |
| 17  | K     | 40    | 0        | 48       | 3       | 0            |
| 17  | L     | 120   | 0        | 145      | 22      | 0            |
| 17  | M     | 40    | 0        | 48       | 6       | 0            |
| 17  | Q     | 80    | 0        | 98       | 9       | 0            |
| 17  | R     | 80    | 0        | 96       | 12      | 0            |
| 17  | S     | 40    | 0        | 47       | 10      | 0            |
| 17  | T     | 40    | 0        | 49       | 6       | 0            |
| 17  | U     | 120   | 0        | 145      | 19      | 0            |
| 17  | V     | 40    | 0        | 49       | 6       | 0            |
| 17  | Y     | 280   | 0        | 337      | 58      | 0            |
| 17  | Z     | 225   | 0        | 271      | 33      | 0            |
| 17  | d     | 40    | 0        | 48       | 0       | 0            |
| 17  | e     | 40    | 0        | 48       | 0       | 0            |
| 17  | f     | 120   | 0        | 145      | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | h     | 80    | 0        | 97       | 0       | 0            |
| 17  | i     | 40    | 0        | 47       | 0       | 0            |
| 18  | A     | 81    | 0        | 108      | 5       | 0            |
| 18  | B     | 39    | 0        | 48       | 0       | 0            |
| 18  | G     | 81    | 0        | 108      | 12      | 0            |
| 18  | H     | 37    | 0        | 44       | 2       | 0            |
| 18  | Y     | 74    | 0        | 94       | 9       | 0            |
| 18  | j     | 28    | 0        | 26       | 0       | 0            |
| 19  | B     | 52    | 0        | 77       | 6       | 0            |
| 19  | H     | 49    | 0        | 68       | 4       | 0            |
| 19  | Z     | 49    | 0        | 68       | 3       | 0            |
| 20  | L     | 1     | 0        | 0        | 0       | 0            |
| 20  | U     | 1     | 0        | 0        | 0       | 0            |
| 20  | h     | 1     | 0        | 0        | 0       | 0            |
| 21  | A     | 9     | 0        | 0        | 0       | 0            |
| 21  | B     | 9     | 0        | 0        | 0       | 0            |
| 21  | C     | 1     | 0        | 0        | 1       | 0            |
| 21  | D     | 2     | 0        | 0        | 0       | 0            |
| 21  | E     | 1     | 0        | 0        | 0       | 0            |
| 21  | G     | 8     | 0        | 0        | 15      | 0            |
| 21  | H     | 3     | 0        | 0        | 0       | 0            |
| 21  | J     | 1     | 0        | 0        | 0       | 0            |
| 21  | K     | 1     | 0        | 0        | 0       | 0            |
| 21  | L     | 5     | 0        | 0        | 0       | 0            |
| 21  | N     | 1     | 0        | 0        | 1       | 0            |
| 21  | O     | 2     | 0        | 0        | 0       | 0            |
| 21  | Q     | 2     | 0        | 0        | 0       | 0            |
| 21  | T     | 1     | 0        | 0        | 0       | 0            |
| 21  | U     | 4     | 0        | 0        | 0       | 0            |
| 21  | W     | 1     | 0        | 0        | 1       | 0            |
| 21  | Y     | 8     | 0        | 0        | 19      | 0            |
| 21  | Z     | 2     | 0        | 0        | 0       | 0            |
| 21  | b     | 4     | 0        | 0        | 0       | 0            |
| 21  | c     | 1     | 0        | 0        | 0       | 0            |
| 21  | d     | 2     | 0        | 0        | 0       | 0            |
| 21  | f     | 1     | 0        | 0        | 0       | 0            |
| 21  | h     | 1     | 0        | 0        | 0       | 0            |
| 21  | j     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 72532 | 0        | 72009    | 3482    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (3482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:819:CLA:HBB1 | 21:G:907:HOH:O    | 1.23                     | 1.26              |
| 1:G:373:HIS:ND1   | 14:G:818:CLA:OBD  | 1.80                     | 1.15              |
| 14:Y:821:CLA:C3B  | 21:Y:904:HOH:O    | 1.92                     | 1.14              |
| 1:A:399:TRP:CD1   | 14:A:828:CLA:HAB  | 1.84                     | 1.12              |
| 2:B:318:PHE:CD1   | 14:B:822:CLA:HAB  | 1.84                     | 1.10              |
| 14:U:1006:CLA:HAB | 14:Z:808:CLA:HMA1 | 1.14                     | 1.10              |
| 9:K:32:TYR:C      | 9:K:34:ILE:N      | 2.07                     | 1.08              |
| 3:C:47:CYS:SG     | 21:C:201:HOH:O    | 2.09                     | 1.08              |
| 14:Z:821:CLA:HAB  | 14:Z:828:CLA:HMD2 | 1.32                     | 1.06              |
| 2:Z:354:HIS:ND1   | 14:Z:815:CLA:OBD  | 1.90                     | 1.04              |
| 1:G:399:TRP:CD1   | 14:G:828:CLA:HAB  | 1.93                     | 1.04              |
| 14:G:803:CLA:OBD  | 14:H:802:CLA:HMB3 | 1.57                     | 1.03              |
| 2:B:14:ASP:OD2    | 2:B:18:ARG:NH1    | 1.91                     | 1.02              |
| 10:U:96:TYR:OH    | 2:Z:698:ARG:NH1   | 1.93                     | 1.01              |
| 14:Y:827:CLA:H8   | 21:Y:904:HOH:O    | 1.61                     | 1.01              |
| 14:B:810:CLA:HMA1 | 14:L:202:CLA:HAB  | 1.43                     | 1.01              |
| 3:N:16:CYS:SG     | 3:N:25:LEU:HD22   | 2.01                     | 1.00              |
| 14:H:808:CLA:HMA1 | 14:H:809:CLA:HAB  | 1.43                     | 1.00              |
| 1:Y:642:SER:OG    | 1:Y:652:ASP:OD2   | 1.79                     | 0.99              |
| 2:B:354:HIS:ND1   | 14:B:817:CLA:OBD  | 1.95                     | 0.99              |
| 1:A:703:SER:O     | 2:B:423:SER:OG    | 1.79                     | 0.98              |
| 14:Y:839:CLA:H2A  | 21:Y:908:HOH:O    | 1.61                     | 0.98              |
| 1:G:217:ILE:HA    | 1:G:221:LEU:HD12  | 1.45                     | 0.96              |
| 1:G:336:PHE:O     | 1:G:432:ARG:NH2   | 1.98                     | 0.96              |
| 1:G:76:HIS:ND1    | 14:G:813:CLA:OBD  | 1.98                     | 0.96              |
| 2:H:70:GLN:NE2    | 14:H:806:CLA:O1D  | 1.99                     | 0.96              |
| 21:G:904:HOH:O    | 14:H:801:CLA:C2C  | 2.14                     | 0.95              |
| 2:Z:28:HIS:ND1    | 14:Z:805:CLA:O1A  | 1.99                     | 0.94              |
| 1:Y:363:MET:HG3   | 14:Y:805:CLA:HED1 | 1.48                     | 0.94              |
| 14:Z:825:CLA:O1D  | 14:Z:826:CLA:HMA1 | 1.66                     | 0.94              |
| 2:B:647:ASN:HD22  | 2:B:649:LEU:H     | 1.14                     | 0.94              |
| 14:G:802:CLA:C2C  | 21:G:904:HOH:O    | 2.16                     | 0.93              |
| 6:Q:40:GLN:NE2    | 8:S:40:PRO:O      | 2.03                     | 0.91              |
| 14:B:835:CLA:C4C  | 14:B:836:CLA:HAB  | 2.01                     | 0.91              |
| 2:Z:292:THR:HG21  | 14:Z:818:CLA:OBD  | 1.70                     | 0.91              |
| 1:A:86:TRP:NE1    | 14:A:828:CLA:OBD  | 2.05                     | 0.90              |
| 2:Z:425:LEU:HG    | 14:Z:837:CLA:HAB  | 1.53                     | 0.90              |
| 1:A:56:HIS:ND1    | 14:A:806:CLA:O1A  | 2.05                     | 0.89              |
| 1:G:121:VAL:HG12  | 14:H:830:CLA:HMD1 | 1.52                     | 0.89              |
| 14:A:828:CLA:H191 | 17:J:103:BCR:H14C | 1.52                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Y:575:ARG:NH1    | 18:Y:852:LHG:O10   | 2.05                     | 0.89              |
| 17:J:104:BCR:HC8   | 17:J:104:BCR:H321  | 1.55                     | 0.89              |
| 10:U:38:ARG:O      | 10:U:46:ARG:NH2    | 2.06                     | 0.89              |
| 17:Z:844:BCR:H23C  | 17:Z:844:BCR:H403  | 1.53                     | 0.89              |
| 17:Y:851:BCR:H403  | 17:Y:851:BCR:H23C  | 1.54                     | 0.88              |
| 1:Y:399:TRP:CD1    | 14:Y:828:CLA:HAB   | 2.07                     | 0.88              |
| 17:R:102:BCR:HC8   | 17:R:102:BCR:H331  | 1.57                     | 0.87              |
| 1:A:451:LEU:HD21   | 14:A:837:CLA:HAB   | 1.57                     | 0.87              |
| 1:G:698:GLN:HE22   | 1:G:720:ARG:HA     | 1.40                     | 0.87              |
| 1:A:121:VAL:HG22   | 14:B:833:CLA:HMD1  | 1.54                     | 0.86              |
| 17:G:854:BCR:H331  | 17:G:854:BCR:HC8   | 1.56                     | 0.86              |
| 2:H:480:LEU:O      | 2:H:482:SER:N      | 2.07                     | 0.86              |
| 1:Y:121:VAL:HG22   | 14:Z:831:CLA:HMD1  | 1.57                     | 0.86              |
| 14:Y:839:CLA:C2A   | 21:Y:908:HOH:O     | 2.21                     | 0.86              |
| 17:S:1104:BCR:H403 | 17:S:1104:BCR:H23C | 1.59                     | 0.85              |
| 17:G:850:BCR:H23C  | 17:G:850:BCR:H403  | 1.57                     | 0.85              |
| 2:B:318:PHE:CE1    | 14:B:822:CLA:HAB   | 2.11                     | 0.85              |
| 2:H:271:ASP:HB3    | 14:H:816:CLA:HMA1  | 1.58                     | 0.84              |
| 14:G:802:CLA:C1C   | 21:G:904:HOH:O     | 2.23                     | 0.84              |
| 14:A:834:CLA:HMD2  | 14:A:835:CLA:HAB   | 1.59                     | 0.84              |
| 12:W:20:LEU:HD13   | 14:W:1701:CLA:HBB1 | 1.59                     | 0.84              |
| 1:Y:57:ASP:O       | 1:Y:60:THR:OG1     | 1.95                     | 0.84              |
| 2:H:325:ILE:HA     | 2:H:328:THR:HG22   | 1.59                     | 0.84              |
| 14:Z:803:CLA:HAB   | 14:Z:805:CLA:CAD   | 2.08                     | 0.83              |
| 14:Y:819:CLA:C4D   | 21:Y:907:HOH:O     | 2.27                     | 0.83              |
| 1:A:149:ALA:HB1    | 14:A:819:CLA:HED1  | 1.61                     | 0.83              |
| 1:A:564:ARG:NH2    | 4:D:14:THR:O       | 2.12                     | 0.83              |
| 1:G:158:LEU:O      | 1:G:161:THR:OG1    | 1.96                     | 0.83              |
| 14:H:801:CLA:HED1  | 14:H:802:CLA:H92   | 1.61                     | 0.83              |
| 1:Y:337:THR:OG1    | 18:Y:853:LHG:O4    | 1.96                     | 0.83              |
| 14:U:1006:CLA:HAB  | 14:Z:808:CLA:CMA   | 2.06                     | 0.83              |
| 1:Y:593:ASP:OD1    | 1:Y:728:ARG:NH1    | 2.12                     | 0.83              |
| 1:A:519:ALA:HB1    | 1:A:625:VAL:HG21   | 1.59                     | 0.83              |
| 10:U:25:GLY:O      | 10:U:29:THR:OG1    | 1.96                     | 0.82              |
| 1:Y:145:GLN:HB3    | 1:Y:380:TYR:HB3    | 1.62                     | 0.82              |
| 14:A:828:CLA:O1D   | 14:A:829:CLA:HMA1  | 1.79                     | 0.82              |
| 2:Z:198:ILE:HG13   | 2:Z:199:PRO:HD3    | 1.62                     | 0.82              |
| 14:A:822:CLA:HBA2  | 9:K:35:GLN:OE1     | 1.80                     | 0.82              |
| 1:Y:399:TRP:NE1    | 14:Y:828:CLA:HAB   | 1.95                     | 0.82              |
| 14:G:802:CLA:H12   | 2:H:430:LEU:HD12   | 1.62                     | 0.81              |
| 21:G:904:HOH:O     | 14:H:801:CLA:C3C   | 2.25                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:Q:65:ILE:HD12   | 14:S:1103:CLA:HMB3 | 1.62                     | 0.81              |
| 2:Z:494:ASN:HD22  | 2:Z:496:GLY:H      | 1.26                     | 0.81              |
| 14:G:819:CLA:HMB1 | 21:G:907:HOH:O     | 1.80                     | 0.81              |
| 14:Y:802:CLA:OBD  | 14:Z:802:CLA:HMB3  | 1.80                     | 0.81              |
| 2:H:339:TRP:HE1   | 14:H:823:CLA:C2B   | 1.94                     | 0.81              |
| 2:H:489:SER:O     | 2:H:497:ASN:ND2    | 2.14                     | 0.81              |
| 2:Z:67:VAL:HG11   | 2:Z:123:TRP:HZ3    | 1.44                     | 0.81              |
| 14:A:802:CLA:CAD  | 14:B:803:CLA:HMB3  | 2.11                     | 0.80              |
| 2:B:596:VAL:HG13  | 14:B:837:CLA:HAB   | 1.64                     | 0.80              |
| 1:Y:450:PHE:HE1   | 14:Y:838:CLA:HAB   | 1.47                     | 0.80              |
| 14:Z:806:CLA:HHB  | 14:Z:807:CLA:HMB3  | 1.63                     | 0.80              |
| 1:A:99:ASN:HD22   | 1:A:110:ILE:HD11   | 1.45                     | 0.79              |
| 10:L:29:THR:O     | 10:L:33:ASN:ND2    | 2.16                     | 0.79              |
| 6:F:60:ALA:HA     | 6:F:64:LEU:HD13    | 1.64                     | 0.79              |
| 14:Y:839:CLA:HMA3 | 21:Y:908:HOH:O     | 1.81                     | 0.79              |
| 2:B:294:PHE:CE2   | 14:B:820:CLA:O1A   | 2.36                     | 0.79              |
| 2:H:28:HIS:ND1    | 14:H:805:CLA:O1A   | 2.13                     | 0.79              |
| 14:A:833:CLA:HAB  | 14:L:201:CLA:HHB   | 1.65                     | 0.79              |
| 14:Y:819:CLA:C3D  | 21:Y:907:HOH:O     | 2.31                     | 0.79              |
| 14:G:828:CLA:O1D  | 14:G:829:CLA:HMA1  | 1.82                     | 0.78              |
| 1:Y:346:GLU:O     | 1:Y:350:THR:OG1    | 1.99                     | 0.78              |
| 17:L:203:BCR:H23C | 17:L:203:BCR:H392  | 1.64                     | 0.78              |
| 21:G:904:HOH:O    | 14:H:801:CLA:CMC   | 2.31                     | 0.78              |
| 2:B:181:LEU:HG    | 14:B:813:CLA:H42   | 1.65                     | 0.78              |
| 14:B:809:CLA:HMC2 | 17:B:848:BCR:H312  | 1.66                     | 0.77              |
| 2:B:360:PRO:HG3   | 14:B:818:CLA:HBA1  | 1.65                     | 0.77              |
| 1:Y:357:ALA:HA    | 1:Y:408:GLY:HA2    | 1.67                     | 0.77              |
| 14:B:826:CLA:HED1 | 17:B:847:BCR:H331  | 1.66                     | 0.77              |
| 2:B:566:ASP:OD2   | 3:C:65:ARG:NH2     | 2.17                     | 0.77              |
| 14:G:828:CLA:H91  | 17:G:854:BCR:H361  | 1.66                     | 0.77              |
| 1:G:681:PHE:CG    | 17:G:850:BCR:H363  | 2.20                     | 0.77              |
| 2:H:360:PRO:HG3   | 14:H:817:CLA:HBA1  | 1.67                     | 0.77              |
| 1:Y:417:VAL:HG21  | 1:Y:574:PHE:HB2    | 1.66                     | 0.77              |
| 1:A:153:THR:HG23  | 1:A:233:ALA:HB1    | 1.67                     | 0.77              |
| 14:B:815:CLA:HMA1 | 17:B:845:BCR:C10   | 2.14                     | 0.77              |
| 2:H:478:ASP:OD1   | 2:H:483:ASN:ND2    | 2.18                     | 0.77              |
| 14:Z:835:CLA:HMB2 | 14:Z:837:CLA:HED1  | 1.65                     | 0.77              |
| 2:H:542:LYS:HE2   | 2:H:546:ASP:OD2    | 1.85                     | 0.76              |
| 14:Y:824:CLA:HMA1 | 14:Y:843:CLA:HAB   | 1.66                     | 0.76              |
| 14:A:808:CLA:HHB  | 14:A:808:CLA:HBB1  | 1.68                     | 0.76              |
| 1:G:550:VAL:HG11  | 14:G:838:CLA:HMB3  | 1.65                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:H:816:CLA:O1D  | 14:H:817:CLA:HMA1 | 1.86                     | 0.76              |
| 9:T:25:PHE:HE2    | 9:T:67:HIS:CE1    | 2.03                     | 0.76              |
| 1:Y:558:LEU:HD21  | 14:Y:821:CLA:H201 | 1.66                     | 0.76              |
| 2:H:301:LYS:NZ    | 2:H:327:GLU:OE2   | 2.17                     | 0.76              |
| 2:H:647:ASN:HD22  | 2:H:649:LEU:H     | 1.31                     | 0.76              |
| 14:A:807:CLA:HBB1 | 14:A:807:CLA:HHC  | 1.67                     | 0.76              |
| 2:B:558:ASP:OD2   | 4:D:122:ASN:ND2   | 2.19                     | 0.76              |
| 9:T:32:TYR:C      | 9:T:34:ILE:N      | 2.39                     | 0.76              |
| 14:Z:806:CLA:HMC2 | 14:Z:806:CLA:H92  | 1.65                     | 0.76              |
| 2:B:339:TRP:HE1   | 14:B:824:CLA:C2B  | 1.98                     | 0.76              |
| 14:H:814:CLA:HBB1 | 17:H:840:BCR:H333 | 1.66                     | 0.76              |
| 17:J:104:BCR:H23C | 17:J:104:BCR:H403 | 1.68                     | 0.76              |
| 2:Z:596:VAL:HG13  | 14:Z:835:CLA:HAB  | 1.67                     | 0.76              |
| 1:G:451:LEU:O     | 1:G:455:SER:HB3   | 1.85                     | 0.76              |
| 17:A:849:BCR:H362 | 14:A:852:CLA:H43  | 1.66                     | 0.76              |
| 14:A:807:CLA:HMB3 | 14:A:808:CLA:HHB  | 1.68                     | 0.75              |
| 17:B:847:BCR:H403 | 17:B:847:BCR:H23C | 1.68                     | 0.75              |
| 1:G:751:ILE:HA    | 1:G:754:VAL:HG22  | 1.69                     | 0.75              |
| 2:H:390:PHE:HZ    | 14:H:824:CLA:HAB  | 1.51                     | 0.75              |
| 17:I:101:BCR:HC8  | 17:I:101:BCR:H321 | 3.16                     | 0.75              |
| 2:B:414:VAL:HG11  | 17:B:846:BCR:H401 | 1.68                     | 0.75              |
| 9:K:65:PHE:HA     | 9:K:68:LEU:CD2    | 2.16                     | 0.75              |
| 2:Z:277:LEU:HD13  | 14:Z:813:CLA:HMC1 | 1.67                     | 0.75              |
| 1:G:57:ASP:OD1    | 1:G:60:THR:OG1    | 2.04                     | 0.75              |
| 9:K:65:PHE:HA     | 9:K:68:LEU:HD22   | 1.68                     | 0.75              |
| 6:Q:55:GLY:HA2    | 6:Q:64:LEU:HD21   | 1.69                     | 0.75              |
| 6:Q:80:VAL:HG23   | 6:Q:109:CYS:HB2   | 1.67                     | 0.75              |
| 14:Y:821:CLA:C4B  | 21:Y:904:HOH:O    | 2.29                     | 0.75              |
| 1:G:35:ASP:OD1    | 1:G:37:THR:OG1    | 2.04                     | 0.74              |
| 14:G:804:CLA:HAB  | 14:G:806:CLA:CAD  | 2.17                     | 0.74              |
| 10:U:19:THR:HG21  | 14:Y:831:CLA:HMA2 | 1.68                     | 0.74              |
| 14:H:834:CLA:HMB2 | 14:H:836:CLA:HED1 | 1.68                     | 0.74              |
| 8:S:5:LEU:HD22    | 8:S:8:LEU:HD12    | 1.69                     | 0.74              |
| 1:Y:117:VAL:HG22  | 1:Y:127:ASN:OD1   | 1.88                     | 0.74              |
| 14:Y:854:CLA:HAB  | 2:Z:588:TRP:CH2   | 2.22                     | 0.74              |
| 2:B:198:ILE:HG13  | 2:B:199:PRO:HD3   | 1.66                     | 0.74              |
| 1:A:19:ASP:OD1    | 1:A:182:LYS:NZ    | 2.15                     | 0.74              |
| 1:A:449:ILE:HD11  | 17:B:848:BCR:H402 | 1.70                     | 0.74              |
| 1:G:356:LEU:O     | 1:G:360:LEU:HB2   | 1.87                     | 0.74              |
| 1:A:215:HIS:CE1   | 1:A:219:VAL:HG21  | 2.22                     | 0.74              |
| 1:G:601:TRP:HH2   | 14:G:803:CLA:HAB  | 1.52                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:G:818:CLA:C2D  | 21:G:907:HOH:O     | 2.36                     | 0.74              |
| 1:Y:219:VAL:HG23  | 1:Y:239:PRO:HB3    | 1.69                     | 0.74              |
| 1:Y:432:ARG:NE    | 14:Y:831:CLA:OBD   | 2.20                     | 0.74              |
| 14:B:827:CLA:O1D  | 14:B:828:CLA:HMA1  | 1.88                     | 0.73              |
| 9:T:22:CYS:HA     | 9:T:25:PHE:CD1     | 2.24                     | 0.73              |
| 14:A:804:CLA:HMA2 | 14:A:811:CLA:HMD2  | 1.70                     | 0.73              |
| 14:Y:832:CLA:HMC2 | 14:Y:838:CLA:H171  | 1.70                     | 0.73              |
| 1:A:371:ALA:HB2   | 1:A:397:HIS:HB2    | 1.70                     | 0.73              |
| 14:A:802:CLA:OBD  | 14:B:803:CLA:HMB3  | 1.89                     | 0.73              |
| 14:A:806:CLA:HBD  | 14:A:806:CLA:HBA2  | 1.69                     | 0.73              |
| 4:D:95:HIS:HB3    | 4:D:96:PRO:HD3     | 1.71                     | 0.73              |
| 1:G:352:TRP:HB3   | 14:G:805:CLA:HAC1  | 1.69                     | 0.73              |
| 2:H:82:ASN:O      | 2:H:84:ARG:NH1     | 2.21                     | 0.73              |
| 14:U:1004:CLA:HAB | 14:Y:834:CLA:H92   | 1.71                     | 0.73              |
| 3:C:4:VAL:HG13    | 3:C:66:VAL:HG12    | 1.69                     | 0.73              |
| 2:Z:390:PHE:HZ    | 14:Z:823:CLA:HAB   | 1.54                     | 0.73              |
| 14:H:803:CLA:CGA  | 14:H:803:CLA:H3A   | 2.18                     | 0.73              |
| 2:B:380:TYR:CD2   | 14:B:827:CLA:HAB   | 2.24                     | 0.73              |
| 14:A:833:CLA:HMA1 | 17:I:101:BCR:H292  | 1.71                     | 0.73              |
| 1:G:564:ARG:O     | 4:O:60:ARG:NH1     | 2.20                     | 0.73              |
| 2:Z:321:PRO:HB2   | 2:Z:323:GLN:HE22   | 1.53                     | 0.73              |
| 9:T:65:PHE:HB2    | 17:T:102:BCR:H24C  | 1.71                     | 0.72              |
| 14:Y:812:CLA:H93  | 14:Y:820:CLA:H41   | 1.70                     | 0.72              |
| 14:A:808:CLA:H91  | 14:A:811:CLA:H191  | 1.71                     | 0.72              |
| 2:H:724:ILE:HD13  | 14:H:826:CLA:HMC2  | 1.70                     | 0.72              |
| 14:Y:818:CLA:H61  | 14:Y:836:CLA:HMA2  | 1.71                     | 0.72              |
| 2:Z:430:LEU:HA    | 14:Z:801:CLA:O2A   | 1.88                     | 0.72              |
| 14:B:825:CLA:HAA2 | 14:B:826:CLA:OBD   | 1.89                     | 0.72              |
| 2:H:513:SER:HB2   | 2:H:516:LEU:HD11   | 1.70                     | 0.72              |
| 1:A:446:TRP:HB2   | 14:A:841:CLA:HED2  | 1.70                     | 0.72              |
| 14:G:825:CLA:HMD2 | 14:G:825:CLA:H142  | 1.72                     | 0.72              |
| 1:G:216:GLN:HE22  | 1:G:301:HIS:HD2    | 1.36                     | 0.72              |
| 1:G:451:LEU:HD21  | 14:G:837:CLA:CAB   | 2.19                     | 0.72              |
| 2:B:647:ASN:ND2   | 2:B:649:LEU:H      | 1.87                     | 0.72              |
| 10:L:130:GLY:HA3  | 17:L:209:BCR:H383  | 1.71                     | 0.72              |
| 1:Y:198:ASN:HD21  | 1:Y:315:TYR:H      | 1.35                     | 0.72              |
| 10:U:130:GLY:HA3  | 17:U:1008:BCR:H383 | 1.70                     | 0.72              |
| 14:A:837:CLA:H202 | 14:L:206:CLA:H193  | 1.71                     | 0.71              |
| 14:Z:806:CLA:HMA1 | 14:Z:807:CLA:HMB3  | 1.72                     | 0.71              |
| 14:Y:808:CLA:C3D  | 14:Y:828:CLA:HBA1  | 2.21                     | 0.71              |
| 1:G:362:MET:HG3   | 14:G:825:CLA:HMB2  | 1.73                     | 0.71              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:O:95:HIS:HB3     | 4:O:96:PRO:HD3     | 1.71                     | 0.71              |
| 14:B:830:CLA:O1A   | 12:X:12:ARG:NH1    | 2.24                     | 0.71              |
| 14:B:806:CLA:HMB1  | 14:B:806:CLA:HBB1  | 1.73                     | 0.71              |
| 1:A:50:ASN:ND2     | 5:E:50:GLY:O       | 2.23                     | 0.71              |
| 14:H:832:CLA:C4C   | 14:H:833:CLA:HAB   | 2.21                     | 0.71              |
| 14:U:1003:CLA:H93  | 14:Y:832:CLA:H11   | 1.72                     | 0.71              |
| 14:Y:855:CLA:HAB   | 2:Z:665:THR:HA     | 1.73                     | 0.71              |
| 1:G:689:PHE:HA     | 15:G:844:PQN:H9    | 1.73                     | 0.71              |
| 14:G:806:CLA:HED1  | 14:G:830:CLA:H52   | 1.73                     | 0.71              |
| 1:G:392:SER:HB3    | 14:G:828:CLA:HMA1  | 1.73                     | 0.71              |
| 14:Y:830:CLA:HMD2  | 18:Y:852:LHG:H281  | 1.72                     | 0.71              |
| 1:G:541:ILE:HD12   | 13:G:801:CL0:H63   | 1.71                     | 0.71              |
| 1:G:152:ILE:HA     | 14:G:814:CLA:HED1  | 1.73                     | 0.71              |
| 14:G:818:CLA:C1D   | 21:G:907:HOH:O     | 2.39                     | 0.71              |
| 1:G:397:HIS:O      | 1:G:401:GLY:N      | 2.20                     | 0.70              |
| 14:G:809:CLA:HMB1  | 14:G:809:CLA:HBB1  | 1.72                     | 0.70              |
| 9:K:35:GLN:HE22    | 17:K:102:BCR:H281  | 1.56                     | 0.70              |
| 14:U:1003:CLA:HMB3 | 14:U:1004:CLA:HBC2 | 1.73                     | 0.70              |
| 2:B:181:LEU:HD21   | 14:B:813:CLA:H11   | 1.73                     | 0.70              |
| 2:B:724:ILE:HD13   | 14:B:827:CLA:HMC2  | 1.72                     | 0.70              |
| 2:H:168:LYS:O      | 2:H:330:ASN:ND2    | 2.15                     | 0.70              |
| 1:A:466:ARG:HB2    | 1:A:474:MET:HE1    | 1.73                     | 0.70              |
| 1:G:143:LEU:HA     | 1:G:146:LEU:HB3    | 1.72                     | 0.70              |
| 17:G:849:BCR:H23C  | 17:G:849:BCR:H382  | 1.73                     | 0.70              |
| 14:Z:825:CLA:CGA   | 14:Z:825:CLA:H3A   | 2.21                     | 0.70              |
| 14:Z:805:CLA:HMB2  | 14:Z:827:CLA:HBB2  | 1.72                     | 0.70              |
| 2:B:206:VAL:HG12   | 2:B:214:THR:HG21   | 1.72                     | 0.70              |
| 1:G:683:TRP:CD2    | 13:G:801:CL0:H5    | 2.26                     | 0.70              |
| 2:H:459:GLU:HG3    | 6:Q:5:LEU:HD11     | 1.73                     | 0.70              |
| 1:Y:199:HIS:O      | 1:Y:203:GLY:N      | 2.25                     | 0.70              |
| 1:Y:465:MET:HG3    | 1:Y:470:ARG:HD3    | 1.73                     | 0.70              |
| 1:A:588:GLN:HG3    | 2:B:673:TRP:HB2    | 1.73                     | 0.70              |
| 1:Y:694:ARG:NH1    | 1:Y:721:ALA:O      | 2.25                     | 0.70              |
| 1:A:399:TRP:HD1    | 14:A:828:CLA:HAB   | 1.53                     | 0.70              |
| 14:B:827:CLA:H3A   | 14:B:827:CLA:CGA   | 2.20                     | 0.70              |
| 8:J:5:LEU:HD23     | 8:J:8:LEU:HD12     | 1.74                     | 0.70              |
| 1:Y:293:TRP:HB2    | 1:Y:296:ASP:HB2    | 1.73                     | 0.70              |
| 17:Y:846:BCR:H23C  | 17:Y:846:BCR:H383  | 1.74                     | 0.70              |
| 2:Z:361:TYR:O      | 2:Z:364:ILE:HG22   | 1.91                     | 0.70              |
| 14:H:801:CLA:H141  | 14:S:1101:CLA:H191 | 1.74                     | 0.70              |
| 1:Y:366:LEU:HD13   | 14:Y:827:CLA:H42   | 1.74                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:424:HIS:O     | 2:H:428:VAL:HG23   | 1.91                     | 0.70              |
| 14:G:803:CLA:HED2 | 2:H:660:HIS:CD2    | 2.27                     | 0.70              |
| 1:Y:121:VAL:CG2   | 14:Z:831:CLA:HMD1  | 2.21                     | 0.70              |
| 1:Y:626:ALA:HB3   | 1:Y:630:THR:HB     | 1.72                     | 0.70              |
| 1:A:464:THR:HG22  | 2:B:654:TRP:HE1    | 1.56                     | 0.69              |
| 17:B:844:BCR:H23C | 17:B:844:BCR:H382  | 1.73                     | 0.69              |
| 1:Y:601:TRP:HE1   | 14:Y:855:CLA:CHD   | 2.05                     | 0.69              |
| 17:G:848:BCR:H403 | 17:G:848:BCR:H23C  | 1.74                     | 0.69              |
| 10:U:29:THR:O     | 10:U:33:ASN:ND2    | 2.25                     | 0.69              |
| 6:Q:101:ILE:HG13  | 8:S:14:LEU:HD12    | 1.75                     | 0.69              |
| 14:Y:828:CLA:H43  | 17:Y:851:BCR:H311  | 1.72                     | 0.69              |
| 2:B:193:LEU:HA    | 2:B:197:ALA:HB3    | 1.75                     | 0.69              |
| 2:H:663:TRP:CE3   | 14:H:802:CLA:HMA1  | 2.27                     | 0.69              |
| 1:Y:674:LEU:HD21  | 2:Z:448:ALA:HB2    | 1.74                     | 0.69              |
| 17:G:850:BCR:H362 | 14:H:801:CLA:H43   | 1.74                     | 0.69              |
| 14:Y:821:CLA:CMD  | 14:Y:822:CLA:HAB   | 2.23                     | 0.69              |
| 14:U:1006:CLA:CAB | 14:Z:808:CLA:HMA1  | 2.08                     | 0.69              |
| 2:B:532:GLY:O     | 2:B:536:THR:HG22   | 1.93                     | 0.69              |
| 17:B:845:BCR:H383 | 17:B:845:BCR:H23C  | 1.73                     | 0.69              |
| 17:M:101:BCR:HC8  | 17:M:101:BCR:H321  | 1.73                     | 0.69              |
| 4:O:100:VAL:HG21  | 4:O:106:ASN:HB2    | 1.74                     | 0.69              |
| 1:A:158:LEU:O     | 1:A:161:THR:OG1    | 2.09                     | 0.69              |
| 14:B:810:CLA:HMA1 | 14:L:202:CLA:CAB   | 2.21                     | 0.69              |
| 2:Z:481:LEU:HA    | 2:Z:489:SER:HB2    | 1.75                     | 0.69              |
| 1:A:486:PHE:HB3   | 14:A:836:CLA:H2    | 1.74                     | 0.69              |
| 2:B:548:ARG:NH1   | 6:F:141:ARG:O      | 2.26                     | 0.69              |
| 14:B:826:CLA:HAB  | 14:B:834:CLA:HMA2  | 1.74                     | 0.69              |
| 6:F:109:CYS:O     | 6:F:112:THR:HG22   | 1.93                     | 0.69              |
| 1:G:86:TRP:HZ3    | 17:G:847:BCR:H401  | 1.58                     | 0.69              |
| 6:Q:90:ASN:O      | 6:Q:90:ASN:ND2     | 2.25                     | 0.69              |
| 1:A:38:LEU:HD13   | 1:A:51:LEU:HA      | 1.75                     | 0.69              |
| 14:A:831:CLA:CBB  | 18:A:851:LHG:H291  | 2.23                     | 0.69              |
| 14:B:833:CLA:H41  | 17:B:851:BCR:H373  | 1.75                     | 0.69              |
| 1:G:59:ASP:HB2    | 1:G:418:ARG:HH12   | 1.58                     | 0.69              |
| 17:U:1007:BCR:HC8 | 17:U:1007:BCR:H331 | 1.75                     | 0.69              |
| 14:J:102:CLA:HED2 | 14:Z:835:CLA:H41   | 151.16                   | 0.69              |
| 1:A:367:SER:OG    | 1:A:397:HIS:O      | 2.11                     | 0.68              |
| 1:G:216:GLN:HE22  | 1:G:301:HIS:CD2    | 2.10                     | 0.68              |
| 17:S:1104:BCR:HC8 | 17:S:1104:BCR:H321 | 1.74                     | 0.68              |
| 13:Y:801:CL0:H13  | 14:Y:854:CLA:CAD   | 2.23                     | 0.68              |
| 14:Y:829:CLA:H52  | 21:Y:907:HOH:O     | 1.92                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:699:GLU:OE1    | 2:H:542:LYS:NZ     | 2.26                     | 0.68              |
| 1:G:380:TYR:CE2    | 14:G:829:CLA:HED2  | 2.29                     | 0.68              |
| 5:P:23:VAL:HA      | 5:P:38:VAL:HA      | 1.76                     | 0.68              |
| 1:Y:76:HIS:ND1     | 14:Y:813:CLA:OBD   | 2.26                     | 0.68              |
| 14:Y:818:CLA:O1D   | 14:Y:819:CLA:HMA1  | 1.93                     | 0.68              |
| 14:Y:840:CLA:HHD   | 17:Z:846:BCR:H383  | 1.74                     | 0.68              |
| 2:Z:390:PHE:CZ     | 14:Z:823:CLA:HAB   | 2.28                     | 0.68              |
| 9:K:43:LEU:HD22    | 9:K:56:LEU:HB3     | 1.75                     | 0.68              |
| 17:U:1007:BCR:H23C | 17:U:1007:BCR:H392 | 1.74                     | 0.68              |
| 10:U:59:ILE:HG22   | 10:U:82:GLY:HA3    | 1.75                     | 0.68              |
| 17:Y:847:BCR:H23C  | 17:Y:847:BCR:H403  | 1.76                     | 0.68              |
| 1:A:451:LEU:HD21   | 14:A:837:CLA:CAB   | 2.23                     | 0.68              |
| 1:G:189:TRP:CZ2    | 14:G:810:CLA:HMA1  | 2.28                     | 0.68              |
| 13:G:801:CL0:O1D   | 14:H:802:CLA:HBB2  | 1.93                     | 0.68              |
| 14:Y:826:CLA:CHB   | 17:Y:850:BCR:H352  | 2.23                     | 0.68              |
| 17:U:1007:BCR:H352 | 14:Y:834:CLA:C2    | 2.24                     | 0.68              |
| 1:A:612:HIS:ND1    | 14:A:836:CLA:HMC2  | 2.09                     | 0.68              |
| 2:B:730:PHE:O      | 2:B:734:SER:OG     | 2.11                     | 0.68              |
| 14:H:807:CLA:HAB   | 14:H:808:CLA:HAA2  | 1.76                     | 0.68              |
| 2:H:651:VAL:HG22   | 14:H:808:CLA:HAC1  | 1.75                     | 0.68              |
| 14:Y:828:CLA:O1D   | 14:Y:829:CLA:HMA1  | 1.94                     | 0.68              |
| 2:Z:630:LEU:O      | 2:Z:634:SER:OG     | 2.08                     | 0.68              |
| 1:Y:201:LEU:O      | 1:Y:308:PHE:HB3    | 1.94                     | 0.68              |
| 14:B:829:CLA:HBB1  | 14:B:829:CLA:HMB1  | 1.75                     | 0.68              |
| 14:A:841:CLA:HBC1  | 15:B:842:PQN:H193  | 1.76                     | 0.68              |
| 1:G:601:TRP:CH2    | 14:G:803:CLA:HAB   | 2.29                     | 0.68              |
| 2:H:354:HIS:ND1    | 14:H:816:CLA:OBD   | 2.27                     | 0.68              |
| 14:H:820:CLA:HBB2  | 14:H:821:CLA:HBC2  | 1.74                     | 0.68              |
| 2:B:525:VAL:HG13   | 14:B:803:CLA:H141  | 1.75                     | 0.67              |
| 2:B:390:PHE:CZ     | 17:B:847:BCR:H373  | 2.29                     | 0.67              |
| 6:Q:22:VAL:O       | 6:Q:34:ARG:NH2     | 2.24                     | 0.67              |
| 2:Z:373:ALA:HB1    | 14:Z:825:CLA:HMA1  | 1.75                     | 0.67              |
| 2:Z:86:ILE:O       | 2:Z:120:TYR:OH     | 2.06                     | 0.67              |
| 1:A:296:ASP:HB3    | 14:A:818:CLA:HMA1  | 1.76                     | 0.67              |
| 2:B:179:ALA:HA     | 2:B:284:ILE:HA     | 1.74                     | 0.67              |
| 2:H:278:ALA:HB2    | 14:H:816:CLA:HAB   | 1.76                     | 0.67              |
| 1:A:602:MET:HG2    | 14:A:826:CLA:HBC1  | 1.75                     | 0.67              |
| 10:U:35:PRO:HG3    | 10:U:49:GLU:CD     | 2.15                     | 0.67              |
| 1:Y:681:PHE:CG     | 17:Y:851:BCR:H363  | 2.30                     | 0.67              |
| 3:C:57:CYS:HA      | 16:C:102:SF4:S4    | 2.34                     | 0.67              |
| 1:G:439:ALA:HA     | 2:H:686:TRP:CZ3    | 2.29                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:100:VAL:O     | 2:H:104:THR:OG1   | 2.11                     | 0.67              |
| 6:F:53:VAL:HG12   | 6:F:63:PHE:HB2    | 1.77                     | 0.67              |
| 1:G:625:VAL:HG12  | 1:G:631:VAL:HG22  | 1.77                     | 0.67              |
| 1:A:366:LEU:HD21  | 14:A:819:CLA:H72  | 1.77                     | 0.67              |
| 1:G:399:TRP:HD1   | 14:G:828:CLA:HAB  | 1.56                     | 0.67              |
| 2:H:626:LEU:HD13  | 14:H:801:CLA:HED3 | 1.77                     | 0.67              |
| 2:H:52:HIS:CE1    | 2:H:56:ILE:HD11   | 2.28                     | 0.67              |
| 1:Y:512:ALA:HA    | 1:Y:528:PRO:HA    | 1.74                     | 0.67              |
| 1:Y:432:ARG:HE    | 14:Y:831:CLA:CAD  | 2.07                     | 0.67              |
| 3:C:33:CYS:SG     | 3:C:34:LYS:N      | 2.67                     | 0.67              |
| 1:G:514:GLY:HA2   | 1:G:528:PRO:HB3   | 1.76                     | 0.67              |
| 1:A:536:PHE:HA    | 14:A:837:CLA:HED1 | 1.76                     | 0.67              |
| 14:Y:803:CLA:H203 | 14:Y:841:CLA:H161 | 1.76                     | 0.67              |
| 2:B:45:ILE:HG21   | 14:B:806:CLA:H201 | 1.75                     | 0.66              |
| 2:B:361:TYR:OH    | 14:B:828:CLA:OBD  | 2.13                     | 0.66              |
| 2:H:219:ALA:HB1   | 2:H:223:PRO:HG2   | 1.77                     | 0.66              |
| 14:B:839:CLA:HBB1 | 14:B:839:CLA:HHC  | 1.77                     | 0.66              |
| 4:D:117:ARG:HH12  | 4:D:123:PRO:HD3   | 1.59                     | 0.66              |
| 1:Y:634:ILE:HG23  | 1:Y:754:VAL:HG11  | 1.76                     | 0.66              |
| 14:A:834:CLA:HED2 | 14:A:835:CLA:HMA3 | 1.76                     | 0.66              |
| 2:B:531:LEU:HD11  | 14:B:801:CLA:O1A  | 1.95                     | 0.66              |
| 1:G:302:LEU:HD13  | 14:G:815:CLA:HMC1 | 1.75                     | 0.66              |
| 14:G:803:CLA:CAD  | 14:H:802:CLA:HMB3 | 2.24                     | 0.66              |
| 2:H:339:TRP:CH2   | 17:H:843:BCR:H372 | 2.31                     | 0.66              |
| 1:Y:476:SER:HB3   | 1:Y:644:ILE:HD12  | 1.78                     | 0.66              |
| 2:B:535:THR:O     | 2:B:539:ILE:HG13  | 1.96                     | 0.66              |
| 2:B:719:PHE:O     | 2:B:723:TYR:HB2   | 1.94                     | 0.66              |
| 14:G:808:CLA:HAB  | 17:G:854:BCR:H363 | 1.76                     | 0.66              |
| 14:G:808:CLA:C3D  | 14:G:828:CLA:HBA1 | 2.25                     | 0.66              |
| 1:G:460:VAL:HG21  | 14:G:833:CLA:HMC3 | 1.76                     | 0.66              |
| 2:Z:714:VAL:O     | 2:Z:718:HIS:ND1   | 2.26                     | 0.66              |
| 1:A:45:THR:HG22   | 1:A:720:ARG:H     | 1.59                     | 0.66              |
| 2:H:494:ASN:HD22  | 2:H:496:GLY:H     | 1.42                     | 0.66              |
| 2:H:60:VAL:O      | 2:H:64:LEU:HD12   | 1.96                     | 0.66              |
| 2:H:349:SER:OG    | 14:H:824:CLA:CAD  | 2.44                     | 0.66              |
| 1:Y:371:ALA:HB2   | 1:Y:397:HIS:HB2   | 1.78                     | 0.66              |
| 14:G:834:CLA:HMD2 | 14:G:835:CLA:HAB  | 1.77                     | 0.66              |
| 1:A:120:ILE:HD12  | 17:J:104:BCR:H313 | 1.78                     | 0.66              |
| 3:N:57:CYS:HA     | 21:N:201:HOH:O    | 1.96                     | 0.66              |
| 2:Z:525:VAL:HG11  | 2:Z:599:TYR:CG    | 2.30                     | 0.66              |
| 1:A:148:ARG:NH2   | 1:A:228:ASP:OD1   | 2.28                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:683:TRP:CG    | 13:A:801:CL0:H5    | 2.31                     | 0.66              |
| 14:B:808:CLA:HHB  | 14:B:809:CLA:HMB3  | 1.78                     | 0.66              |
| 14:G:802:CLA:H51  | 14:G:802:CLA:HMA1  | 1.78                     | 0.66              |
| 2:H:25:ALA:HB2    | 19:H:846:LMG:H121  | 1.77                     | 0.66              |
| 1:Y:120:ILE:O     | 1:Y:121:VAL:HG12   | 1.94                     | 0.66              |
| 2:B:600:TRP:HB2   | 14:B:837:CLA:HMC1  | 1.78                     | 0.65              |
| 14:G:805:CLA:HMC3 | 14:G:830:CLA:HMA1  | 1.76                     | 0.65              |
| 2:H:414:VAL:HG21  | 17:H:843:BCR:H401  | 1.77                     | 0.65              |
| 1:Y:34:PHE:HB2    | 1:Y:61:HIS:CG      | 2.31                     | 0.65              |
| 2:H:73:PHE:HB3    | 2:H:131:ASN:ND2    | 2.09                     | 0.65              |
| 1:A:118:TRP:HB3   | 17:J:104:BCR:HC21  | 1.78                     | 0.65              |
| 14:V:1201:CLA:H2A | 14:V:1201:CLA:HED2 | 1.78                     | 0.65              |
| 1:A:542:HIS:HE1   | 1:A:612:HIS:ND1    | 1.94                     | 0.65              |
| 1:G:237:PRO:HG3   | 1:G:248:LEU:HD21   | 1.79                     | 0.65              |
| 14:L:201:CLA:H152 | 17:L:203:BCR:H372  | 1.78                     | 0.65              |
| 17:A:849:BCR:H403 | 17:A:849:BCR:H23C  | 1.78                     | 0.65              |
| 2:H:227:GLY:O     | 14:H:815:CLA:H43   | 1.96                     | 0.65              |
| 2:B:373:ALA:HB1   | 14:B:827:CLA:HMA1  | 1.78                     | 0.65              |
| 2:B:662:VAL:HG22  | 14:B:841:CLA:HMB3  | 1.77                     | 0.65              |
| 14:G:802:CLA:H142 | 17:G:850:BCR:C40   | 2.27                     | 0.65              |
| 9:K:24:LEU:HD23   | 9:K:70:ALA:HA      | 1.77                     | 0.65              |
| 14:L:206:CLA:HMA2 | 17:L:209:BCR:H341  | 1.79                     | 0.65              |
| 5:P:5:SER:O       | 5:P:23:VAL:HG12    | 1.97                     | 0.65              |
| 1:Y:738:GLY:O     | 1:Y:742:THR:OG1    | 2.15                     | 0.65              |
| 14:Y:839:CLA:CMA  | 21:Y:908:HOH:O     | 2.39                     | 0.65              |
| 1:A:357:ALA:HA    | 1:A:408:GLY:HA2    | 1.78                     | 0.65              |
| 14:G:824:CLA:H62  | 17:G:849:BCR:H363  | 1.77                     | 0.65              |
| 1:Y:36:ARG:NH2    | 1:Y:60:THR:O       | 2.29                     | 0.65              |
| 2:Z:650:SER:HB3   | 14:Z:808:CLA:HBC1  | 1.79                     | 0.65              |
| 2:B:196:VAL:O     | 2:B:199:PRO:HD2    | 1.95                     | 0.65              |
| 1:G:58:PHE:HE1    | 14:G:804:CLA:HED1  | 1.62                     | 0.65              |
| 8:S:3:HIS:O       | 8:S:6:THR:OG1      | 2.14                     | 0.65              |
| 1:Y:257:ASP:OD2   | 1:Y:262:SER:OG     | 2.15                     | 0.65              |
| 14:Y:802:CLA:CAD  | 14:Z:802:CLA:HMB3  | 2.27                     | 0.65              |
| 14:Z:823:CLA:H101 | 17:Z:845:BCR:H333  | 1.78                     | 0.65              |
| 14:H:805:CLA:H92  | 14:H:828:CLA:H91   | 1.78                     | 0.65              |
| 2:Z:57:PHE:HB2    | 2:Z:145:ALA:HB2    | 1.77                     | 0.65              |
| 2:Z:651:VAL:HG21  | 14:Z:807:CLA:HAC1  | 1.78                     | 0.65              |
| 14:Z:831:CLA:H52  | 17:Z:846:BCR:H312  | 1.79                     | 0.65              |
| 1:A:660:GLN:HG2   | 1:A:750:ARG:HA     | 1.78                     | 0.64              |
| 1:A:680:HIS:HB3   | 14:A:852:CLA:HBD   | 1.79                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D:117:ARG:NH2    | 4:D:122:ASN:OD1   | 2.29                     | 0.64              |
| 14:H:818:CLA:HBA1  | 14:H:823:CLA:CBB  | 2.26                     | 0.64              |
| 10:L:6:LYS:HG3     | 10:L:18:SER:HB3   | 1.79                     | 0.64              |
| 1:A:237:PRO:HG3    | 1:A:248:LEU:HD21  | 1.80                     | 0.64              |
| 1:A:196:MET:HE2    | 14:A:813:CLA:HBC2 | 1.78                     | 0.64              |
| 14:A:820:CLA:HMA1  | 9:K:61:ALA:HB2    | 1.79                     | 0.64              |
| 14:A:826:CLA:CHB   | 17:A:848:BCR:H352 | 2.27                     | 0.64              |
| 3:C:60:ASP:OD2     | 5:E:14:SER:OG     | 2.11                     | 0.64              |
| 1:G:488:GLN:NE2    | 1:G:531:LEU:O     | 2.31                     | 0.64              |
| 1:G:450:PHE:HE2    | 14:G:837:CLA:HAB  | 1.60                     | 0.64              |
| 1:Y:352:TRP:HB3    | 14:Y:805:CLA:HAC1 | 1.79                     | 0.64              |
| 14:Y:842:CLA:HHD   | 17:Y:856:BCR:H383 | 1.78                     | 0.64              |
| 1:A:189:TRP:CZ2    | 14:A:810:CLA:HMA1 | 2.32                     | 0.64              |
| 14:U:1003:CLA:H101 | 14:Y:832:CLA:H42  | 1.78                     | 0.64              |
| 3:C:9:THR:HG23     | 3:C:63:SER:OG     | 1.98                     | 0.64              |
| 14:G:821:CLA:HED2  | 14:G:824:CLA:HED2 | 1.78                     | 0.64              |
| 17:G:854:BCR:H331  | 17:G:854:BCR:C8   | 2.23                     | 0.64              |
| 14:Z:832:CLA:ND    | 14:Z:833:CLA:HAB  | 2.13                     | 0.64              |
| 14:B:840:CLA:HBB2  | 15:B:842:PQN:H141 | 1.78                     | 0.64              |
| 1:G:212:TRP:N      | 14:G:814:CLA:HAB  | 2.13                     | 0.64              |
| 14:H:824:CLA:HMA1  | 17:H:844:BCR:H14C | 1.80                     | 0.64              |
| 9:K:39:LYS:HG3     | 9:K:59:LEU:HD22   | 1.78                     | 0.64              |
| 14:Z:801:CLA:H3A   | 14:Z:801:CLA:CGA  | 2.28                     | 0.64              |
| 1:A:106:ASP:O      | 1:A:110:ILE:HG22  | 1.98                     | 0.64              |
| 1:A:738:GLY:O      | 1:A:742:THR:OG1   | 2.15                     | 0.64              |
| 14:A:808:CLA:HMC2  | 14:A:828:CLA:H141 | 1.79                     | 0.64              |
| 14:B:829:CLA:H112  | 19:B:849:LMG:H202 | 1.80                     | 0.64              |
| 14:G:808:CLA:HHC   | 14:G:808:CLA:HBB1 | 1.80                     | 0.64              |
| 17:H:844:BCR:H23C  | 17:H:844:BCR:H403 | 1.79                     | 0.64              |
| 10:U:86:ILE:O      | 10:U:90:THR:HG23  | 1.98                     | 0.64              |
| 14:G:803:CLA:H2    | 2:H:661:LEU:HD22  | 1.80                     | 0.64              |
| 14:Z:824:CLA:HAB   | 14:Z:832:CLA:HMA2 | 1.80                     | 0.64              |
| 2:Z:443:ASN:HB3    | 2:Z:455:GLN:HE21  | 1.63                     | 0.64              |
| 1:A:400:ILE:HG21   | 14:A:829:CLA:HAB  | 1.80                     | 0.64              |
| 6:F:27:ASP:OD2     | 6:F:33:LYS:NZ     | 2.28                     | 0.64              |
| 2:B:475:TYR:HB3    | 6:F:3:ALA:HA      | 1.79                     | 0.64              |
| 1:Y:642:SER:O      | 1:Y:648:GLY:HA3   | 1.97                     | 0.64              |
| 14:B:819:CLA:HMB2  | 14:B:824:CLA:HMA3 | 1.79                     | 0.64              |
| 2:H:676:TYR:OH     | 14:H:803:CLA:OBD  | 2.16                     | 0.64              |
| 8:S:31:ARG:NH1     | 14:S:1102:CLA:O1D | 2.30                     | 0.64              |
| 14:Y:827:CLA:C8    | 21:Y:904:HOH:O    | 2.31                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:Z:446:VAL:HG13   | 2:Z:454:LYS:HB2    | 1.80                     | 0.64              |
| 14:Z:839:CLA:HMC1  | 14:Z:839:CLA:HBC2  | 1.80                     | 0.64              |
| 1:A:300:HIS:CE1    | 1:A:304:ILE:HG13   | 2.32                     | 0.63              |
| 1:G:683:TRP:CE3    | 13:G:801:CL0:H4    | 2.33                     | 0.63              |
| 14:H:825:CLA:HMB1  | 14:H:825:CLA:HBB1  | 1.80                     | 0.63              |
| 1:Y:313:HIS:CE1    | 17:Y:846:BCR:H363  | 2.33                     | 0.63              |
| 2:B:664:ALA:O      | 14:B:804:CLA:HAB   | 1.98                     | 0.63              |
| 1:G:675:LEU:HD21   | 14:G:828:CLA:H143  | 1.79                     | 0.63              |
| 1:G:460:VAL:CG2    | 14:G:833:CLA:HMC3  | 2.28                     | 0.63              |
| 17:J:103:BCR:HC8   | 17:J:103:BCR:H321  | 1.79                     | 0.63              |
| 6:Q:56:ARG:HG2     | 12:W:31:PHE:HE1    | 1.62                     | 0.63              |
| 1:Y:27:LYS:HD3     | 14:Y:811:CLA:HMA2  | 1.80                     | 0.63              |
| 2:B:500:LEU:HG     | 2:B:504:LEU:HD12   | 1.80                     | 0.63              |
| 2:H:503:TRP:CZ2    | 14:H:831:CLA:HED1  | 2.34                     | 0.63              |
| 8:J:22:THR:HA      | 8:J:25:ILE:HD12    | 1.79                     | 0.63              |
| 1:Y:313:HIS:HE1    | 17:Y:846:BCR:H363  | 1.62                     | 0.63              |
| 1:A:460:VAL:O      | 1:A:464:THR:HG23   | 1.97                     | 0.63              |
| 14:G:826:CLA:HAB   | 17:G:849:BCR:H311  | 1.81                     | 0.63              |
| 9:K:65:PHE:O       | 9:K:68:LEU:HD23    | 1.98                     | 0.63              |
| 1:Y:46:THR:HA      | 1:Y:49:TRP:HD1     | 1.63                     | 0.63              |
| 2:Z:264:THR:HG22   | 2:Z:363:PHE:CZ     | 2.34                     | 0.63              |
| 14:B:830:CLA:H3A   | 14:B:831:CLA:OBD   | 1.99                     | 0.63              |
| 1:G:272:TRP:CH2    | 14:G:817:CLA:HBB1  | 2.34                     | 0.63              |
| 1:Y:680:HIS:HB3    | 14:Y:854:CLA:HBD   | 1.79                     | 0.63              |
| 1:A:395:THR:HG22   | 1:A:610:ILE:HB     | 1.79                     | 0.63              |
| 1:G:588:GLN:HG3    | 2:H:673:TRP:HB2    | 1.81                     | 0.63              |
| 14:H:828:CLA:HMB1  | 14:H:828:CLA:HBB1  | 1.80                     | 0.63              |
| 14:V:1201:CLA:HMB2 | 17:V:1202:BCR:H333 | 1.80                     | 0.63              |
| 14:Y:806:CLA:H151  | 14:Y:829:CLA:HBB2  | 1.81                     | 0.63              |
| 2:Z:72:ASN:O       | 2:Z:76:TRP:HB2     | 1.98                     | 0.63              |
| 1:A:683:TRP:CD2    | 13:A:801:CL0:H5    | 2.34                     | 0.63              |
| 1:A:392:SER:HB2    | 14:A:828:CLA:HMA1  | 1.80                     | 0.63              |
| 17:B:847:BCR:H311  | 17:B:847:BCR:HC8   | 1.79                     | 0.63              |
| 14:G:802:CLA:H141  | 14:S:1101:CLA:H201 | 1.81                     | 0.63              |
| 2:H:156:LEU:O      | 2:H:161:ARG:NH1    | 2.29                     | 0.63              |
| 17:U:1005:BCR:C8   | 17:U:1005:BCR:H331 | 2.29                     | 0.63              |
| 14:Z:817:CLA:H41   | 17:Z:845:BCR:H353  | 1.80                     | 0.63              |
| 1:A:650:LEU:HD23   | 2:B:638:ILE:HD11   | 1.79                     | 0.63              |
| 2:H:275:HIS:HB2    | 14:H:816:CLA:C1B   | 2.28                     | 0.63              |
| 14:Y:841:CLA:H91   | 17:Z:846:BCR:C19   | 2.29                     | 0.63              |
| 14:Y:855:CLA:H201  | 14:Z:839:CLA:H62   | 1.81                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:97:PHE:HB3    | 1:G:116:VAL:HG23  | 1.80                     | 0.63              |
| 2:H:60:VAL:HG13   | 2:H:141:LEU:HD13  | 1.79                     | 0.63              |
| 1:A:514:GLY:HA2   | 1:A:528:PRO:HB3   | 1.80                     | 0.62              |
| 2:B:383:GLY:HA3   | 2:B:589:MET:HE2   | 1.80                     | 0.62              |
| 1:G:280:THR:OG1   | 1:G:281:PHE:N     | 2.32                     | 0.62              |
| 14:H:836:CLA:HBB1 | 14:H:836:CLA:HHC  | 1.80                     | 0.62              |
| 14:Y:804:CLA:HBC2 | 14:Y:830:CLA:H43  | 1.80                     | 0.62              |
| 14:Z:805:CLA:HBB1 | 14:Z:805:CLA:HMB1 | 1.81                     | 0.62              |
| 14:B:819:CLA:CMB  | 14:B:824:CLA:HMA3 | 2.29                     | 0.62              |
| 2:H:674:ARG:HD2   | 2:H:707:SER:HA    | 1.80                     | 0.62              |
| 14:H:808:CLA:CMA  | 14:H:809:CLA:HAB  | 2.25                     | 0.62              |
| 7:I:21:LEU:HD13   | 2:Z:146:SER:O     | 58.64                    | 0.62              |
| 1:Y:699:GLU:OE1   | 2:Z:542:LYS:NZ    | 2.22                     | 0.62              |
| 14:Z:804:CLA:O1A  | 14:Z:804:CLA:HMA2 | 1.99                     | 0.62              |
| 17:F:201:BCR:H383 | 17:F:201:BCR:H23C | 1.81                     | 0.62              |
| 2:Z:166:TRP:HD1   | 14:Z:810:CLA:HED3 | 1.63                     | 0.62              |
| 1:A:375:TYR:OH    | 14:A:836:CLA:HBC3 | 1.99                     | 0.62              |
| 2:B:472:LYS:HG2   | 2:B:475:TYR:CE2   | 2.34                     | 0.62              |
| 1:G:581:PRO:HD2   | 3:N:51:LYS:HG3    | 1.80                     | 0.62              |
| 1:G:718:GLN:NE2   | 5:P:15:TYR:OH     | 2.33                     | 0.62              |
| 14:A:806:CLA:HBC2 | 14:A:828:CLA:HMD1 | 1.81                     | 0.62              |
| 14:A:840:CLA:HBA1 | 18:A:850:LHG:H171 | 1.81                     | 0.62              |
| 14:A:852:CLA:HAB  | 2:B:588:TRP:CH2   | 2.35                     | 0.62              |
| 1:G:400:ILE:HG23  | 14:G:806:CLA:H143 | 1.82                     | 0.62              |
| 2:H:318:PHE:HB2   | 14:H:822:CLA:HMA1 | 1.80                     | 0.62              |
| 2:B:354:HIS:HB3   | 14:B:817:CLA:HED2 | 1.82                     | 0.62              |
| 1:G:583:ARG:HG2   | 3:N:48:VAL:HG13   | 1.81                     | 0.62              |
| 2:Z:303:MET:HA    | 14:Z:820:CLA:O1D  | 2.00                     | 0.62              |
| 2:B:536:THR:HB    | 2:B:588:TRP:HB3   | 1.80                     | 0.62              |
| 2:H:178:LEU:HA    | 2:H:182:PHE:HB2   | 1.81                     | 0.62              |
| 14:Z:833:CLA:C4C  | 14:Z:834:CLA:HAB  | 2.30                     | 0.62              |
| 14:A:827:CLA:HMA1 | 14:A:834:CLA:H52  | 1.82                     | 0.62              |
| 1:G:220:SER:O     | 1:G:224:ASN:ND2   | 2.33                     | 0.62              |
| 14:H:803:CLA:H121 | 17:H:845:BCR:H362 | 1.81                     | 0.62              |
| 14:G:807:CLA:CBB  | 17:G:854:BCR:H392 | 2.29                     | 0.62              |
| 1:A:99:ASN:ND2    | 1:A:110:ILE:HD11  | 2.13                     | 0.62              |
| 1:A:511:VAL:HG23  | 1:A:526:MET:HG3   | 1.82                     | 0.62              |
| 17:A:845:BCR:H362 | 17:A:846:BCR:C11  | 2.30                     | 0.62              |
| 2:B:304:MET:HG3   | 2:B:322:HIS:O     | 2.00                     | 0.62              |
| 1:G:384:ALA:HB1   | 1:G:525:ALA:O     | 1.99                     | 0.62              |
| 14:H:831:CLA:HBB1 | 14:H:831:CLA:HMB1 | 1.80                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Y:850:BCR:H382 | 17:Y:850:BCR:H23C | 1.81                     | 0.62              |
| 14:A:834:CLA:HMD2 | 14:A:835:CLA:CAB  | 2.30                     | 0.61              |
| 2:B:498:VAL:O     | 2:B:501:PRO:HD2   | 2.00                     | 0.61              |
| 10:L:35:PRO:HB2   | 10:L:50:VAL:HG23  | 1.81                     | 0.61              |
| 1:Y:84:PHE:CZ     | 14:Y:805:CLA:H91  | 2.34                     | 0.61              |
| 2:Z:652:TRP:HE3   | 2:Z:729:ALA:HA    | 1.64                     | 0.61              |
| 14:Z:817:CLA:H111 | 14:Z:821:CLA:H41  | 1.81                     | 0.61              |
| 14:B:830:CLA:HBB2 | 14:B:839:CLA:HBB1 | 1.82                     | 0.61              |
| 14:H:808:CLA:H52  | 14:H:826:CLA:H193 | 1.82                     | 0.61              |
| 2:H:166:TRP:CZ2   | 14:H:810:CLA:HMA1 | 2.34                     | 0.61              |
| 2:Z:430:LEU:HD11  | 17:Z:846:BCR:H402 | 1.82                     | 0.61              |
| 2:H:397:LEU:HD12  | 2:H:544:ALA:O     | 2.01                     | 0.61              |
| 1:Y:592:TRP:O     | 1:Y:595:VAL:HG22  | 1.99                     | 0.61              |
| 2:B:385:LEU:HD21  | 14:B:807:CLA:H142 | 1.81                     | 0.61              |
| 14:B:825:CLA:HMA1 | 17:B:847:BCR:H14C | 1.83                     | 0.61              |
| 1:G:366:LEU:HD13  | 14:G:827:CLA:H42  | 1.81                     | 0.61              |
| 14:G:807:CLA:CAB  | 17:G:854:BCR:H392 | 2.30                     | 0.61              |
| 3:N:16:CYS:HB2    | 16:N:102:SF4:S4   | 2.41                     | 0.61              |
| 14:A:823:CLA:HMB3 | 14:A:842:CLA:C2C  | 2.30                     | 0.61              |
| 2:B:294:PHE:O     | 2:B:296:ILE:N     | 2.33                     | 0.61              |
| 2:B:580:ASP:OD1   | 2:B:712:ARG:NH1   | 2.33                     | 0.61              |
| 14:B:805:CLA:HAB  | 14:B:807:CLA:CAD  | 2.30                     | 0.61              |
| 13:G:801:CL0:H15  | 13:G:801:CL0:H11  | 1.81                     | 0.61              |
| 2:H:334:HIS:CE1   | 14:H:828:CLA:HED1 | 2.35                     | 0.61              |
| 2:B:44:LYS:NZ     | 11:M:29:LEU:O     | 2.31                     | 0.61              |
| 4:O:60:ARG:HB2    | 4:O:63:GLN:HG3    | 1.82                     | 0.61              |
| 14:Z:835:CLA:HBB1 | 14:Z:835:CLA:HMB1 | 1.81                     | 0.61              |
| 2:B:401:TYR:O     | 4:D:126:SER:OG    | 2.19                     | 0.61              |
| 1:G:275:TYR:CE1   | 14:G:815:CLA:HMD2 | 2.35                     | 0.61              |
| 1:G:307:LEU:HD12  | 14:G:818:CLA:HBC2 | 1.83                     | 0.61              |
| 14:Y:806:CLA:HMA1 | 14:Y:830:CLA:CAB  | 2.31                     | 0.61              |
| 1:Y:337:THR:HG21  | 18:Y:853:LHG:O1   | 2.00                     | 0.61              |
| 1:A:56:HIS:ND1    | 14:A:805:CLA:HAB  | 2.16                     | 0.61              |
| 14:A:852:CLA:H11  | 2:B:622:LEU:HD12  | 1.82                     | 0.61              |
| 1:G:308:PHE:HE1   | 14:G:821:CLA:HAB  | 1.64                     | 0.61              |
| 2:H:487:ILE:HG22  | 14:H:832:CLA:HMD3 | 1.81                     | 0.61              |
| 1:Y:202:ALA:HB2   | 1:Y:312:GLY:HA3   | 1.82                     | 0.61              |
| 14:Y:829:CLA:C3D  | 14:Y:829:CLA:H51  | 2.31                     | 0.61              |
| 2:Z:301:LYS:NZ    | 2:Z:327:GLU:OE2   | 2.33                     | 0.61              |
| 14:Z:811:CLA:H143 | 14:Z:826:CLA:HMD2 | 1.81                     | 0.61              |
| 1:G:466:ARG:NH2   | 1:G:645:THR:HG21  | 2.15                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:I:21:LEU:O       | 7:I:25:VAL:HG23    | 2.01                     | 0.61              |
| 1:Y:450:PHE:CE1    | 14:Y:838:CLA:HAB   | 2.33                     | 0.61              |
| 14:Y:807:CLA:HMA1  | 14:Y:808:CLA:HMB3  | 1.82                     | 0.61              |
| 2:Z:640:GLY:HA2    | 2:Z:647:ASN:HD21   | 1.66                     | 0.61              |
| 1:A:431:ASP:OD1    | 4:D:46:ALA:N       | 2.32                     | 0.61              |
| 14:A:804:CLA:H91   | 17:J:104:BCR:H381  | 1.82                     | 0.61              |
| 2:B:339:TRP:CE2    | 14:B:826:CLA:H91   | 2.36                     | 0.61              |
| 14:G:826:CLA:O1A   | 14:G:836:CLA:HMA1  | 2.01                     | 0.61              |
| 14:U:1003:CLA:HMA1 | 14:U:1004:CLA:HBC1 | 1.82                     | 0.61              |
| 10:U:65:LEU:HB3    | 14:Y:834:CLA:HMA2  | 1.81                     | 0.61              |
| 2:Z:219:ALA:HB1    | 2:Z:223:PRO:HG2    | 1.83                     | 0.61              |
| 2:Z:318:PHE:HB2    | 14:Z:821:CLA:HMA1  | 1.83                     | 0.61              |
| 10:U:35:PRO:HG2    | 14:U:1003:CLA:HED2 | 1.83                     | 0.61              |
| 14:Y:855:CLA:CAB   | 2:Z:665:THR:HG22   | 2.31                     | 0.61              |
| 1:A:189:TRP:CZ2    | 14:A:813:CLA:HAC2  | 2.36                     | 0.60              |
| 2:B:442:HIS:CD2    | 2:B:456:ILE:HG13   | 2.36                     | 0.60              |
| 1:G:733:ALA:HA     | 18:G:851:LHG:H341  | 1.83                     | 0.60              |
| 14:Y:826:CLA:H71   | 14:Y:835:CLA:HAB   | 1.81                     | 0.60              |
| 1:Y:392:SER:HB2    | 14:Y:828:CLA:HMA1  | 1.83                     | 0.60              |
| 2:Z:178:LEU:O      | 2:Z:283:PHE:HB3    | 2.00                     | 0.60              |
| 1:A:323:HIS:HB3    | 1:A:328:ILE:HD11   | 1.83                     | 0.60              |
| 14:A:833:CLA:H41   | 14:A:841:CLA:HBC2  | 1.82                     | 0.60              |
| 2:B:210:ASN:O      | 2:B:214:THR:HG22   | 2.00                     | 0.60              |
| 2:B:491:ALA:HB2    | 2:B:497:ASN:HD21   | 1.66                     | 0.60              |
| 1:G:280:THR:OG1    | 1:G:282:ASN:ND2    | 2.34                     | 0.60              |
| 1:G:535:ASP:O      | 1:G:539:HIS:ND1    | 2.32                     | 0.60              |
| 1:Y:683:TRP:CG     | 13:Y:801:CL0:H5    | 2.36                     | 0.60              |
| 2:Z:188:ALA:O      | 14:Z:812:CLA:HMC3  | 2.01                     | 0.60              |
| 13:A:801:CL0:H13   | 14:A:852:CLA:CAD   | 2.31                     | 0.60              |
| 2:B:387:VAL:HG11   | 2:B:586:MET:HG2    | 1.83                     | 0.60              |
| 2:B:53:LEU:HD22    | 14:B:813:CLA:HED2  | 1.82                     | 0.60              |
| 14:B:808:CLA:H122  | 17:I:101:BCR:HC21  | 1.82                     | 0.60              |
| 1:Y:601:TRP:HE1    | 14:Y:855:CLA:C1D   | 2.14                     | 0.60              |
| 2:Z:200:GLU:OE2    | 2:Z:205:HIS:CE1    | 2.53                     | 0.60              |
| 1:A:79:HIS:CD2     | 14:A:805:CLA:HMA1  | 2.37                     | 0.60              |
| 14:H:808:CLA:HMA1  | 14:H:809:CLA:CAB   | 2.26                     | 0.60              |
| 14:T:101:CLA:HMC1  | 14:T:101:CLA:HBC3  | 1.84                     | 0.60              |
| 14:Y:818:CLA:HBB1  | 14:Y:818:CLA:HMB1  | 1.82                     | 0.60              |
| 2:B:236:PRO:HA     | 2:B:252:ALA:HB3    | 1.82                     | 0.60              |
| 14:A:822:CLA:HBA2  | 9:K:35:GLN:CD      | 2.21                     | 0.60              |
| 14:U:1002:CLA:H202 | 14:U:1002:CLA:CGA  | 2.32                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:Y:817:CLA:HMC1 | 14:Y:817:CLA:HBC2  | 1.83                     | 0.60              |
| 14:A:837:CLA:HBB2 | 14:A:838:CLA:HBC3  | 1.84                     | 0.60              |
| 14:A:852:CLA:HMD3 | 14:B:803:CLA:O1A   | 2.01                     | 0.60              |
| 14:G:818:CLA:HMB1 | 14:G:818:CLA:HBB1  | 1.84                     | 0.60              |
| 17:H:841:BCR:H23C | 17:H:841:BCR:H382  | 1.84                     | 0.60              |
| 6:Q:1:ASP:N       | 6:Q:5:LEU:O        | 2.22                     | 0.60              |
| 14:B:803:CLA:HHC  | 14:B:803:CLA:HBB1  | 1.83                     | 0.60              |
| 1:G:375:TYR:CZ    | 14:G:836:CLA:HBC3  | 2.36                     | 0.60              |
| 2:Z:447:VAL:HG13  | 2:Z:452:PRO:HG3    | 1.83                     | 0.60              |
| 5:E:39:ARG:HA     | 5:E:57:THR:HG22    | 1.84                     | 0.60              |
| 1:Y:149:ALA:HB2   | 1:Y:381:PRO:HD2    | 1.83                     | 0.60              |
| 1:Y:344:LEU:HA    | 1:Y:347:VAL:HB     | 1.84                     | 0.60              |
| 17:Z:843:BCR:H23C | 17:Z:843:BCR:H383  | 1.82                     | 0.60              |
| 1:A:543:ALA:HB1   | 14:A:837:CLA:HMB3  | 1.83                     | 0.60              |
| 14:B:810:CLA:HMB3 | 14:L:202:CLA:CHC   | 2.32                     | 0.60              |
| 3:N:51:LYS:O      | 3:N:55:THR:HG23    | 2.01                     | 0.60              |
| 17:U:1007:BCR:C8  | 17:U:1007:BCR:H331 | 2.32                     | 0.60              |
| 1:Y:74:SER:HA     | 1:Y:77:PHE:HD2     | 1.66                     | 0.60              |
| 1:A:123:GLN:O     | 1:A:126:LEU:HG     | 2.02                     | 0.59              |
| 14:A:826:CLA:HBB2 | 17:A:848:BCR:H311  | 1.81                     | 0.59              |
| 1:A:142:GLY:O     | 14:A:829:CLA:HED1  | 2.02                     | 0.59              |
| 2:H:710:GLN:HG3   | 19:H:846:LMG:H111  | 1.82                     | 0.59              |
| 1:A:683:TRP:O     | 1:A:686:SER:OG     | 2.11                     | 0.59              |
| 14:A:803:CLA:HMB1 | 14:A:803:CLA:HBB1  | 1.84                     | 0.59              |
| 1:A:744:TRP:NE1   | 14:A:828:CLA:O1A   | 2.35                     | 0.59              |
| 2:H:29:ASP:OD2    | 2:H:32:SER:OG      | 2.13                     | 0.59              |
| 14:G:842:CLA:H61  | 14:H:837:CLA:H43   | 1.84                     | 0.59              |
| 4:O:10:TYR:OH     | 4:O:44:ALA:O       | 2.19                     | 0.59              |
| 10:U:37:TYR:O     | 10:U:39:GLN:NE2    | 2.34                     | 0.59              |
| 1:Y:279:LEU:HD22  | 1:Y:299:HIS:HA     | 1.84                     | 0.59              |
| 1:G:403:PHE:O     | 14:G:830:CLA:HMC1  | 2.02                     | 0.59              |
| 2:H:465:PHE:CG    | 12:W:30:TYR:HD1    | 2.20                     | 0.59              |
| 2:Z:181:LEU:HD13  | 14:Z:811:CLA:HBB   | 1.84                     | 0.59              |
| 2:B:693:LEU:HD23  | 10:L:37:TYR:HE2    | 1.67                     | 0.59              |
| 1:A:268:PHE:HA    | 14:K:101:CLA:HAC1  | 1.83                     | 0.59              |
| 14:Y:829:CLA:C7   | 21:Y:907:HOH:O     | 2.51                     | 0.59              |
| 14:Y:833:CLA:H41  | 14:Y:842:CLA:HBC2  | 1.82                     | 0.59              |
| 17:Y:848:BCR:HC8  | 17:Y:848:BCR:H321  | 1.84                     | 0.59              |
| 14:A:829:CLA:H92  | 14:A:829:CLA:HMD2  | 1.84                     | 0.59              |
| 14:A:831:CLA:HMA1 | 14:A:832:CLA:O1D   | 2.02                     | 0.59              |
| 14:A:840:CLA:HHC  | 14:A:840:CLA:HBB1  | 1.83                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:391:ALA:O      | 2:B:395:ILE:HG13  | 2.02                     | 0.59              |
| 13:G:801:CL0:H13   | 14:H:801:CLA:CAD  | 2.32                     | 0.59              |
| 14:Z:832:CLA:C1D   | 14:Z:833:CLA:HAB  | 2.32                     | 0.59              |
| 14:B:837:CLA:HMB2  | 14:B:839:CLA:HED1 | 1.85                     | 0.59              |
| 1:A:44:THR:OG1     | 5:E:52:ALA:O      | 2.12                     | 0.59              |
| 2:H:518:ILE:HG22   | 2:H:522:ASP:OD2   | 2.02                     | 0.59              |
| 1:Y:740:ILE:HG21   | 14:Y:828:CLA:HMC2 | 1.83                     | 0.59              |
| 14:Y:843:CLA:HBB1  | 14:Y:843:CLA:HMB1 | 1.84                     | 0.59              |
| 14:Z:807:CLA:HAB   | 14:Z:808:CLA:HAA2 | 1.83                     | 0.59              |
| 1:A:681:PHE:CG     | 17:A:849:BCR:H363 | 2.38                     | 0.59              |
| 2:B:663:TRP:CE3    | 14:B:803:CLA:HMA1 | 2.38                     | 0.59              |
| 2:B:664:ALA:C      | 14:B:804:CLA:HAB  | 2.23                     | 0.59              |
| 14:B:819:CLA:H52   | 14:B:824:CLA:H91  | 1.84                     | 0.59              |
| 14:G:819:CLA:CBB   | 21:G:907:HOH:O    | 2.05                     | 0.59              |
| 1:Y:511:VAL:HG21   | 1:Y:518:VAL:HG23  | 1.85                     | 0.59              |
| 1:Y:565:LEU:HD13   | 2:Z:678:GLN:HG2   | 1.83                     | 0.59              |
| 1:Y:84:PHE:CE2     | 14:Y:805:CLA:H91  | 2.37                     | 0.59              |
| 14:Y:855:CLA:HAB   | 2:Z:665:THR:CA    | 2.32                     | 0.59              |
| 14:Y:854:CLA:CAB   | 2:Z:588:TRP:CH2   | 2.84                     | 0.59              |
| 14:Z:827:CLA:H2A   | 14:Z:827:CLA:HED2 | 1.84                     | 0.59              |
| 2:H:677:TRP:CH2    | 15:H:839:PQN:H2M3 | 2.37                     | 0.59              |
| 2:H:583:TYR:CE1    | 2:H:712:ARG:HB3   | 2.38                     | 0.59              |
| 3:N:20:CYS:HA      | 16:N:101:SF4:S4   | 2.43                     | 0.59              |
| 17:Y:849:BCR:H23C  | 17:Y:849:BCR:H403 | 1.85                     | 0.59              |
| 2:Z:329:TYR:HB3    | 14:Z:822:CLA:HBC3 | 1.83                     | 0.59              |
| 2:Z:470:HIS:HB3    | 14:Z:832:CLA:HED1 | 1.85                     | 0.59              |
| 1:A:523:LYS:HA     | 1:A:624:THR:HA    | 1.85                     | 0.59              |
| 2:H:728:ALA:O      | 2:H:732:ILE:HG12  | 2.03                     | 0.59              |
| 1:Y:683:TRP:CD2    | 13:Y:801:CL0:H5   | 2.38                     | 0.59              |
| 1:A:437:ARG:HH12   | 1:A:562:SER:HB2   | 1.68                     | 0.58              |
| 4:D:10:TYR:HD1     | 4:D:47:ALA:HB2    | 1.68                     | 0.58              |
| 2:H:119:VAL:HG22   | 2:H:123:TRP:CZ2   | 2.37                     | 0.58              |
| 2:H:276:HIS:HA     | 2:H:279:ILE:HG12  | 1.84                     | 0.58              |
| 1:Y:612:HIS:ND1    | 14:Y:837:CLA:HMC2 | 2.18                     | 0.58              |
| 1:A:79:HIS:NE2     | 14:A:805:CLA:HMA1 | 2.18                     | 0.58              |
| 5:E:23:VAL:HG12    | 5:E:38:VAL:HG22   | 1.83                     | 0.58              |
| 14:G:818:CLA:H43   | 14:G:834:CLA:HAA2 | 1.85                     | 0.58              |
| 2:H:318:PHE:CD1    | 14:H:821:CLA:HAB  | 2.38                     | 0.58              |
| 8:S:28:GLU:CD      | 8:S:31:ARG:NH2    | 2.56                     | 0.58              |
| 14:U:1004:CLA:HAB  | 14:Y:834:CLA:C9   | 2.33                     | 0.58              |
| 14:U:1004:CLA:HBB2 | 14:Y:833:CLA:HMC2 | 1.85                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:Y:444:LEU:HD13   | 14:Y:839:CLA:C3B  | 2.32                     | 0.58              |
| 1:A:579:ASP:OD2    | 3:C:52:ARG:NH2    | 2.32                     | 0.58              |
| 2:B:419:GLU:OE2    | 6:F:141:ARG:NH2   | 2.35                     | 0.58              |
| 14:B:806:CLA:O1A   | 14:B:806:CLA:HMA2 | 2.03                     | 0.58              |
| 1:G:237:PRO:HG2    | 1:G:242:PHE:CZ    | 2.38                     | 0.58              |
| 14:G:818:CLA:CHD   | 21:G:907:HOH:O    | 2.50                     | 0.58              |
| 2:H:662:VAL:HG22   | 14:H:838:CLA:HMB3 | 1.85                     | 0.58              |
| 14:Y:808:CLA:CHC   | 14:Y:809:CLA:HMD2 | 2.33                     | 0.58              |
| 14:A:841:CLA:HHC   | 14:A:841:CLA:HBB1 | 1.85                     | 0.58              |
| 14:B:835:CLA:CHD   | 14:B:836:CLA:HAB  | 2.33                     | 0.58              |
| 14:G:802:CLA:CGA   | 14:G:802:CLA:H3A  | 2.32                     | 0.58              |
| 2:Z:176:HIS:HB3    | 14:Z:811:CLA:CAB  | 2.33                     | 0.58              |
| 2:Z:351:VAL:HG12   | 14:Z:816:CLA:C2   | 2.33                     | 0.58              |
| 1:G:309:ILE:HG22   | 1:G:313:HIS:HE1   | 1.69                     | 0.58              |
| 1:G:698:GLN:NE2    | 1:G:720:ARG:HA    | 2.16                     | 0.58              |
| 14:H:826:CLA:H3A   | 14:H:826:CLA:CGA  | 2.33                     | 0.58              |
| 9:K:63:THR:O       | 9:K:67:HIS:ND1    | 2.36                     | 0.58              |
| 9:T:43:LEU:HG      | 9:T:57:PRO:HD2    | 1.84                     | 0.58              |
| 17:V:1202:BCR:H321 | 17:V:1202:BCR:HC8 | 1.84                     | 0.58              |
| 1:Y:527:MET:HB2    | 1:Y:528:PRO:HD2   | 1.86                     | 0.58              |
| 1:Y:602:MET:HG2    | 14:Y:826:CLA:HBC1 | 1.86                     | 0.58              |
| 14:Z:801:CLA:HMA1  | 14:Z:801:CLA:H51  | 1.85                     | 0.58              |
| 2:H:73:PHE:HB3     | 2:H:131:ASN:HD21  | 1.69                     | 0.58              |
| 2:H:721:VAL:O      | 2:H:725:LEU:HG    | 2.03                     | 0.58              |
| 1:Y:324:SER:O      | 1:Y:327:GLU:N     | 2.37                     | 0.58              |
| 1:Y:329:LEU:HD12   | 1:Y:345:TYR:HB2   | 1.84                     | 0.58              |
| 1:Y:681:PHE:CD2    | 17:Y:851:BCR:H363 | 2.38                     | 0.58              |
| 14:Y:854:CLA:H42   | 2:Z:441:VAL:HG22  | 1.85                     | 0.58              |
| 1:A:79:HIS:CE1     | 14:A:805:CLA:HMA1 | 2.38                     | 0.58              |
| 2:H:466:ILE:HD11   | 14:H:834:CLA:C2   | 2.34                     | 0.58              |
| 14:L:205:CLA:C1B   | 14:L:206:CLA:HED1 | 2.33                     | 0.58              |
| 3:N:33:CYS:SG      | 3:N:34:LYS:N      | 2.76                     | 0.58              |
| 1:Y:386:ASP:OD2    | 1:Y:389:THR:HG23  | 2.04                     | 0.58              |
| 1:Y:619:SER:OG     | 1:Y:639:PHE:HB2   | 2.04                     | 0.58              |
| 1:A:189:TRP:CD1    | 14:A:812:CLA:HED2 | 2.39                     | 0.58              |
| 1:A:189:TRP:CE2    | 14:A:813:CLA:HAC2 | 2.39                     | 0.58              |
| 1:G:702:GLU:O      | 1:G:705:VAL:HG22  | 2.04                     | 0.58              |
| 14:H:805:CLA:HED1  | 14:H:828:CLA:H43  | 1.85                     | 0.58              |
| 14:H:809:CLA:O2A   | 10:U:148:ILE:HG23 | 2.04                     | 0.58              |
| 1:Y:689:PHE:HA     | 15:Y:844:PQN:H9   | 1.84                     | 0.58              |
| 1:A:253:TYR:HB2    | 1:A:258:TRP:HZ2   | 1.68                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:A:846:BCR:HC8   | 17:A:846:BCR:H321 | 1.85                     | 0.58              |
| 14:H:806:CLA:HBB   | 14:H:807:CLA:HMB3 | 1.84                     | 0.58              |
| 17:S:1104:BCR:H403 | 17:S:1104:BCR:C23 | 2.33                     | 0.58              |
| 2:Z:166:TRP:CD1    | 14:Z:810:CLA:HED3 | 2.39                     | 0.58              |
| 1:A:218:HIS:O      | 1:A:222:PRO:HG2   | 2.03                     | 0.58              |
| 1:A:255:LYS:NZ     | 1:A:273:ALA:O     | 2.31                     | 0.58              |
| 1:A:651:ARG:HB2    | 2:B:638:ILE:HG13  | 1.86                     | 0.58              |
| 14:H:832:CLA:NC    | 14:H:833:CLA:HAB  | 2.18                     | 0.58              |
| 17:L:208:BCR:C23   | 17:L:208:BCR:H403 | 2.33                     | 0.58              |
| 2:Z:724:ILE:HD13   | 14:Z:825:CLA:HMC2 | 1.86                     | 0.58              |
| 14:A:818:CLA:H62   | 14:A:835:CLA:HMA2 | 1.85                     | 0.57              |
| 14:B:832:CLA:HAB   | 14:B:833:CLA:HMB2 | 1.86                     | 0.57              |
| 14:B:838:CLA:HMB2  | 14:B:839:CLA:C2D  | 2.33                     | 0.57              |
| 1:G:593:ASP:HA     | 1:G:596:PHE:HB3   | 1.86                     | 0.57              |
| 14:G:819:CLA:H202  | 14:G:834:CLA:H51  | 1.85                     | 0.57              |
| 10:L:62:TRP:O      | 10:L:66:GLY:HA3   | 2.03                     | 0.57              |
| 1:Y:399:TRP:HE1    | 14:Y:828:CLA:HAB  | 1.67                     | 0.57              |
| 14:Y:806:CLA:HMA1  | 14:Y:830:CLA:HAB  | 1.86                     | 0.57              |
| 14:Y:840:CLA:HMB1  | 14:Y:840:CLA:HBB1 | 1.85                     | 0.57              |
| 2:Z:126:ILE:HG22   | 14:Z:816:CLA:HED2 | 1.85                     | 0.57              |
| 2:B:288:HIS:O      | 14:B:820:CLA:HED1 | 2.04                     | 0.57              |
| 2:B:548:ARG:HD3    | 6:F:141:ARG:OXT   | 2.04                     | 0.57              |
| 2:H:239:ALA:O      | 2:H:262:PRO:HG2   | 2.04                     | 0.57              |
| 14:Y:831:CLA:HMB2  | 14:Y:832:CLA:C1D  | 2.34                     | 0.57              |
| 2:Z:45:ILE:HG21    | 14:Z:804:CLA:H201 | 1.85                     | 0.57              |
| 1:A:216:GLN:O      | 1:A:220:SER:OG    | 2.09                     | 0.57              |
| 1:A:701:ILE:HA     | 1:A:704:ILE:HD12  | 1.86                     | 0.57              |
| 2:B:667:PHE:HB3    | 14:B:804:CLA:HMC3 | 1.85                     | 0.57              |
| 1:G:699:GLU:O      | 1:G:702:GLU:HB2   | 2.04                     | 0.57              |
| 2:H:341:LEU:HG     | 14:H:804:CLA:HED1 | 1.87                     | 0.57              |
| 2:H:668:MET:O      | 2:H:672:SER:OG    | 2.18                     | 0.57              |
| 17:I:101:BCR:C31   | 14:Z:806:CLA:H203 | 68.03                    | 0.57              |
| 11:M:22:ALA:O      | 11:M:26:SER:OG    | 2.22                     | 0.57              |
| 3:N:23:ASP:HB3     | 4:O:61:LYS:HE2    | 1.85                     | 0.57              |
| 1:Y:461:HIS:CE1    | 1:Y:465:MET:HE1   | 2.38                     | 0.57              |
| 1:Y:487:ALA:O      | 1:Y:491:GLN:HG3   | 2.04                     | 0.57              |
| 2:Z:243:PHE:CD1    | 2:Z:264:THR:HG21  | 2.39                     | 0.57              |
| 2:Z:592:THR:O      | 2:Z:596:VAL:HG23  | 2.03                     | 0.57              |
| 2:Z:652:TRP:O      | 2:Z:656:PHE:HB2   | 2.04                     | 0.57              |
| 14:Z:827:CLA:HMB1  | 14:Z:827:CLA:HBB1 | 1.85                     | 0.57              |
| 14:A:821:CLA:HMA2  | 14:A:825:CLA:C1C  | 2.35                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:663:TRP:CD2    | 14:B:803:CLA:HMA2  | 2.40                     | 0.57              |
| 6:F:100:ILE:HG22   | 8:J:10:THR:HG22    | 1.86                     | 0.57              |
| 2:H:318:PHE:HA     | 14:H:821:CLA:CAB   | 2.34                     | 0.57              |
| 2:H:122:TRP:HA     | 2:H:361:TYR:CD1    | 2.39                     | 0.57              |
| 2:H:440:TYR:CZ     | 2:H:524:LEU:HB3    | 2.40                     | 0.57              |
| 2:H:548:ARG:NH2    | 4:O:124:ASN:OD1    | 2.37                     | 0.57              |
| 14:H:835:CLA:CMA   | 14:H:836:CLA:HED2  | 2.34                     | 0.57              |
| 17:I:101:BCR:H382  | 17:I:101:BCR:H23C  | 1.85                     | 0.57              |
| 1:Y:677:LEU:HB3    | 14:Y:854:CLA:H2    | 1.87                     | 0.57              |
| 1:A:162:ALA:O      | 1:A:166:LEU:HG     | 2.05                     | 0.57              |
| 1:G:399:TRP:HB3    | 14:G:828:CLA:HMC3  | 1.86                     | 0.57              |
| 2:H:198:ILE:HG12   | 2:H:269:LEU:HB3    | 1.86                     | 0.57              |
| 2:H:347:ILE:HA     | 2:H:350:LEU:HB3    | 1.86                     | 0.57              |
| 10:U:63:VAL:HG22   | 10:U:75:ASN:HA     | 1.87                     | 0.57              |
| 2:Z:269:LEU:HD12   | 2:Z:269:LEU:H      | 1.70                     | 0.57              |
| 1:A:367:SER:O      | 1:A:397:HIS:HB3    | 2.05                     | 0.57              |
| 1:G:445:ASN:ND2    | 14:H:803:CLA:HED3  | 2.20                     | 0.57              |
| 2:H:640:GLY:HA2    | 2:H:647:ASN:HD21   | 1.69                     | 0.57              |
| 1:Y:362:MET:O      | 1:Y:366:LEU:HB2    | 2.05                     | 0.57              |
| 1:Y:456:PHE:CE1    | 14:Y:802:CLA:HMA1  | 2.39                     | 0.57              |
| 14:Y:819:CLA:CHA   | 21:Y:907:HOH:O     | 2.49                     | 0.57              |
| 2:B:217:HIS:HB2    | 2:B:253:ILE:HD13   | 1.86                     | 0.57              |
| 14:B:821:CLA:C2B   | 14:B:822:CLA:HMD2  | 2.35                     | 0.57              |
| 1:G:674:LEU:O      | 14:H:801:CLA:H62   | 2.05                     | 0.57              |
| 2:H:443:ASN:HB3    | 2:H:455:GLN:HE21   | 1.70                     | 0.57              |
| 7:I:19:CYS:HB3     | 14:L:202:CLA:HBB2  | 1.86                     | 0.57              |
| 2:H:453:GLU:HA     | 6:Q:48:LEU:HD22    | 1.86                     | 0.57              |
| 1:Y:294:LEU:HA     | 1:Y:297:THR:HG22   | 1.85                     | 0.57              |
| 1:Y:661:VAL:HG21   | 1:Y:746:PHE:HA     | 1.86                     | 0.57              |
| 2:Z:62:GLY:HA3     | 14:Z:806:CLA:HAB   | 1.86                     | 0.57              |
| 1:G:281:PHE:O      | 1:G:505:ALA:HA     | 2.04                     | 0.57              |
| 1:G:365:SER:O      | 1:G:369:ILE:HG13   | 2.04                     | 0.57              |
| 14:G:804:CLA:HBC1  | 18:G:851:LHG:H142  | 1.86                     | 0.57              |
| 1:G:536:PHE:HA     | 14:G:837:CLA:HED2  | 1.87                     | 0.57              |
| 2:H:525:VAL:HG11   | 2:H:599:TYR:HB2    | 1.86                     | 0.57              |
| 17:R:101:BCR:H23C  | 17:R:101:BCR:H382  | 1.85                     | 0.57              |
| 17:U:1005:BCR:H392 | 17:U:1005:BCR:H23C | 1.87                     | 0.57              |
| 1:Y:471:PRO:HA     | 1:Y:474:MET:HE2    | 1.85                     | 0.57              |
| 1:Y:56:HIS:CG      | 14:Y:805:CLA:HAB   | 2.40                     | 0.57              |
| 1:Y:321:ILE:HB     | 14:Y:822:CLA:HMD1  | 1.87                     | 0.57              |
| 14:Z:805:CLA:HHB   | 14:Z:827:CLA:CBB   | 2.35                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:Z:596:VAL:CG1    | 14:Z:835:CLA:HAB   | 2.33                     | 0.57              |
| 1:A:14:VAL:CG2     | 14:A:810:CLA:HMA2  | 2.35                     | 0.57              |
| 14:A:811:CLA:HBB1  | 14:A:811:CLA:HHC   | 1.85                     | 0.57              |
| 1:G:443:HIS:O      | 1:G:447:VAL:HG23   | 2.04                     | 0.57              |
| 14:G:805:CLA:H62   | 14:G:813:CLA:H12   | 1.87                     | 0.57              |
| 14:G:821:CLA:HMB3  | 14:G:825:CLA:HED2  | 1.87                     | 0.57              |
| 1:G:97:PHE:O       | 1:G:114:ALA:HA     | 2.05                     | 0.57              |
| 2:H:241:HIS:CE1    | 2:H:249:ALA:HB2    | 2.39                     | 0.57              |
| 2:H:677:TRP:CZ2    | 15:H:839:PQN:H2M3  | 2.40                     | 0.57              |
| 4:O:67:LEU:O       | 4:O:71:GLN:HB2     | 2.04                     | 0.57              |
| 14:H:806:CLA:HED2  | 7:R:11:PRO:HB3     | 1.87                     | 0.57              |
| 1:Y:297:THR:O      | 1:Y:301:HIS:CD2    | 2.58                     | 0.57              |
| 14:Z:806:CLA:HMA1  | 14:Z:807:CLA:CMB   | 2.34                     | 0.57              |
| 14:B:825:CLA:C2B   | 17:B:847:BCR:H363  | 2.35                     | 0.57              |
| 14:G:818:CLA:H101  | 14:G:818:CLA:HMC2  | 1.86                     | 0.57              |
| 2:H:193:LEU:HA     | 2:H:197:ALA:HB3    | 1.87                     | 0.57              |
| 2:H:442:HIS:CD2    | 2:H:456:ILE:HG13   | 2.40                     | 0.57              |
| 14:V:1201:CLA:HBB1 | 14:V:1201:CLA:HMB1 | 1.87                     | 0.57              |
| 14:A:806:CLA:HMA1  | 14:A:830:CLA:HAB   | 1.86                     | 0.56              |
| 14:A:806:CLA:H91   | 18:A:850:LHG:H331  | 1.87                     | 0.56              |
| 2:B:663:TRP:CE2    | 14:B:803:CLA:HMA2  | 2.40                     | 0.56              |
| 1:G:157:GLN:O      | 1:G:161:THR:HG23   | 2.04                     | 0.56              |
| 1:G:223:ILE:HG23   | 1:G:236:ILE:HD13   | 1.87                     | 0.56              |
| 1:Y:484:PRO:HD2    | 1:Y:488:GLN:NE2    | 2.20                     | 0.56              |
| 2:Z:380:TYR:CD1    | 14:Z:825:CLA:HAB   | 2.40                     | 0.56              |
| 2:Z:625:TRP:O      | 2:Z:629:TYR:HB3    | 2.04                     | 0.56              |
| 17:A:848:BCR:H382  | 17:A:848:BCR:H23C  | 1.86                     | 0.56              |
| 14:H:807:CLA:HMC3  | 14:H:808:CLA:C3D   | 2.35                     | 0.56              |
| 14:H:835:CLA:H93   | 14:H:836:CLA:HBC1  | 1.87                     | 0.56              |
| 1:Y:497:ALA:HB3    | 1:Y:498:PRO:HD3    | 1.86                     | 0.56              |
| 2:Z:351:VAL:HG12   | 14:Z:816:CLA:C3    | 2.35                     | 0.56              |
| 2:Z:542:LYS:HD3    | 2:Z:543:GLY:N      | 2.20                     | 0.56              |
| 2:B:149:LEU:HD22   | 11:M:22:ALA:HA     | 1.86                     | 0.56              |
| 2:B:651:VAL:HG21   | 14:B:809:CLA:HAC1  | 1.86                     | 0.56              |
| 14:H:822:CLA:HAB   | 14:H:829:CLA:HMD2  | 1.87                     | 0.56              |
| 17:L:209:BCR:C38   | 17:L:209:BCR:H23C  | 2.35                     | 0.56              |
| 2:H:555:ASP:OD2    | 3:N:65:ARG:NH1     | 2.38                     | 0.56              |
| 8:S:41:LEU:HA      | 14:S:1103:CLA:HED1 | 1.86                     | 0.56              |
| 1:Y:70:ARG:HG2     | 1:Y:184:ALA:HB1    | 1.87                     | 0.56              |
| 2:Z:139:ILE:O      | 2:Z:142:LEU:HB2    | 2.05                     | 0.56              |
| 2:Z:202:ARG:HH21   | 2:Z:237:ASP:CG     | 2.09                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Z:67:VAL:HG11   | 2:Z:123:TRP:CZ3   | 2.32                     | 0.56              |
| 14:Z:804:CLA:H142 | 14:Z:822:CLA:CAD  | 2.35                     | 0.56              |
| 2:B:60:VAL:HG23   | 2:B:141:LEU:HD12  | 1.86                     | 0.56              |
| 11:M:13:VAL:HA    | 11:M:16:LEU:HD12  | 1.86                     | 0.56              |
| 14:L:205:CLA:HMD1 | 10:U:94:ALA:HB3   | 1.86                     | 0.56              |
| 14:Y:843:CLA:HBC2 | 14:Y:843:CLA:HHD  | 1.88                     | 0.56              |
| 2:Z:339:TRP:CH2   | 17:Z:844:BCR:H372 | 2.39                     | 0.56              |
| 2:Z:428:VAL:O     | 2:Z:432:LEU:N     | 2.37                     | 0.56              |
| 1:Y:697:TRP:HZ3   | 14:Z:801:CLA:O1D  | 1.88                     | 0.56              |
| 14:Z:806:CLA:HMA1 | 14:Z:807:CLA:C2B  | 2.35                     | 0.56              |
| 14:A:805:CLA:H41  | 14:A:805:CLA:H72  | 1.87                     | 0.56              |
| 14:A:808:CLA:C3D  | 14:A:828:CLA:HBA1 | 2.35                     | 0.56              |
| 14:A:837:CLA:CBB  | 14:A:838:CLA:HBC3 | 2.35                     | 0.56              |
| 1:G:357:ALA:HA    | 1:G:408:GLY:HA2   | 1.87                     | 0.56              |
| 1:G:519:ALA:HB1   | 1:G:625:VAL:HG21  | 1.85                     | 0.56              |
| 6:Q:17:ARG:NH2    | 6:Q:46:ASP:O      | 2.32                     | 0.56              |
| 14:U:1004:CLA:CBB | 14:Y:833:CLA:HMC2 | 2.36                     | 0.56              |
| 1:Y:433:VAL:HA    | 1:Y:436:HIS:CE1   | 2.41                     | 0.56              |
| 2:Z:647:ASN:HD22  | 2:Z:649:LEU:H     | 1.53                     | 0.56              |
| 1:A:302:LEU:HD13  | 14:A:815:CLA:HMC1 | 1.87                     | 0.56              |
| 14:A:805:CLA:H142 | 17:A:846:BCR:H372 | 1.86                     | 0.56              |
| 3:C:28:VAL:HG12   | 4:D:109:ARG:HB3   | 1.87                     | 0.56              |
| 1:G:141:SER:CB    | 1:G:143:LEU:HG    | 2.36                     | 0.56              |
| 1:G:460:VAL:O     | 1:G:464:THR:OG1   | 2.22                     | 0.56              |
| 1:G:649:TRP:O     | 1:G:653:PHE:HB3   | 2.06                     | 0.56              |
| 1:G:593:ASP:OD1   | 1:G:728:ARG:NH1   | 2.39                     | 0.56              |
| 2:H:441:VAL:HG22  | 14:H:801:CLA:H42  | 1.86                     | 0.56              |
| 2:H:50:PHE:CE1    | 14:H:810:CLA:HBB1 | 2.41                     | 0.56              |
| 17:T:102:BCR:H331 | 17:T:102:BCR:C8   | 2.35                     | 0.56              |
| 1:Y:224:ASN:O     | 1:Y:228:ASP:N     | 2.37                     | 0.56              |
| 1:Y:561:ARG:HD2   | 1:Y:570:ALA:HB2   | 1.88                     | 0.56              |
| 14:U:1006:CLA:CHC | 14:Z:808:CLA:HMB3 | 2.35                     | 0.56              |
| 2:Z:360:PRO:HG3   | 14:Z:816:CLA:HBA1 | 1.86                     | 0.56              |
| 14:Z:832:CLA:HBB1 | 14:Z:832:CLA:HMB1 | 1.86                     | 0.56              |
| 2:B:260:PHE:CZ    | 2:B:358:LEU:HD23  | 2.40                     | 0.56              |
| 14:A:802:CLA:H2   | 2:B:661:LEU:HD22  | 1.88                     | 0.56              |
| 1:G:683:TRP:CG    | 13:G:801:CL0:H5   | 2.40                     | 0.56              |
| 2:H:414:VAL:HA    | 2:H:417:HIS:CE1   | 2.40                     | 0.56              |
| 17:H:842:BCR:H383 | 17:H:842:BCR:H23C | 1.87                     | 0.56              |
| 1:Y:416:MET:O     | 1:Y:420:TYR:HB3   | 2.04                     | 0.56              |
| 14:J:102:CLA:HBC3 | 14:Z:837:CLA:HBC2 | 145.65                   | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:699:GLU:HB2   | 2:B:542:LYS:NZ    | 2.20                     | 0.56              |
| 14:H:835:CLA:H3A  | 14:H:836:CLA:OBD  | 2.05                     | 0.56              |
| 1:Y:345:TYR:O     | 1:Y:349:THR:HG22  | 2.05                     | 0.56              |
| 1:Y:354:ALA:HB1   | 17:Y:849:BCR:H313 | 1.88                     | 0.56              |
| 1:A:354:ALA:HB2   | 1:A:415:PHE:CD1   | 2.41                     | 0.56              |
| 1:A:24:SER:O      | 14:A:811:CLA:HMA1 | 2.06                     | 0.56              |
| 2:B:459:GLU:HG3   | 6:F:5:LEU:HD21    | 1.87                     | 0.56              |
| 14:B:834:CLA:HMD2 | 14:B:835:CLA:C1C  | 2.35                     | 0.56              |
| 1:G:216:GLN:OE1   | 1:G:297:THR:OG1   | 2.22                     | 0.56              |
| 3:N:53:CYS:HB2    | 3:N:64:ILE:HD13   | 1.88                     | 0.56              |
| 1:Y:141:SER:OG    | 14:Y:808:CLA:O1D  | 2.18                     | 0.56              |
| 2:Z:652:TRP:CE3   | 2:Z:729:ALA:HA    | 2.40                     | 0.56              |
| 1:A:456:PHE:HE1   | 14:A:802:CLA:HMA1 | 1.69                     | 0.56              |
| 14:A:839:CLA:HHC  | 14:A:839:CLA:HBB1 | 1.87                     | 0.56              |
| 2:B:304:MET:HG2   | 2:B:325:ILE:HG22  | 1.88                     | 0.56              |
| 2:B:379:GLN:HA    | 2:B:379:GLN:OE1   | 2.06                     | 0.56              |
| 2:B:431:PHE:CD2   | 14:B:838:CLA:HBB2 | 2.40                     | 0.56              |
| 2:B:368:HIS:CE1   | 2:B:608:TRP:CD1   | 2.94                     | 0.56              |
| 4:D:123:PRO:HB3   | 4:D:127:GLN:NE2   | 2.20                     | 0.56              |
| 1:G:289:THR:HB    | 1:G:381:PRO:HB3   | 1.88                     | 0.56              |
| 14:G:821:CLA:HMB2 | 14:G:825:CLA:HMA3 | 1.88                     | 0.56              |
| 14:H:816:CLA:H43  | 14:H:831:CLA:CGD  | 2.36                     | 0.56              |
| 14:H:820:CLA:CBB  | 14:H:821:CLA:HBC2 | 2.35                     | 0.56              |
| 3:N:4:VAL:HG12    | 3:N:66:VAL:HG13   | 1.88                     | 0.56              |
| 1:Y:307:LEU:HD12  | 14:Y:818:CLA:HBC2 | 1.86                     | 0.56              |
| 17:Y:848:BCR:H383 | 17:Y:848:BCR:C23  | 2.35                     | 0.56              |
| 14:Z:828:CLA:HAC2 | 17:Z:844:BCR:H402 | 1.88                     | 0.56              |
| 1:A:433:VAL:HA    | 1:A:436:HIS:CE1   | 2.42                     | 0.56              |
| 2:H:566:ASP:OD2   | 3:N:65:ARG:NH2    | 2.38                     | 0.56              |
| 2:H:390:PHE:CZ    | 14:H:824:CLA:HAB  | 2.38                     | 0.56              |
| 14:H:814:CLA:C1C  | 17:H:840:BCR:H312 | 2.35                     | 0.56              |
| 1:Y:651:ARG:HA    | 1:Y:655:TRP:HB3   | 1.87                     | 0.56              |
| 14:Y:807:CLA:CGD  | 14:Y:809:CLA:HED1 | 2.36                     | 0.56              |
| 2:Z:425:LEU:CG    | 14:Z:837:CLA:HAB  | 2.31                     | 0.56              |
| 2:B:375:TYR:CE2   | 2:B:379:GLN:HG3   | 2.41                     | 0.55              |
| 2:B:469:ALA:O     | 2:B:481:LEU:HD12  | 2.06                     | 0.55              |
| 1:G:683:TRP:CE3   | 13:G:801:CL0:CMA  | 2.89                     | 0.55              |
| 14:H:807:CLA:O1A  | 14:H:826:CLA:HAA1 | 2.07                     | 0.55              |
| 10:L:57:PHE:O     | 10:L:60:GLY:N     | 2.36                     | 0.55              |
| 10:L:137:PHE:CE2  | 10:U:79:LEU:HD23  | 2.41                     | 0.55              |
| 1:Y:86:TRP:CD1    | 14:Y:806:CLA:HBC1 | 2.41                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:647:ASN:HD22  | 2:B:657:LEU:HD11  | 1.70                     | 0.55              |
| 2:B:472:LYS:HG2   | 2:B:475:TYR:HE2   | 1.71                     | 0.55              |
| 6:F:84:TYR:O      | 6:F:88:VAL:HG22   | 2.05                     | 0.55              |
| 1:G:531:LEU:HD23  | 1:G:535:ASP:OD2   | 2.05                     | 0.55              |
| 1:G:313:HIS:HB3   | 14:G:820:CLA:HED1 | 1.88                     | 0.55              |
| 10:L:66:GLY:O     | 10:L:69:ARG:HG2   | 2.06                     | 0.55              |
| 1:Y:592:TRP:CD1   | 14:Y:830:CLA:HMD1 | 2.41                     | 0.55              |
| 1:A:223:ILE:HG22  | 1:A:227:LEU:HD12  | 1.89                     | 0.55              |
| 1:A:336:PHE:O     | 1:A:432:ARG:NH2   | 2.40                     | 0.55              |
| 14:A:802:CLA:HED2 | 2:B:660:HIS:CD2   | 2.41                     | 0.55              |
| 1:A:31:PRO:HB3    | 14:A:803:CLA:HAC1 | 1.88                     | 0.55              |
| 2:B:490:THR:O     | 2:B:495:TYR:HA    | 2.06                     | 0.55              |
| 1:A:685:PHE:HA    | 14:B:801:CLA:HAB  | 1.87                     | 0.55              |
| 2:H:199:PRO:HB3   | 2:H:204:GLN:OE1   | 2.06                     | 0.55              |
| 2:H:253:ILE:O     | 2:H:254:LEU:HD23  | 2.07                     | 0.55              |
| 5:P:24:ALA:N      | 5:P:37:ILE:O      | 2.35                     | 0.55              |
| 2:Z:428:VAL:HA    | 2:Z:431:PHE:HB3   | 1.89                     | 0.55              |
| 2:B:122:TRP:CZ2   | 14:B:813:CLA:H191 | 2.42                     | 0.55              |
| 4:D:95:HIS:CB     | 4:D:96:PRO:HD3    | 2.34                     | 0.55              |
| 2:H:622:LEU:HD13  | 14:H:801:CLA:HMA2 | 1.88                     | 0.55              |
| 14:H:805:CLA:HBB2 | 14:H:827:CLA:HMC2 | 1.87                     | 0.55              |
| 1:Y:97:PHE:O      | 1:Y:114:ALA:HA    | 2.07                     | 0.55              |
| 1:A:433:VAL:HG21  | 14:A:824:CLA:HMC3 | 1.88                     | 0.55              |
| 1:A:744:TRP:O     | 1:A:748:LEU:HG    | 2.07                     | 0.55              |
| 1:G:648:GLY:O     | 1:G:652:ASP:N     | 2.39                     | 0.55              |
| 2:H:278:ALA:CB    | 14:H:816:CLA:HAB  | 2.37                     | 0.55              |
| 14:H:814:CLA:HMA1 | 17:H:842:BCR:C10  | 2.36                     | 0.55              |
| 14:A:841:CLA:H151 | 10:L:85:LEU:HD11  | 1.88                     | 0.55              |
| 1:Y:580:GLY:O     | 1:Y:586:THR:OG1   | 2.11                     | 0.55              |
| 1:G:26:GLU:HA     | 8:S:3:HIS:CG      | 2.41                     | 0.55              |
| 14:G:806:CLA:HMA1 | 14:G:830:CLA:HAB  | 1.89                     | 0.55              |
| 17:G:846:BCR:H321 | 17:G:846:BCR:HC8  | 1.89                     | 0.55              |
| 6:Q:34:ARG:NH1    | 8:S:35:ASP:OD2    | 2.36                     | 0.55              |
| 1:Y:143:LEU:O     | 1:Y:147:TRP:N     | 2.35                     | 0.55              |
| 1:Y:437:ARG:HH22  | 1:Y:562:SER:HB2   | 1.72                     | 0.55              |
| 1:A:618:GLN:OE1   | 1:A:657:GLN:NE2   | 2.39                     | 0.55              |
| 2:B:367:ASP:O     | 2:B:371:MET:HG2   | 2.07                     | 0.55              |
| 2:B:434:PHE:HZ    | 17:F:201:BCR:H372 | 1.72                     | 0.55              |
| 2:B:46:PHE:O      | 2:B:49:HIS:HB2    | 2.06                     | 0.55              |
| 1:A:651:ARG:HD3   | 2:B:639:ASN:ND2   | 2.22                     | 0.55              |
| 1:G:360:LEU:HD23  | 1:G:407:GLY:C     | 2.27                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:30:PHE:HB3    | 2:H:36:MET:HE3    | 1.88                     | 0.55              |
| 14:Y:821:CLA:C2B  | 21:Y:904:HOH:O    | 2.36                     | 0.55              |
| 14:Y:841:CLA:HMB1 | 14:Y:841:CLA:HBB1 | 1.89                     | 0.55              |
| 1:A:203:GLY:HA2   | 14:A:820:CLA:HBC1 | 1.89                     | 0.55              |
| 17:A:846:BCR:C8   | 17:A:846:BCR:H321 | 2.37                     | 0.55              |
| 2:B:427:TRP:O     | 2:B:431:PHE:N     | 2.37                     | 0.55              |
| 2:B:678:GLN:OE1   | 2:B:705:ALA:N     | 2.33                     | 0.55              |
| 1:G:307:LEU:HB3   | 14:G:821:CLA:HMC1 | 1.89                     | 0.55              |
| 14:G:829:CLA:HMD2 | 14:G:829:CLA:H92  | 1.87                     | 0.55              |
| 1:G:685:PHE:HZ    | 14:G:841:CLA:HBC2 | 1.71                     | 0.55              |
| 14:H:824:CLA:C2B  | 17:H:844:BCR:H363 | 2.36                     | 0.55              |
| 14:H:835:CLA:H18  | 17:Q:204:BCR:H383 | 1.89                     | 0.55              |
| 9:K:61:ALA:HA     | 9:K:64:SER:OG     | 2.07                     | 0.55              |
| 9:T:76:GLY:O      | 9:T:77:LEU:HD12   | 2.07                     | 0.55              |
| 1:Y:66:GLU:HG3    | 1:Y:187:LEU:H     | 1.71                     | 0.55              |
| 14:Y:815:CLA:HMB1 | 14:Y:815:CLA:HBB1 | 1.88                     | 0.55              |
| 14:Y:823:CLA:HBC1 | 14:Y:827:CLA:H141 | 1.89                     | 0.55              |
| 17:Y:848:BCR:H23C | 17:Y:848:BCR:H383 | 1.88                     | 0.55              |
| 14:Z:813:CLA:NC   | 17:Z:841:BCR:H312 | 2.22                     | 0.55              |
| 1:A:201:LEU:O     | 1:A:308:PHE:HB3   | 2.07                     | 0.55              |
| 14:B:817:CLA:O1D  | 14:B:818:CLA:HMA1 | 2.08                     | 0.55              |
| 5:E:7:VAL:HB      | 5:E:65:VAL:HB     | 1.89                     | 0.55              |
| 1:G:121:VAL:HG12  | 14:H:830:CLA:CMD  | 2.33                     | 0.55              |
| 14:G:819:CLA:H121 | 14:G:821:CLA:CBB  | 2.37                     | 0.55              |
| 2:H:589:MET:O     | 2:H:593:ILE:HG12  | 2.06                     | 0.55              |
| 14:A:832:CLA:OBD  | 10:L:19:THR:HG21  | 2.07                     | 0.55              |
| 14:L:206:CLA:HAC2 | 17:L:208:BCR:H382 | 1.87                     | 0.55              |
| 6:Q:72:TYR:OH     | 6:Q:114:PHE:O     | 2.16                     | 0.55              |
| 1:Y:625:VAL:HG22  | 1:Y:631:VAL:HG22  | 1.88                     | 0.55              |
| 2:Z:14:ASP:OD1    | 2:Z:16:THR:HG22   | 2.06                     | 0.55              |
| 2:Z:661:LEU:O     | 2:Z:665:THR:HG23  | 2.07                     | 0.55              |
| 2:Z:354:HIS:CE1   | 14:Z:815:CLA:OBD  | 2.58                     | 0.55              |
| 2:B:395:ILE:HG12  | 2:B:561:TYR:CD2   | 2.41                     | 0.54              |
| 2:B:663:TRP:CD2   | 14:B:803:CLA:CMA  | 2.91                     | 0.54              |
| 1:A:468:PHE:CE2   | 2:B:94:GLN:HB3    | 2.42                     | 0.54              |
| 6:F:42:LEU:HD22   | 6:F:52:VAL:HG21   | 1.88                     | 0.54              |
| 2:H:361:TYR:CE2   | 14:H:827:CLA:HED2 | 2.42                     | 0.54              |
| 2:H:480:LEU:HD12  | 2:H:488:ALA:HB2   | 1.89                     | 0.54              |
| 2:H:54:ALA:CB     | 2:H:149:LEU:HG    | 2.37                     | 0.54              |
| 2:H:633:ASN:HB3   | 2:H:734:SER:HB2   | 1.89                     | 0.54              |
| 1:Y:213:ALA:HA    | 1:Y:216:GLN:HB2   | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y:674:LEU:HD13  | 2:Z:445:VAL:HG22  | 1.89                     | 0.54              |
| 14:A:818:CLA:H2   | 14:A:827:CLA:HBB2 | 1.88                     | 0.54              |
| 2:B:194:ILE:HD13  | 14:B:815:CLA:CAC  | 2.37                     | 0.54              |
| 1:G:216:GLN:HA    | 1:G:220:SER:HB3   | 1.90                     | 0.54              |
| 14:L:206:CLA:HMB3 | 14:L:207:CLA:HBC2 | 1.88                     | 0.54              |
| 17:Q:204:BCR:H331 | 17:Q:204:BCR:C8   | 2.37                     | 0.54              |
| 8:S:11:ALA:N      | 8:S:12:PRO:HD2    | 2.21                     | 0.54              |
| 9:T:20:ILE:HD12   | 9:T:21:LEU:HB2    | 1.90                     | 0.54              |
| 1:Y:149:ALA:HB2   | 1:Y:381:PRO:CD    | 2.36                     | 0.54              |
| 2:Z:243:PHE:CE1   | 2:Z:269:LEU:HD11  | 2.43                     | 0.54              |
| 2:Z:424:HIS:O     | 2:Z:428:VAL:HG22  | 2.08                     | 0.54              |
| 1:A:604:ASN:O     | 1:A:608:VAL:HG23  | 2.07                     | 0.54              |
| 1:A:699:GLU:O     | 1:A:702:GLU:HB2   | 2.06                     | 0.54              |
| 2:B:494:ASN:HD22  | 2:B:496:GLY:H     | 1.54                     | 0.54              |
| 3:C:64:ILE:HB     | 16:C:102:SF4:S3   | 2.48                     | 0.54              |
| 1:G:379:PRO:HG3   | 14:G:819:CLA:CBA  | 2.37                     | 0.54              |
| 1:G:79:HIS:CD2    | 14:G:805:CLA:HMA1 | 2.43                     | 0.54              |
| 14:H:808:CLA:H202 | 17:R:102:BCR:H311 | 1.88                     | 0.54              |
| 9:T:24:LEU:O      | 9:T:69:LEU:HD21   | 2.07                     | 0.54              |
| 1:Y:690:LEU:HB3   | 2:Z:671:ILE:HG12  | 1.88                     | 0.54              |
| 1:Y:177:TRP:HB2   | 14:Y:811:CLA:HMC3 | 1.89                     | 0.54              |
| 2:Z:114:ILE:O     | 14:Z:807:CLA:HMD3 | 2.06                     | 0.54              |
| 2:Z:92:ASP:OD1    | 2:Z:94:GLN:NE2    | 2.34                     | 0.54              |
| 2:B:27:ALA:O      | 2:B:33:HIS:HE1    | 1.91                     | 0.54              |
| 17:B:845:BCR:H321 | 17:B:845:BCR:HC8  | 1.88                     | 0.54              |
| 1:G:448:CYS:O     | 1:G:452:GLY:N     | 2.41                     | 0.54              |
| 14:G:816:CLA:HMB1 | 17:G:846:BCR:H343 | 1.88                     | 0.54              |
| 8:J:11:ALA:N      | 8:J:12:PRO:HD2    | 2.23                     | 0.54              |
| 2:Z:375:TYR:CE2   | 2:Z:379:GLN:HG3   | 2.42                     | 0.54              |
| 1:A:20:PRO:HD3    | 1:A:182:LYS:O     | 2.06                     | 0.54              |
| 1:G:23:THR:HG22   | 1:G:181:HIS:CG    | 2.42                     | 0.54              |
| 17:G:847:BCR:H383 | 17:G:847:BCR:C23  | 2.38                     | 0.54              |
| 10:L:49:GLU:HB2   | 14:L:205:CLA:HED2 | 1.88                     | 0.54              |
| 1:Y:461:HIS:CE1   | 1:Y:465:MET:CE    | 2.91                     | 0.54              |
| 14:Y:829:CLA:C6   | 21:Y:907:HOH:O    | 2.55                     | 0.54              |
| 17:Y:847:BCR:H331 | 17:Y:847:BCR:C8   | 2.38                     | 0.54              |
| 6:F:103:VAL:CG1   | 6:F:104:PRO:HD3   | 2.38                     | 0.54              |
| 1:G:178:PHE:O     | 1:G:182:LYS:HB2   | 2.07                     | 0.54              |
| 17:G:850:BCR:H403 | 17:G:850:BCR:C23  | 2.35                     | 0.54              |
| 2:H:200:GLU:HG2   | 2:H:205:HIS:HA    | 1.90                     | 0.54              |
| 2:H:87:ALA:O      | 14:H:807:CLA:HED1 | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:Z:256:PHE:O      | 2:Z:498:VAL:HG12  | 2.08                     | 0.54              |
| 1:A:541:ILE:HD12   | 13:A:801:CL0:H60  | 1.89                     | 0.54              |
| 2:H:451:THR:HG22   | 6:Q:22:VAL:CG1    | 2.38                     | 0.54              |
| 17:H:845:BCR:H331  | 17:H:845:BCR:C8   | 2.36                     | 0.54              |
| 1:Y:356:LEU:O      | 1:Y:360:LEU:HB2   | 2.08                     | 0.54              |
| 1:Y:375:TYR:CZ     | 14:Y:837:CLA:HBC3 | 2.43                     | 0.54              |
| 17:Y:847:BCR:H331  | 17:Y:847:BCR:HC8  | 1.90                     | 0.54              |
| 14:Y:833:CLA:H171  | 14:Z:838:CLA:HMB2 | 1.90                     | 0.54              |
| 1:A:583:ARG:O      | 2:B:674:ARG:NH1   | 2.40                     | 0.54              |
| 4:D:20:ALA:HA      | 4:D:23:THR:HB     | 1.90                     | 0.54              |
| 6:F:54:ASP:HB3     | 6:F:56:ARG:HG3    | 1.88                     | 0.54              |
| 2:H:85:PRO:HG2     | 2:H:115:ALA:O     | 2.08                     | 0.54              |
| 17:R:101:BCR:C8    | 17:R:101:BCR:H331 | 2.37                     | 0.54              |
| 14:Y:842:CLA:HMB1  | 2:Z:697:VAL:HG21  | 1.89                     | 0.54              |
| 1:A:435:ARG:NH1    | 4:D:12:GLY:O      | 2.37                     | 0.54              |
| 1:A:82:VAL:HG11    | 14:A:806:CLA:HMD2 | 1.89                     | 0.54              |
| 2:B:194:ILE:HD13   | 14:B:815:CLA:C3C  | 2.38                     | 0.54              |
| 14:H:824:CLA:HAA2  | 14:H:825:CLA:OBD  | 2.08                     | 0.54              |
| 10:L:106:SER:OG    | 10:L:107:SER:N    | 2.40                     | 0.54              |
| 4:O:58:PHE:HB3     | 4:O:63:GLN:HE21   | 1.73                     | 0.54              |
| 17:R:102:BCR:C23   | 17:R:102:BCR:H403 | 2.38                     | 0.54              |
| 17:U:1005:BCR:H403 | 17:U:1005:BCR:C23 | 2.38                     | 0.54              |
| 1:Y:443:HIS:O      | 1:Y:447:VAL:HG23  | 2.08                     | 0.54              |
| 14:Y:808:CLA:HMC2  | 14:Y:828:CLA:H141 | 1.89                     | 0.54              |
| 1:Y:210:LEU:HD21   | 17:Y:847:BCR:H373 | 1.90                     | 0.54              |
| 2:Z:354:HIS:HE1    | 14:Z:815:CLA:HMD1 | 1.73                     | 0.54              |
| 2:Z:586:MET:HG3    | 2:Z:716:LEU:HD21  | 1.88                     | 0.54              |
| 17:A:847:BCR:H403  | 17:A:847:BCR:H23C | 1.89                     | 0.54              |
| 17:F:201:BCR:H23C  | 17:F:201:BCR:C38  | 2.38                     | 0.54              |
| 1:G:59:ASP:HB2     | 1:G:418:ARG:NH1   | 2.22                     | 0.54              |
| 2:H:350:LEU:HD23   | 14:H:817:CLA:H41  | 1.90                     | 0.54              |
| 2:H:128:MET:CE     | 14:H:813:CLA:HMA2 | 2.38                     | 0.54              |
| 14:K:103:CLA:HED2  | 14:K:103:CLA:H2A  | 1.89                     | 0.54              |
| 1:Y:24:SER:O       | 14:Y:811:CLA:HMA1 | 2.08                     | 0.54              |
| 14:Y:830:CLA:HBB1  | 14:Y:830:CLA:HMB1 | 1.89                     | 0.54              |
| 2:Z:42:TYR:OH      | 2:Z:168:LYS:NZ    | 2.38                     | 0.54              |
| 14:Z:806:CLA:CMA   | 14:Z:807:CLA:HMB3 | 2.37                     | 0.54              |
| 1:A:193:VAL:HG21   | 1:A:349:THR:HG22  | 1.90                     | 0.53              |
| 1:G:442:SER:O      | 14:G:842:CLA:HED2 | 2.06                     | 0.53              |
| 14:G:806:CLA:H201  | 18:G:851:LHG:H221 | 1.88                     | 0.53              |
| 14:H:817:CLA:HBB1  | 14:H:817:CLA:HMB1 | 1.90                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:H:828:CLA:H41   | 14:V:1201:CLA:HBC3 | 1.89                     | 0.53              |
| 14:H:835:CLA:HMA1  | 14:H:836:CLA:HED2  | 1.89                     | 0.53              |
| 5:P:7:VAL:N        | 5:P:21:GLY:O       | 2.41                     | 0.53              |
| 14:U:1002:CLA:HBA1 | 17:U:1008:BCR:H363 | 1.90                     | 0.53              |
| 2:Z:237:ASP:HB3    | 2:Z:241:HIS:CD2    | 2.43                     | 0.53              |
| 1:A:148:ARG:HG2    | 1:A:381:PRO:HG2    | 1.89                     | 0.53              |
| 1:A:348:LEU:HD12   | 14:A:825:CLA:HMC2  | 1.90                     | 0.53              |
| 14:A:806:CLA:H151  | 14:A:829:CLA:HBB2  | 1.89                     | 0.53              |
| 1:A:86:TRP:HA      | 14:A:807:CLA:HBB2  | 1.89                     | 0.53              |
| 17:B:851:BCR:H393  | 17:B:851:BCR:H271  | 1.90                     | 0.53              |
| 14:G:839:CLA:O1A   | 2:H:427:TRP:CD1    | 2.61                     | 0.53              |
| 8:S:28:GLU:OE2     | 8:S:31:ARG:NH2     | 2.41                     | 0.53              |
| 17:U:1007:BCR:H372 | 14:Y:834:CLA:H152  | 1.90                     | 0.53              |
| 14:Y:813:CLA:HMB1  | 14:Y:813:CLA:HBB1  | 1.90                     | 0.53              |
| 17:Z:843:BCR:H23C  | 17:Z:843:BCR:C38   | 2.37                     | 0.53              |
| 1:A:375:TYR:CZ     | 14:A:836:CLA:HBC3  | 2.43                     | 0.53              |
| 2:B:318:PHE:CD1    | 14:B:822:CLA:CAB   | 2.76                     | 0.53              |
| 2:B:470:HIS:O      | 2:B:503:TRP:NE1    | 2.40                     | 0.53              |
| 2:B:711:ALA:HB2    | 15:B:842:PQN:C7    | 2.39                     | 0.53              |
| 5:E:17:TYR:O       | 6:F:137:THR:OG1    | 2.19                     | 0.53              |
| 1:G:425:ASN:OD1    | 1:G:428:ASN:ND2    | 2.41                     | 0.53              |
| 14:G:802:CLA:H192  | 14:H:801:CLA:H171  | 1.90                     | 0.53              |
| 2:H:387:VAL:HG11   | 2:H:586:MET:HE2    | 1.91                     | 0.53              |
| 10:U:110:PRO:O     | 10:U:113:THR:OG1   | 2.11                     | 0.53              |
| 14:Y:803:CLA:HMA2  | 14:Y:803:CLA:O1A   | 2.07                     | 0.53              |
| 1:A:308:PHE:CE1    | 14:A:821:CLA:HAB   | 2.44                     | 0.53              |
| 14:A:829:CLA:C1    | 17:A:846:BCR:H24C  | 2.38                     | 0.53              |
| 14:A:833:CLA:H93   | 14:B:840:CLA:H52   | 1.90                     | 0.53              |
| 2:H:303:MET:HA     | 14:H:821:CLA:O1D   | 2.07                     | 0.53              |
| 8:J:31:ARG:NE      | 17:J:104:BCR:H312  | 2.24                     | 0.53              |
| 2:Z:275:HIS:CE1    | 14:Z:816:CLA:HMB3  | 2.44                     | 0.53              |
| 1:A:14:VAL:HG23    | 14:A:810:CLA:HMA2  | 1.90                     | 0.53              |
| 14:A:818:CLA:O1D   | 14:A:819:CLA:HMA1  | 2.08                     | 0.53              |
| 14:B:804:CLA:H143  | 17:B:848:BCR:H362  | 1.89                     | 0.53              |
| 1:G:379:PRO:HG3    | 14:G:819:CLA:HBA1  | 1.91                     | 0.53              |
| 1:G:407:GLY:O      | 1:G:410:ALA:HB3    | 2.08                     | 0.53              |
| 1:G:606:ILE:HA     | 1:G:609:VAL:HB     | 1.91                     | 0.53              |
| 1:G:740:ILE:HG21   | 14:G:828:CLA:HMC2  | 1.91                     | 0.53              |
| 14:G:818:CLA:O1D   | 14:G:819:CLA:HHB   | 2.08                     | 0.53              |
| 2:H:648:ASN:H      | 2:H:648:ASN:HD22   | 1.56                     | 0.53              |
| 2:H:70:GLN:HE22    | 14:H:806:CLA:CGD   | 2.18                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:91:TRP:HB3    | 7:R:15:ILE:HG12    | 1.91                     | 0.53              |
| 14:Y:842:CLA:HHD  | 17:Y:856:BCR:C38   | 2.39                     | 0.53              |
| 2:Z:47:ALA:CB     | 2:Z:156:LEU:HG     | 2.39                     | 0.53              |
| 2:Z:239:ALA:HB1   | 2:Z:262:PRO:HG2    | 1.90                     | 0.53              |
| 14:A:812:CLA:O1D  | 14:A:813:CLA:HMC1  | 2.09                     | 0.53              |
| 2:B:282:LEU:HD21  | 14:B:817:CLA:H203  | 1.89                     | 0.53              |
| 14:B:811:CLA:O1D  | 14:B:811:CLA:H2A   | 2.08                     | 0.53              |
| 6:F:72:TYR:OH     | 6:F:114:PHE:O      | 2.24                     | 0.53              |
| 2:H:651:VAL:HG22  | 14:H:808:CLA:HHD   | 1.90                     | 0.53              |
| 2:H:687:ALA:O     | 2:H:691:THR:HG23   | 2.09                     | 0.53              |
| 2:H:654:TRP:CE3   | 17:H:845:BCR:HC41  | 2.44                     | 0.53              |
| 10:L:47:GLY:O     | 10:L:124:PHE:HA    | 2.09                     | 0.53              |
| 3:N:24:VAL:O      | 3:N:42:PRO:HD2     | 2.08                     | 0.53              |
| 17:Y:851:BCR:H362 | 14:Y:854:CLA:H43   | 1.91                     | 0.53              |
| 2:Z:537:THR:HG21  | 14:Z:837:CLA:HMB3  | 1.91                     | 0.53              |
| 14:Z:812:CLA:HBB1 | 14:Z:812:CLA:HMB1  | 1.90                     | 0.53              |
| 1:A:38:LEU:CD1    | 1:A:51:LEU:HA      | 2.37                     | 0.53              |
| 1:A:457:GLY:HA3   | 14:L:201:CLA:HAB   | 1.91                     | 0.53              |
| 2:B:122:TRP:CZ2   | 14:B:813:CLA:H201  | 2.44                     | 0.53              |
| 7:I:22:MET:O      | 7:I:26:VAL:HG22    | 2.09                     | 0.53              |
| 6:Q:60:ALA:HA     | 6:Q:64:LEU:HD13    | 1.90                     | 0.53              |
| 17:V:1202:BCR:C32 | 17:V:1202:BCR:HC8  | 2.39                     | 0.53              |
| 14:Y:841:CLA:CGA  | 14:Y:841:CLA:C1A   | 2.86                     | 0.53              |
| 14:Y:855:CLA:CBC  | 2:Z:671:ILE:HB     | 2.39                     | 0.53              |
| 2:Z:649:LEU:HA    | 2:Z:652:TRP:HD1    | 1.73                     | 0.53              |
| 1:A:204:LEU:HD13  | 14:A:813:CLA:HHB   | 1.89                     | 0.53              |
| 1:A:463:ASP:CG    | 1:A:646:ILE:H      | 2.12                     | 0.53              |
| 2:B:166:TRP:CE2   | 14:B:813:CLA:HAC2  | 2.44                     | 0.53              |
| 2:B:504:LEU:O     | 2:B:508:ASN:ND2    | 2.40                     | 0.53              |
| 3:C:80:TYR:OXT    | 4:D:20:ALA:HB2     | 2.09                     | 0.53              |
| 1:G:31:PRO:HB3    | 14:S:1101:CLA:HAC1 | 1.91                     | 0.53              |
| 14:H:818:CLA:HMB2 | 14:H:823:CLA:HMA3  | 1.91                     | 0.53              |
| 10:L:33:ASN:O     | 10:L:38:ARG:NH1    | 2.37                     | 0.53              |
| 1:G:713:VAL:HA    | 6:Q:85:LEU:HD22    | 1.91                     | 0.53              |
| 14:Y:802:CLA:H42  | 2:Z:657:LEU:HB2    | 1.90                     | 0.53              |
| 2:Z:677:TRP:CZ2   | 15:Z:840:PQN:H2M3  | 2.43                     | 0.53              |
| 2:Z:48:SER:OG     | 14:Z:803:CLA:HMA1  | 2.08                     | 0.53              |
| 14:Z:815:CLA:O1D  | 14:Z:816:CLA:HMA1  | 2.09                     | 0.53              |
| 2:B:133:ASP:CG    | 2:B:205:HIS:HE2    | 2.13                     | 0.53              |
| 14:B:801:CLA:H51  | 14:B:801:CLA:HMA1  | 1.90                     | 0.53              |
| 14:G:803:CLA:CAD  | 14:H:802:CLA:CMB   | 2.87                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:177:TRP:HB2   | 14:G:811:CLA:HMC3 | 1.91                     | 0.53              |
| 17:H:841:BCR:H313 | 17:H:842:BCR:HC31 | 1.90                     | 0.53              |
| 14:A:832:CLA:HED1 | 10:L:16:HIS:CD2   | 2.44                     | 0.53              |
| 7:R:7:ALA:O       | 7:R:10:LEU:HG     | 2.09                     | 0.53              |
| 1:Y:336:PHE:CD2   | 18:Y:853:LHG:HC42 | 2.44                     | 0.53              |
| 1:Y:438:ASP:O     | 1:Y:442:SER:OG    | 2.19                     | 0.53              |
| 14:Y:803:CLA:H43  | 14:Y:841:CLA:H122 | 1.91                     | 0.53              |
| 13:A:801:CL0:CGD  | 13:A:801:CL0:H8   | 2.39                     | 0.53              |
| 2:B:75:GLN:O      | 2:B:83:THR:HG21   | 2.09                     | 0.53              |
| 14:B:832:CLA:HMB1 | 14:B:832:CLA:HBB1 | 1.91                     | 0.53              |
| 1:A:564:ARG:O     | 4:D:60:ARG:NH1    | 2.42                     | 0.53              |
| 1:G:539:HIS:HB2   | 14:G:837:CLA:HED1 | 1.91                     | 0.53              |
| 14:H:807:CLA:H92  | 14:H:828:CLA:H202 | 1.91                     | 0.53              |
| 2:H:166:TRP:HD1   | 14:H:811:CLA:HED2 | 1.74                     | 0.53              |
| 14:H:808:CLA:H192 | 7:R:23:PRO:HA     | 1.90                     | 0.53              |
| 1:Y:14:VAL:HA     | 1:Y:189:TRP:CD1   | 2.44                     | 0.53              |
| 1:Y:460:VAL:HG23  | 14:Y:834:CLA:HMC3 | 1.91                     | 0.53              |
| 2:Z:256:PHE:HZ    | 14:Z:815:CLA:H72  | 1.74                     | 0.53              |
| 1:A:410:ALA:O     | 1:A:414:ILE:HG13  | 2.09                     | 0.52              |
| 2:B:677:TRP:CH2   | 15:B:842:PQN:H2M3 | 2.44                     | 0.52              |
| 1:G:684:ALA:C     | 14:G:802:CLA:HAB  | 2.30                     | 0.52              |
| 2:H:340:HIS:CD2   | 14:H:823:CLA:HAA1 | 2.44                     | 0.52              |
| 9:K:76:GLY:O      | 14:K:103:CLA:HMB3 | 2.09                     | 0.52              |
| 10:L:6:LYS:NZ     | 10:L:18:SER:OG    | 2.30                     | 0.52              |
| 9:T:25:PHE:O      | 9:T:29:LEU:HG     | 2.09                     | 0.52              |
| 14:Y:833:CLA:HAB  | 14:Y:834:CLA:HHB  | 1.91                     | 0.52              |
| 17:Y:851:BCR:C40  | 17:Y:851:BCR:H23C | 2.35                     | 0.52              |
| 14:Z:825:CLA:H3A  | 14:Z:825:CLA:O1A  | 2.09                     | 0.52              |
| 14:B:805:CLA:HMC3 | 14:B:807:CLA:HED2 | 1.90                     | 0.52              |
| 2:B:706:LEU:HB2   | 15:B:842:PQN:C6   | 2.39                     | 0.52              |
| 1:G:188:GLU:O     | 1:G:192:ASN:ND2   | 2.42                     | 0.52              |
| 1:G:344:LEU:HA    | 1:G:347:VAL:HB    | 1.91                     | 0.52              |
| 1:G:261:PHE:CE2   | 14:G:815:CLA:H43  | 2.44                     | 0.52              |
| 2:H:425:LEU:HD13  | 2:H:538:LEU:HA    | 1.91                     | 0.52              |
| 1:Y:432:ARG:O     | 1:Y:436:HIS:ND1   | 2.42                     | 0.52              |
| 1:A:358:ILE:O     | 1:A:361:ALA:HB3   | 2.08                     | 0.52              |
| 13:A:801:CL0:H13  | 14:A:852:CLA:HMD1 | 1.91                     | 0.52              |
| 14:B:835:CLA:NC   | 14:B:836:CLA:HAB  | 2.23                     | 0.52              |
| 1:G:309:ILE:O     | 1:G:313:HIS:ND1   | 2.43                     | 0.52              |
| 14:G:821:CLA:CMB  | 14:G:825:CLA:HED2 | 2.39                     | 0.52              |
| 2:H:119:VAL:HG22  | 2:H:123:TRP:CE2   | 2.44                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:188:ALA:HA    | 14:H:814:CLA:HAB  | 1.91                     | 0.52              |
| 14:H:830:CLA:H2A  | 14:H:830:CLA:HED2 | 1.91                     | 0.52              |
| 1:Y:535:ASP:O     | 1:Y:539:HIS:ND1   | 2.25                     | 0.52              |
| 14:Y:829:CLA:C5   | 21:Y:907:HOH:O    | 2.53                     | 0.52              |
| 14:Y:840:CLA:HBC1 | 15:Y:844:PQN:H191 | 1.90                     | 0.52              |
| 17:Y:846:BCR:H23C | 17:Y:846:BCR:C38  | 2.37                     | 0.52              |
| 17:Y:849:BCR:H372 | 18:Y:853:LHG:H262 | 1.91                     | 0.52              |
| 2:Z:9:GLN:HA      | 2:Z:12:ALA:HB3    | 1.91                     | 0.52              |
| 2:Z:706:LEU:HB3   | 2:Z:710:GLN:HG2   | 1.91                     | 0.52              |
| 2:Z:726:THR:HB    | 14:Z:802:CLA:O1D  | 2.09                     | 0.52              |
| 2:B:128:MET:O     | 2:B:129:ARG:NH1   | 2.42                     | 0.52              |
| 2:B:166:TRP:CZ2   | 14:B:811:CLA:HMA1 | 2.45                     | 0.52              |
| 4:D:54:ASN:N      | 4:D:54:ASN:HD22   | 2.07                     | 0.52              |
| 21:G:904:HOH:O    | 14:H:801:CLA:CAC  | 2.53                     | 0.52              |
| 14:L:205:CLA:OBD  | 10:U:91:ALA:HA    | 2.09                     | 0.52              |
| 1:Y:541:ILE:HG23  | 13:Y:801:CL0:H70  | 1.90                     | 0.52              |
| 14:Y:804:CLA:HMC3 | 14:Y:806:CLA:HED3 | 1.91                     | 0.52              |
| 14:A:812:CLA:C3D  | 14:A:813:CLA:HMC3 | 2.39                     | 0.52              |
| 2:B:618:SER:O     | 2:B:624:GLY:HA3   | 2.10                     | 0.52              |
| 14:G:803:CLA:H3A  | 14:G:803:CLA:O1A  | 2.10                     | 0.52              |
| 14:G:838:CLA:HMB1 | 14:G:838:CLA:HBB1 | 1.91                     | 0.52              |
| 14:G:824:CLA:C6   | 17:G:849:BCR:H363 | 2.40                     | 0.52              |
| 2:H:164:LEU:HA    | 2:H:167:PHE:HD2   | 1.75                     | 0.52              |
| 2:H:663:TRP:CD2   | 14:H:802:CLA:CMA  | 2.92                     | 0.52              |
| 17:H:840:BCR:H382 | 17:H:840:BCR:H23C | 1.90                     | 0.52              |
| 7:I:5:TYR:OH      | 7:I:11:PRO:HG2    | 2.09                     | 0.52              |
| 9:K:71:ALA:O      | 9:K:75:SER:OG     | 2.27                     | 0.52              |
| 4:O:61:LYS:O      | 4:O:65:LEU:HD12   | 2.10                     | 0.52              |
| 14:T:103:CLA:H2A  | 14:T:103:CLA:HED2 | 1.91                     | 0.52              |
| 1:Y:509:ALA:HB1   | 14:Y:827:CLA:HBB2 | 1.90                     | 0.52              |
| 2:Z:207:GLY:O     | 2:Z:211:PHE:HB3   | 2.09                     | 0.52              |
| 2:Z:126:ILE:CG2   | 14:Z:816:CLA:HED2 | 2.38                     | 0.52              |
| 2:B:351:VAL:O     | 2:B:355:MET:HG3   | 2.10                     | 0.52              |
| 2:B:435:HIS:HB2   | 17:B:851:BCR:HC42 | 1.91                     | 0.52              |
| 14:H:808:CLA:H191 | 7:R:27:MET:HG3    | 1.92                     | 0.52              |
| 14:H:805:CLA:HMB2 | 14:H:828:CLA:HBB2 | 1.90                     | 0.52              |
| 6:F:41:ALA:HB2    | 8:J:38:PHE:CZ     | 2.44                     | 0.52              |
| 10:L:38:ARG:NH2   | 10:L:49:GLU:OE1   | 2.39                     | 0.52              |
| 6:Q:54:ASP:OD2    | 6:Q:56:ARG:NE     | 2.43                     | 0.52              |
| 1:G:319:TRP:HD1   | 9:T:42:GLY:HA3    | 1.74                     | 0.52              |
| 17:U:1007:BCR:C33 | 17:U:1007:BCR:HC8 | 2.38                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:Y:842:CLA:HBB1 | 14:Y:842:CLA:HHC  | 1.91                     | 0.52              |
| 2:Z:235:ASN:HD21  | 2:Z:251:THR:HG23  | 1.74                     | 0.52              |
| 2:Z:60:VAL:HG12   | 2:Z:64:LEU:CD1    | 2.39                     | 0.52              |
| 1:Y:690:LEU:HD13  | 2:Z:671:ILE:HD13  | 1.92                     | 0.52              |
| 1:A:211:ALA:HB2   | 17:A:845:BCR:H363 | 1.90                     | 0.52              |
| 1:G:484:PRO:HD3   | 1:G:536:PHE:HB2   | 1.91                     | 0.52              |
| 2:H:376:THR:HG23  | 2:H:597:THR:HG21  | 1.90                     | 0.52              |
| 2:H:320:MET:CE    | 18:H:847:LHG:O4   | 2.58                     | 0.52              |
| 10:L:35:PRO:HG3   | 10:L:49:GLU:CD    | 2.29                     | 0.52              |
| 1:Y:58:PHE:CE2    | 14:Y:804:CLA:HED1 | 2.44                     | 0.52              |
| 2:Z:315:GLU:O     | 2:Z:321:PRO:HA    | 2.09                     | 0.52              |
| 14:Z:801:CLA:H3A  | 14:Z:801:CLA:O1A  | 2.09                     | 0.52              |
| 1:A:237:PRO:HG2   | 1:A:242:PHE:CE2   | 2.45                     | 0.52              |
| 1:G:575:ARG:NH1   | 18:G:851:LHG:O10  | 2.43                     | 0.52              |
| 14:G:820:CLA:CMA  | 9:T:61:ALA:HB2    | 2.40                     | 0.52              |
| 2:H:475:TYR:HB3   | 6:Q:3:ALA:HA      | 1.91                     | 0.52              |
| 14:H:803:CLA:H112 | 17:H:845:BCR:H362 | 1.90                     | 0.52              |
| 14:H:807:CLA:C3D  | 14:H:826:CLA:HBA1 | 2.40                     | 0.52              |
| 14:H:826:CLA:O1D  | 14:H:827:CLA:HMA1 | 2.10                     | 0.52              |
| 17:G:850:BCR:H382 | 14:H:830:CLA:CBB  | 2.39                     | 0.52              |
| 3:N:25:LEU:HD21   | 3:N:64:ILE:HD11   | 1.90                     | 0.52              |
| 17:G:846:BCR:H382 | 17:T:102:BCR:H323 | 1.92                     | 0.52              |
| 2:B:206:VAL:CG1   | 2:B:214:THR:HG21  | 2.39                     | 0.52              |
| 2:B:181:LEU:CG    | 14:B:813:CLA:H42  | 2.38                     | 0.52              |
| 1:G:19:ASP:HA     | 1:G:181:HIS:O     | 2.09                     | 0.52              |
| 1:G:280:THR:HG23  | 1:G:296:ASP:OD1   | 2.10                     | 0.52              |
| 1:G:346:GLU:HA    | 1:G:349:THR:HG22  | 1.92                     | 0.52              |
| 1:G:578:CYS:HB2   | 1:G:586:THR:O     | 2.10                     | 0.52              |
| 2:H:375:TYR:CE2   | 2:H:379:GLN:HG3   | 2.44                     | 0.52              |
| 2:H:361:TYR:CD2   | 14:H:827:CLA:HED2 | 2.45                     | 0.52              |
| 14:A:841:CLA:H91  | 17:L:208:BCR:H392 | 1.91                     | 0.52              |
| 17:L:208:BCR:H23C | 17:L:208:BCR:H403 | 1.92                     | 0.52              |
| 1:Y:520:VAL:HG12  | 1:Y:525:ALA:HB2   | 1.90                     | 0.52              |
| 1:Y:302:LEU:HD11  | 14:Y:817:CLA:HAB  | 1.91                     | 0.52              |
| 1:Y:201:LEU:HD21  | 14:Y:821:CLA:C3B  | 2.40                     | 0.52              |
| 1:Y:380:TYR:OH    | 14:Y:829:CLA:OBD  | 2.19                     | 0.52              |
| 2:Z:177:HIS:HA    | 2:Z:181:LEU:HB3   | 1.92                     | 0.52              |
| 1:A:340:GLY:O     | 1:A:429:VAL:N     | 2.43                     | 0.52              |
| 16:A:844:SF4:S3   | 2:B:574:CYS:HB3   | 2.49                     | 0.52              |
| 14:B:826:CLA:HED1 | 17:B:847:BCR:C33  | 2.37                     | 0.52              |
| 2:B:84:ARG:HA     | 2:B:84:ARG:NE     | 2.25                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:650:LEU:HD22  | 2:H:657:LEU:HD21  | 1.92                     | 0.52              |
| 14:G:804:CLA:HED2 | 14:G:804:CLA:H2A  | 1.92                     | 0.52              |
| 17:K:102:BCR:C8   | 17:K:102:BCR:H331 | 2.40                     | 0.52              |
| 10:L:54:HIS:O     | 10:L:58:LEU:HD13  | 2.08                     | 0.52              |
| 7:R:5:TYR:OH      | 7:R:11:PRO:HG2    | 2.10                     | 0.52              |
| 1:Y:510:SER:HB2   | 1:Y:513:PHE:CE2   | 2.45                     | 0.52              |
| 1:Y:737:LEU:HD22  | 14:Y:841:CLA:HMA1 | 1.92                     | 0.52              |
| 14:Z:807:CLA:C1A  | 14:Z:807:CLA:CGA  | 2.88                     | 0.52              |
| 14:Z:817:CLA:HMB2 | 14:Z:822:CLA:HMA3 | 1.90                     | 0.52              |
| 1:A:376:ALA:HA    | 1:A:526:MET:CE    | 2.40                     | 0.51              |
| 14:B:802:CLA:H43  | 14:B:832:CLA:HAA2 | 1.93                     | 0.51              |
| 17:B:847:BCR:H321 | 17:B:847:BCR:C8   | 2.40                     | 0.51              |
| 3:C:74:ARG:NH2    | 4:D:25:GLU:OE1    | 2.42                     | 0.51              |
| 6:F:8:CYS:HB3     | 6:F:14:PHE:CD2    | 2.45                     | 0.51              |
| 2:B:150:PHE:CZ    | 14:G:843:CLA:H11  | 2.45                     | 0.51              |
| 2:H:380:TYR:CD2   | 14:H:826:CLA:HAB  | 2.46                     | 0.51              |
| 14:H:816:CLA:H42  | 14:H:831:CLA:HAA2 | 1.92                     | 0.51              |
| 9:K:65:PHE:CD1    | 9:K:68:LEU:HD21   | 2.45                     | 0.51              |
| 14:H:808:CLA:H141 | 17:R:102:BCR:H322 | 1.92                     | 0.51              |
| 1:Y:537:MET:CE    | 1:Y:644:ILE:HA    | 2.40                     | 0.51              |
| 1:Y:78:GLY:O      | 1:Y:82:VAL:HG23   | 2.10                     | 0.51              |
| 2:Z:221:LEU:HG    | 2:Z:225:PHE:CE2   | 2.45                     | 0.51              |
| 2:Z:46:PHE:CE2    | 2:Z:50:PHE:HE2    | 2.28                     | 0.51              |
| 1:A:577:PRO:HB3   | 1:A:724:ILE:HB    | 1.91                     | 0.51              |
| 1:A:360:LEU:HD21  | 14:A:830:CLA:CBB  | 2.40                     | 0.51              |
| 2:B:390:PHE:HZ    | 14:B:825:CLA:HAB  | 1.74                     | 0.51              |
| 3:C:53:CYS:HB2    | 3:C:64:ILE:HD13   | 1.93                     | 0.51              |
| 14:G:819:CLA:CGA  | 14:G:819:CLA:H3A  | 2.40                     | 0.51              |
| 14:G:823:CLA:HMB3 | 14:G:843:CLA:C2C  | 2.41                     | 0.51              |
| 2:H:194:ILE:HG23  | 2:H:253:ILE:HB    | 1.93                     | 0.51              |
| 2:H:292:THR:HG21  | 14:H:819:CLA:OBD  | 2.10                     | 0.51              |
| 14:Y:810:CLA:HMB1 | 14:Y:810:CLA:HBB1 | 1.91                     | 0.51              |
| 2:Z:414:VAL:HG11  | 17:Z:844:BCR:H401 | 1.91                     | 0.51              |
| 2:Z:677:TRP:CH2   | 15:Z:840:PQN:H2M3 | 2.44                     | 0.51              |
| 1:A:319:TRP:CZ3   | 14:A:812:CLA:HMA1 | 2.45                     | 0.51              |
| 2:B:27:ALA:O      | 2:B:33:HIS:CE1    | 2.63                     | 0.51              |
| 2:B:462:PHE:HB2   | 14:B:838:CLA:OBD  | 2.11                     | 0.51              |
| 2:B:59:TRP:HA     | 14:B:808:CLA:HBB2 | 1.93                     | 0.51              |
| 1:G:552:ILE:HG12  | 14:H:803:CLA:HMD1 | 1.93                     | 0.51              |
| 1:G:602:MET:HG2   | 14:G:826:CLA:HBC1 | 1.92                     | 0.51              |
| 14:G:813:CLA:CAD  | 14:G:825:CLA:H92  | 2.39                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y:679:ALA:HB1   | 1:Y:742:THR:OG1   | 2.10                     | 0.51              |
| 14:Y:819:CLA:CAD  | 21:Y:907:HOH:O    | 2.58                     | 0.51              |
| 1:Y:539:HIS:HB2   | 14:Y:838:CLA:HED1 | 1.92                     | 0.51              |
| 17:Y:851:BCR:HC8  | 17:Y:851:BCR:H323 | 1.90                     | 0.51              |
| 2:Z:55:ILE:HG23   | 14:Z:806:CLA:H141 | 1.92                     | 0.51              |
| 14:Y:855:CLA:HBC1 | 2:Z:671:ILE:HB    | 1.92                     | 0.51              |
| 14:Z:826:CLA:H12  | 17:Z:842:BCR:H393 | 1.93                     | 0.51              |
| 14:A:803:CLA:HBB2 | 14:A:811:CLA:H122 | 1.93                     | 0.51              |
| 6:F:116:TRP:CG    | 6:F:117:PRO:HD3   | 2.46                     | 0.51              |
| 1:G:216:GLN:NE2   | 1:G:301:HIS:HD2   | 2.06                     | 0.51              |
| 1:G:681:PHE:CD1   | 17:G:850:BCR:H363 | 2.44                     | 0.51              |
| 10:L:57:PHE:CE1   | 10:L:58:LEU:HD12  | 2.45                     | 0.51              |
| 2:Z:467:GLN:NE2   | 2:Z:515:PHE:HB3   | 2.25                     | 0.51              |
| 2:Z:173:ARG:NE    | 14:Z:822:CLA:HMD1 | 2.25                     | 0.51              |
| 14:B:818:CLA:H141 | 14:B:819:CLA:H101 | 1.92                     | 0.51              |
| 15:B:842:PQN:H192 | 17:B:848:BCR:H23C | 1.91                     | 0.51              |
| 4:D:73:ARG:N      | 4:D:74:PRO:HD2    | 2.25                     | 0.51              |
| 1:G:297:THR:HA    | 1:G:300:HIS:HB3   | 1.91                     | 0.51              |
| 2:H:119:VAL:CG2   | 2:H:123:TRP:CZ2   | 2.94                     | 0.51              |
| 14:H:811:CLA:O1D  | 14:H:812:CLA:HMC1 | 2.10                     | 0.51              |
| 12:X:11:PHE:O     | 12:X:14:PHE:HB3   | 2.10                     | 0.51              |
| 1:Y:289:THR:OG1   | 1:Y:382:TYR:N     | 2.44                     | 0.51              |
| 14:Y:833:CLA:O2A  | 14:Y:842:CLA:H42  | 2.10                     | 0.51              |
| 2:Z:334:HIS:O     | 2:Z:392:HIS:HB3   | 2.10                     | 0.51              |
| 1:A:336:PHE:CE1   | 10:L:4:LEU:HD13   | 2.46                     | 0.51              |
| 14:A:812:CLA:HHD  | 14:A:812:CLA:HBC2 | 1.91                     | 0.51              |
| 14:A:839:CLA:HMD1 | 6:F:85:LEU:HD11   | 1.93                     | 0.51              |
| 1:G:195:SER:O     | 1:G:199:HIS:ND1   | 2.29                     | 0.51              |
| 2:H:300:ILE:HG23  | 14:H:818:CLA:HED3 | 1.91                     | 0.51              |
| 2:H:466:ILE:HG12  | 14:H:831:CLA:HMC3 | 1.92                     | 0.51              |
| 2:B:109:SER:OG    | 7:I:4:SER:HB2     | 2.09                     | 0.51              |
| 1:A:480:ILE:HD11  | 10:L:69:ARG:HH21  | 1.76                     | 0.51              |
| 3:N:13:CYS:O      | 3:N:14:THR:HG22   | 2.10                     | 0.51              |
| 1:G:90:MET:HE2    | 14:G:808:CLA:HAA2 | 1.93                     | 0.51              |
| 2:H:440:TYR:CD2   | 14:H:802:CLA:H203 | 2.45                     | 0.51              |
| 2:H:542:LYS:CE    | 2:H:546:ASP:OD2   | 2.57                     | 0.51              |
| 2:H:665:THR:HA    | 14:H:803:CLA:HAB  | 1.91                     | 0.51              |
| 1:Y:384:ALA:HB1   | 1:Y:525:ALA:O     | 2.11                     | 0.51              |
| 14:Y:805:CLA:H41  | 14:Y:805:CLA:H72  | 1.92                     | 0.51              |
| 2:Z:443:ASN:HA    | 2:Z:455:GLN:HG2   | 1.92                     | 0.51              |
| 2:Z:447:VAL:HG22  | 2:Z:452:PRO:HA    | 1.91                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:42:PRO:HB3    | 1:A:47:TRP:CE3    | 2.46                     | 0.51              |
| 2:B:29:ASP:OD2    | 2:B:32:SER:OG     | 2.23                     | 0.51              |
| 2:B:336:GLN:O     | 2:B:340:HIS:ND1   | 2.44                     | 0.51              |
| 2:B:453:GLU:HA    | 6:F:48:LEU:HD22   | 1.93                     | 0.51              |
| 1:G:319:TRP:O     | 1:G:321:ILE:N     | 2.43                     | 0.51              |
| 1:G:387:TYR:HB3   | 1:G:751:ILE:HD11  | 1.92                     | 0.51              |
| 1:Y:58:PHE:CD1    | 14:Y:805:CLA:HMC2 | 2.46                     | 0.51              |
| 1:Y:281:PHE:CE1   | 14:Y:836:CLA:HED1 | 2.45                     | 0.51              |
| 17:Y:846:BCR:H331 | 17:Y:846:BCR:C8   | 2.41                     | 0.51              |
| 2:Z:122:TRP:HH2   | 17:Z:843:BCR:H391 | 1.76                     | 0.51              |
| 2:Z:288:HIS:CE1   | 17:Z:841:BCR:H363 | 2.45                     | 0.51              |
| 1:A:201:LEU:O     | 1:A:206:GLY:N     | 2.44                     | 0.51              |
| 1:A:329:LEU:HD21  | 14:A:821:CLA:HED1 | 1.93                     | 0.51              |
| 1:A:389:THR:HG22  | 1:A:393:LEU:HD11  | 1.93                     | 0.51              |
| 1:A:575:ARG:HG3   | 1:A:592:TRP:CD1   | 2.45                     | 0.51              |
| 1:A:744:TRP:CD2   | 17:A:849:BCR:H313 | 2.46                     | 0.51              |
| 1:A:308:PHE:HE1   | 14:A:821:CLA:HAB  | 1.75                     | 0.51              |
| 15:A:843:PQN:H172 | 15:A:843:PQN:H141 | 1.93                     | 0.51              |
| 1:G:683:TRP:CD2   | 13:G:801:CL0:CMA  | 2.94                     | 0.51              |
| 2:H:602:TRP:CD2   | 2:H:629:TYR:HB2   | 2.46                     | 0.51              |
| 9:T:38:GLY:O      | 9:T:41:PRO:HD2    | 2.11                     | 0.51              |
| 1:Y:421:ASP:HB3   | 1:Y:424:MET:HB2   | 1.92                     | 0.51              |
| 2:Z:122:TRP:CH2   | 17:Z:843:BCR:H391 | 2.45                     | 0.51              |
| 14:A:834:CLA:C4D  | 14:A:835:CLA:HMB3 | 2.41                     | 0.51              |
| 14:A:841:CLA:H61  | 14:B:840:CLA:H43  | 1.91                     | 0.51              |
| 2:B:433:GLY:O     | 2:B:437:LEU:HB3   | 2.10                     | 0.51              |
| 2:H:70:GLN:OE1    | 2:H:89:ALA:N      | 2.41                     | 0.51              |
| 9:T:24:LEU:HG     | 9:T:70:ALA:HA     | 1.93                     | 0.51              |
| 1:Y:387:TYR:N     | 1:Y:388:PRO:CD    | 2.74                     | 0.51              |
| 1:Y:14:VAL:HG23   | 14:Y:810:CLA:HMA2 | 1.93                     | 0.51              |
| 1:A:648:GLY:HA2   | 1:A:651:ARG:NH2   | 2.26                     | 0.50              |
| 14:A:813:CLA:HBB1 | 14:A:813:CLA:HMB1 | 1.92                     | 0.50              |
| 1:A:193:VAL:CG1   | 14:A:825:CLA:HHD  | 2.41                     | 0.50              |
| 14:A:829:CLA:C2   | 17:A:846:BCR:H24C | 2.41                     | 0.50              |
| 14:B:809:CLA:H72  | 14:B:829:CLA:H202 | 1.92                     | 0.50              |
| 1:G:77:PHE:CZ     | 14:G:813:CLA:HED1 | 2.46                     | 0.50              |
| 1:G:599:LEU:HD21  | 14:G:830:CLA:HBC1 | 1.91                     | 0.50              |
| 2:H:418:LYS:O     | 2:H:422:ILE:HG13  | 2.12                     | 0.50              |
| 2:H:596:VAL:O     | 2:H:599:TYR:HB3   | 2.12                     | 0.50              |
| 2:H:350:LEU:CD2   | 14:H:817:CLA:H41  | 2.40                     | 0.50              |
| 9:K:24:LEU:HD22   | 9:K:73:VAL:HG11   | 1.92                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:O:61:LYS:HG2    | 4:O:65:LEU:CD1    | 2.41                     | 0.50              |
| 14:Y:855:CLA:H3A  | 14:Y:855:CLA:CGA  | 2.41                     | 0.50              |
| 2:Z:539:ILE:HG12  | 14:Z:801:CLA:HMD1 | 1.92                     | 0.50              |
| 2:Z:76:TRP:CD1    | 2:Z:83:THR:HB     | 2.46                     | 0.50              |
| 2:Z:466:ILE:HG12  | 14:Z:832:CLA:HMC3 | 1.93                     | 0.50              |
| 1:A:352:TRP:CE2   | 14:A:825:CLA:H18  | 2.46                     | 0.50              |
| 1:A:302:LEU:HD13  | 14:A:815:CLA:CMC  | 2.41                     | 0.50              |
| 14:B:808:CLA:H3A  | 14:B:809:CLA:HMB3 | 1.93                     | 0.50              |
| 1:G:94:GLY:HA2    | 1:G:98:SER:HB3    | 1.94                     | 0.50              |
| 2:H:168:LYS:HD3   | 2:H:331:ASN:ND2   | 2.26                     | 0.50              |
| 2:H:503:TRP:CE2   | 14:H:831:CLA:HED1 | 2.46                     | 0.50              |
| 17:H:848:BCR:C8   | 17:H:848:BCR:H331 | 2.41                     | 0.50              |
| 14:B:841:CLA:H151 | 10:L:92:CYS:SG    | 2.51                     | 0.50              |
| 9:T:34:ILE:O      | 9:T:34:ILE:HG22   | 2.11                     | 0.50              |
| 1:Y:289:THR:HA    | 1:Y:520:VAL:HG21  | 1.93                     | 0.50              |
| 14:Y:805:CLA:H191 | 14:Y:813:CLA:C15  | 2.41                     | 0.50              |
| 14:Y:826:CLA:C1B  | 17:Y:850:BCR:H352 | 2.41                     | 0.50              |
| 1:A:444:LEU:HD13  | 14:A:838:CLA:CAB  | 2.41                     | 0.50              |
| 1:A:651:ARG:CD    | 2:B:639:ASN:HD21  | 2.23                     | 0.50              |
| 14:A:812:CLA:H41  | 14:A:812:CLA:H72  | 1.94                     | 0.50              |
| 1:G:21:VAL:HG23   | 1:G:181:HIS:HA    | 1.92                     | 0.50              |
| 1:G:45:THR:HG22   | 1:G:720:ARG:H     | 1.76                     | 0.50              |
| 2:H:52:HIS:CE1    | 14:H:804:CLA:HMA1 | 2.47                     | 0.50              |
| 14:H:806:CLA:HMB3 | 14:H:807:CLA:HMA1 | 1.94                     | 0.50              |
| 10:L:110:PRO:O    | 10:L:113:THR:OG1  | 2.26                     | 0.50              |
| 7:R:33:TYR:HH     | 11:V:30:TYR:HH    | 1.59                     | 0.50              |
| 10:U:111:LEU:HD11 | 10:U:120:PHE:CD1  | 2.47                     | 0.50              |
| 1:Y:17:ASP:OD1    | 1:Y:186:LYS:NZ    | 2.43                     | 0.50              |
| 2:Z:89:ALA:HA     | 2:Z:112:VAL:HG12  | 1.92                     | 0.50              |
| 14:B:835:CLA:CHA  | 14:B:836:CLA:HMB3 | 2.42                     | 0.50              |
| 1:G:244:LEU:O     | 1:G:244:LEU:HG    | 2.11                     | 0.50              |
| 2:H:332:SER:OG    | 2:H:396:PHE:HD1   | 1.94                     | 0.50              |
| 2:H:361:TYR:O     | 2:H:364:ILE:HG22  | 2.11                     | 0.50              |
| 17:J:103:BCR:C38  | 17:J:103:BCR:H23C | 2.41                     | 0.50              |
| 1:Y:254:PRO:C     | 1:Y:256:VAL:H     | 2.15                     | 0.50              |
| 1:A:706:TRP:CD1   | 2:B:419:GLU:HG3   | 2.46                     | 0.50              |
| 14:A:832:CLA:HMA1 | 2:B:691:THR:OG1   | 2.11                     | 0.50              |
| 14:B:804:CLA:CGA  | 14:B:804:CLA:H3A  | 2.42                     | 0.50              |
| 14:B:825:CLA:HBA1 | 14:B:826:CLA:O1D  | 2.11                     | 0.50              |
| 1:A:121:VAL:CG2   | 14:B:833:CLA:HMD1 | 2.35                     | 0.50              |
| 4:D:36:GLU:HG2    | 4:D:50:ARG:HA     | 1.92                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F:73:ILE:O       | 6:F:76:TRP:HB3     | 2.11                     | 0.50              |
| 1:G:80:LEU:HD12    | 14:G:813:CLA:HED3  | 1.94                     | 0.50              |
| 2:H:379:GLN:HE21   | 2:H:596:VAL:HG11   | 1.75                     | 0.50              |
| 1:Y:217:ILE:HA     | 1:Y:221:LEU:HD12   | 1.93                     | 0.50              |
| 1:Y:543:ALA:O      | 1:Y:547:HIS:HD2    | 1.95                     | 0.50              |
| 14:Y:821:CLA:H62   | 14:Y:825:CLA:HMB1  | 1.94                     | 0.50              |
| 2:Z:189:TRP:CZ3    | 2:Z:192:HIS:CD2    | 3.00                     | 0.50              |
| 14:Z:817:CLA:CMB   | 14:Z:822:CLA:HMA3  | 2.41                     | 0.50              |
| 14:Z:812:CLA:HMA1  | 17:Z:843:BCR:H292  | 1.93                     | 0.50              |
| 2:B:516:LEU:O      | 2:B:518:ILE:HG23   | 2.12                     | 0.50              |
| 2:B:551:LYS:NZ     | 6:F:138:VAL:O      | 2.44                     | 0.50              |
| 2:B:353:GLN:NE2    | 14:B:825:CLA:OBD   | 2.39                     | 0.50              |
| 14:G:804:CLA:HBA1  | 14:G:811:CLA:ND    | 2.27                     | 0.50              |
| 1:G:681:PHE:HB2    | 14:H:801:CLA:O1A   | 2.12                     | 0.50              |
| 14:V:1201:CLA:HMC1 | 14:V:1201:CLA:HBC2 | 1.93                     | 0.50              |
| 1:Y:429:VAL:HG23   | 14:Y:824:CLA:HBC3  | 1.94                     | 0.50              |
| 2:Z:5:PRO:HG2      | 2:Z:11:LEU:HB2     | 1.93                     | 0.50              |
| 1:A:548:VAL:O      | 1:A:552:ILE:HG13   | 2.12                     | 0.50              |
| 2:B:557:LYS:NZ     | 2:B:558:ASP:OD1    | 2.43                     | 0.50              |
| 6:F:87:ALA:HB1     | 6:F:105:LEU:HD21   | 1.94                     | 0.50              |
| 1:G:272:TRP:CG     | 14:G:817:CLA:HMB2  | 2.46                     | 0.50              |
| 2:H:274:HIS:ND1    | 14:H:816:CLA:HMB1  | 2.26                     | 0.50              |
| 14:H:824:CLA:H92   | 14:H:831:CLA:CAB   | 2.42                     | 0.50              |
| 11:V:15:ALA:O      | 11:V:18:PRO:HD2    | 2.12                     | 0.50              |
| 1:A:38:LEU:HA      | 1:A:47:TRP:HE1     | 1.76                     | 0.50              |
| 2:B:668:MET:HG2    | 15:B:842:PQN:O1    | 2.11                     | 0.50              |
| 1:G:201:LEU:O      | 1:G:308:PHE:HB3    | 2.11                     | 0.50              |
| 2:H:222:ALA:HB3    | 2:H:223:PRO:HD3    | 1.94                     | 0.50              |
| 2:H:432:LEU:HD21   | 14:H:835:CLA:C3B   | 2.42                     | 0.50              |
| 2:H:532:GLY:HA3    | 2:H:592:THR:HG23   | 1.93                     | 0.50              |
| 2:H:22:TYR:HH      | 2:H:707:SER:HG     | 1.52                     | 0.50              |
| 14:H:803:CLA:CGA   | 14:H:803:CLA:C3A   | 2.86                     | 0.50              |
| 7:I:20:TRP:O       | 7:I:24:THR:HG22    | 2.10                     | 0.50              |
| 2:Z:525:VAL:HG11   | 2:Z:599:TYR:HB2    | 1.94                     | 0.50              |
| 1:A:249:MET:O      | 1:A:252:LEU:N      | 2.43                     | 0.50              |
| 1:A:300:HIS:NE2    | 14:A:819:CLA:C1B   | 2.75                     | 0.50              |
| 3:C:16:CYS:HB3     | 16:C:102:SF4:S4    | 2.51                     | 0.50              |
| 3:C:28:VAL:HG21    | 4:D:111:ALA:HB2    | 1.93                     | 0.50              |
| 1:G:141:SER:HB2    | 1:G:143:LEU:HG     | 1.94                     | 0.50              |
| 1:G:167:VAL:O      | 1:G:171:LEU:HD13   | 2.12                     | 0.50              |
| 1:G:221:LEU:N      | 1:G:222:PRO:HD2    | 2.27                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:82:VAL:HG21   | 14:G:811:CLA:H141  | 1.93                     | 0.50              |
| 2:H:325:ILE:HA    | 2:H:328:THR:CG2    | 2.39                     | 0.50              |
| 2:H:387:VAL:HG21  | 2:H:589:MET:HG2    | 1.93                     | 0.50              |
| 2:H:586:MET:HG2   | 2:H:716:LEU:HD21   | 1.94                     | 0.50              |
| 14:H:817:CLA:HBC2 | 14:H:827:CLA:H91   | 1.94                     | 0.50              |
| 1:A:28:TRP:HE3    | 8:J:7:TYR:CG       | 2.30                     | 0.50              |
| 14:H:834:CLA:C4   | 14:W:1701:CLA:HED2 | 2.41                     | 0.50              |
| 2:Z:497:ASN:O     | 2:Z:498:VAL:HB     | 2.12                     | 0.50              |
| 1:A:236:ILE:HD12  | 1:A:237:PRO:O      | 2.12                     | 0.49              |
| 1:A:376:ALA:O     | 1:A:378:PRO:HD3    | 2.12                     | 0.49              |
| 1:A:78:GLY:O      | 1:A:81:ALA:HB3     | 2.12                     | 0.49              |
| 1:A:16:VAL:HG21   | 14:A:810:CLA:HED3  | 1.93                     | 0.49              |
| 1:A:486:PHE:CE2   | 14:A:837:CLA:H42   | 2.47                     | 0.49              |
| 2:B:354:HIS:HD1   | 14:B:817:CLA:CAD   | 2.12                     | 0.49              |
| 2:B:333:LEU:HD22  | 14:B:806:CLA:H203  | 1.93                     | 0.49              |
| 4:D:60:ARG:NH2    | 4:D:62:GLU:OE1     | 2.44                     | 0.49              |
| 4:D:95:HIS:O      | 4:D:97:LYS:N       | 2.41                     | 0.49              |
| 14:G:833:CLA:H2A  | 14:G:833:CLA:O2D   | 2.12                     | 0.49              |
| 14:H:829:CLA:O1D  | 14:H:829:CLA:H2A   | 2.12                     | 0.49              |
| 14:L:201:CLA:H171 | 14:L:206:CLA:HMB2  | 1.94                     | 0.49              |
| 17:L:209:BCR:H362 | 14:U:1006:CLA:H151 | 1.93                     | 0.49              |
| 1:Y:278:PHE:CE2   | 1:Y:279:LEU:HG     | 2.47                     | 0.49              |
| 14:Y:804:CLA:HAB  | 14:Y:806:CLA:CAD   | 2.42                     | 0.49              |
| 2:Z:440:TYR:CE2   | 2:Z:524:LEU:HB3    | 2.47                     | 0.49              |
| 2:Z:470:HIS:CD2   | 2:Z:515:PHE:CZ     | 3.00                     | 0.49              |
| 1:A:456:PHE:CD1   | 14:A:802:CLA:HMB3  | 2.47                     | 0.49              |
| 1:A:575:ARG:NH2   | 14:A:830:CLA:O1D   | 2.33                     | 0.49              |
| 2:B:425:LEU:HG    | 14:B:839:CLA:CAB   | 2.42                     | 0.49              |
| 2:B:598:PHE:HE2   | 14:B:803:CLA:H93   | 1.77                     | 0.49              |
| 2:B:59:TRP:CZ3    | 14:B:807:CLA:HMC1  | 2.47                     | 0.49              |
| 14:B:801:CLA:CGA  | 14:B:801:CLA:H3A   | 2.42                     | 0.49              |
| 2:B:361:TYR:CE2   | 14:B:828:CLA:HED2  | 2.47                     | 0.49              |
| 14:B:838:CLA:H42  | 14:B:838:CLA:NC    | 2.27                     | 0.49              |
| 3:C:49:GLY:HA2    | 16:C:101:SF4:S2    | 2.52                     | 0.49              |
| 1:G:196:MET:HB2   | 14:G:813:CLA:HBC2  | 1.94                     | 0.49              |
| 2:H:594:GLY:O     | 2:H:598:PHE:CD1    | 2.65                     | 0.49              |
| 7:I:19:CYS:HB3    | 14:L:202:CLA:CBB   | 2.42                     | 0.49              |
| 4:O:28:ALA:O      | 4:O:83:TYR:N       | 2.27                     | 0.49              |
| 4:O:36:GLU:HA     | 4:O:49:MET:O       | 2.12                     | 0.49              |
| 9:T:22:CYS:HA     | 9:T:25:PHE:HD1     | 1.71                     | 0.49              |
| 14:Y:827:CLA:HHC  | 14:Y:827:CLA:HBB1  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Y:846:BCR:H331 | 17:Y:846:BCR:HC8  | 1.94                     | 0.49              |
| 2:Z:184:VAL:HG13  | 17:Z:842:BCR:HC31 | 1.93                     | 0.49              |
| 10:U:92:CYS:SG    | 14:Z:839:CLA:H151 | 2.52                     | 0.49              |
| 1:A:148:ARG:HG2   | 1:A:224:ASN:HD21  | 1.77                     | 0.49              |
| 1:A:408:GLY:O     | 1:A:412:GLY:N     | 2.44                     | 0.49              |
| 1:A:415:PHE:CD1   | 1:A:419:ASP:HB2   | 2.46                     | 0.49              |
| 13:A:801:CL0:H13  | 14:A:852:CLA:OBD  | 2.11                     | 0.49              |
| 1:A:204:LEU:HD11  | 14:A:813:CLA:H42  | 1.95                     | 0.49              |
| 1:A:444:LEU:HD13  | 14:A:838:CLA:C3B  | 2.43                     | 0.49              |
| 1:G:581:PRO:HD3   | 2:H:567:GLY:HA2   | 1.94                     | 0.49              |
| 14:G:802:CLA:H142 | 17:G:850:BCR:H401 | 1.94                     | 0.49              |
| 1:A:13:ARG:H      | 14:A:812:CLA:HED1 | 1.78                     | 0.49              |
| 1:A:178:PHE:CE2   | 1:A:183:ARG:HB2   | 2.47                     | 0.49              |
| 1:A:463:ASP:OD2   | 1:A:646:ILE:N     | 2.38                     | 0.49              |
| 1:A:497:ALA:N     | 1:A:498:PRO:HD2   | 2.27                     | 0.49              |
| 2:B:242:VAL:HB    | 2:B:245:THR:OG1   | 2.12                     | 0.49              |
| 2:B:604:HIS:HA    | 2:B:607:VAL:HG22  | 1.94                     | 0.49              |
| 14:G:827:CLA:HMA1 | 14:G:834:CLA:H52  | 1.94                     | 0.49              |
| 14:H:807:CLA:C1A  | 14:H:807:CLA:CGA  | 2.90                     | 0.49              |
| 2:H:318:PHE:CD1   | 14:H:821:CLA:CAB  | 2.95                     | 0.49              |
| 14:J:102:CLA:HBB1 | 14:J:102:CLA:HMB1 | 2.36                     | 0.49              |
| 9:K:29:LEU:O      | 9:K:32:TYR:HB3    | 2.12                     | 0.49              |
| 14:L:202:CLA:HED1 | 17:L:203:BCR:H331 | 1.95                     | 0.49              |
| 11:M:9:TYR:HB3    | 17:M:101:BCR:H401 | 1.93                     | 0.49              |
| 10:U:43:PRO:HB3   | 10:U:111:LEU:CD1  | 2.43                     | 0.49              |
| 2:Z:246:ALA:O     | 2:Z:248:GLY:N     | 2.45                     | 0.49              |
| 2:Z:516:LEU:HB3   | 2:Z:603:LYS:HE3   | 1.95                     | 0.49              |
| 1:A:19:ASP:N      | 1:A:20:PRO:HD3    | 2.28                     | 0.49              |
| 1:A:682:ILE:HD11  | 14:A:840:CLA:CMB  | 2.43                     | 0.49              |
| 2:B:133:ASP:OD2   | 2:B:205:HIS:NE2   | 2.40                     | 0.49              |
| 2:B:239:ALA:HA    | 2:B:262:PRO:HG2   | 1.95                     | 0.49              |
| 1:G:275:TYR:CZ    | 14:G:815:CLA:HMD2 | 2.48                     | 0.49              |
| 2:H:335:PHE:O     | 2:H:339:TRP:HB2   | 2.11                     | 0.49              |
| 2:H:50:PHE:HE1    | 14:H:810:CLA:HBB1 | 1.78                     | 0.49              |
| 2:Z:525:VAL:HG11  | 2:Z:599:TYR:CB    | 2.42                     | 0.49              |
| 2:Z:166:TRP:CZ2   | 14:Z:809:CLA:HMA1 | 2.47                     | 0.49              |
| 14:Z:817:CLA:H43  | 14:Z:824:CLA:H112 | 1.94                     | 0.49              |
| 1:A:511:VAL:HG23  | 1:A:526:MET:CG    | 2.42                     | 0.49              |
| 1:A:56:HIS:ND1    | 14:A:806:CLA:CGA  | 2.73                     | 0.49              |
| 2:B:658:PHE:O     | 2:B:662:VAL:HG23  | 2.13                     | 0.49              |
| 2:B:667:PHE:HB3   | 14:B:804:CLA:CMC  | 2.42                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:B:805:CLA:HMC3 | 14:B:807:CLA:OBD   | 2.12                     | 0.49              |
| 14:B:832:CLA:CAB  | 14:B:833:CLA:HMB2  | 2.42                     | 0.49              |
| 4:D:117:ARG:NH1   | 4:D:123:PRO:HD3    | 2.27                     | 0.49              |
| 1:G:200:HIS:HA    | 1:G:204:LEU:HB3    | 1.95                     | 0.49              |
| 1:G:341:HIS:ND1   | 1:G:429:VAL:HG21   | 2.26                     | 0.49              |
| 1:G:531:LEU:HA    | 1:G:535:ASP:OD2    | 2.12                     | 0.49              |
| 1:G:534:ALA:HA    | 1:G:537:MET:HE2    | 1.93                     | 0.49              |
| 2:H:361:TYR:HB2   | 2:H:364:ILE:HD12   | 1.94                     | 0.49              |
| 14:H:824:CLA:H51  | 14:H:825:CLA:HED1  | 1.94                     | 0.49              |
| 14:Y:806:CLA:HBC3 | 14:Y:828:CLA:HMD1  | 1.94                     | 0.49              |
| 14:Y:802:CLA:H42  | 2:Z:657:LEU:CB     | 2.43                     | 0.49              |
| 1:A:460:VAL:HG12  | 14:A:802:CLA:H12   | 1.94                     | 0.49              |
| 1:A:718:GLN:NE2   | 5:E:15:TYR:OH      | 2.45                     | 0.49              |
| 2:B:654:TRP:CE3   | 17:B:848:BCR:HC41  | 2.47                     | 0.49              |
| 14:G:804:CLA:HAC2 | 18:G:851:LHG:H161  | 1.94                     | 0.49              |
| 2:H:179:ALA:HA    | 2:H:284:ILE:HA     | 1.94                     | 0.49              |
| 2:H:254:LEU:HD11  | 2:H:277:LEU:HD23   | 1.95                     | 0.49              |
| 2:H:176:HIS:CG    | 14:H:812:CLA:HMC2  | 2.48                     | 0.49              |
| 2:H:95:PHE:HD2    | 2:H:100:VAL:HG12   | 1.76                     | 0.49              |
| 17:L:203:BCR:C20  | 14:L:206:CLA:HAB   | 2.43                     | 0.49              |
| 8:S:31:ARG:NE     | 17:S:1104:BCR:H312 | 2.27                     | 0.49              |
| 2:Z:430:LEU:HD23  | 14:Z:801:CLA:O2A   | 2.12                     | 0.49              |
| 2:Z:600:TRP:HB2   | 14:Z:835:CLA:HMC1  | 1.94                     | 0.49              |
| 14:A:807:CLA:CGD  | 14:A:809:CLA:HED1  | 2.42                     | 0.49              |
| 14:A:839:CLA:CHB  | 15:A:843:PQN:H242  | 2.43                     | 0.49              |
| 2:B:654:TRP:CZ3   | 17:B:848:BCR:HC41  | 2.47                     | 0.49              |
| 2:H:172:SER:HB2   | 2:H:292:THR:HG22   | 1.94                     | 0.49              |
| 2:H:318:PHE:HA    | 14:H:821:CLA:CBB   | 2.43                     | 0.49              |
| 14:H:829:CLA:O1A  | 12:W:12:ARG:NH1    | 2.45                     | 0.49              |
| 14:H:824:CLA:H93  | 17:H:844:BCR:H333  | 1.94                     | 0.49              |
| 17:J:104:BCR:HC8  | 17:J:104:BCR:C32   | 2.35                     | 0.49              |
| 14:B:840:CLA:H151 | 10:L:88:VAL:HG11   | 1.93                     | 0.49              |
| 10:U:30:PHE:CZ    | 14:U:1002:CLA:HBB2 | 2.47                     | 0.49              |
| 7:I:29:LEU:HD12   | 2:Z:156:LEU:CD1    | 64.18                    | 0.49              |
| 2:Z:347:ILE:O     | 2:Z:351:VAL:HG13   | 2.13                     | 0.49              |
| 14:Z:833:CLA:HED2 | 14:Z:834:CLA:HMA3  | 1.95                     | 0.49              |
| 1:A:662:ILE:HA    | 2:B:623:MET:SD     | 2.53                     | 0.49              |
| 14:A:806:CLA:HED3 | 14:A:830:CLA:H52   | 1.95                     | 0.49              |
| 17:A:849:BCR:H321 | 17:A:849:BCR:HC8   | 1.95                     | 0.49              |
| 2:B:317:PRO:HD2   | 2:B:322:HIS:HB2    | 1.95                     | 0.49              |
| 2:B:424:HIS:O     | 2:B:428:VAL:HG12   | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:B:827:CLA:C2D  | 14:B:828:CLA:CMB   | 2.90                     | 0.49              |
| 2:B:460:PRO:HB2   | 14:B:838:CLA:HED2  | 1.93                     | 0.49              |
| 1:G:118:TRP:CD2   | 17:S:1104:BCR:H323 | 2.47                     | 0.49              |
| 1:G:470:ARG:NH2   | 1:G:473:ASP:OD2    | 2.37                     | 0.49              |
| 2:H:166:TRP:CE2   | 14:H:810:CLA:HMA1  | 2.48                     | 0.49              |
| 2:H:166:TRP:CD1   | 14:H:811:CLA:HED2  | 2.48                     | 0.49              |
| 14:A:820:CLA:CMA  | 9:K:61:ALA:HB2     | 2.43                     | 0.49              |
| 11:V:9:TYR:HB3    | 17:V:1202:BCR:H401 | 1.93                     | 0.49              |
| 1:Y:445:ASN:O     | 1:Y:449:ILE:HG13   | 2.13                     | 0.49              |
| 14:Y:832:CLA:HBB1 | 14:Y:832:CLA:HMB1  | 1.93                     | 0.49              |
| 2:Z:652:TRP:O     | 2:Z:729:ALA:HB1    | 2.12                     | 0.49              |
| 2:Z:388:GLY:HA3   | 14:Z:827:CLA:C2C   | 2.42                     | 0.49              |
| 2:B:430:LEU:HD12  | 14:B:801:CLA:H12   | 1.94                     | 0.49              |
| 14:B:809:CLA:HAB  | 14:B:810:CLA:HAA2  | 1.95                     | 0.49              |
| 6:F:1:ASP:N       | 6:F:5:LEU:O        | 2.27                     | 0.49              |
| 14:G:824:CLA:HMC1 | 14:G:824:CLA:HBC2  | 1.95                     | 0.49              |
| 1:G:713:VAL:O     | 14:G:840:CLA:HMD3  | 2.13                     | 0.49              |
| 1:G:337:THR:HG21  | 18:G:852:LHG:O1    | 2.13                     | 0.49              |
| 2:H:395:ILE:HG12  | 2:H:561:TYR:CG     | 2.47                     | 0.49              |
| 2:H:680:LEU:O     | 2:H:683:THR:OG1    | 2.20                     | 0.49              |
| 2:H:288:HIS:O     | 14:H:819:CLA:HED1  | 2.13                     | 0.49              |
| 17:I:101:BCR:H351 | 17:I:101:BCR:H15C  | 1.61                     | 0.49              |
| 9:K:56:LEU:HG     | 9:K:57:PRO:HD3     | 1.95                     | 0.49              |
| 10:L:21:ILE:O     | 10:L:21:ILE:HG22   | 2.12                     | 0.49              |
| 2:Z:707:SER:H     | 2:Z:710:GLN:HE21   | 1.58                     | 0.49              |
| 14:Z:806:CLA:C3A  | 14:Z:807:CLA:HMB3  | 2.43                     | 0.49              |
| 1:A:283:GLY:N     | 1:A:296:ASP:OD2    | 2.44                     | 0.48              |
| 14:A:839:CLA:H43  | 8:J:14:LEU:O       | 2.13                     | 0.48              |
| 14:B:808:CLA:HMA1 | 14:B:809:CLA:HMB3  | 1.94                     | 0.48              |
| 14:A:802:CLA:H93  | 14:B:841:CLA:CBB   | 2.43                     | 0.48              |
| 3:C:40:SER:OG     | 4:D:112:VAL:HG23   | 2.13                     | 0.48              |
| 1:G:217:ILE:HD13  | 1:G:278:PHE:HE2    | 1.77                     | 0.48              |
| 1:G:210:LEU:CD2   | 14:G:815:CLA:HAB   | 2.42                     | 0.48              |
| 2:H:589:MET:SD    | 2:H:590:LEU:N      | 2.86                     | 0.48              |
| 2:H:722:GLY:O     | 2:H:726:THR:OG1    | 2.26                     | 0.48              |
| 6:Q:116:TRP:N     | 6:Q:117:PRO:CD     | 2.76                     | 0.48              |
| 8:S:15:ALA:O      | 8:S:19:MET:HB2     | 2.13                     | 0.48              |
| 10:U:50:VAL:O     | 10:U:54:HIS:ND1    | 2.46                     | 0.48              |
| 1:Y:197:LEU:HD12  | 1:Y:325:LEU:HD11   | 1.95                     | 0.48              |
| 1:Y:722:LEU:HD22  | 1:Y:726:GLN:NE2    | 2.28                     | 0.48              |
| 14:Y:824:CLA:HMA1 | 14:Y:843:CLA:CAB   | 2.41                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:Y:816:CLA:HBB2 | 17:Y:847:BCR:C35  | 2.43                     | 0.48              |
| 17:Y:851:BCR:C32  | 17:Y:851:BCR:HC8  | 2.43                     | 0.48              |
| 2:Z:454:LYS:HG2   | 14:Z:831:CLA:HED3 | 1.94                     | 0.48              |
| 1:A:593:ASP:HA    | 1:A:596:PHE:HB3   | 1.94                     | 0.48              |
| 14:A:806:CLA:H191 | 18:A:850:LHG:H211 | 1.95                     | 0.48              |
| 2:B:369:THR:HG22  | 2:B:732:ILE:HD13  | 1.95                     | 0.48              |
| 2:B:59:TRP:CE3    | 2:B:60:VAL:HG13   | 2.48                     | 0.48              |
| 2:B:188:ALA:HA    | 14:B:815:CLA:HAB  | 1.95                     | 0.48              |
| 3:C:15:GLN:HA     | 3:C:18:ARG:HG2    | 1.94                     | 0.48              |
| 6:F:139:SER:O     | 6:F:141:ARG:NH1   | 2.46                     | 0.48              |
| 14:G:830:CLA:H2A  | 14:G:830:CLA:O2D  | 2.13                     | 0.48              |
| 1:G:337:THR:HG22  | 18:G:852:LHG:O4   | 2.14                     | 0.48              |
| 14:G:807:CLA:HBB2 | 17:G:854:BCR:H392 | 1.94                     | 0.48              |
| 2:H:172:SER:O     | 2:H:176:HIS:ND1   | 2.42                     | 0.48              |
| 2:H:240:SER:O     | 2:H:248:GLY:HA3   | 2.12                     | 0.48              |
| 3:N:64:ILE:HB     | 16:N:102:SF4:S3   | 2.53                     | 0.48              |
| 14:G:841:CLA:H193 | 8:S:19:MET:HG3    | 1.96                     | 0.48              |
| 1:Y:411:HIS:HA    | 1:Y:414:ILE:HD12  | 1.95                     | 0.48              |
| 14:Y:825:CLA:HBD  | 14:Y:825:CLA:HAA2 | 1.95                     | 0.48              |
| 17:Y:850:BCR:H382 | 17:Y:850:BCR:C23  | 2.43                     | 0.48              |
| 14:A:825:CLA:HMA1 | 14:A:827:CLA:H61  | 1.95                     | 0.48              |
| 1:G:202:ALA:HB2   | 1:G:312:GLY:HA3   | 1.95                     | 0.48              |
| 2:H:139:ILE:O     | 2:H:143:ILE:HG12  | 2.13                     | 0.48              |
| 3:N:6:ILE:HG13    | 3:N:64:ILE:HG13   | 1.94                     | 0.48              |
| 1:Y:416:MET:O     | 1:Y:561:ARG:HD3   | 2.14                     | 0.48              |
| 1:Y:71:LYS:HE2    | 14:Y:811:CLA:OBD  | 2.13                     | 0.48              |
| 14:A:826:CLA:CBB  | 17:A:848:BCR:H311 | 2.43                     | 0.48              |
| 2:B:334:HIS:CE1   | 2:B:395:ILE:HG21  | 2.49                     | 0.48              |
| 2:B:480:LEU:HD21  | 12:X:29:TYR:CE2   | 2.48                     | 0.48              |
| 2:B:395:ILE:HG12  | 2:B:561:TYR:CG    | 2.48                     | 0.48              |
| 4:D:7:PRO:O       | 4:D:50:ARG:NH1    | 2.47                     | 0.48              |
| 1:G:237:PRO:CG    | 1:G:248:LEU:HD21  | 2.44                     | 0.48              |
| 1:G:45:THR:HG21   | 14:G:840:CLA:HBB1 | 1.95                     | 0.48              |
| 13:G:801:CL0:H13  | 14:H:801:CLA:OBD  | 2.13                     | 0.48              |
| 10:L:75:ASN:ND2   | 10:L:139:LEU:HB3  | 2.28                     | 0.48              |
| 2:B:149:LEU:HB3   | 11:M:21:LEU:O     | 2.13                     | 0.48              |
| 1:Y:329:LEU:CD1   | 1:Y:345:TYR:HB2   | 2.43                     | 0.48              |
| 14:Z:824:CLA:HED2 | 17:Z:845:BCR:C33  | 2.43                     | 0.48              |
| 1:A:159:TYR:CE2   | 1:A:163:ILE:HD11  | 2.49                     | 0.48              |
| 1:A:619:SER:O     | 1:A:633:HIS:ND1   | 2.45                     | 0.48              |
| 14:A:836:CLA:HMB1 | 14:A:836:CLA:HBB1 | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:A:841:CLA:HHD  | 17:B:848:BCR:H383 | 1.95                     | 0.48              |
| 14:G:809:CLA:CAB  | 14:H:830:CLA:HMD2 | 2.44                     | 0.48              |
| 1:Y:468:PHE:O     | 2:Z:96:GLY:N      | 2.42                     | 0.48              |
| 1:Y:534:ALA:O     | 1:Y:538:VAL:HG23  | 2.13                     | 0.48              |
| 1:Y:743:THR:HG22  | 13:Y:801:CL0:OBD  | 2.13                     | 0.48              |
| 1:Y:683:TRP:CE3   | 13:Y:801:CL0:H4   | 2.49                     | 0.48              |
| 14:Y:828:CLA:HMB1 | 14:Y:828:CLA:HBB1 | 1.95                     | 0.48              |
| 1:Y:487:ALA:HA    | 14:Y:837:CLA:HBA1 | 1.94                     | 0.48              |
| 2:Z:369:THR:O     | 2:Z:372:ALA:HB3   | 2.14                     | 0.48              |
| 2:Z:615:PHE:O     | 2:Z:619:SER:OG    | 2.19                     | 0.48              |
| 14:Z:826:CLA:HBA2 | 14:Z:826:CLA:H3A  | 1.63                     | 0.48              |
| 1:A:270:PHE:CD2   | 14:K:101:CLA:HMD2 | 2.49                     | 0.48              |
| 14:A:819:CLA:HMB1 | 14:A:819:CLA:HBB1 | 1.95                     | 0.48              |
| 2:B:236:PRO:O     | 2:B:250:GLY:HA3   | 2.13                     | 0.48              |
| 2:B:189:TRP:CZ2   | 14:B:818:CLA:OBD  | 2.66                     | 0.48              |
| 1:G:141:SER:HB3   | 1:G:143:LEU:HG    | 1.95                     | 0.48              |
| 1:G:313:HIS:CE1   | 17:T:102:BCR:H363 | 2.48                     | 0.48              |
| 1:G:344:LEU:HD23  | 14:G:824:CLA:HMD3 | 1.95                     | 0.48              |
| 2:H:522:ASP:HB3   | 2:H:526:HIS:CD2   | 2.48                     | 0.48              |
| 2:H:582:PHE:CE1   | 2:H:586:MET:HE3   | 2.49                     | 0.48              |
| 14:H:818:CLA:HBA1 | 14:H:823:CLA:HBB1 | 1.95                     | 0.48              |
| 2:H:59:TRP:NE1    | 14:H:826:CLA:OBD  | 2.46                     | 0.48              |
| 7:I:30:LEU:HA     | 7:I:33:TYR:HB3    | 1.96                     | 0.48              |
| 10:L:131:SER:HA   | 10:L:134:VAL:HG12 | 1.95                     | 0.48              |
| 1:Y:360:LEU:HD13  | 1:Y:407:GLY:HA3   | 1.96                     | 0.48              |
| 1:Y:675:LEU:HD21  | 14:Y:828:CLA:H143 | 1.95                     | 0.48              |
| 2:Z:359:PRO:HB2   | 2:Z:364:ILE:CG2   | 2.44                     | 0.48              |
| 2:Z:443:ASN:O     | 2:Z:447:VAL:HG23  | 2.13                     | 0.48              |
| 1:A:522:GLY:O     | 1:A:625:VAL:HG22  | 2.14                     | 0.48              |
| 1:A:683:TRP:CD2   | 13:A:801:CL0:CMA  | 2.97                     | 0.48              |
| 2:B:239:ALA:O     | 2:B:262:PRO:HG2   | 2.14                     | 0.48              |
| 14:A:840:CLA:H142 | 17:F:201:BCR:C16  | 2.44                     | 0.48              |
| 1:G:285:LEU:HD21  | 1:G:378:PRO:HD2   | 1.95                     | 0.48              |
| 14:G:830:CLA:HBB1 | 14:G:830:CLA:HMB1 | 1.95                     | 0.48              |
| 2:H:582:PHE:CE1   | 2:H:586:MET:CE    | 2.97                     | 0.48              |
| 14:H:820:CLA:C3D  | 17:H:840:BCR:H393 | 2.43                     | 0.48              |
| 1:A:118:TRP:CE3   | 17:J:104:BCR:H323 | 2.49                     | 0.48              |
| 4:O:5:GLY:HA2     | 4:O:53:GLU:HG2    | 1.96                     | 0.48              |
| 10:U:76:LEU:O     | 10:U:79:LEU:N     | 2.47                     | 0.48              |
| 1:Y:273:ALA:O     | 1:Y:276:SER:OG    | 2.32                     | 0.48              |
| 14:Y:805:CLA:H201 | 14:Y:813:CLA:C15  | 2.43                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Z:637:LEU:HD22  | 2:Z:730:PHE:HA    | 1.95                     | 0.48              |
| 14:Z:802:CLA:HBA2 | 14:Z:802:CLA:H3A  | 1.64                     | 0.48              |
| 2:Z:663:TRP:CE2   | 14:Z:802:CLA:HMA2 | 2.49                     | 0.48              |
| 17:A:849:BCR:C32  | 17:A:849:BCR:HC8  | 2.44                     | 0.48              |
| 1:A:744:TRP:CE3   | 17:A:849:BCR:H313 | 2.49                     | 0.48              |
| 2:B:60:VAL:HG23   | 2:B:141:LEU:CD1   | 2.43                     | 0.48              |
| 2:B:721:VAL:HA    | 19:B:849:LMG:H432 | 1.95                     | 0.48              |
| 2:B:393:GLY:HA2   | 17:B:847:BCR:H393 | 1.95                     | 0.48              |
| 14:G:804:CLA:HAB  | 14:G:806:CLA:CBD  | 2.44                     | 0.48              |
| 14:G:826:CLA:HAB  | 17:G:849:BCR:C8   | 2.44                     | 0.48              |
| 2:H:117:SER:HA    | 14:H:826:CLA:HMA2 | 1.96                     | 0.48              |
| 2:H:481:LEU:HD22  | 2:H:500:LEU:HD21  | 1.96                     | 0.48              |
| 17:K:102:BCR:H15C | 17:K:102:BCR:H351 | 1.62                     | 0.48              |
| 6:Q:99:ILE:O      | 8:S:11:ALA:N      | 2.43                     | 0.48              |
| 1:Y:368:ILE:HG13  | 1:Y:401:GLY:HA3   | 1.96                     | 0.48              |
| 14:Y:803:CLA:C20  | 14:Z:801:CLA:H141 | 2.44                     | 0.48              |
| 14:Y:823:CLA:HBD  | 14:Y:823:CLA:HAA1 | 1.96                     | 0.48              |
| 2:B:428:VAL:HA    | 2:B:431:PHE:HB3   | 1.96                     | 0.48              |
| 2:B:592:THR:O     | 2:B:595:TRP:N     | 2.47                     | 0.48              |
| 2:B:72:ASN:O      | 2:B:76:TRP:N      | 2.47                     | 0.48              |
| 14:B:810:CLA:H203 | 7:I:26:VAL:HG23   | 1.95                     | 0.48              |
| 6:F:55:GLY:HA2    | 6:F:64:LEU:HD11   | 1.95                     | 0.48              |
| 1:G:196:MET:HE2   | 14:G:813:CLA:HBC2 | 1.95                     | 0.48              |
| 1:G:413:ALA:O     | 1:G:416:MET:HB2   | 2.13                     | 0.48              |
| 14:G:818:CLA:H42  | 14:G:827:CLA:HAB  | 1.96                     | 0.48              |
| 14:G:839:CLA:HMC3 | 14:G:840:CLA:ND   | 2.29                     | 0.48              |
| 2:B:4:PHE:HB2     | 7:I:34:ILE:HA     | 1.95                     | 0.48              |
| 17:T:102:BCR:H331 | 17:T:102:BCR:HC8  | 1.95                     | 0.48              |
| 17:Y:851:BCR:H403 | 17:Y:851:BCR:C23  | 2.35                     | 0.48              |
| 2:Z:202:ARG:NE    | 2:Z:237:ASP:OD1   | 2.35                     | 0.48              |
| 2:Z:358:LEU:O     | 14:Z:815:CLA:HED1 | 2.14                     | 0.48              |
| 2:Z:480:LEU:O     | 2:Z:482:SER:N     | 2.45                     | 0.48              |
| 2:Z:380:TYR:HH    | 2:Z:723:TYR:HE1   | 1.60                     | 0.48              |
| 14:Y:802:CLA:HMD1 | 14:Z:802:CLA:CMB  | 2.42                     | 0.48              |
| 1:A:460:VAL:HG23  | 14:L:201:CLA:HMC3 | 1.96                     | 0.48              |
| 1:A:675:LEU:HD11  | 14:A:828:CLA:H143 | 1.96                     | 0.48              |
| 2:B:86:ILE:HG23   | 2:B:112:VAL:HG22  | 1.95                     | 0.48              |
| 1:G:348:LEU:HB3   | 14:G:825:CLA:HBC3 | 1.95                     | 0.48              |
| 1:G:56:HIS:CD2    | 14:G:805:CLA:HBB2 | 2.48                     | 0.48              |
| 14:G:822:CLA:CMD  | 17:T:102:BCR:H392 | 2.44                     | 0.48              |
| 1:G:337:THR:HG21  | 18:G:852:LHG:C1   | 2.44                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:654:TRP:HE3    | 17:H:845:BCR:HC41  | 1.79                     | 0.48              |
| 17:H:848:BCR:H15C  | 17:H:848:BCR:H351  | 1.69                     | 0.48              |
| 17:L:203:BCR:C39   | 17:L:203:BCR:H23C  | 2.37                     | 0.48              |
| 2:B:149:LEU:HD21   | 17:M:101:BCR:H342  | 1.95                     | 0.48              |
| 4:O:42:PRO:HD2     | 4:O:58:PHE:CZ      | 2.49                     | 0.48              |
| 1:G:717:ILE:HD11   | 6:Q:95:ASN:O       | 2.14                     | 0.48              |
| 1:Y:237:PRO:HG2    | 1:Y:242:PHE:CZ     | 2.49                     | 0.48              |
| 1:Y:387:TYR:HD2    | 1:Y:755:GLY:HA3    | 1.79                     | 0.48              |
| 2:Z:31:GLU:OE1     | 2:Z:334:HIS:NE2    | 2.47                     | 0.48              |
| 1:A:103:TRP:CG     | 1:A:144:PHE:HD2    | 2.31                     | 0.47              |
| 1:A:660:GLN:CG     | 1:A:750:ARG:HA     | 2.44                     | 0.47              |
| 1:A:602:MET:CG     | 14:A:826:CLA:HBC1  | 2.43                     | 0.47              |
| 14:A:827:CLA:H172  | 14:A:834:CLA:H91   | 1.96                     | 0.47              |
| 2:B:479:THR:HG21   | 12:X:29:TYR:O      | 2.13                     | 0.47              |
| 2:B:491:ALA:HB2    | 2:B:497:ASN:ND2    | 2.29                     | 0.47              |
| 14:B:825:CLA:HBB1  | 14:B:825:CLA:HMB1  | 1.96                     | 0.47              |
| 14:G:805:CLA:H162  | 14:G:813:CLA:H51   | 1.96                     | 0.47              |
| 17:G:848:BCR:H351  | 17:G:848:BCR:H15C  | 1.62                     | 0.47              |
| 2:H:339:TRP:CZ3    | 17:H:843:BCR:H372  | 2.48                     | 0.47              |
| 9:K:43:LEU:HA      | 9:K:58:GLU:OE1     | 2.14                     | 0.47              |
| 17:L:209:BCR:H383  | 17:L:209:BCR:H23C  | 1.95                     | 0.47              |
| 14:S:1102:CLA:HMC3 | 17:S:1104:BCR:H352 | 1.96                     | 0.47              |
| 1:Y:392:SER:CB     | 14:Y:828:CLA:HMA1  | 2.44                     | 0.47              |
| 14:Y:826:CLA:O1A   | 14:Y:837:CLA:HMA1  | 2.13                     | 0.47              |
| 2:Z:450:GLY:C      | 2:Z:452:PRO:HD3    | 2.33                     | 0.47              |
| 14:A:818:CLA:C4    | 14:A:827:CLA:HMB1  | 2.44                     | 0.47              |
| 2:B:22:TYR:O       | 2:B:26:MET:HG3     | 2.14                     | 0.47              |
| 14:B:816:CLA:HBB1  | 14:B:816:CLA:HMB1  | 1.96                     | 0.47              |
| 1:G:351:SER:OG     | 1:G:419:ASP:OD2    | 2.19                     | 0.47              |
| 14:G:809:CLA:HMC3  | 2:H:445:VAL:HG13   | 1.95                     | 0.47              |
| 2:H:425:LEU:HG     | 14:H:836:CLA:CAB   | 2.44                     | 0.47              |
| 2:H:339:TRP:HH2    | 17:H:843:BCR:H372  | 1.78                     | 0.47              |
| 2:H:677:TRP:HZ3    | 17:H:845:BCR:H391  | 1.78                     | 0.47              |
| 17:J:104:BCR:C23   | 17:J:104:BCR:H403  | 2.41                     | 0.47              |
| 9:K:55:GLY:HA3     | 9:K:59:LEU:HD11    | 1.96                     | 0.47              |
| 14:H:809:CLA:HBB2  | 7:R:19:CYS:HB3     | 1.96                     | 0.47              |
| 1:Y:216:GLN:HA     | 1:Y:220:SER:HB3    | 1.96                     | 0.47              |
| 1:Y:337:THR:HG22   | 1:Y:340:GLY:HA2    | 1.95                     | 0.47              |
| 2:Z:136:GLN:HE22   | 2:Z:208:TRP:HE1    | 1.63                     | 0.47              |
| 2:Z:22:TYR:O       | 2:Z:26:MET:HG3     | 2.14                     | 0.47              |
| 2:Z:697:VAL:O      | 2:Z:697:VAL:HG23   | 2.15                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:Z:806:CLA:HMA2 | 14:Z:808:CLA:HED1  | 1.97                     | 0.47              |
| 1:A:101:GLU:HG3   | 1:A:155:GLU:HG3    | 1.95                     | 0.47              |
| 1:A:399:TRP:CD1   | 14:A:828:CLA:CAB   | 2.77                     | 0.47              |
| 1:A:348:LEU:CD1   | 14:A:825:CLA:HMC2  | 2.44                     | 0.47              |
| 2:B:260:PHE:CE1   | 2:B:358:LEU:HD23   | 2.49                     | 0.47              |
| 2:B:396:PHE:CD1   | 2:B:400:ASP:HB2    | 2.49                     | 0.47              |
| 1:G:199:HIS:O     | 1:G:203:GLY:N      | 2.48                     | 0.47              |
| 1:G:332:HIS:HE1   | 14:G:823:CLA:NA    | 2.11                     | 0.47              |
| 1:G:743:THR:HG22  | 13:G:801:CL0:OBD   | 2.13                     | 0.47              |
| 1:G:687:LEU:HB2   | 14:G:802:CLA:HMC3  | 1.95                     | 0.47              |
| 14:G:811:CLA:H171 | 14:S:1101:CLA:HBB1 | 1.96                     | 0.47              |
| 17:G:847:BCR:H321 | 17:G:847:BCR:HC8   | 1.96                     | 0.47              |
| 2:H:491:ALA:HB1   | 2:H:494:ASN:HD21   | 1.79                     | 0.47              |
| 2:H:50:PHE:CD2    | 2:H:152:GLY:HA2    | 2.49                     | 0.47              |
| 14:G:853:CLA:OBD  | 14:H:829:CLA:H3A   | 2.14                     | 0.47              |
| 1:Y:257:ASP:O     | 1:Y:258:TRP:HB2    | 2.14                     | 0.47              |
| 2:Z:203:GLY:N     | 2:Z:244:GLY:O      | 2.46                     | 0.47              |
| 1:A:451:LEU:CD2   | 14:A:837:CLA:HAB   | 2.36                     | 0.47              |
| 2:B:110:ASN:HB3   | 7:I:3:GLY:HA2      | 1.96                     | 0.47              |
| 2:B:434:PHE:CZ    | 17:F:201:BCR:H372  | 2.50                     | 0.47              |
| 2:B:372:ALA:HA    | 2:B:600:TRP:CZ3    | 2.50                     | 0.47              |
| 3:C:62:LEU:HD12   | 3:C:65:ARG:NE      | 2.30                     | 0.47              |
| 1:G:601:TRP:HE1   | 14:H:803:CLA:C1D   | 2.28                     | 0.47              |
| 14:G:818:CLA:HMD3 | 21:G:907:HOH:O     | 2.13                     | 0.47              |
| 14:G:841:CLA:H172 | 8:S:19:MET:HG3     | 1.96                     | 0.47              |
| 2:H:202:ARG:NH2   | 2:H:252:ALA:O      | 2.29                     | 0.47              |
| 17:B:851:BCR:H401 | 8:J:33:TYR:CD1     | 2.50                     | 0.47              |
| 10:L:16:HIS:CD2   | 10:L:17:LEU:H      | 2.33                     | 0.47              |
| 6:Q:94:ALA:O      | 6:Q:98:GLU:HG3     | 2.14                     | 0.47              |
| 17:R:102:BCR:H331 | 17:R:102:BCR:C8    | 2.30                     | 0.47              |
| 9:T:55:GLY:HA3    | 9:T:59:LEU:HD11    | 1.95                     | 0.47              |
| 1:Y:449:ILE:HG12  | 14:Y:855:CLA:HBA2  | 1.96                     | 0.47              |
| 17:Y:856:BCR:H351 | 17:Y:856:BCR:H15C  | 1.70                     | 0.47              |
| 2:Z:198:ILE:HA    | 2:Z:201:SER:HB3    | 1.96                     | 0.47              |
| 2:Z:542:LYS:HE2   | 2:Z:546:ASP:OD2    | 2.14                     | 0.47              |
| 14:Y:854:CLA:HMB3 | 14:Z:802:CLA:H201  | 1.95                     | 0.47              |
| 1:A:464:THR:HG22  | 2:B:654:TRP:NE1    | 2.27                     | 0.47              |
| 14:A:808:CLA:HBA2 | 14:A:808:CLA:H3A   | 1.56                     | 0.47              |
| 14:A:824:CLA:H3A  | 14:A:824:CLA:O1A   | 2.13                     | 0.47              |
| 2:B:17:THR:HG21   | 14:B:840:CLA:HBB1  | 1.97                     | 0.47              |
| 14:B:835:CLA:C1A  | 14:B:836:CLA:HMB3  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:116:TRP:N     | 6:F:117:PRO:CD    | 2.77                     | 0.47              |
| 1:G:614:SER:O     | 1:G:618:GLN:HG3   | 2.15                     | 0.47              |
| 1:G:387:TYR:CE2   | 1:G:622:TRP:HB3   | 2.50                     | 0.47              |
| 14:G:839:CLA:H122 | 14:G:839:CLA:HAB  | 1.96                     | 0.47              |
| 2:H:332:SER:O     | 2:H:336:GLN:HG3   | 2.14                     | 0.47              |
| 5:P:6:LYS:HD2     | 5:P:22:THR:HG22   | 1.95                     | 0.47              |
| 6:Q:76:TRP:O      | 6:Q:80:VAL:HG12   | 2.14                     | 0.47              |
| 1:Y:168:MET:O     | 1:Y:172:MET:HG2   | 2.14                     | 0.47              |
| 2:Z:377:HIS:O     | 2:Z:381:ILE:HG12  | 2.15                     | 0.47              |
| 2:Z:467:GLN:OE1   | 2:Z:475:TYR:OH    | 2.16                     | 0.47              |
| 1:A:551:LEU:O     | 1:A:555:LYS:HB2   | 2.15                     | 0.47              |
| 2:B:2:THR:HG21    | 2:B:19:ARG:NH1    | 2.29                     | 0.47              |
| 2:B:275:HIS:CE1   | 14:B:818:CLA:C2B  | 2.98                     | 0.47              |
| 14:B:837:CLA:HMB1 | 14:B:837:CLA:HBB1 | 1.96                     | 0.47              |
| 17:B:851:BCR:H391 | 8:J:33:TYR:CD1    | 2.48                     | 0.47              |
| 5:E:23:VAL:HA     | 5:E:38:VAL:HA     | 1.96                     | 0.47              |
| 1:G:403:PHE:CZ    | 1:G:736:LEU:HD13  | 2.49                     | 0.47              |
| 14:G:825:CLA:H42  | 14:G:829:CLA:C19  | 2.45                     | 0.47              |
| 2:H:397:LEU:O     | 2:H:401:TYR:HB3   | 2.15                     | 0.47              |
| 2:H:693:LEU:O     | 2:H:696:LEU:HB2   | 2.14                     | 0.47              |
| 14:H:830:CLA:HMB2 | 14:Q:201:CLA:CAB  | 2.45                     | 0.47              |
| 14:H:832:CLA:CHA  | 14:H:833:CLA:HMB3 | 2.45                     | 0.47              |
| 17:L:208:BCR:H15C | 17:L:208:BCR:H351 | 1.77                     | 0.47              |
| 2:Z:105:GLN:CD    | 2:Z:114:ILE:HD11  | 2.35                     | 0.47              |
| 14:Y:832:CLA:HHB  | 2:Z:691:THR:HG22  | 1.95                     | 0.47              |
| 1:A:45:THR:CG2    | 1:A:720:ARG:H     | 2.26                     | 0.47              |
| 1:A:48:ILE:HD13   | 14:A:839:CLA:HMB3 | 1.97                     | 0.47              |
| 14:A:805:CLA:CAD  | 14:A:825:CLA:H93  | 2.45                     | 0.47              |
| 2:B:253:ILE:HG13  | 2:B:254:LEU:HG    | 1.96                     | 0.47              |
| 14:B:814:CLA:HBC2 | 14:B:814:CLA:HMC1 | 1.97                     | 0.47              |
| 14:B:827:CLA:HBC3 | 19:B:849:LMG:H422 | 1.96                     | 0.47              |
| 14:B:833:CLA:H2A  | 14:B:833:CLA:HED2 | 1.95                     | 0.47              |
| 2:H:494:ASN:HD22  | 2:H:496:GLY:N     | 2.11                     | 0.47              |
| 1:G:694:ARG:NH1   | 2:H:572:GLY:O     | 2.47                     | 0.47              |
| 14:H:808:CLA:HMB3 | 14:H:809:CLA:CHC  | 2.44                     | 0.47              |
| 14:H:835:CLA:C4C  | 14:H:835:CLA:H42  | 2.45                     | 0.47              |
| 17:J:103:BCR:H15C | 17:J:103:BCR:H351 | 1.63                     | 0.47              |
| 14:K:103:CLA:H2A  | 14:K:103:CLA:CED  | 2.45                     | 0.47              |
| 1:G:426:GLN:NE2   | 4:O:48:VAL:CG2    | 2.78                     | 0.47              |
| 10:U:54:HIS:HA    | 10:U:57:PHE:CE2   | 2.50                     | 0.47              |
| 1:Y:399:TRP:HB3   | 14:Y:828:CLA:HMC3 | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:Y:808:CLA:H91  | 14:Y:811:CLA:H191 | 1.95                     | 0.47              |
| 17:Y:846:BCR:H351 | 17:Y:846:BCR:H15C | 1.58                     | 0.47              |
| 2:Z:188:ALA:HB2   | 14:Z:813:CLA:HBB2 | 1.96                     | 0.47              |
| 2:Z:255:THR:HG23  | 2:Z:271:ASP:OD1   | 2.14                     | 0.47              |
| 2:Z:437:LEU:O     | 2:Z:441:VAL:HG23  | 2.14                     | 0.47              |
| 2:Z:589:MET:HA    | 14:Z:823:CLA:HBC1 | 1.97                     | 0.47              |
| 2:Z:377:HIS:HB2   | 14:Z:825:CLA:C1B  | 2.44                     | 0.47              |
| 1:A:304:ILE:HD12  | 14:A:819:CLA:HAB  | 1.97                     | 0.47              |
| 2:B:50:PHE:HB3    | 2:B:148:ALA:O     | 2.15                     | 0.47              |
| 14:B:825:CLA:O2A  | 14:B:837:CLA:HMA1 | 2.15                     | 0.47              |
| 14:B:838:CLA:H121 | 14:B:838:CLA:HMC2 | 1.96                     | 0.47              |
| 3:C:76:MET:HB2    | 3:C:78:LEU:HG     | 1.96                     | 0.47              |
| 1:G:606:ILE:O     | 1:G:609:VAL:HB    | 2.15                     | 0.47              |
| 1:G:722:LEU:HD11  | 14:G:841:CLA:HMD3 | 1.95                     | 0.47              |
| 1:G:405:VAL:HG13  | 17:G:849:BCR:H342 | 1.97                     | 0.47              |
| 2:H:117:SER:HB2   | 14:H:827:CLA:HMA2 | 1.96                     | 0.47              |
| 2:H:187:LEU:HB2   | 2:H:280:ALA:HB1   | 1.96                     | 0.47              |
| 2:H:336:GLN:O     | 2:H:340:HIS:ND1   | 2.48                     | 0.47              |
| 2:H:368:HIS:HB3   | 2:H:608:TRP:CE3   | 2.50                     | 0.47              |
| 14:H:837:CLA:HBB2 | 15:H:839:PQN:H141 | 1.96                     | 0.47              |
| 17:I:101:BCR:H382 | 17:I:101:BCR:C23  | 2.45                     | 0.47              |
| 8:J:28:GLU:OE1    | 8:J:28:GLU:HA     | 2.15                     | 0.47              |
| 17:B:851:BCR:C21  | 8:J:36:LEU:HD13   | 2.45                     | 0.47              |
| 1:Y:164:GLY:O     | 17:Y:847:BCR:H313 | 2.15                     | 0.47              |
| 1:Y:451:LEU:HD21  | 14:Y:838:CLA:CAB  | 2.45                     | 0.47              |
| 1:Y:608:VAL:HG21  | 13:Y:801:CL0:H66  | 1.96                     | 0.47              |
| 2:Z:677:TRP:O     | 2:Z:680:LEU:N     | 2.48                     | 0.47              |
| 14:Z:808:CLA:H93  | 14:Z:827:CLA:H193 | 1.97                     | 0.47              |
| 2:B:655:MET:CG    | 2:B:725:LEU:HD22  | 2.45                     | 0.47              |
| 14:B:807:CLA:HMB1 | 14:B:807:CLA:HBB1 | 1.97                     | 0.47              |
| 4:D:28:ALA:HB2    | 4:D:57:TYR:CD1    | 2.49                     | 0.47              |
| 4:D:5:GLY:HA3     | 4:D:55:LEU:HB2    | 1.97                     | 0.47              |
| 1:G:319:TRP:HB3   | 9:T:58:GLU:HG3    | 1.97                     | 0.47              |
| 1:G:79:HIS:O      | 1:G:83:VAL:HG23   | 2.15                     | 0.47              |
| 14:G:810:CLA:HMC1 | 14:G:810:CLA:HBC2 | 1.95                     | 0.47              |
| 2:H:110:ASN:ND2   | 7:R:4:SER:H       | 2.13                     | 0.47              |
| 2:H:200:GLU:OE2   | 2:H:205:HIS:CE1   | 2.68                     | 0.47              |
| 17:H:842:BCR:H321 | 17:H:842:BCR:HC8  | 1.97                     | 0.47              |
| 14:G:842:CLA:HHD  | 17:H:845:BCR:H383 | 1.96                     | 0.47              |
| 10:U:58:LEU:HD13  | 10:U:85:LEU:CD2   | 2.45                     | 0.47              |
| 1:Y:13:ARG:HD2    | 1:Y:15:VAL:HG22   | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y:140:THR:HG21  | 1:Y:748:LEU:HD22  | 1.97                     | 0.47              |
| 2:Z:166:TRP:CE2   | 14:Z:809:CLA:HMA1 | 2.50                     | 0.47              |
| 14:Z:828:CLA:HAB  | 14:Z:837:CLA:HBB2 | 1.97                     | 0.47              |
| 1:A:31:PRO:HG2    | 1:A:47:TRP:HH2    | 1.79                     | 0.47              |
| 2:B:150:PHE:HZ    | 14:G:843:CLA:H11  | 1.80                     | 0.47              |
| 2:B:238:THR:HG22  | 2:B:240:SER:H     | 1.80                     | 0.47              |
| 2:B:492:TRP:HZ3   | 14:B:836:CLA:HMD3 | 1.80                     | 0.47              |
| 6:F:117:PRO:O     | 6:F:121:LEU:HG    | 2.15                     | 0.47              |
| 1:G:352:TRP:HB3   | 14:G:805:CLA:CAC  | 2.40                     | 0.47              |
| 1:G:608:VAL:HA    | 1:G:611:PHE:HB2   | 1.97                     | 0.47              |
| 14:G:834:CLA:H91  | 17:G:849:BCR:H372 | 1.96                     | 0.47              |
| 14:G:830:CLA:H161 | 17:G:850:BCR:H342 | 1.96                     | 0.47              |
| 14:H:821:CLA:HBC1 | 14:H:822:CLA:H102 | 1.97                     | 0.47              |
| 10:U:75:ASN:ND2   | 10:U:139:LEU:HB3  | 2.29                     | 0.47              |
| 1:Y:14:VAL:HA     | 1:Y:189:TRP:HD1   | 1.80                     | 0.47              |
| 1:Y:214:GLY:O     | 1:Y:218:HIS:HB2   | 2.15                     | 0.47              |
| 1:Y:372:GLN:HE22  | 14:Y:837:CLA:CHC  | 2.28                     | 0.47              |
| 14:Y:832:CLA:HHB  | 2:Z:691:THR:CG2   | 2.45                     | 0.47              |
| 17:Y:851:BCR:H402 | 14:Z:801:CLA:H142 | 1.96                     | 0.47              |
| 1:A:654:LEU:HD13  | 14:B:803:CLA:CBB  | 2.45                     | 0.47              |
| 14:B:832:CLA:H121 | 6:F:71:LEU:HD22   | 1.97                     | 0.47              |
| 1:G:68:ILE:O      | 1:G:72:ILE:HG13   | 2.14                     | 0.47              |
| 1:G:79:HIS:CG     | 14:G:805:CLA:HMA1 | 2.50                     | 0.47              |
| 14:G:811:CLA:HBA2 | 14:G:811:CLA:H3A  | 1.61                     | 0.47              |
| 14:G:818:CLA:HAA1 | 14:G:827:CLA:HBB2 | 1.97                     | 0.47              |
| 2:H:530:ALA:HA    | 14:H:836:CLA:HED3 | 1.97                     | 0.47              |
| 2:H:181:LEU:HD22  | 14:H:812:CLA:CHB  | 2.44                     | 0.47              |
| 2:H:173:ARG:HB2   | 14:H:812:CLA:HBC2 | 1.97                     | 0.47              |
| 7:I:17:VAL:O      | 7:I:22:MET:HB2    | 2.15                     | 0.47              |
| 10:U:131:SER:HA   | 10:U:134:VAL:HG12 | 1.96                     | 0.47              |
| 1:Y:219:VAL:CG2   | 1:Y:239:PRO:HB3   | 2.42                     | 0.47              |
| 1:Y:543:ALA:O     | 1:Y:547:HIS:CD2   | 2.68                     | 0.47              |
| 14:Y:809:CLA:HBB1 | 14:Y:809:CLA:HMB1 | 1.97                     | 0.47              |
| 2:Z:648:ASN:OD1   | 2:Z:649:LEU:HG    | 2.14                     | 0.47              |
| 2:Z:586:MET:HB3   | 2:Z:716:LEU:HD11  | 1.96                     | 0.47              |
| 1:A:587:CYS:O     | 2:B:675:GLY:HA3   | 2.15                     | 0.46              |
| 14:A:829:CLA:H12  | 17:A:846:BCR:H24C | 1.95                     | 0.46              |
| 1:A:650:LEU:HD23  | 2:B:638:ILE:CD1   | 2.45                     | 0.46              |
| 1:G:88:SER:OG     | 1:G:165:GLY:HA3   | 2.15                     | 0.46              |
| 1:G:301:HIS:HE1   | 14:G:819:CLA:NA   | 2.12                     | 0.46              |
| 17:G:849:BCR:H393 | 17:G:849:BCR:H271 | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:663:TRP:CD2   | 14:H:802:CLA:HMA1  | 2.48                     | 0.46              |
| 17:H:844:BCR:H311 | 17:H:844:BCR:HC8   | 1.95                     | 0.46              |
| 2:B:92:ASP:H      | 7:I:1:MET:HE1      | 1.79                     | 0.46              |
| 1:A:28:TRP:HB3    | 8:J:7:TYR:HB2      | 1.97                     | 0.46              |
| 14:U:1002:CLA:CBA | 17:U:1008:BCR:H363 | 2.45                     | 0.46              |
| 1:Y:348:LEU:HD12  | 14:Y:825:CLA:HMC2  | 1.97                     | 0.46              |
| 1:Y:456:PHE:O     | 1:Y:460:VAL:HG22   | 2.16                     | 0.46              |
| 1:Y:34:PHE:HB2    | 1:Y:61:HIS:CD2     | 2.49                     | 0.46              |
| 1:Y:683:TRP:O     | 1:Y:686:SER:N      | 2.48                     | 0.46              |
| 1:Y:140:THR:HG21  | 1:Y:748:LEU:CD2    | 2.45                     | 0.46              |
| 14:Y:840:CLA:H3A  | 14:Y:840:CLA:HBA2  | 1.69                     | 0.46              |
| 2:Z:378:HIS:O     | 2:Z:382:ALA:N      | 2.46                     | 0.46              |
| 2:Z:441:VAL:HG11  | 14:Z:831:CLA:HMC1  | 1.97                     | 0.46              |
| 17:Z:845:BCR:H351 | 17:Z:845:BCR:H15C  | 1.56                     | 0.46              |
| 1:A:696:TYR:O     | 2:B:542:LYS:NZ     | 2.42                     | 0.46              |
| 1:A:356:LEU:HD11  | 14:A:830:CLA:CBB   | 2.45                     | 0.46              |
| 1:A:694:ARG:HD3   | 2:B:572:GLY:HA3    | 1.97                     | 0.46              |
| 14:B:818:CLA:HBB1 | 14:B:818:CLA:HMB1  | 1.98                     | 0.46              |
| 2:B:503:TRP:NE1   | 14:B:834:CLA:HED1  | 2.30                     | 0.46              |
| 1:G:405:VAL:HG11  | 14:G:826:CLA:C2C   | 2.45                     | 0.46              |
| 1:G:98:SER:HB2    | 1:G:144:PHE:CZ     | 2.51                     | 0.46              |
| 2:H:347:ILE:HA    | 2:H:350:LEU:CB     | 2.45                     | 0.46              |
| 2:H:427:TRP:CD1   | 14:Q:201:CLA:HED2  | 2.50                     | 0.46              |
| 14:H:807:CLA:HAB  | 14:H:808:CLA:CAA   | 2.41                     | 0.46              |
| 14:H:827:CLA:HBC2 | 14:H:827:CLA:HHD   | 1.98                     | 0.46              |
| 14:H:835:CLA:HMB2 | 14:H:836:CLA:C2D   | 2.45                     | 0.46              |
| 17:H:840:BCR:H351 | 17:H:840:BCR:H15C  | 1.72                     | 0.46              |
| 8:J:20:THR:HG23   | 17:J:104:BCR:H351  | 1.97                     | 0.46              |
| 3:N:22:THR:HG22   | 4:O:62:GLU:HB2     | 1.98                     | 0.46              |
| 3:N:71:GLU:HB3    | 3:N:76:MET:HG3     | 1.95                     | 0.46              |
| 2:Z:49:HIS:ND1    | 14:Z:811:CLA:OBD   | 2.48                     | 0.46              |
| 1:A:46:THR:O      | 1:A:49:TRP:N       | 2.48                     | 0.46              |
| 1:A:677:LEU:O     | 14:A:852:CLA:HBA1  | 2.15                     | 0.46              |
| 14:A:826:CLA:HAB  | 17:A:848:BCR:C8    | 2.44                     | 0.46              |
| 14:A:852:CLA:H42  | 2:B:441:VAL:HG13   | 1.98                     | 0.46              |
| 2:B:414:VAL:HA    | 2:B:417:HIS:CE1    | 2.50                     | 0.46              |
| 2:B:426:SER:HB2   | 14:B:801:CLA:HED2  | 1.97                     | 0.46              |
| 2:B:49:HIS:HB3    | 14:B:813:CLA:O1D   | 2.15                     | 0.46              |
| 1:G:219:VAL:HG13  | 1:G:239:PRO:HB3    | 1.98                     | 0.46              |
| 1:G:358:ILE:HG22  | 1:G:359:ASN:HD22   | 1.79                     | 0.46              |
| 1:G:359:ASN:C     | 14:G:805:CLA:HED1  | 2.35                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:375:TYR:OH     | 14:G:836:CLA:HBC3  | 2.15                     | 0.46              |
| 2:H:275:HIS:HB2    | 14:H:816:CLA:CHB   | 2.46                     | 0.46              |
| 2:H:583:TYR:CD1    | 2:H:712:ARG:HB3    | 2.49                     | 0.46              |
| 5:P:45:TYR:O       | 5:P:46:THR:C       | 2.54                     | 0.46              |
| 9:T:69:LEU:HA      | 14:T:103:CLA:HBC2  | 1.96                     | 0.46              |
| 1:Y:503:PRO:HG3    | 14:Y:836:CLA:CMD   | 2.45                     | 0.46              |
| 14:Y:816:CLA:HBB2  | 17:Y:847:BCR:H352  | 1.97                     | 0.46              |
| 2:Z:530:ALA:O      | 2:Z:534:HIS:ND1    | 2.42                     | 0.46              |
| 14:Z:807:CLA:H2    | 14:Z:807:CLA:H102  | 1.98                     | 0.46              |
| 1:A:58:PHE:CE2     | 14:A:805:CLA:HMC2  | 2.51                     | 0.46              |
| 1:A:746:PHE:CD2    | 13:A:801:CL0:H25   | 2.50                     | 0.46              |
| 14:A:819:CLA:H93   | 14:A:829:CLA:H171  | 1.97                     | 0.46              |
| 14:A:831:CLA:O2D   | 10:L:5:VAL:HG11    | 2.14                     | 0.46              |
| 14:A:834:CLA:C3D   | 14:A:835:CLA:HMB3  | 2.45                     | 0.46              |
| 1:A:86:TRP:O       | 1:A:90:MET:HG2     | 2.16                     | 0.46              |
| 2:B:11:LEU:HD22    | 2:B:19:ARG:HA      | 1.97                     | 0.46              |
| 2:B:91:TRP:N       | 14:B:810:CLA:O1D   | 2.48                     | 0.46              |
| 1:A:42:PRO:HG3     | 6:F:99:ILE:HD13    | 1.98                     | 0.46              |
| 14:G:821:CLA:ND    | 14:G:827:CLA:H142  | 2.31                     | 0.46              |
| 14:G:831:CLA:HBB2  | 14:G:838:CLA:HMC2  | 1.97                     | 0.46              |
| 14:G:842:CLA:HBB1  | 14:G:842:CLA:H93   | 1.97                     | 0.46              |
| 1:G:569:LYS:NZ     | 2:H:679:GLU:OE2    | 2.41                     | 0.46              |
| 14:H:805:CLA:CED   | 14:H:828:CLA:H43   | 2.46                     | 0.46              |
| 14:B:810:CLA:CMB   | 14:L:202:CLA:CHC   | 2.94                     | 0.46              |
| 14:A:841:CLA:H92   | 14:L:206:CLA:HMC1  | 1.97                     | 0.46              |
| 7:R:14:PHE:O       | 7:R:18:VAL:HG23    | 2.15                     | 0.46              |
| 17:U:1008:BCR:H351 | 17:U:1008:BCR:H15C | 1.70                     | 0.46              |
| 1:Y:224:ASN:OD1    | 1:Y:294:LEU:HD22   | 2.15                     | 0.46              |
| 1:Y:662:ILE:HD13   | 13:Y:801:CL0:H22   | 1.98                     | 0.46              |
| 14:U:1006:CLA:OBD  | 14:Y:834:CLA:HBA2  | 2.14                     | 0.46              |
| 2:Z:605:LEU:O      | 2:Z:609:GLU:HG3    | 2.14                     | 0.46              |
| 2:Z:385:LEU:HD21   | 14:Z:805:CLA:H142  | 1.97                     | 0.46              |
| 15:Z:840:PQN:H162  | 15:Z:840:PQN:H193  | 1.70                     | 0.46              |
| 1:A:279:LEU:HB3    | 1:A:299:HIS:CD2    | 2.51                     | 0.46              |
| 1:A:387:TYR:CZ     | 1:A:622:TRP:HB3    | 2.51                     | 0.46              |
| 14:A:822:CLA:HBA2  | 9:K:35:GLN:CG      | 2.46                     | 0.46              |
| 14:A:840:CLA:H193  | 8:J:19:MET:HG3     | 1.98                     | 0.46              |
| 2:B:390:PHE:CD2    | 2:B:540:LEU:HD13   | 2.50                     | 0.46              |
| 14:B:821:CLA:C3B   | 14:B:822:CLA:HMD2  | 2.45                     | 0.46              |
| 3:C:7:TYR:CD1      | 4:D:115:VAL:HB     | 2.51                     | 0.46              |
| 6:F:116:TRP:CD1    | 6:F:117:PRO:HD3    | 2.50                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:672:TYR:CE1   | 1:G:748:LEU:HD12  | 2.50                     | 0.46              |
| 1:G:219:VAL:HG11  | 14:G:814:CLA:O1D  | 2.16                     | 0.46              |
| 14:G:829:CLA:H162 | 14:G:829:CLA:H112 | 1.97                     | 0.46              |
| 1:G:429:VAL:HG13  | 14:G:831:CLA:CMD  | 2.45                     | 0.46              |
| 14:H:838:CLA:O1A  | 15:H:839:PQN:H302 | 2.16                     | 0.46              |
| 14:K:101:CLA:HBC3 | 14:K:101:CLA:HMC1 | 1.98                     | 0.46              |
| 6:Q:33:LYS:HA     | 6:Q:33:LYS:HD2    | 1.76                     | 0.46              |
| 2:Z:304:MET:HG3   | 2:Z:322:HIS:O     | 2.15                     | 0.46              |
| 2:Z:487:ILE:HA    | 2:Z:490:THR:OG1   | 2.14                     | 0.46              |
| 14:Z:819:CLA:CBB  | 14:Z:820:CLA:HBC2 | 2.45                     | 0.46              |
| 14:Y:840:CLA:C2B  | 14:Z:830:CLA:H41  | 2.46                     | 0.46              |
| 2:Z:86:ILE:HG23   | 2:Z:112:VAL:HB    | 1.96                     | 0.46              |
| 1:A:193:VAL:HG11  | 14:A:825:CLA:HAC2 | 1.96                     | 0.46              |
| 2:B:86:ILE:CG2    | 2:B:112:VAL:HG22  | 2.46                     | 0.46              |
| 1:A:670:SER:HB3   | 2:B:448:ALA:HB1   | 1.97                     | 0.46              |
| 1:A:442:SER:HB3   | 2:B:683:THR:O     | 2.15                     | 0.46              |
| 2:B:723:TYR:HE2   | 14:B:803:CLA:CGA  | 2.28                     | 0.46              |
| 2:B:21:TRP:CZ3    | 15:B:842:PQN:H293 | 2.51                     | 0.46              |
| 3:C:1:ALA:N       | 3:C:70:ALA:O      | 2.41                     | 0.46              |
| 5:E:36:VAL:HG23   | 5:E:36:VAL:O      | 2.16                     | 0.46              |
| 1:G:13:ARG:HB3    | 1:G:188:GLU:OE1   | 2.16                     | 0.46              |
| 1:G:77:PHE:CE1    | 14:G:813:CLA:HED1 | 2.51                     | 0.46              |
| 1:G:450:PHE:CE2   | 14:G:837:CLA:HAB  | 2.47                     | 0.46              |
| 14:G:840:CLA:CBB  | 15:G:844:PQN:H141 | 2.46                     | 0.46              |
| 1:G:86:TRP:CZ3    | 17:G:847:BCR:H401 | 2.46                     | 0.46              |
| 17:J:103:BCR:C32  | 17:J:103:BCR:HC8  | 2.44                     | 0.46              |
| 2:B:696:LEU:HD11  | 10:L:36:ALA:HB1   | 1.98                     | 0.46              |
| 1:G:583:ARG:NH2   | 4:O:62:GLU:OE2    | 2.42                     | 0.46              |
| 17:Q:204:BCR:H24C | 17:Q:204:BCR:H371 | 1.69                     | 0.46              |
| 14:U:1006:CLA:CHC | 14:Z:808:CLA:CMB  | 2.93                     | 0.46              |
| 1:Y:300:HIS:NE2   | 14:Y:819:CLA:C2B  | 2.79                     | 0.46              |
| 1:Y:314:MET:O     | 1:Y:323:HIS:N     | 2.42                     | 0.46              |
| 2:Z:121:HIS:O     | 2:Z:125:THR:OG1   | 2.31                     | 0.46              |
| 2:Z:339:TRP:CE2   | 14:Z:824:CLA:H91  | 2.51                     | 0.46              |
| 14:Z:818:CLA:H3A  | 14:Z:818:CLA:HBA2 | 1.71                     | 0.46              |
| 17:Z:843:BCR:H15C | 17:Z:843:BCR:H351 | 1.65                     | 0.46              |
| 1:A:54:LEU:O      | 1:A:61:HIS:NE2    | 2.48                     | 0.46              |
| 1:A:556:GLY:HA3   | 1:A:594:HIS:CG    | 2.51                     | 0.46              |
| 2:B:75:GLN:O      | 2:B:78:GLN:CG     | 2.64                     | 0.46              |
| 14:B:814:CLA:HMB1 | 14:B:814:CLA:HBB1 | 1.97                     | 0.46              |
| 2:B:582:PHE:HE1   | 14:B:829:CLA:HAC2 | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:B:847:BCR:H371 | 17:B:847:BCR:H24C | 1.72                     | 0.46              |
| 1:G:662:ILE:HG22  | 2:H:623:MET:SD    | 2.55                     | 0.46              |
| 1:G:52:HIS:O      | 14:G:830:CLA:H11  | 2.15                     | 0.46              |
| 2:H:332:SER:HB2   | 2:H:400:ASP:HB3   | 1.97                     | 0.46              |
| 14:H:806:CLA:HMB3 | 14:H:807:CLA:HBB  | 1.98                     | 0.46              |
| 2:H:419:GLU:CD    | 6:Q:141:ARG:HH22  | 2.19                     | 0.46              |
| 17:R:102:BCR:H392 | 17:R:102:BCR:H23C | 1.98                     | 0.46              |
| 2:H:92:ASP:N      | 7:R:1:MET:HE1     | 2.30                     | 0.46              |
| 1:Y:249:MET:O     | 1:Y:251:GLU:N     | 2.48                     | 0.46              |
| 1:Y:563:SER:HB2   | 1:Y:566:ILE:O     | 2.16                     | 0.46              |
| 14:Y:805:CLA:H191 | 14:Y:813:CLA:H143 | 1.98                     | 0.46              |
| 14:Y:832:CLA:HMB1 | 14:Y:842:CLA:HAA2 | 1.98                     | 0.46              |
| 17:Y:849:BCR:C8   | 17:Y:849:BCR:H331 | 2.44                     | 0.46              |
| 14:Y:854:CLA:HMB3 | 14:Z:802:CLA:H191 | 1.97                     | 0.46              |
| 1:A:591:GLY:O     | 1:A:595:VAL:HG23  | 2.16                     | 0.46              |
| 1:A:682:ILE:CD1   | 14:A:840:CLA:HMB3 | 2.46                     | 0.46              |
| 2:B:579:TRP:O     | 2:B:582:PHE:HB3   | 2.15                     | 0.46              |
| 14:B:813:CLA:H151 | 14:B:828:CLA:HMD2 | 1.97                     | 0.46              |
| 3:C:20:CYS:HA     | 16:C:101:SF4:S4   | 2.56                     | 0.46              |
| 1:G:378:PRO:HG2   | 1:G:384:ALA:HB2   | 1.98                     | 0.46              |
| 17:G:854:BCR:HC8  | 17:G:854:BCR:C33  | 2.39                     | 0.46              |
| 10:L:36:ALA:HB2   | 14:L:206:CLA:HMD1 | 1.98                     | 0.46              |
| 2:H:451:THR:HG22  | 6:Q:22:VAL:HG13   | 1.98                     | 0.46              |
| 17:R:101:BCR:H15C | 17:R:101:BCR:H351 | 1.73                     | 0.46              |
| 2:Z:668:MET:O     | 2:Z:672:SER:OG    | 2.26                     | 0.46              |
| 2:Z:674:ARG:HG3   | 2:Z:706:LEU:O     | 2.16                     | 0.46              |
| 1:A:347:VAL:CG2   | 1:A:425:ASN:HD21  | 2.29                     | 0.46              |
| 1:A:682:ILE:HG23  | 1:A:734:HIS:HD2   | 1.81                     | 0.46              |
| 14:A:806:CLA:HMA1 | 14:A:830:CLA:CAB  | 2.45                     | 0.46              |
| 14:A:811:CLA:CBB  | 14:A:811:CLA:HHC  | 2.46                     | 0.46              |
| 2:B:689:GLU:O     | 2:B:695:ASN:OD1   | 2.34                     | 0.46              |
| 2:B:467:GLN:NE2   | 14:B:837:CLA:HMD1 | 2.30                     | 0.46              |
| 1:G:12:VAL:N      | 1:G:318:ASN:OD1   | 2.49                     | 0.46              |
| 1:G:736:LEU:HD12  | 18:G:851:LHG:H332 | 1.98                     | 0.46              |
| 1:G:429:VAL:HG12  | 14:G:824:CLA:HMC3 | 1.97                     | 0.46              |
| 17:H:841:BCR:H371 | 17:H:841:BCR:H24C | 1.73                     | 0.46              |
| 9:K:65:PHE:HD1    | 9:K:68:LEU:HD21   | 1.81                     | 0.46              |
| 1:Y:447:VAL:O     | 1:Y:451:LEU:HG    | 2.16                     | 0.46              |
| 1:Y:392:SER:HA    | 14:Y:828:CLA:HMB3 | 1.97                     | 0.46              |
| 1:Y:733:ALA:HA    | 18:Y:852:LHG:H342 | 1.97                     | 0.46              |
| 2:Z:479:THR:N     | 2:Z:482:SER:OG    | 2.49                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:Y:832:CLA:HMA1 | 2:Z:691:THR:HG23  | 1.98                     | 0.46              |
| 2:Z:530:ALA:HB1   | 14:Z:836:CLA:HMB3 | 1.98                     | 0.46              |
| 2:B:17:THR:HG22   | 2:B:704:VAL:HG22  | 1.98                     | 0.46              |
| 2:B:75:GLN:O      | 2:B:78:GLN:HG2    | 2.16                     | 0.46              |
| 14:B:810:CLA:H203 | 7:I:26:VAL:CG2    | 2.46                     | 0.46              |
| 14:B:825:CLA:CMA  | 17:B:847:BCR:H14C | 2.46                     | 0.46              |
| 1:G:224:ASN:CB    | 1:G:294:LEU:HD13  | 2.46                     | 0.46              |
| 14:G:814:CLA:CMC  | 14:G:815:CLA:HBB1 | 2.46                     | 0.46              |
| 17:G:846:BCR:H15C | 17:G:846:BCR:H351 | 1.55                     | 0.46              |
| 17:G:850:BCR:H15C | 17:G:850:BCR:H351 | 1.84                     | 0.46              |
| 2:H:178:LEU:O     | 2:H:183:GLY:N     | 2.49                     | 0.46              |
| 14:H:809:CLA:HHC  | 14:H:809:CLA:CBB  | 2.46                     | 0.46              |
| 2:H:93:PRO:HB3    | 10:U:149:MET:HA   | 1.97                     | 0.46              |
| 14:L:206:CLA:HMA1 | 14:L:207:CLA:HBC1 | 1.98                     | 0.46              |
| 1:Y:458:LEU:HD22  | 1:Y:475:PHE:CE2   | 2.51                     | 0.46              |
| 1:Y:582:GLY:O     | 1:Y:586:THR:HG23  | 2.15                     | 0.46              |
| 14:Y:821:CLA:HMB2 | 14:Y:825:CLA:HMA3 | 1.98                     | 0.46              |
| 1:Y:99:ASN:O      | 1:Y:103:TRP:N     | 2.47                     | 0.46              |
| 2:Z:440:TYR:HB3   | 2:Z:622:LEU:HD11  | 1.97                     | 0.46              |
| 2:Z:52:HIS:CE1    | 14:Z:804:CLA:HMA1 | 2.51                     | 0.46              |
| 2:Z:730:PHE:CD2   | 14:Z:802:CLA:HMD1 | 2.50                     | 0.46              |
| 14:Z:811:CLA:HBB1 | 14:Z:811:CLA:HMB1 | 1.98                     | 0.46              |
| 2:B:339:TRP:CZ2   | 14:B:826:CLA:H91  | 2.50                     | 0.45              |
| 2:B:669:PHE:HB3   | 2:B:711:ALA:O     | 2.17                     | 0.45              |
| 14:B:815:CLA:HMB3 | 17:B:845:BCR:C12  | 2.46                     | 0.45              |
| 1:G:541:ILE:CD1   | 13:G:801:CL0:H63  | 2.41                     | 0.45              |
| 1:G:71:LYS:HG2    | 14:G:811:CLA:OBD  | 2.16                     | 0.45              |
| 14:G:839:CLA:C2B  | 14:Q:201:CLA:H41  | 2.46                     | 0.45              |
| 17:G:849:BCR:H382 | 17:G:849:BCR:C23  | 2.44                     | 0.45              |
| 14:H:804:CLA:H3A  | 14:H:804:CLA:HBA1 | 1.77                     | 0.45              |
| 14:H:806:CLA:HMA1 | 14:H:807:CLA:C2B  | 2.46                     | 0.45              |
| 3:N:60:ASP:H      | 5:P:58:ASN:CG     | 2.18                     | 0.45              |
| 4:O:42:PRO:HD2    | 4:O:58:PHE:HZ     | 1.81                     | 0.45              |
| 8:S:27:ILE:HG21   | 17:S:1104:BCR:C10 | 2.46                     | 0.45              |
| 17:Y:847:BCR:H15C | 17:Y:847:BCR:H351 | 1.67                     | 0.45              |
| 2:Z:246:ALA:O     | 2:Z:249:ALA:N     | 2.33                     | 0.45              |
| 14:Z:804:CLA:HBA1 | 14:Z:804:CLA:H3A  | 1.66                     | 0.45              |
| 14:Z:824:CLA:HED2 | 17:Z:845:BCR:H332 | 1.98                     | 0.45              |
| 1:A:58:PHE:CD2    | 14:A:805:CLA:HMC2 | 2.51                     | 0.45              |
| 14:A:807:CLA:HHB  | 14:A:808:CLA:HMB3 | 1.99                     | 0.45              |
| 14:A:803:CLA:H172 | 14:A:840:CLA:H161 | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:177:HIS:HA    | 2:B:181:LEU:HB3    | 1.97                     | 0.45              |
| 2:B:473:LEU:HD21  | 2:B:482:SER:HA     | 1.98                     | 0.45              |
| 2:B:376:THR:HG22  | 2:B:597:THR:CG2    | 2.46                     | 0.45              |
| 2:B:681:ILE:O     | 2:B:685:VAL:HG23   | 2.17                     | 0.45              |
| 2:B:667:PHE:CB    | 14:B:804:CLA:HMC3  | 2.46                     | 0.45              |
| 2:B:353:GLN:HE22  | 14:B:837:CLA:C4B   | 2.30                     | 0.45              |
| 1:G:237:PRO:HG2   | 1:G:242:PHE:CE2    | 2.52                     | 0.45              |
| 1:G:353:HIS:HB3   | 1:G:411:HIS:HB3    | 1.99                     | 0.45              |
| 1:G:272:TRP:HB3   | 14:G:817:CLA:HHB   | 1.98                     | 0.45              |
| 14:G:827:CLA:HMA3 | 17:G:849:BCR:H382  | 1.98                     | 0.45              |
| 14:G:835:CLA:HAA1 | 14:G:835:CLA:HBD   | 1.98                     | 0.45              |
| 17:L:209:BCR:H15C | 17:L:209:BCR:H351  | 1.78                     | 0.45              |
| 10:L:41:LEU:HD22  | 10:L:45:LEU:HD23   | 1.99                     | 0.45              |
| 6:Q:73:ILE:O      | 6:Q:77:ILE:HG13    | 2.15                     | 0.45              |
| 8:S:10:THR:C      | 8:S:12:PRO:HD2     | 2.36                     | 0.45              |
| 1:Y:308:PHE:O     | 1:Y:312:GLY:N      | 2.48                     | 0.45              |
| 1:Y:607:SER:O     | 1:Y:610:ILE:HG12   | 2.16                     | 0.45              |
| 1:Y:407:GLY:CA    | 14:Y:830:CLA:C2C   | 2.95                     | 0.45              |
| 2:Z:681:ILE:HA    | 2:Z:684:LEU:HD12   | 1.98                     | 0.45              |
| 2:Z:354:HIS:CE1   | 14:Z:815:CLA:HMD1  | 2.51                     | 0.45              |
| 14:Z:832:CLA:C1A  | 14:Z:832:CLA:HED2  | 2.46                     | 0.45              |
| 14:A:826:CLA:H92  | 14:A:838:CLA:H41   | 1.97                     | 0.45              |
| 2:B:176:HIS:HB3   | 14:B:813:CLA:CAB   | 2.45                     | 0.45              |
| 2:B:390:PHE:CE2   | 17:B:847:BCR:H373  | 2.50                     | 0.45              |
| 2:B:677:TRP:HZ3   | 14:B:804:CLA:O1D   | 2.00                     | 0.45              |
| 2:B:21:TRP:HZ3    | 15:B:842:PQN:H293  | 1.81                     | 0.45              |
| 4:D:9:LEU:HD23    | 4:D:50:ARG:NH1     | 2.31                     | 0.45              |
| 1:G:103:TRP:CD1   | 1:G:107:PRO:HA     | 2.51                     | 0.45              |
| 1:G:405:VAL:HG13  | 17:G:849:BCR:C34   | 2.46                     | 0.45              |
| 14:G:839:CLA:H161 | 6:Q:81:GLY:HA2     | 1.98                     | 0.45              |
| 2:H:677:TRP:CZ3   | 17:H:845:BCR:H391  | 2.52                     | 0.45              |
| 7:I:20:TRP:O      | 7:I:23:PRO:HG2     | 2.17                     | 0.45              |
| 8:J:1:MET:HB3     | 8:J:4:PHE:HB3      | 1.97                     | 0.45              |
| 4:O:36:GLU:HG2    | 4:O:50:ARG:HA      | 1.97                     | 0.45              |
| 6:Q:70:PHE:CD1    | 17:Q:202:BCR:H343  | 2.51                     | 0.45              |
| 17:R:102:BCR:H23C | 17:R:102:BCR:H403  | 1.98                     | 0.45              |
| 8:S:31:ARG:HE     | 17:S:1104:BCR:H312 | 1.82                     | 0.45              |
| 14:Y:829:CLA:HMB1 | 14:Y:829:CLA:HBB1  | 1.99                     | 0.45              |
| 2:Z:443:ASN:HB3   | 2:Z:455:GLN:NE2    | 2.29                     | 0.45              |
| 17:Z:846:BCR:H24C | 17:Z:846:BCR:H371  | 1.73                     | 0.45              |
| 1:A:548:VAL:HG11  | 1:A:601:TRP:CH2    | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:A:834:CLA:HED2 | 14:A:835:CLA:CMA  | 2.43                     | 0.45              |
| 14:A:841:CLA:H41  | 14:A:841:CLA:H62  | 1.78                     | 0.45              |
| 14:A:802:CLA:H41  | 2:B:654:TRP:NE1   | 2.31                     | 0.45              |
| 5:E:44:ASN:OD1    | 5:E:54:GLY:O      | 2.33                     | 0.45              |
| 1:G:349:THR:O     | 14:G:825:CLA:H203 | 2.17                     | 0.45              |
| 14:G:825:CLA:HBA1 | 14:G:829:CLA:H201 | 1.97                     | 0.45              |
| 14:G:838:CLA:C2   | 14:G:838:CLA:O1A  | 2.65                     | 0.45              |
| 17:G:847:BCR:HC8  | 17:G:847:BCR:H311 | 1.99                     | 0.45              |
| 1:G:744:TRP:CE2   | 17:G:850:BCR:H313 | 2.51                     | 0.45              |
| 2:H:140:PHE:CG    | 14:H:813:CLA:H12  | 2.51                     | 0.45              |
| 14:G:853:CLA:HMD1 | 14:H:829:CLA:HBA1 | 1.97                     | 0.45              |
| 14:H:832:CLA:C1A  | 14:H:833:CLA:HMB3 | 2.47                     | 0.45              |
| 4:O:117:ARG:HD2   | 4:O:122:ASN:ND2   | 2.32                     | 0.45              |
| 17:U:1007:BCR:C38 | 14:Y:834:CLA:H193 | 2.47                     | 0.45              |
| 1:Y:185:PRO:O     | 1:Y:190:PHE:HE2   | 1.99                     | 0.45              |
| 1:Y:200:HIS:O     | 1:Y:204:LEU:HB3   | 2.17                     | 0.45              |
| 1:A:376:ALA:HA    | 1:A:526:MET:HE3   | 1.99                     | 0.45              |
| 17:A:847:BCR:H15C | 17:A:847:BCR:H351 | 1.81                     | 0.45              |
| 2:B:301:LYS:NZ    | 2:B:327:GLU:OE2   | 2.47                     | 0.45              |
| 2:B:459:GLU:OE1   | 2:B:464:GLN:NE2   | 2.40                     | 0.45              |
| 3:C:37:GLN:OE1    | 4:D:105:VAL:HG22  | 2.17                     | 0.45              |
| 6:F:103:VAL:N     | 6:F:104:PRO:CD    | 2.80                     | 0.45              |
| 1:G:77:PHE:HB3    | 1:G:172:MET:O     | 2.15                     | 0.45              |
| 14:G:803:CLA:OBD  | 14:H:802:CLA:CMB  | 2.47                     | 0.45              |
| 1:G:90:MET:HE1    | 14:G:808:CLA:HED2 | 1.98                     | 0.45              |
| 14:G:808:CLA:CAD  | 14:G:828:CLA:HBA1 | 2.47                     | 0.45              |
| 14:G:829:CLA:H111 | 17:G:847:BCR:H383 | 1.98                     | 0.45              |
| 2:H:185:SER:OG    | 17:H:841:BCR:H351 | 2.16                     | 0.45              |
| 2:H:724:ILE:HD13  | 14:H:826:CLA:CMC  | 2.44                     | 0.45              |
| 1:Y:221:LEU:HD23  | 1:Y:221:LEU:HA    | 1.81                     | 0.45              |
| 1:Y:601:TRP:CH2   | 14:Y:802:CLA:HAB  | 2.50                     | 0.45              |
| 14:Y:826:CLA:HBA2 | 14:Y:826:CLA:H3A  | 1.77                     | 0.45              |
| 2:Z:181:LEU:HG    | 14:Z:811:CLA:H42  | 1.98                     | 0.45              |
| 2:Z:254:LEU:O     | 2:Z:255:THR:HB    | 2.16                     | 0.45              |
| 14:A:812:CLA:C1A  | 14:A:812:CLA:CGA  | 2.94                     | 0.45              |
| 14:A:821:CLA:CMD  | 14:A:822:CLA:HAB  | 2.47                     | 0.45              |
| 14:A:828:CLA:C9   | 17:J:103:BCR:H361 | 2.47                     | 0.45              |
| 1:A:719:PRO:HB2   | 14:A:839:CLA:HMC3 | 1.97                     | 0.45              |
| 2:B:200:GLU:CD    | 2:B:205:HIS:HA    | 2.37                     | 0.45              |
| 2:B:637:LEU:HD13  | 2:B:733:ALA:HB3   | 1.99                     | 0.45              |
| 14:B:807:CLA:H143 | 14:B:828:CLA:HBB2 | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:565:LEU:HD11  | 1:G:583:ARG:HB3   | 1.97                     | 0.45              |
| 1:G:576:PHE:CE2   | 1:G:589:VAL:HG23  | 2.52                     | 0.45              |
| 14:G:807:CLA:HAB  | 17:G:854:BCR:H392 | 1.98                     | 0.45              |
| 2:H:238:THR:OG1   | 2:H:248:GLY:O     | 2.22                     | 0.45              |
| 14:G:828:CLA:H122 | 14:H:801:CLA:H161 | 1.97                     | 0.45              |
| 14:H:802:CLA:H91  | 14:H:802:CLA:H111 | 1.86                     | 0.45              |
| 14:H:819:CLA:HBA2 | 14:H:819:CLA:H3A  | 1.71                     | 0.45              |
| 14:H:821:CLA:HMB1 | 14:H:821:CLA:HBB1 | 1.99                     | 0.45              |
| 17:I:101:BCR:H341 | 2:Z:58:LEU:CD1    | 62.16                    | 0.45              |
| 14:A:822:CLA:HAA1 | 9:K:35:GLN:HG2    | 1.98                     | 0.45              |
| 4:O:50:ARG:N      | 4:O:54:ASN:HD21   | 2.14                     | 0.45              |
| 1:Y:217:ILE:HD13  | 1:Y:278:PHE:CE2   | 2.51                     | 0.45              |
| 14:Y:821:CLA:HMA2 | 14:Y:825:CLA:C1C  | 2.46                     | 0.45              |
| 14:Y:855:CLA:H52  | 14:Y:855:CLA:HMB2 | 1.99                     | 0.45              |
| 2:Z:7:PHE:CD1     | 2:Z:33:HIS:CD2    | 3.05                     | 0.45              |
| 2:Z:614:GLN:O     | 2:Z:618:SER:HB2   | 2.17                     | 0.45              |
| 14:Z:822:CLA:H2A  | 14:Z:822:CLA:HED2 | 1.99                     | 0.45              |
| 14:Z:825:CLA:CGA  | 14:Z:825:CLA:C3A  | 2.93                     | 0.45              |
| 14:Z:834:CLA:HBC2 | 14:Z:834:CLA:HHD  | 1.99                     | 0.45              |
| 1:A:726:GLN:O     | 1:A:730:VAL:HG23  | 2.16                     | 0.45              |
| 13:A:801:CL0:CMB  | 14:A:852:CLA:HMD1 | 2.47                     | 0.45              |
| 5:E:62:LEU:HD23   | 5:E:62:LEU:HA     | 1.83                     | 0.45              |
| 14:B:802:CLA:H121 | 14:F:202:CLA:HAC1 | 1.97                     | 0.45              |
| 1:G:617:MET:O     | 1:G:622:TRP:N     | 2.45                     | 0.45              |
| 1:G:78:GLY:HA3    | 14:G:811:CLA:HBC1 | 1.98                     | 0.45              |
| 17:G:847:BCR:H23C | 17:G:847:BCR:H383 | 1.99                     | 0.45              |
| 2:H:555:ASP:CG    | 3:N:65:ARG:HH12   | 2.20                     | 0.45              |
| 6:Q:103:VAL:HG22  | 8:S:14:LEU:HD11   | 1.98                     | 0.45              |
| 1:Y:219:VAL:O     | 1:Y:222:PRO:HD2   | 2.17                     | 0.45              |
| 1:Y:550:VAL:HG13  | 17:Y:850:BCR:H313 | 1.98                     | 0.45              |
| 2:Z:42:TYR:CE2    | 2:Z:333:LEU:HD21  | 2.51                     | 0.45              |
| 2:Z:564:PRO:HB3   | 2:Z:708:ILE:HB    | 1.97                     | 0.45              |
| 1:Y:464:THR:HG22  | 2:Z:654:TRP:HE1   | 1.81                     | 0.45              |
| 2:Z:710:GLN:HA    | 19:Z:847:LMG:O9   | 2.17                     | 0.45              |
| 14:Z:832:CLA:C1D  | 14:Z:833:CLA:CAB  | 2.94                     | 0.45              |
| 1:A:103:TRP:CG    | 1:A:144:PHE:CD2   | 3.05                     | 0.45              |
| 1:A:392:SER:O     | 1:A:396:HIS:HB2   | 2.16                     | 0.45              |
| 1:A:681:PHE:O     | 1:A:685:PHE:N     | 2.44                     | 0.45              |
| 1:A:303:ALA:HA    | 14:A:817:CLA:HMC3 | 1.99                     | 0.45              |
| 2:B:664:ALA:O     | 2:B:667:PHE:HB2   | 2.17                     | 0.45              |
| 1:G:356:LEU:O     | 1:G:360:LEU:CB    | 2.63                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:646:ILE:HG21  | 14:G:803:CLA:HMA2  | 1.99                     | 0.45              |
| 17:G:850:BCR:HC8  | 17:G:850:BCR:C32   | 2.46                     | 0.45              |
| 14:G:808:CLA:H12  | 17:G:854:BCR:H371  | 1.98                     | 0.45              |
| 2:H:596:VAL:HG22  | 14:H:834:CLA:HAB   | 1.99                     | 0.45              |
| 14:H:801:CLA:C7   | 14:H:801:CLA:H41   | 2.47                     | 0.45              |
| 14:H:827:CLA:H142 | 17:H:842:BCR:H372  | 1.99                     | 0.45              |
| 14:H:824:CLA:H111 | 17:H:844:BCR:H312  | 1.99                     | 0.45              |
| 10:L:53:ALA:O     | 10:L:57:PHE:HE2    | 2.00                     | 0.45              |
| 10:U:87:LEU:HA    | 10:U:87:LEU:HD23   | 1.78                     | 0.45              |
| 14:Y:819:CLA:H193 | 14:Y:819:CLA:H102  | 1.97                     | 0.45              |
| 14:Y:821:CLA:H72  | 17:Y:850:BCR:H14C  | 1.98                     | 0.45              |
| 14:Y:841:CLA:HMC2 | 14:Z:801:CLA:H101  | 1.99                     | 0.45              |
| 17:Y:849:BCR:H15C | 17:Y:849:BCR:H351  | 1.74                     | 0.45              |
| 2:Z:228:ASN:O     | 2:Z:231:VAL:HG22   | 2.16                     | 0.45              |
| 1:A:189:TRP:HH2   | 14:A:810:CLA:HMB3  | 1.82                     | 0.45              |
| 1:A:387:TYR:N     | 1:A:388:PRO:HD2    | 2.32                     | 0.45              |
| 1:A:535:ASP:O     | 1:A:539:HIS:ND1    | 2.50                     | 0.45              |
| 2:B:665:THR:HA    | 14:B:804:CLA:HAB   | 1.99                     | 0.45              |
| 14:B:830:CLA:HMA1 | 14:B:831:CLA:O1D   | 2.17                     | 0.45              |
| 14:B:834:CLA:HMD2 | 14:B:835:CLA:CHC   | 2.47                     | 0.45              |
| 17:B:851:BCR:H391 | 8:J:33:TYR:HD1     | 1.82                     | 0.45              |
| 1:G:340:GLY:O     | 1:G:429:VAL:HG23   | 2.17                     | 0.45              |
| 17:G:850:BCR:H382 | 14:H:830:CLA:HBB2  | 1.99                     | 0.45              |
| 2:H:387:VAL:HG13  | 2:H:540:LEU:HD21   | 1.99                     | 0.45              |
| 2:H:651:VAL:HG11  | 14:H:807:CLA:HAC1  | 1.98                     | 0.45              |
| 2:H:360:PRO:CG    | 14:H:817:CLA:HBA1  | 2.41                     | 0.45              |
| 14:L:207:CLA:HMB1 | 14:L:207:CLA:HBB1  | 1.98                     | 0.45              |
| 10:L:26:LEU:O     | 10:L:29:THR:HG22   | 2.17                     | 0.45              |
| 6:Q:60:ALA:O      | 6:Q:65:ILE:HG12    | 2.17                     | 0.45              |
| 14:H:828:CLA:C4   | 14:V:1201:CLA:HBC3 | 2.47                     | 0.45              |
| 1:Y:336:PHE:HD2   | 18:Y:853:LHG:HC42  | 1.82                     | 0.45              |
| 1:Y:641:GLN:HA    | 1:Y:644:ILE:HD13   | 1.99                     | 0.45              |
| 2:Z:492:TRP:O     | 2:Z:495:TYR:CE1    | 2.70                     | 0.45              |
| 2:Z:497:ASN:O     | 2:Z:499:TRP:CE3    | 2.69                     | 0.45              |
| 2:Z:56:ILE:O      | 2:Z:59:TRP:HB3     | 2.16                     | 0.45              |
| 17:Z:842:BCR:H351 | 17:Z:842:BCR:H15C  | 1.80                     | 0.45              |
| 2:Z:92:ASP:O      | 2:Z:94:GLN:N       | 2.50                     | 0.45              |
| 1:A:371:ALA:HB2   | 1:A:397:HIS:CB     | 2.43                     | 0.45              |
| 1:A:353:HIS:CE1   | 1:A:414:ILE:HG21   | 2.52                     | 0.45              |
| 1:A:484:PRO:HG2   | 1:A:488:GLN:HG3    | 1.99                     | 0.45              |
| 1:A:682:ILE:HD12  | 17:A:849:BCR:H353  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:291:ARG:HA    | 2:B:297:GLY:HA3   | 1.98                     | 0.45              |
| 2:B:589:MET:O     | 2:B:593:ILE:HG12  | 2.17                     | 0.45              |
| 14:B:805:CLA:HBC1 | 19:B:849:LMG:H181 | 1.98                     | 0.45              |
| 6:F:96:GLU:O      | 6:F:100:ILE:HG12  | 2.17                     | 0.45              |
| 1:G:59:ASP:CB     | 1:G:418:ARG:HH12  | 2.29                     | 0.45              |
| 14:G:805:CLA:H41  | 17:G:847:BCR:H292 | 1.98                     | 0.45              |
| 1:G:90:MET:CE     | 14:G:808:CLA:HED2 | 2.47                     | 0.45              |
| 14:G:839:CLA:H71  | 14:Q:201:CLA:H42  | 1.98                     | 0.45              |
| 14:G:821:CLA:H191 | 17:G:848:BCR:HC21 | 1.98                     | 0.45              |
| 2:H:615:PHE:O     | 2:H:619:SER:N     | 2.43                     | 0.45              |
| 14:H:834:CLA:O1A  | 14:H:835:CLA:HBD  | 2.17                     | 0.45              |
| 4:O:43:THR:HG23   | 4:O:58:PHE:HE1    | 1.82                     | 0.45              |
| 1:Y:385:THR:OG1   | 1:Y:520:VAL:HG13  | 2.16                     | 0.45              |
| 14:Y:841:CLA:H41  | 14:Y:841:CLA:H62  | 1.73                     | 0.45              |
| 2:Z:184:VAL:HG23  | 14:Z:818:CLA:HAC1 | 1.99                     | 0.45              |
| 2:Z:337:LEU:N     | 14:Z:804:CLA:HMD3 | 2.31                     | 0.45              |
| 2:Z:550:SER:O     | 2:Z:553:MET:N     | 2.50                     | 0.45              |
| 2:Z:713:LEU:HD22  | 19:Z:847:LMG:O10  | 2.17                     | 0.45              |
| 2:Z:339:TRP:CZ3   | 14:Z:821:CLA:HBC2 | 2.51                     | 0.45              |
| 14:A:817:CLA:OBD  | 14:A:835:CLA:HED2 | 2.17                     | 0.44              |
| 14:B:801:CLA:H91  | 14:B:801:CLA:H111 | 1.71                     | 0.44              |
| 14:B:805:CLA:HMD2 | 17:L:208:BCR:HC31 | 1.99                     | 0.44              |
| 6:F:132:LYS:HD2   | 6:F:135:GLU:OE1   | 2.16                     | 0.44              |
| 6:F:17:ARG:NH2    | 6:F:46:ASP:O      | 2.42                     | 0.44              |
| 1:G:164:GLY:C     | 1:G:167:VAL:HG12  | 2.37                     | 0.44              |
| 1:G:282:ASN:O     | 1:G:506:ALA:HB3   | 2.17                     | 0.44              |
| 14:G:821:CLA:CMB  | 14:G:825:CLA:HMA3 | 2.47                     | 0.44              |
| 17:G:854:BCR:H321 | 17:G:854:BCR:HC7  | 1.80                     | 0.44              |
| 2:H:662:VAL:HG11  | 2:H:721:VAL:CG2   | 2.48                     | 0.44              |
| 8:J:40:PRO:O      | 8:J:41:LEU:HB2    | 2.17                     | 0.44              |
| 1:Y:392:SER:O     | 1:Y:396:HIS:HB3   | 2.17                     | 0.44              |
| 2:Z:195:HIS:O     | 2:Z:199:PRO:HG2   | 2.16                     | 0.44              |
| 2:Z:699:TRP:HA    | 14:Z:838:CLA:O1D  | 2.17                     | 0.44              |
| 1:A:651:ARG:HE    | 1:A:652:ASP:CG    | 2.19                     | 0.44              |
| 14:A:828:CLA:H93  | 17:J:103:BCR:H361 | 1.99                     | 0.44              |
| 1:A:722:LEU:N     | 15:A:843:PQN:O4   | 2.42                     | 0.44              |
| 2:B:170:ALA:O     | 2:B:174:LEU:HD12  | 2.17                     | 0.44              |
| 2:B:625:TRP:O     | 2:B:629:TYR:HB3   | 2.16                     | 0.44              |
| 1:A:467:ALA:HB2   | 2:B:641:TYR:CD1   | 2.52                     | 0.44              |
| 14:B:802:CLA:C2B  | 14:B:832:CLA:H41  | 2.47                     | 0.44              |
| 14:B:834:CLA:HBB1 | 14:B:834:CLA:HMB1 | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:50:CYS:HB2    | 3:C:52:ARG:HG3     | 1.98                     | 0.44              |
| 4:D:52:GLY:O      | 4:D:54:ASN:ND2     | 2.50                     | 0.44              |
| 1:G:447:VAL:HG12  | 1:G:451:LEU:HG     | 1.99                     | 0.44              |
| 1:G:80:LEU:CD1    | 14:G:813:CLA:HED3  | 2.48                     | 0.44              |
| 1:G:296:ASP:HB3   | 14:G:818:CLA:HMA1  | 1.99                     | 0.44              |
| 14:G:821:CLA:H52  | 14:G:824:CLA:H92   | 1.98                     | 0.44              |
| 2:H:461:VAL:HA    | 2:H:464:GLN:HB2    | 1.99                     | 0.44              |
| 2:H:480:LEU:HD12  | 2:H:488:ALA:CB     | 2.47                     | 0.44              |
| 2:H:652:TRP:O     | 2:H:729:ALA:HB1    | 2.16                     | 0.44              |
| 14:G:803:CLA:H143 | 14:H:809:CLA:HBC3  | 1.98                     | 0.44              |
| 17:M:101:BCR:H15C | 17:M:101:BCR:H351  | 1.76                     | 0.44              |
| 6:Q:84:TYR:CD1    | 6:Q:105:LEU:CD2    | 3.00                     | 0.44              |
| 14:Q:201:CLA:HBB1 | 17:Q:202:BCR:H323  | 1.98                     | 0.44              |
| 14:Y:821:CLA:H161 | 17:Y:849:BCR:HC8   | 1.98                     | 0.44              |
| 1:Y:461:HIS:HE1   | 14:Y:834:CLA:C1A   | 2.30                     | 0.44              |
| 1:A:683:TRP:CE3   | 13:A:801:CL0:H4    | 2.53                     | 0.44              |
| 14:A:805:CLA:H2A  | 14:A:805:CLA:O1D   | 2.16                     | 0.44              |
| 14:A:806:CLA:HBC2 | 14:A:828:CLA:CMD   | 2.47                     | 0.44              |
| 14:A:832:CLA:HBB1 | 14:A:832:CLA:HMB1  | 1.99                     | 0.44              |
| 2:B:493:PRO:HB2   | 14:B:836:CLA:O1D   | 2.18                     | 0.44              |
| 2:B:685:VAL:HG13  | 2:B:699:TRP:CH2    | 2.52                     | 0.44              |
| 14:B:813:CLA:H41  | 14:B:813:CLA:H62   | 1.58                     | 0.44              |
| 2:B:596:VAL:CG2   | 14:B:837:CLA:HBB2  | 2.48                     | 0.44              |
| 5:E:17:TYR:O      | 6:F:137:THR:HA     | 2.17                     | 0.44              |
| 1:G:310:ILE:O     | 14:G:822:CLA:HAC1  | 2.17                     | 0.44              |
| 1:G:429:VAL:HG13  | 14:G:831:CLA:HMD3  | 1.99                     | 0.44              |
| 1:G:604:ASN:OD1   | 13:G:801:CL0:H37   | 2.17                     | 0.44              |
| 14:G:839:CLA:HMA2 | 14:G:853:CLA:HMB3  | 1.97                     | 0.44              |
| 2:H:489:SER:C     | 2:H:497:ASN:HD21   | 2.20                     | 0.44              |
| 2:H:691:THR:O     | 2:H:695:ASN:OD1    | 2.35                     | 0.44              |
| 2:H:663:TRP:CD2   | 14:H:802:CLA:HMA2  | 2.52                     | 0.44              |
| 9:K:24:LEU:HD22   | 9:K:73:VAL:CG1     | 2.48                     | 0.44              |
| 5:P:10:LEU:HB2    | 5:P:64:GLU:O       | 2.17                     | 0.44              |
| 7:R:27:MET:HG2    | 17:R:102:BCR:C10   | 2.48                     | 0.44              |
| 10:U:134:VAL:HB   | 17:U:1008:BCR:H403 | 1.98                     | 0.44              |
| 12:W:13:THR:HA    | 12:W:16:ALA:HB3    | 1.99                     | 0.44              |
| 12:X:25:LEU:O     | 12:X:29:TYR:HD1    | 2.00                     | 0.44              |
| 1:Y:15:VAL:HG11   | 1:Y:186:LYS:HD2    | 1.98                     | 0.44              |
| 14:Y:805:CLA:H72  | 17:Y:848:BCR:H402  | 1.99                     | 0.44              |
| 14:Y:821:CLA:HMA2 | 14:Y:825:CLA:NC    | 2.32                     | 0.44              |
| 1:Y:306:VAL:HG22  | 17:Y:846:BCR:C35   | 2.47                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Z:172:SER:O     | 2:Z:176:HIS:ND1   | 2.44                     | 0.44              |
| 2:Z:223:PRO:HA    | 2:Z:226:THR:OG1   | 2.16                     | 0.44              |
| 1:A:522:GLY:O     | 1:A:625:VAL:CG2   | 2.66                     | 0.44              |
| 2:B:239:ALA:CA    | 2:B:262:PRO:HG2   | 2.47                     | 0.44              |
| 2:B:443:ASN:ND2   | 2:B:455:GLN:OE1   | 2.51                     | 0.44              |
| 3:C:60:ASP:HB2    | 5:E:58:ASN:CG     | 2.38                     | 0.44              |
| 1:G:79:HIS:CE1    | 14:G:805:CLA:HMA1 | 2.53                     | 0.44              |
| 14:G:802:CLA:HMC2 | 21:G:904:HOH:O    | 2.17                     | 0.44              |
| 1:G:86:TRP:CD1    | 14:G:806:CLA:HBC1 | 2.53                     | 0.44              |
| 1:G:210:LEU:HD23  | 14:G:815:CLA:HAB  | 1.99                     | 0.44              |
| 14:G:821:CLA:C1D  | 14:G:827:CLA:H142 | 2.48                     | 0.44              |
| 14:G:829:CLA:H111 | 17:G:847:BCR:C38  | 2.48                     | 0.44              |
| 14:H:810:CLA:HBB1 | 14:H:810:CLA:HHC  | 1.99                     | 0.44              |
| 7:I:22:MET:N      | 7:I:23:PRO:HD2    | 2.32                     | 0.44              |
| 3:N:42:PRO:HG2    | 3:N:43:ARG:HG3    | 1.98                     | 0.44              |
| 1:Y:207:LEU:HD11  | 14:Y:820:CLA:HBC1 | 1.99                     | 0.44              |
| 1:Y:79:HIS:HB2    | 14:Y:805:CLA:HMB2 | 1.99                     | 0.44              |
| 2:Z:298:HIS:CE1   | 14:Z:820:CLA:OBD  | 2.70                     | 0.44              |
| 2:Z:388:GLY:HA2   | 14:Z:827:CLA:C3C  | 2.48                     | 0.44              |
| 1:A:120:ILE:O     | 1:A:122:GLY:N     | 2.49                     | 0.44              |
| 1:A:64:ASP:O      | 1:A:68:ILE:HG13   | 2.16                     | 0.44              |
| 14:A:814:CLA:HBD  | 14:A:814:CLA:HBA1 | 2.00                     | 0.44              |
| 14:A:828:CLA:H8   | 17:A:849:BCR:H343 | 1.99                     | 0.44              |
| 2:B:437:LEU:O     | 2:B:441:VAL:HG23  | 2.17                     | 0.44              |
| 2:B:481:LEU:HD22  | 2:B:500:LEU:HD11  | 1.99                     | 0.44              |
| 2:B:440:TYR:OH    | 2:B:525:VAL:HG22  | 2.18                     | 0.44              |
| 2:B:727:TYR:HB2   | 14:B:803:CLA:HED3 | 1.99                     | 0.44              |
| 14:B:832:CLA:H3A  | 14:B:832:CLA:HBA2 | 1.73                     | 0.44              |
| 17:B:845:BCR:H351 | 17:B:845:BCR:H15C | 1.68                     | 0.44              |
| 14:B:833:CLA:C4   | 17:B:851:BCR:H373 | 2.46                     | 0.44              |
| 2:H:327:GLU:N     | 2:H:327:GLU:OE1   | 2.50                     | 0.44              |
| 2:H:660:HIS:CE1   | 2:H:726:THR:HG23  | 2.52                     | 0.44              |
| 14:H:810:CLA:H3A  | 14:H:810:CLA:HBA2 | 1.57                     | 0.44              |
| 2:H:207:GLY:HA2   | 14:H:813:CLA:OBD  | 2.17                     | 0.44              |
| 14:H:818:CLA:HBA2 | 14:H:818:CLA:H3A  | 1.71                     | 0.44              |
| 12:W:17:VAL:O     | 12:W:21:ALA:N     | 2.36                     | 0.44              |
| 1:Y:321:ILE:CD1   | 14:Y:820:CLA:HED2 | 2.48                     | 0.44              |
| 1:Y:448:CYS:O     | 1:Y:544:PHE:HE1   | 2.01                     | 0.44              |
| 1:Y:697:TRP:CZ3   | 14:Z:801:CLA:O1D  | 2.69                     | 0.44              |
| 14:Y:805:CLA:HMC3 | 14:Y:830:CLA:HMA1 | 2.00                     | 0.44              |
| 14:Y:843:CLA:H3A  | 14:Y:843:CLA:HBA2 | 1.67                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:45:THR:OG1     | 14:A:839:CLA:C2B   | 2.66                     | 0.44              |
| 1:A:548:VAL:HG11   | 1:A:601:TRP:CZ2    | 2.53                     | 0.44              |
| 14:A:813:CLA:C2    | 14:A:813:CLA:HMA2  | 2.47                     | 0.44              |
| 14:A:827:CLA:HED1  | 14:A:834:CLA:CAB   | 2.48                     | 0.44              |
| 15:A:843:PQN:C17   | 15:A:843:PQN:H141  | 2.47                     | 0.44              |
| 2:B:348:THR:HG21   | 2:B:381:ILE:HG22   | 1.99                     | 0.44              |
| 3:C:24:VAL:HG21    | 3:C:47:CYS:HA      | 2.00                     | 0.44              |
| 1:G:149:ALA:O      | 1:G:220:SER:OG     | 2.27                     | 0.44              |
| 1:G:695:GLY:HA3    | 2:H:576:ILE:HB     | 1.98                     | 0.44              |
| 1:G:692:SER:OG     | 14:G:802:CLA:HBC3  | 2.18                     | 0.44              |
| 14:G:805:CLA:H172  | 17:G:846:BCR:H321  | 1.98                     | 0.44              |
| 14:G:829:CLA:H61   | 14:G:829:CLA:H41   | 1.80                     | 0.44              |
| 14:G:853:CLA:HAC1  | 14:H:836:CLA:HBC3  | 2.00                     | 0.44              |
| 2:H:217:HIS:HB2    | 2:H:253:ILE:HD13   | 2.00                     | 0.44              |
| 2:H:443:ASN:O      | 2:H:447:VAL:HG23   | 2.17                     | 0.44              |
| 17:I:101:BCR:H371  | 17:I:101:BCR:H24C  | 2.03                     | 0.44              |
| 6:Q:85:LEU:HD21    | 6:Q:89:ARG:NH2     | 2.33                     | 0.44              |
| 14:Y:808:CLA:HMB1  | 14:Y:808:CLA:HBB1  | 1.99                     | 0.44              |
| 1:Y:279:LEU:HB2    | 14:Y:817:CLA:HMA3  | 1.99                     | 0.44              |
| 17:Y:849:BCR:H371  | 17:Y:849:BCR:H24C  | 1.86                     | 0.44              |
| 2:Z:337:LEU:HD23   | 2:Z:392:HIS:CE1    | 2.53                     | 0.44              |
| 2:Z:62:GLY:HA3     | 14:Z:806:CLA:CAB   | 2.47                     | 0.44              |
| 14:Z:810:CLA:O1D   | 14:Z:811:CLA:HMC1  | 2.18                     | 0.44              |
| 14:Z:829:CLA:HBC2  | 14:Z:829:CLA:HHD   | 2.00                     | 0.44              |
| 1:A:244:LEU:C      | 1:A:246:PRO:HD3    | 2.38                     | 0.44              |
| 1:A:284:GLY:O      | 1:A:292:LEU:HD23   | 2.16                     | 0.44              |
| 1:A:52:HIS:HA      | 1:A:55:ALA:HB2     | 1.99                     | 0.44              |
| 14:A:826:CLA:HAA2  | 14:A:827:CLA:OBD   | 2.18                     | 0.44              |
| 2:B:303:MET:HA     | 14:B:822:CLA:O1D   | 2.18                     | 0.44              |
| 15:B:842:PQN:H2M1  | 15:B:842:PQN:H111  | 1.82                     | 0.44              |
| 17:B:843:BCR:H351  | 17:B:843:BCR:H15C  | 1.66                     | 0.44              |
| 5:E:12:PRO:HA      | 5:E:17:TYR:CD1     | 2.53                     | 0.44              |
| 6:F:52:VAL:HG12    | 6:F:54:ASP:HB2     | 2.00                     | 0.44              |
| 1:G:647:ASN:O      | 1:G:650:LEU:HB3    | 2.18                     | 0.44              |
| 14:G:832:CLA:CBB   | 14:G:833:CLA:O1A   | 2.66                     | 0.44              |
| 14:G:802:CLA:C1    | 2:H:430:LEU:HD12   | 2.38                     | 0.44              |
| 2:H:706:LEU:HD22   | 2:H:710:GLN:NE2    | 2.32                     | 0.44              |
| 14:H:820:CLA:HBB1  | 14:H:820:CLA:HMB1  | 1.99                     | 0.44              |
| 2:H:674:ARG:HA     | 15:H:839:PQN:C7    | 2.47                     | 0.44              |
| 14:S:1101:CLA:HMB1 | 14:S:1101:CLA:HBB1 | 1.99                     | 0.44              |
| 9:T:20:ILE:HD13    | 9:T:74:VAL:HG21    | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y:356:LEU:N     | 14:Y:805:CLA:HMD3 | 2.32                     | 0.44              |
| 1:Y:42:PRO:HB2    | 1:Y:717:ILE:HD13  | 1.99                     | 0.44              |
| 14:Y:840:CLA:O2D  | 14:Y:840:CLA:H2A  | 2.18                     | 0.44              |
| 2:Z:484:PRO:HA    | 2:Z:489:SER:OG    | 2.17                     | 0.44              |
| 2:Z:591:ASN:HA    | 2:Z:723:TYR:OH    | 2.18                     | 0.44              |
| 2:Z:650:SER:CB    | 14:Z:808:CLA:HBC1 | 2.45                     | 0.44              |
| 2:Z:377:HIS:HB2   | 14:Z:825:CLA:CHB  | 2.47                     | 0.44              |
| 14:Z:832:CLA:HMD2 | 14:Z:833:CLA:C1C  | 2.48                     | 0.44              |
| 17:Z:844:BCR:C23  | 17:Z:844:BCR:H403 | 2.37                     | 0.44              |
| 1:A:86:TRP:CD1    | 14:A:806:CLA:HBC1 | 2.53                     | 0.44              |
| 2:B:304:MET:CG    | 2:B:325:ILE:HG22  | 2.48                     | 0.44              |
| 2:B:390:PHE:HB2   | 2:B:540:LEU:HD22  | 2.00                     | 0.44              |
| 2:B:63:SER:O      | 2:B:67:VAL:HG23   | 2.17                     | 0.44              |
| 2:B:333:LEU:HD13  | 14:B:806:CLA:HAC1 | 2.00                     | 0.44              |
| 2:B:86:ILE:HD11   | 2:B:108:ALA:HB2   | 2.00                     | 0.44              |
| 4:D:9:LEU:HB2     | 4:D:48:VAL:CG2    | 2.47                     | 0.44              |
| 1:G:226:LEU:HD22  | 1:G:231:VAL:HG21  | 1.99                     | 0.44              |
| 1:G:538:VAL:HG22  | 1:G:542:HIS:CE1   | 2.53                     | 0.44              |
| 2:H:222:ALA:O     | 2:H:226:THR:HG23  | 2.17                     | 0.44              |
| 14:H:801:CLA:H72  | 14:H:801:CLA:H41  | 2.00                     | 0.44              |
| 14:H:813:CLA:HBB1 | 14:H:813:CLA:HMB1 | 1.98                     | 0.44              |
| 14:H:817:CLA:HBA2 | 14:H:817:CLA:H3A  | 1.53                     | 0.44              |
| 14:H:818:CLA:CMB  | 14:H:823:CLA:HMA3 | 2.48                     | 0.44              |
| 7:I:33:TYR:OH     | 11:M:30:TYR:CZ    | 2.71                     | 0.44              |
| 8:J:23:ALA:O      | 8:J:27:ILE:HD12   | 2.17                     | 0.44              |
| 1:G:423:ALA:HB2   | 4:O:38:VAL:HG11   | 1.99                     | 0.44              |
| 13:Y:801:CL0:H15  | 13:Y:801:CL0:H11  | 1.99                     | 0.44              |
| 1:Y:196:MET:HE2   | 14:Y:813:CLA:HBC2 | 2.00                     | 0.44              |
| 1:Y:740:ILE:HG22  | 17:Y:851:BCR:HC31 | 2.00                     | 0.44              |
| 2:Z:199:PRO:O     | 2:Z:204:GLN:HB2   | 2.18                     | 0.44              |
| 2:Z:239:ALA:CB    | 2:Z:262:PRO:HG2   | 2.47                     | 0.44              |
| 2:Z:347:ILE:HA    | 2:Z:350:LEU:HB3   | 1.99                     | 0.44              |
| 2:Z:537:THR:O     | 2:Z:541:VAL:HG23  | 2.18                     | 0.44              |
| 1:A:106:ASP:O     | 1:A:108:THR:N     | 2.48                     | 0.44              |
| 1:A:369:ILE:HA    | 14:A:826:CLA:HED2 | 2.00                     | 0.44              |
| 14:A:804:CLA:HAB  | 14:A:806:CLA:CAD  | 2.48                     | 0.44              |
| 2:B:577:SER:HB3   | 2:B:580:ASP:OD2   | 2.18                     | 0.44              |
| 2:B:655:MET:HG3   | 2:B:725:LEU:HD22  | 2.00                     | 0.44              |
| 14:A:852:CLA:HED1 | 14:B:803:CLA:H92  | 1.99                     | 0.44              |
| 2:B:59:TRP:CE3    | 14:B:807:CLA:HMC1 | 2.52                     | 0.44              |
| 2:B:256:PHE:HZ    | 14:B:817:CLA:H72  | 1.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:B:826:CLA:H111 | 14:B:826:CLA:H72   | 1.86                     | 0.44              |
| 2:B:503:TRP:CE2   | 14:B:834:CLA:HED1  | 2.52                     | 0.44              |
| 2:B:533:LEU:HD12  | 14:B:839:CLA:HED3  | 2.00                     | 0.44              |
| 14:B:828:CLA:H12  | 17:B:844:BCR:H393  | 1.99                     | 0.44              |
| 4:D:132:GLY:O     | 4:D:134:LYS:HD2    | 2.18                     | 0.44              |
| 4:D:71:GLN:O      | 4:D:74:PRO:HG2     | 2.18                     | 0.44              |
| 1:G:391:LEU:HD11  | 1:G:614:SER:OG     | 2.18                     | 0.44              |
| 2:H:121:HIS:CD2   | 2:H:364:ILE:HA     | 2.53                     | 0.44              |
| 2:H:564:PRO:HA    | 2:H:709:VAL:HG13   | 2.00                     | 0.44              |
| 1:G:714:ALA:O     | 6:Q:89:ARG:NH2     | 2.50                     | 0.44              |
| 1:Y:297:THR:O     | 1:Y:301:HIS:HD2    | 1.97                     | 0.44              |
| 14:Y:839:CLA:HMB1 | 14:Y:839:CLA:HBB1  | 1.99                     | 0.44              |
| 2:Z:198:ILE:CG1   | 2:Z:199:PRO:HD3    | 2.40                     | 0.44              |
| 2:Z:222:ALA:HB3   | 2:Z:223:PRO:HD3    | 1.99                     | 0.44              |
| 2:Z:547:ALA:O     | 2:Z:556:LYS:HB3    | 2.17                     | 0.44              |
| 2:Z:638:ILE:HD12  | 2:Z:638:ILE:HA     | 1.86                     | 0.44              |
| 1:A:167:VAL:O     | 1:A:171:LEU:HD12   | 2.18                     | 0.43              |
| 14:A:840:CLA:H172 | 8:J:19:MET:SD      | 2.58                     | 0.43              |
| 2:B:275:HIS:NE2   | 14:B:818:CLA:C1B   | 2.80                     | 0.43              |
| 2:B:427:TRP:HB2   | 14:B:802:CLA:HED2  | 1.99                     | 0.43              |
| 14:B:804:CLA:H111 | 17:B:848:BCR:H362  | 1.99                     | 0.43              |
| 2:B:254:LEU:HD11  | 14:B:815:CLA:CAC   | 2.48                     | 0.43              |
| 1:G:120:ILE:HD12  | 17:S:1104:BCR:H313 | 1.99                     | 0.43              |
| 1:G:466:ARG:O     | 2:H:646:THR:HG22   | 2.18                     | 0.43              |
| 1:G:617:MET:HB3   | 1:G:622:TRP:CD2    | 2.53                     | 0.43              |
| 2:H:497:ASN:O     | 2:H:499:TRP:CD2    | 2.71                     | 0.43              |
| 2:H:580:ASP:HA    | 2:H:583:TYR:HB3    | 1.99                     | 0.43              |
| 14:H:812:CLA:HBB1 | 14:H:812:CLA:HMB1  | 2.00                     | 0.43              |
| 17:I:101:BCR:H331 | 17:I:101:BCR:C8    | 2.48                     | 0.43              |
| 10:L:39:GLN:HA    | 10:L:39:GLN:OE1    | 2.18                     | 0.43              |
| 17:R:102:BCR:H351 | 17:R:102:BCR:H15C  | 1.58                     | 0.43              |
| 1:Y:659:SER:HB2   | 1:Y:660:GLN:NE2    | 2.33                     | 0.43              |
| 1:Y:736:LEU:O     | 1:Y:740:ILE:HG13   | 2.18                     | 0.43              |
| 14:Y:806:CLA:H41  | 18:Y:852:LHG:H272  | 2.00                     | 0.43              |
| 14:Y:811:CLA:C4A  | 14:Y:811:CLA:HBA2  | 2.47                     | 0.43              |
| 2:Z:43:GLN:NE2    | 2:Z:161:ARG:HB3    | 2.33                     | 0.43              |
| 2:Z:494:ASN:HB3   | 14:Z:834:CLA:HED3  | 1.99                     | 0.43              |
| 2:Z:320:MET:CE    | 14:Z:828:CLA:HMD1  | 2.48                     | 0.43              |
| 1:A:527:MET:HB2   | 1:A:528:PRO:HD2    | 2.00                     | 0.43              |
| 1:A:610:ILE:CD1   | 1:A:743:THR:HG21   | 2.48                     | 0.43              |
| 1:A:323:HIS:HE1   | 14:A:822:CLA:ND    | 2.17                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:291:ARG:NH1    | 2:B:295:GLY:O      | 2.51                     | 0.43              |
| 4:D:81:LYS:HB3     | 4:D:93:LEU:CD2     | 2.47                     | 0.43              |
| 1:G:255:LYS:NZ     | 1:G:273:ALA:O      | 2.50                     | 0.43              |
| 1:G:317:THR:HG21   | 14:G:820:CLA:OBD   | 2.18                     | 0.43              |
| 2:H:319:ASN:HD21   | 18:H:847:LHG:C2    | 2.31                     | 0.43              |
| 17:H:841:BCR:H15C  | 17:H:841:BCR:H351  | 1.69                     | 0.43              |
| 14:J:102:CLA:H62   | 14:J:102:CLA:H41   | 1.75                     | 0.43              |
| 4:O:83:TYR:CE2     | 4:O:93:LEU:HG      | 2.53                     | 0.43              |
| 14:Y:817:CLA:CGA   | 14:Y:817:CLA:C1A   | 2.97                     | 0.43              |
| 2:Z:261:HIS:HA     | 2:Z:262:PRO:HD3    | 1.89                     | 0.43              |
| 14:Z:816:CLA:H61   | 14:Z:816:CLA:H41   | 1.73                     | 0.43              |
| 2:Z:296:ILE:HB     | 14:Z:819:CLA:HMD1  | 2.00                     | 0.43              |
| 1:A:354:ALA:HB1    | 17:A:847:BCR:H313  | 2.00                     | 0.43              |
| 14:B:808:CLA:C3A   | 14:B:809:CLA:HMB3  | 2.46                     | 0.43              |
| 2:B:293:GLN:OE1    | 14:B:812:CLA:HMA2  | 2.17                     | 0.43              |
| 14:B:813:CLA:HBB1  | 14:B:813:CLA:HMB1  | 1.99                     | 0.43              |
| 14:B:821:CLA:HMB2  | 14:B:822:CLA:H42   | 2.01                     | 0.43              |
| 1:G:329:LEU:HB3    | 1:G:341:HIS:O      | 2.18                     | 0.43              |
| 1:G:589:VAL:HG13   | 2:H:675:GLY:HA3    | 2.00                     | 0.43              |
| 1:G:300:HIS:NE2    | 14:G:819:CLA:C2B   | 2.81                     | 0.43              |
| 14:G:831:CLA:H3A   | 14:G:831:CLA:HBA1  | 1.82                     | 0.43              |
| 14:H:823:CLA:H41   | 14:H:823:CLA:H62   | 1.76                     | 0.43              |
| 14:H:824:CLA:HMB3  | 17:H:844:BCR:C16   | 2.48                     | 0.43              |
| 1:G:270:PHE:CD1    | 14:T:101:CLA:HMD2  | 2.54                     | 0.43              |
| 10:U:20:PRO:HA     | 10:U:24:SER:HB2    | 1.99                     | 0.43              |
| 17:V:1202:BCR:H24C | 17:V:1202:BCR:H371 | 1.86                     | 0.43              |
| 11:V:4:THR:O       | 11:V:8:VAL:HG23    | 2.18                     | 0.43              |
| 1:Y:117:VAL:HG13   | 1:Y:127:ASN:HD21   | 1.83                     | 0.43              |
| 1:Y:128:GLY:O      | 1:Y:130:VAL:HG13   | 2.19                     | 0.43              |
| 1:Y:285:LEU:HD11   | 1:Y:526:MET:HB3    | 1.99                     | 0.43              |
| 1:Y:512:ALA:HB1    | 1:Y:529:ILE:HG13   | 1.99                     | 0.43              |
| 1:Y:744:TRP:CD1    | 17:Y:851:BCR:H313  | 2.53                     | 0.43              |
| 14:Y:825:CLA:HBB1  | 14:Y:825:CLA:HMB1  | 2.00                     | 0.43              |
| 1:Y:446:TRP:HD1    | 14:Y:842:CLA:O1A   | 2.01                     | 0.43              |
| 2:Z:677:TRP:O      | 2:Z:678:GLN:C      | 2.55                     | 0.43              |
| 1:Y:565:LEU:HB2    | 2:Z:682:GLU:OE2    | 2.18                     | 0.43              |
| 14:Z:825:CLA:CGD   | 14:Z:826:CLA:HMA1  | 2.44                     | 0.43              |
| 14:Z:832:CLA:HAA1  | 14:Z:833:CLA:HMB3  | 1.99                     | 0.43              |
| 1:A:410:ALA:HA     | 1:A:595:VAL:HG21   | 2.00                     | 0.43              |
| 1:A:439:ALA:HB2    | 2:B:686:TRP:CH2    | 2.53                     | 0.43              |
| 1:A:654:LEU:HD11   | 13:A:801:CL0:H43   | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:89:ALA:HA     | 2:B:112:VAL:HG23  | 2.00                     | 0.43              |
| 2:B:664:ALA:HB3   | 14:B:804:CLA:HBB2 | 1.99                     | 0.43              |
| 2:B:24:ILE:HA     | 14:B:805:CLA:HMD3 | 2.00                     | 0.43              |
| 14:B:819:CLA:CMD  | 14:B:821:CLA:HAB  | 2.47                     | 0.43              |
| 17:B:848:BCR:H15C | 17:B:848:BCR:H351 | 1.55                     | 0.43              |
| 1:G:323:HIS:CE1   | 14:G:823:CLA:OBD  | 2.70                     | 0.43              |
| 1:G:50:ASN:HA     | 1:G:53:ALA:HB3    | 2.00                     | 0.43              |
| 1:G:511:VAL:HG23  | 1:G:526:MET:HG3   | 1.99                     | 0.43              |
| 14:G:804:CLA:HAA1 | 14:G:811:CLA:H2   | 1.99                     | 0.43              |
| 1:G:399:TRP:NE1   | 14:G:828:CLA:HAB  | 2.29                     | 0.43              |
| 17:H:840:BCR:C8   | 17:H:840:BCR:H331 | 2.48                     | 0.43              |
| 14:B:808:CLA:O1A  | 7:I:14:PHE:HB3    | 2.18                     | 0.43              |
| 1:A:464:THR:HG21  | 14:L:201:CLA:HBC3 | 2.00                     | 0.43              |
| 4:O:39:PHE:CD1    | 4:O:49:MET:HB3    | 2.54                     | 0.43              |
| 4:O:82:ILE:HG22   | 4:O:94:ILE:HD11   | 2.01                     | 0.43              |
| 14:H:809:CLA:H11  | 10:U:148:ILE:HD13 | 2.00                     | 0.43              |
| 1:Y:379:PRO:HG3   | 14:Y:819:CLA:CBA  | 2.48                     | 0.43              |
| 10:U:69:ARG:NH2   | 1:Y:473:ASP:HA    | 2.34                     | 0.43              |
| 1:Y:487:ALA:HB2   | 14:Y:838:CLA:O1D  | 2.18                     | 0.43              |
| 14:Y:819:CLA:C10  | 14:Y:819:CLA:H193 | 2.48                     | 0.43              |
| 1:Y:379:PRO:HG3   | 14:Y:819:CLA:HBA1 | 2.01                     | 0.43              |
| 17:Y:848:BCR:H371 | 17:Y:848:BCR:H24C | 1.79                     | 0.43              |
| 2:Z:151:ALA:HB2   | 14:Z:809:CLA:HBC2 | 1.99                     | 0.43              |
| 2:Z:179:ALA:HB2   | 2:Z:287:GLY:HA3   | 2.00                     | 0.43              |
| 14:Z:805:CLA:H62  | 14:Z:805:CLA:H92  | 1.79                     | 0.43              |
| 14:Z:823:CLA:H122 | 14:Z:835:CLA:H121 | 2.00                     | 0.43              |
| 1:A:435:ARG:HA    | 4:D:13:SER:HB2    | 2.01                     | 0.43              |
| 1:A:409:ALA:HB1   | 1:A:553:LEU:HB3   | 1.98                     | 0.43              |
| 2:B:332:SER:O     | 2:B:336:GLN:HG3   | 2.18                     | 0.43              |
| 2:B:53:LEU:HA     | 2:B:53:LEU:HD12   | 1.86                     | 0.43              |
| 2:B:688:HIS:HE1   | 2:B:697:VAL:O     | 2.01                     | 0.43              |
| 14:B:805:CLA:HBB1 | 14:B:805:CLA:HMB1 | 2.00                     | 0.43              |
| 17:B:844:BCR:C38  | 17:B:844:BCR:H23C | 2.44                     | 0.43              |
| 2:B:98:ALA:O      | 2:B:102:ALA:N     | 2.51                     | 0.43              |
| 1:G:219:VAL:O     | 1:G:223:ILE:HG13  | 2.18                     | 0.43              |
| 1:G:650:LEU:HD22  | 2:H:657:LEU:CD2   | 2.48                     | 0.43              |
| 2:H:525:VAL:HG11  | 2:H:599:TYR:CG    | 2.54                     | 0.43              |
| 6:Q:132:LYS:O     | 6:Q:135:GLU:N     | 2.45                     | 0.43              |
| 6:Q:63:PHE:C      | 6:Q:66:PRO:HD2    | 2.38                     | 0.43              |
| 1:Y:127:ASN:HB3   | 1:Y:135:HIS:HB3   | 2.00                     | 0.43              |
| 14:Y:833:CLA:C4   | 14:Y:842:CLA:HBC2 | 2.48                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:A:848:BCR:H371 | 17:A:848:BCR:H24C  | 1.78                     | 0.43              |
| 2:B:242:VAL:HG13  | 2:B:263:GLN:HE22   | 1.83                     | 0.43              |
| 2:B:626:LEU:O     | 2:B:630:LEU:HB2    | 2.18                     | 0.43              |
| 4:D:27:TYR:O      | 4:D:58:PHE:N       | 2.45                     | 0.43              |
| 1:G:356:LEU:HD11  | 1:G:360:LEU:HD13   | 2.01                     | 0.43              |
| 1:G:451:LEU:HB3   | 1:G:544:PHE:HB2    | 2.00                     | 0.43              |
| 1:G:537:MET:HE1   | 1:G:644:ILE:HA     | 2.00                     | 0.43              |
| 14:G:806:CLA:O1A  | 14:G:830:CLA:HMB2  | 2.18                     | 0.43              |
| 17:G:846:BCR:H311 | 17:G:846:BCR:C8    | 2.49                     | 0.43              |
| 2:H:526:HIS:NE2   | 2:H:599:TYR:OH     | 2.47                     | 0.43              |
| 1:G:681:PHE:HA    | 14:H:801:CLA:HAA1  | 2.01                     | 0.43              |
| 2:H:128:MET:HE2   | 14:H:813:CLA:HMA2  | 2.00                     | 0.43              |
| 14:L:205:CLA:HMD1 | 10:U:94:ALA:CB     | 2.49                     | 0.43              |
| 17:H:848:BCR:H271 | 8:S:40:PRO:HG2     | 2.00                     | 0.43              |
| 10:U:11:ASP:OD2   | 10:U:14:VAL:HG13   | 2.19                     | 0.43              |
| 1:Y:444:LEU:HB3   | 1:Y:551:LEU:HD12   | 2.00                     | 0.43              |
| 14:Y:811:CLA:HBA1 | 14:Y:811:CLA:H3A   | 1.84                     | 0.43              |
| 17:Y:850:BCR:H331 | 17:Y:850:BCR:C8    | 2.49                     | 0.43              |
| 14:Y:855:CLA:HMD1 | 2:Z:676:TYR:OH     | 2.18                     | 0.43              |
| 17:I:101:BCR:H311 | 14:Z:806:CLA:H203  | 67.11                    | 0.43              |
| 14:Z:836:CLA:HBD  | 14:Z:836:CLA:HAA1  | 1.99                     | 0.43              |
| 1:A:164:GLY:HA3   | 14:A:814:CLA:H43   | 2.00                     | 0.43              |
| 1:A:601:TRP:CH2   | 14:A:802:CLA:CAB   | 3.01                     | 0.43              |
| 14:A:804:CLA:HBA1 | 14:A:804:CLA:H3A   | 1.68                     | 0.43              |
| 2:B:537:THR:HG21  | 14:B:839:CLA:HMB3  | 2.00                     | 0.43              |
| 17:B:851:BCR:H371 | 17:B:851:BCR:H24C  | 1.79                     | 0.43              |
| 4:D:36:GLU:HA     | 4:D:49:MET:O       | 2.17                     | 0.43              |
| 1:G:361:ALA:HB2   | 1:G:408:GLY:HA3    | 2.01                     | 0.43              |
| 1:G:578:CYS:HB3   | 1:G:587:CYS:HA     | 2.01                     | 0.43              |
| 1:G:75:ALA:O      | 1:G:79:HIS:N       | 2.46                     | 0.43              |
| 13:G:801:CL0:H66  | 14:G:803:CLA:C2B   | 2.48                     | 0.43              |
| 2:H:706:LEU:O     | 15:H:839:PQN:H6    | 2.19                     | 0.43              |
| 9:K:61:ALA:O      | 9:K:65:PHE:N       | 2.48                     | 0.43              |
| 4:O:85:ILE:HD13   | 4:O:91:THR:HG23    | 1.99                     | 0.43              |
| 10:U:30:PHE:HZ    | 14:U:1002:CLA:HBB2 | 1.83                     | 0.43              |
| 1:Y:167:VAL:O     | 1:Y:171:LEU:HB2    | 2.19                     | 0.43              |
| 1:Y:216:GLN:OE1   | 1:Y:297:THR:HG23   | 2.18                     | 0.43              |
| 14:Y:805:CLA:HMB3 | 14:Y:806:CLA:HAA2  | 1.99                     | 0.43              |
| 1:Y:174:PHE:HD2   | 14:Y:810:CLA:CBC   | 2.31                     | 0.43              |
| 2:Z:438:GLY:O     | 2:Z:442:HIS:N      | 2.45                     | 0.43              |
| 2:Z:414:VAL:HG11  | 17:Z:844:BCR:C29   | 2.49                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:23:THR:O      | 1:A:23:THR:HG23   | 2.19                     | 0.43              |
| 1:A:58:PHE:CE1    | 14:A:804:CLA:HED1 | 2.54                     | 0.43              |
| 14:A:840:CLA:H41  | 14:A:840:CLA:H62  | 1.82                     | 0.43              |
| 2:B:42:TYR:CE2    | 2:B:333:LEU:HD21  | 2.54                     | 0.43              |
| 2:B:606:GLY:O     | 2:B:611:ASN:N     | 2.52                     | 0.43              |
| 14:B:824:CLA:HBB1 | 14:B:824:CLA:HMB1 | 2.00                     | 0.43              |
| 5:E:6:LYS:HD2     | 5:E:22:THR:HG22   | 2.01                     | 0.43              |
| 1:G:256:VAL:HG13  | 1:G:258:TRP:CE2   | 2.54                     | 0.43              |
| 1:G:615:TRP:CD2   | 1:G:639:PHE:HD1   | 2.36                     | 0.43              |
| 1:G:647:ASN:O     | 1:G:650:LEU:N     | 2.51                     | 0.43              |
| 14:G:842:CLA:H62  | 14:G:842:CLA:H41  | 1.71                     | 0.43              |
| 2:H:11:LEU:HD11   | 2:H:26:MET:HE3    | 1.99                     | 0.43              |
| 2:H:54:ALA:HB2    | 2:H:149:LEU:HG    | 2.00                     | 0.43              |
| 2:H:439:LEU:HD22  | 2:H:456:ILE:HD12  | 1.99                     | 0.43              |
| 2:H:462:PHE:O     | 2:H:466:ILE:HG13  | 2.19                     | 0.43              |
| 2:H:527:HIS:NE2   | 17:H:848:BCR:H322 | 2.34                     | 0.43              |
| 2:H:7:PHE:C       | 2:H:7:PHE:CD1     | 2.92                     | 0.43              |
| 17:H:844:BCR:H15C | 17:H:844:BCR:H351 | 1.73                     | 0.43              |
| 8:J:26:LEU:CD2    | 17:J:103:BCR:HC7  | 2.48                     | 0.43              |
| 10:L:35:PRO:CG    | 14:L:206:CLA:HED2 | 2.48                     | 0.43              |
| 3:N:22:THR:OG1    | 3:N:46:ASP:O      | 2.31                     | 0.43              |
| 7:R:18:VAL:O      | 7:R:23:PRO:HD3    | 2.19                     | 0.43              |
| 10:U:30:PHE:O     | 10:U:34:LEU:HD13  | 2.19                     | 0.43              |
| 1:Y:182:LYS:HA    | 1:Y:182:LYS:HD3   | 1.82                     | 0.43              |
| 1:Y:482:LEU:HB2   | 1:Y:533:THR:HG23  | 2.00                     | 0.43              |
| 1:Y:58:PHE:HD2    | 1:Y:61:HIS:CE1    | 2.37                     | 0.43              |
| 1:Y:694:ARG:HG3   | 1:Y:722:LEU:O     | 2.19                     | 0.43              |
| 14:Y:854:CLA:HMB3 | 14:Z:802:CLA:C18  | 2.48                     | 0.43              |
| 14:Z:833:CLA:C1A  | 14:Z:834:CLA:HMB3 | 2.49                     | 0.43              |
| 1:A:319:TRP:CH2   | 14:A:812:CLA:HMA1 | 2.54                     | 0.43              |
| 14:A:819:CLA:H3A  | 14:A:819:CLA:CGA  | 2.45                     | 0.43              |
| 14:A:839:CLA:HBD  | 14:A:839:CLA:HAA2 | 2.01                     | 0.43              |
| 2:B:459:GLU:O     | 2:B:461:VAL:N     | 2.52                     | 0.43              |
| 2:B:685:VAL:HG22  | 2:B:703:PRO:HG2   | 2.01                     | 0.43              |
| 14:B:809:CLA:H91  | 14:B:809:CLA:H112 | 1.81                     | 0.43              |
| 4:D:31:TRP:CD1    | 4:D:77:ILE:HG21   | 2.54                     | 0.43              |
| 6:F:103:VAL:HG13  | 6:F:104:PRO:HD3   | 2.01                     | 0.43              |
| 1:G:325:LEU:O     | 1:G:329:LEU:HG    | 2.19                     | 0.43              |
| 1:G:691:PHE:O     | 2:H:583:TYR:OH    | 2.27                     | 0.43              |
| 2:H:390:PHE:CD2   | 2:H:540:LEU:HD13  | 2.53                     | 0.43              |
| 21:G:904:HOH:O    | 14:H:801:CLA:HAC2 | 2.16                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:H:528:ALA:HB2    | 14:H:802:CLA:H171 | 2.00                     | 0.43              |
| 14:H:809:CLA:HHC   | 14:H:809:CLA:HBB1 | 2.00                     | 0.43              |
| 4:O:83:TYR:HD2     | 4:O:91:THR:HG22   | 1.84                     | 0.43              |
| 9:T:25:PHE:CE2     | 9:T:67:HIS:CE1    | 2.94                     | 0.43              |
| 1:Y:531:LEU:HD22   | 1:Y:535:ASP:HB3   | 2.01                     | 0.43              |
| 17:U:1007:BCR:H372 | 14:Y:834:CLA:C15  | 2.49                     | 0.43              |
| 1:Y:696:TYR:CE1    | 2:Z:542:LYS:HD2   | 2.53                     | 0.43              |
| 2:Z:618:SER:O      | 2:Z:624:GLY:HA3   | 2.19                     | 0.43              |
| 2:Z:275:HIS:NE2    | 14:Z:816:CLA:C2B  | 2.81                     | 0.43              |
| 14:Z:819:CLA:HBB2  | 14:Z:820:CLA:HBC2 | 2.01                     | 0.43              |
| 14:Z:832:CLA:HMD2  | 14:Z:833:CLA:CHC  | 2.49                     | 0.43              |
| 1:A:58:PHE:HE1     | 14:A:804:CLA:HED1 | 1.83                     | 0.43              |
| 14:A:811:CLA:HBA2  | 14:A:811:CLA:H3A  | 1.83                     | 0.43              |
| 14:A:817:CLA:H61   | 14:A:817:CLA:H41  | 1.67                     | 0.43              |
| 1:G:380:TYR:HA     | 1:G:381:PRO:HD3   | 1.91                     | 0.43              |
| 1:G:85:ILE:CD1     | 14:G:809:CLA:H201 | 2.49                     | 0.43              |
| 14:H:809:CLA:HED2  | 14:H:809:CLA:H12  | 2.01                     | 0.43              |
| 14:A:808:CLA:H101  | 17:J:103:BCR:H372 | 2.00                     | 0.43              |
| 9:K:62:THR:O       | 9:K:66:GLY:N      | 2.42                     | 0.43              |
| 2:B:693:LEU:HD12   | 17:L:203:BCR:H272 | 2.01                     | 0.43              |
| 10:L:62:TRP:HB2    | 10:L:78:GLY:HA2   | 2.00                     | 0.43              |
| 5:P:11:ARG:HG2     | 5:P:13:GLU:OE1    | 2.19                     | 0.43              |
| 2:H:551:LYS:N      | 6:Q:139:SER:OG    | 2.52                     | 0.43              |
| 14:Q:201:CLA:HBA2  | 14:Q:201:CLA:H3A  | 1.48                     | 0.43              |
| 10:U:90:THR:HG22   | 10:U:124:PHE:HD2  | 1.84                     | 0.43              |
| 1:Y:284:GLY:O      | 1:Y:285:LEU:HD23  | 2.19                     | 0.43              |
| 1:Y:444:LEU:HD23   | 1:Y:551:LEU:HA    | 1.99                     | 0.43              |
| 14:Y:828:CLA:HBA2  | 14:Y:828:CLA:H3A  | 1.59                     | 0.43              |
| 2:Z:187:LEU:HB2    | 2:Z:280:ALA:HB1   | 2.00                     | 0.43              |
| 2:Z:236:PRO:HA     | 2:Z:252:ALA:HB3   | 2.01                     | 0.43              |
| 2:Z:243:PHE:HE1    | 2:Z:269:LEU:HD11  | 1.83                     | 0.43              |
| 2:Z:504:LEU:HA     | 2:Z:507:ILE:HG22  | 2.00                     | 0.43              |
| 2:Z:60:VAL:HG12    | 2:Z:64:LEU:HD12   | 2.01                     | 0.43              |
| 14:Y:803:CLA:H201  | 14:Z:801:CLA:H141 | 2.00                     | 0.43              |
| 2:Z:358:LEU:HD11   | 14:Z:824:CLA:HMC2 | 2.00                     | 0.43              |
| 2:Z:454:LYS:HE3    | 14:Z:831:CLA:O1D  | 2.19                     | 0.43              |
| 1:A:693:GLY:HA3    | 2:B:574:CYS:HB2   | 2.00                     | 0.42              |
| 2:B:726:THR:HB     | 14:B:803:CLA:O1D  | 2.18                     | 0.42              |
| 1:G:29:ALA:HB2     | 8:S:6:THR:OG1     | 2.19                     | 0.42              |
| 2:H:291:ARG:CZ     | 2:H:299:SER:HB2   | 2.49                     | 0.42              |
| 2:H:367:ASP:O      | 2:H:370:THR:HG22  | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:431:PHE:HA    | 14:Q:201:CLA:O1D   | 2.19                     | 0.42              |
| 14:H:830:CLA:H71  | 14:H:830:CLA:H41   | 2.01                     | 0.42              |
| 17:H:843:BCR:H15C | 17:H:843:BCR:H351  | 1.72                     | 0.42              |
| 2:H:527:HIS:CD2   | 17:H:848:BCR:H322  | 2.54                     | 0.42              |
| 17:J:103:BCR:H383 | 17:J:103:BCR:H23C  | 2.00                     | 0.42              |
| 17:M:101:BCR:H383 | 17:M:101:BCR:C23   | 2.49                     | 0.42              |
| 3:N:20:CYS:SG     | 3:N:24:VAL:HB      | 2.59                     | 0.42              |
| 8:S:13:VAL:O      | 8:S:17:ILE:HG13    | 2.18                     | 0.42              |
| 8:S:28:GLU:OE1    | 8:S:31:ARG:NH2     | 2.52                     | 0.42              |
| 10:U:33:ASN:HB3   | 14:U:1002:CLA:HAC1 | 2.01                     | 0.42              |
| 14:H:829:CLA:CGA  | 12:W:12:ARG:NH1    | 2.82                     | 0.42              |
| 12:W:9:TYR:N      | 21:W:1801:HOH:O    | 2.51                     | 0.42              |
| 1:Y:450:PHE:O     | 1:Y:454:HIS:ND1    | 2.52                     | 0.42              |
| 14:Y:818:CLA:H3A  | 14:Y:818:CLA:HBA2  | 1.72                     | 0.42              |
| 14:Y:812:CLA:HBB1 | 14:Y:820:CLA:HBC2  | 2.00                     | 0.42              |
| 1:Y:464:THR:HG21  | 14:Y:834:CLA:HBC3  | 2.01                     | 0.42              |
| 2:Z:122:TRP:HB2   | 14:Z:826:CLA:CED   | 2.49                     | 0.42              |
| 2:Z:129:ARG:HD3   | 2:Z:129:ARG:HA     | 1.74                     | 0.42              |
| 2:Z:24:ILE:HG22   | 14:Z:827:CLA:C4    | 2.49                     | 0.42              |
| 1:A:120:ILE:C     | 1:A:122:GLY:H      | 2.23                     | 0.42              |
| 1:A:140:THR:HB    | 1:A:392:SER:OG     | 2.18                     | 0.42              |
| 14:A:840:CLA:H41  | 15:A:843:PQN:H191  | 2.01                     | 0.42              |
| 14:A:852:CLA:C1C  | 14:B:801:CLA:HBB1  | 2.49                     | 0.42              |
| 2:B:241:HIS:HD2   | 2:B:261:HIS:HE1    | 1.67                     | 0.42              |
| 2:B:360:PRO:HG3   | 14:B:818:CLA:CBA   | 2.43                     | 0.42              |
| 2:B:529:ILE:O     | 2:B:532:GLY:N      | 2.52                     | 0.42              |
| 2:B:539:ILE:HD13  | 14:B:801:CLA:HMD2  | 2.01                     | 0.42              |
| 14:B:806:CLA:H193 | 14:B:813:CLA:HMD1  | 2.01                     | 0.42              |
| 14:B:811:CLA:HBA2 | 14:B:811:CLA:H3A   | 1.77                     | 0.42              |
| 2:B:85:PRO:O      | 2:B:115:ALA:N      | 2.52                     | 0.42              |
| 3:C:5:LYS:HD3     | 3:C:5:LYS:HA       | 1.89                     | 0.42              |
| 1:G:24:SER:O      | 14:G:811:CLA:HMA1  | 2.18                     | 0.42              |
| 1:G:278:PHE:O     | 1:G:279:LEU:HD23   | 2.18                     | 0.42              |
| 1:G:522:GLY:O     | 1:G:625:VAL:HG22   | 2.18                     | 0.42              |
| 14:G:825:CLA:H42  | 14:G:829:CLA:H193  | 2.01                     | 0.42              |
| 14:G:830:CLA:H171 | 14:G:830:CLA:H13   | 1.89                     | 0.42              |
| 2:H:255:THR:HG22  | 2:H:270:THR:HB     | 2.02                     | 0.42              |
| 14:H:808:CLA:HMB1 | 14:H:808:CLA:HBB1  | 2.01                     | 0.42              |
| 14:H:832:CLA:CHD  | 14:H:833:CLA:HAB   | 2.49                     | 0.42              |
| 2:H:684:LEU:O     | 14:H:837:CLA:HBC1  | 2.18                     | 0.42              |
| 14:A:832:CLA:HED1 | 10:L:16:HIS:HD2    | 1.82                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:Q:202:BCR:C38   | 17:Q:202:BCR:H23C  | 2.49                     | 0.42              |
| 17:Q:202:BCR:H15C  | 17:Q:202:BCR:H351  | 1.78                     | 0.42              |
| 9:T:65:PHE:O       | 9:T:68:LEU:HG      | 2.19                     | 0.42              |
| 17:U:1008:BCR:H24C | 17:U:1008:BCR:H371 | 1.77                     | 0.42              |
| 1:Y:148:ARG:O      | 1:Y:224:ASN:ND2    | 2.40                     | 0.42              |
| 1:Y:453:PHE:O      | 14:Y:834:CLA:HBB2  | 2.19                     | 0.42              |
| 1:Y:86:TRP:NE1     | 14:Y:806:CLA:HBC1  | 2.33                     | 0.42              |
| 1:Y:307:LEU:O      | 14:Y:821:CLA:HBC2  | 2.19                     | 0.42              |
| 14:A:817:CLA:HBC1  | 14:A:818:CLA:HMC2  | 2.00                     | 0.42              |
| 14:A:824:CLA:HMA1  | 14:A:842:CLA:HAB   | 2.01                     | 0.42              |
| 2:B:195:HIS:O      | 2:B:206:VAL:HG21   | 2.19                     | 0.42              |
| 2:B:236:PRO:HB2    | 2:B:237:ASP:H      | 1.69                     | 0.42              |
| 14:B:810:CLA:H18   | 14:B:810:CLA:H152  | 1.78                     | 0.42              |
| 14:G:804:CLA:HMA2  | 14:G:811:CLA:HMD2  | 2.00                     | 0.42              |
| 14:G:809:CLA:H93   | 14:G:809:CLA:H111  | 1.83                     | 0.42              |
| 1:G:214:GLY:HA3    | 14:G:814:CLA:HMC3  | 2.00                     | 0.42              |
| 14:G:824:CLA:CBB   | 14:G:831:CLA:HMD2  | 2.50                     | 0.42              |
| 2:H:207:GLY:N      | 2:H:210:ASN:OD1    | 2.52                     | 0.42              |
| 2:H:435:HIS:O      | 2:H:439:LEU:N      | 2.38                     | 0.42              |
| 2:H:337:LEU:HD21   | 14:H:828:CLA:C2B   | 2.50                     | 0.42              |
| 17:H:845:BCR:H15C  | 17:H:845:BCR:H351  | 1.74                     | 0.42              |
| 6:Q:80:VAL:HG23    | 6:Q:109:CYS:CB     | 2.42                     | 0.42              |
| 10:U:80:ILE:CG2    | 14:U:1006:CLA:H93  | 2.49                     | 0.42              |
| 1:Y:261:PHE:HB3    | 21:Y:902:HOH:O     | 2.19                     | 0.42              |
| 1:Y:452:GLY:HA3    | 14:Y:855:CLA:O1A   | 2.19                     | 0.42              |
| 1:Y:683:TRP:CD2    | 13:Y:801:CLO:CMA   | 3.02                     | 0.42              |
| 14:Y:806:CLA:CBC   | 14:Y:828:CLA:HMD1  | 2.49                     | 0.42              |
| 14:Y:841:CLA:H141  | 14:Y:841:CLA:H162  | 1.88                     | 0.42              |
| 14:Y:834:CLA:CMC   | 14:Y:855:CLA:H91   | 2.49                     | 0.42              |
| 17:Y:856:BCR:H331  | 17:Y:856:BCR:C8    | 2.49                     | 0.42              |
| 1:Y:89:GLY:HA2     | 14:Y:807:CLA:HMC3  | 2.01                     | 0.42              |
| 2:Z:50:PHE:O       | 2:Z:148:ALA:HB1    | 2.20                     | 0.42              |
| 2:Z:200:GLU:OE2    | 2:Z:205:HIS:CD2    | 2.72                     | 0.42              |
| 2:Z:555:ASP:HB2    | 2:Z:558:ASP:OD2    | 2.19                     | 0.42              |
| 14:Z:811:CLA:H121  | 14:Z:811:CLA:H8    | 1.71                     | 0.42              |
| 2:Z:467:GLN:NE2    | 14:Z:835:CLA:HMD1  | 2.34                     | 0.42              |
| 14:A:819:CLA:HBC2  | 14:A:829:CLA:H121  | 2.01                     | 0.42              |
| 14:A:827:CLA:C4C   | 14:A:836:CLA:HED1  | 2.49                     | 0.42              |
| 2:B:566:ASP:HB3    | 2:B:573:THR:HG21   | 2.02                     | 0.42              |
| 14:B:841:CLA:HBC2  | 14:B:841:CLA:HMC1  | 2.01                     | 0.42              |
| 4:D:7:PRO:HB3      | 10:L:13:PHE:HZ     | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:280:THR:HG22  | 1:G:295:SER:OG    | 2.17                     | 0.42              |
| 1:G:341:HIS:CE1   | 1:G:429:VAL:HG21  | 2.55                     | 0.42              |
| 1:G:437:ARG:CZ    | 4:O:44:ALA:HB2    | 2.49                     | 0.42              |
| 2:H:9:GLN:N       | 2:H:34:ASP:OD2    | 2.47                     | 0.42              |
| 2:H:361:TYR:O     | 2:H:364:ILE:CG2   | 2.67                     | 0.42              |
| 2:H:397:LEU:HA    | 2:H:401:TYR:HB2   | 2.02                     | 0.42              |
| 2:H:518:ILE:HG23  | 14:H:834:CLA:HMD2 | 2.00                     | 0.42              |
| 1:G:695:GLY:O     | 2:H:576:ILE:HG13  | 2.20                     | 0.42              |
| 2:H:589:MET:SD    | 2:H:590:LEU:HG    | 2.59                     | 0.42              |
| 14:H:803:CLA:H112 | 14:H:803:CLA:H72  | 1.83                     | 0.42              |
| 6:Q:65:ILE:HB     | 6:Q:66:PRO:HD3    | 2.01                     | 0.42              |
| 1:Y:159:TYR:O     | 1:Y:163:ILE:HG12  | 2.19                     | 0.42              |
| 1:Y:177:TRP:HB2   | 14:Y:811:CLA:CMC  | 2.48                     | 0.42              |
| 1:Y:375:TYR:CE1   | 14:Y:837:CLA:HBC3 | 2.55                     | 0.42              |
| 2:Z:441:VAL:HB    | 14:Z:831:CLA:HMC3 | 2.01                     | 0.42              |
| 2:Z:561:TYR:O     | 2:Z:579:TRP:HB2   | 2.18                     | 0.42              |
| 2:Z:604:HIS:HB3   | 2:Z:608:TRP:CE2   | 2.53                     | 0.42              |
| 2:Z:194:ILE:HD13  | 14:Z:813:CLA:HAC2 | 2.00                     | 0.42              |
| 1:A:37:THR:OG1    | 1:A:38:LEU:N      | 2.52                     | 0.42              |
| 14:A:803:CLA:H111 | 8:J:19:MET:HB3    | 2.02                     | 0.42              |
| 14:A:826:CLA:H11  | 14:A:837:CLA:HBA1 | 2.02                     | 0.42              |
| 2:B:186:SER:HA    | 2:B:189:TRP:HB3   | 2.02                     | 0.42              |
| 14:B:802:CLA:O1A  | 14:B:832:CLA:O2D  | 2.38                     | 0.42              |
| 4:D:131:THR:O     | 4:D:133:LYS:N     | 2.52                     | 0.42              |
| 1:G:592:TRP:O     | 1:G:595:VAL:HB    | 2.18                     | 0.42              |
| 13:G:801:CL0:O2A  | 14:G:803:CLA:HMD3 | 2.19                     | 0.42              |
| 14:G:808:CLA:H3A  | 14:G:808:CLA:HBA2 | 1.81                     | 0.42              |
| 1:G:307:LEU:HD21  | 14:G:817:CLA:H141 | 2.02                     | 0.42              |
| 14:G:817:CLA:HBC1 | 14:G:818:CLA:HMC2 | 2.01                     | 0.42              |
| 7:I:29:LEU:HD12   | 2:Z:156:LEU:HD12  | 63.51                    | 0.42              |
| 1:Y:709:ASN:OD1   | 1:Y:714:ALA:HB3   | 2.19                     | 0.42              |
| 14:Y:829:CLA:HMD2 | 14:Y:829:CLA:H71  | 2.00                     | 0.42              |
| 17:Y:850:BCR:H371 | 17:Y:850:BCR:H24C | 1.73                     | 0.42              |
| 1:A:283:GLY:O     | 1:A:507:ALA:HB3   | 2.19                     | 0.42              |
| 14:B:825:CLA:C1B  | 17:B:847:BCR:H363 | 2.48                     | 0.42              |
| 14:B:825:CLA:HMB3 | 17:B:847:BCR:C17  | 2.50                     | 0.42              |
| 1:A:583:ARG:HG3   | 3:C:48:VAL:CG1    | 2.49                     | 0.42              |
| 1:A:583:ARG:HA    | 3:C:76:MET:HA     | 2.01                     | 0.42              |
| 1:G:433:VAL:HG21  | 14:G:824:CLA:CMC  | 2.50                     | 0.42              |
| 14:G:802:CLA:H141 | 14:G:802:CLA:H161 | 1.72                     | 0.42              |
| 14:G:810:CLA:HBB1 | 14:G:810:CLA:HMB1 | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:207:LEU:HD11  | 14:G:820:CLA:HBC1 | 2.02                     | 0.42              |
| 14:G:824:CLA:O2D  | 14:G:824:CLA:HAA1 | 2.19                     | 0.42              |
| 7:I:18:VAL:O      | 7:I:23:PRO:HD3    | 2.19                     | 0.42              |
| 4:O:37:GLN:NE2    | 4:O:77:ILE:HD11   | 2.34                     | 0.42              |
| 17:Q:204:BCR:H271 | 14:W:1701:CLA:O2A | 2.19                     | 0.42              |
| 6:Q:84:TYR:CD1    | 6:Q:105:LEU:HD23  | 2.54                     | 0.42              |
| 6:Q:84:TYR:CD2    | 6:Q:84:TYR:C      | 2.93                     | 0.42              |
| 1:G:268:PHE:HA    | 14:T:101:CLA:HAC1 | 2.01                     | 0.42              |
| 10:U:131:SER:O    | 10:U:134:VAL:HG12 | 2.18                     | 0.42              |
| 10:U:58:LEU:HD13  | 10:U:85:LEU:HD22  | 2.02                     | 0.42              |
| 1:Y:210:LEU:CD2   | 17:Y:847:BCR:H373 | 2.49                     | 0.42              |
| 1:Y:332:HIS:O     | 1:Y:341:HIS:ND1   | 2.53                     | 0.42              |
| 1:Y:330:GLU:HG2   | 1:Y:342:LYS:HA    | 2.01                     | 0.42              |
| 1:Y:409:ALA:HB1   | 1:Y:553:LEU:HB3   | 2.00                     | 0.42              |
| 14:Z:809:CLA:H41  | 14:Z:809:CLA:H62  | 1.72                     | 0.42              |
| 2:Z:277:LEU:CD1   | 14:Z:813:CLA:HMC1 | 2.44                     | 0.42              |
| 2:Z:230:GLY:HA2   | 14:Z:814:CLA:HAA2 | 2.02                     | 0.42              |
| 2:Z:388:GLY:CA    | 14:Z:827:CLA:C3C  | 2.97                     | 0.42              |
| 17:Z:846:BCR:H15C | 17:Z:846:BCR:H351 | 1.81                     | 0.42              |
| 2:B:325:ILE:HA    | 2:B:328:THR:HG22  | 2.02                     | 0.42              |
| 2:B:425:LEU:HD21  | 14:B:839:CLA:C3B  | 2.50                     | 0.42              |
| 2:B:303:MET:HE2   | 14:B:823:CLA:HED2 | 2.01                     | 0.42              |
| 14:B:825:CLA:H3A  | 14:B:825:CLA:HBA2 | 1.78                     | 0.42              |
| 1:G:212:TRP:CA    | 14:G:814:CLA:HAB  | 2.49                     | 0.42              |
| 2:H:622:LEU:HD13  | 14:H:801:CLA:CMA  | 2.48                     | 0.42              |
| 10:L:6:LYS:O      | 10:L:18:SER:N     | 2.53                     | 0.42              |
| 17:L:203:BCR:H351 | 17:L:203:BCR:H15C | 1.60                     | 0.42              |
| 1:Y:392:SER:O     | 1:Y:396:HIS:CB    | 2.68                     | 0.42              |
| 1:Y:464:THR:HG22  | 2:Z:654:TRP:NE1   | 2.35                     | 0.42              |
| 1:Y:553:LEU:O     | 1:Y:557:VAL:HG23  | 2.19                     | 0.42              |
| 1:Y:592:TRP:NE1   | 14:Y:830:CLA:HMD1 | 2.35                     | 0.42              |
| 1:Y:653:PHE:O     | 1:Y:657:GLN:HG3   | 2.20                     | 0.42              |
| 1:Y:664:SER:OG    | 1:Y:673:GLY:HA3   | 2.20                     | 0.42              |
| 1:Y:45:THR:HB     | 1:Y:719:PRO:HA    | 2.02                     | 0.42              |
| 14:Y:808:CLA:H112 | 14:Y:830:CLA:H192 | 2.02                     | 0.42              |
| 14:Y:833:CLA:HBA1 | 14:Y:833:CLA:H3A  | 1.84                     | 0.42              |
| 2:Z:332:SER:O     | 2:Z:336:GLN:HG3   | 2.19                     | 0.42              |
| 14:Z:838:CLA:HAB  | 15:Z:840:PQN:H193 | 2.02                     | 0.42              |
| 1:A:214:GLY:O     | 1:A:218:HIS:HD2   | 2.01                     | 0.42              |
| 1:A:221:LEU:HB2   | 1:A:222:PRO:HD3   | 2.01                     | 0.42              |
| 1:A:59:ASP:CB     | 1:A:418:ARG:HH12  | 2.32                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:607:SER:O     | 1:A:610:ILE:HG12  | 2.19                     | 0.42              |
| 1:A:677:LEU:HD21  | 2:B:626:LEU:HD22  | 2.02                     | 0.42              |
| 14:A:826:CLA:H2   | 14:A:836:CLA:HMA2 | 2.02                     | 0.42              |
| 14:B:841:CLA:H161 | 14:B:841:CLA:H202 | 1.78                     | 0.42              |
| 17:B:843:BCR:H331 | 17:B:843:BCR:C8   | 2.49                     | 0.42              |
| 4:D:9:LEU:HB2     | 4:D:48:VAL:HG23   | 2.01                     | 0.42              |
| 1:G:21:VAL:HG23   | 1:G:181:HIS:ND1   | 2.34                     | 0.42              |
| 1:G:618:GLN:O     | 1:G:634:ILE:HB    | 2.20                     | 0.42              |
| 1:G:674:LEU:HD21  | 2:H:448:ALA:HB2   | 2.02                     | 0.42              |
| 1:G:90:MET:HE3    | 1:G:90:MET:HA     | 2.02                     | 0.42              |
| 2:H:200:GLU:OE1   | 2:H:205:HIS:CD2   | 2.73                     | 0.42              |
| 2:H:649:LEU:HA    | 2:H:652:TRP:HD1   | 1.85                     | 0.42              |
| 2:H:668:MET:HB2   | 14:H:803:CLA:C1C  | 2.50                     | 0.42              |
| 14:H:805:CLA:H162 | 14:H:827:CLA:HBB2 | 2.01                     | 0.42              |
| 2:H:286:ALA:HB2   | 14:H:818:CLA:C2C  | 2.49                     | 0.42              |
| 14:H:822:CLA:CMD  | 14:H:823:CLA:HAB  | 2.49                     | 0.42              |
| 8:J:17:ILE:O      | 8:J:20:THR:N      | 2.52                     | 0.42              |
| 10:L:107:SER:O    | 10:L:108:SER:C    | 2.57                     | 0.42              |
| 2:H:20:ILE:CD1    | 7:R:34:ILE:HD12   | 2.50                     | 0.42              |
| 10:U:16:HIS:CD2   | 10:U:17:LEU:H     | 2.37                     | 0.42              |
| 1:Y:140:THR:HA    | 1:Y:389:THR:HG22  | 2.00                     | 0.42              |
| 14:Y:808:CLA:H18  | 14:Y:830:CLA:H201 | 2.01                     | 0.42              |
| 17:Y:850:BCR:H351 | 17:Y:850:BCR:H15C | 1.66                     | 0.42              |
| 14:Y:855:CLA:HAB  | 2:Z:665:THR:N     | 2.34                     | 0.42              |
| 2:Z:203:GLY:CA    | 2:Z:244:GLY:O     | 2.67                     | 0.42              |
| 2:Z:355:MET:HE2   | 2:Z:374:LEU:HD13  | 2.02                     | 0.42              |
| 2:Z:360:PRO:HG3   | 14:Z:816:CLA:CBA  | 2.48                     | 0.42              |
| 2:Z:388:GLY:N     | 14:Z:827:CLA:HAC1 | 2.34                     | 0.42              |
| 17:Z:844:BCR:H15C | 17:Z:844:BCR:H351 | 1.60                     | 0.42              |
| 2:Z:92:ASP:C      | 2:Z:94:GLN:H      | 2.23                     | 0.42              |
| 1:A:565:LEU:HD11  | 1:A:583:ARG:HB3   | 2.01                     | 0.42              |
| 1:A:583:ARG:HG3   | 3:C:48:VAL:HG13   | 2.01                     | 0.42              |
| 1:A:662:ILE:HB    | 2:B:627:ARG:HB2   | 2.01                     | 0.42              |
| 14:A:816:CLA:HBC2 | 14:A:816:CLA:HMC1 | 2.00                     | 0.42              |
| 2:B:222:ALA:HB3   | 2:B:223:PRO:HD3   | 2.02                     | 0.42              |
| 2:B:430:LEU:HG    | 2:B:434:PHE:CE2   | 2.55                     | 0.42              |
| 14:B:832:CLA:HBC2 | 14:B:832:CLA:HHD  | 2.01                     | 0.42              |
| 2:B:435:HIS:CB    | 17:B:851:BCR:HC42 | 2.49                     | 0.42              |
| 2:B:86:ILE:O      | 2:B:120:TYR:OH    | 2.23                     | 0.42              |
| 14:B:832:CLA:CAB  | 17:F:201:BCR:H323 | 2.50                     | 0.42              |
| 1:G:675:LEU:HD11  | 14:G:828:CLA:C14  | 2.50                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:699:GLU:HG2   | 2:H:550:SER:OG     | 2.20                     | 0.42              |
| 14:G:808:CLA:CHC  | 14:G:809:CLA:HMD2  | 2.49                     | 0.42              |
| 14:G:808:CLA:HMC2 | 14:G:828:CLA:H141  | 2.01                     | 0.42              |
| 2:H:548:ARG:HH22  | 4:O:124:ASN:CG     | 2.23                     | 0.42              |
| 2:H:181:LEU:HG    | 14:H:812:CLA:H43   | 2.01                     | 0.42              |
| 9:K:21:LEU:O      | 9:K:25:PHE:HE1     | 2.03                     | 0.42              |
| 3:N:13:CYS:C      | 3:N:15:GLN:H       | 2.23                     | 0.42              |
| 1:Y:575:ARG:HA    | 1:Y:592:TRP:HB2    | 2.01                     | 0.42              |
| 1:Y:677:LEU:O     | 1:Y:680:HIS:N      | 2.47                     | 0.42              |
| 14:Y:803:CLA:H191 | 14:Y:854:CLA:H141  | 2.02                     | 0.42              |
| 1:Y:90:MET:HE1    | 14:Y:808:CLA:H2A   | 2.02                     | 0.42              |
| 14:Y:814:CLA:H42  | 14:Y:816:CLA:HMB2  | 2.01                     | 0.42              |
| 14:Z:822:CLA:HMB3 | 14:Z:822:CLA:C10   | 2.49                     | 0.42              |
| 2:Z:427:TRP:CE2   | 14:Z:829:CLA:HAB   | 2.55                     | 0.42              |
| 14:Z:838:CLA:HAA1 | 14:Z:838:CLA:HBD   | 2.02                     | 0.42              |
| 1:A:45:THR:OG1    | 14:A:839:CLA:C3B   | 2.68                     | 0.42              |
| 14:A:807:CLA:HMB3 | 14:A:808:CLA:HMA1  | 2.01                     | 0.42              |
| 14:B:830:CLA:HMA1 | 14:B:831:CLA:CGD   | 2.50                     | 0.42              |
| 3:C:61:PHE:CD2    | 4:D:119:ILE:HG21   | 2.55                     | 0.42              |
| 4:D:31:TRP:HZ2    | 4:D:49:MET:HB2     | 1.85                     | 0.42              |
| 1:G:352:TRP:CE2   | 14:G:825:CLA:H18   | 2.55                     | 0.42              |
| 14:G:802:CLA:H202 | 14:G:841:CLA:H2    | 2.02                     | 0.42              |
| 1:G:215:HIS:HB2   | 14:G:814:CLA:C1C   | 2.50                     | 0.42              |
| 17:G:849:BCR:H351 | 17:G:849:BCR:H15C  | 1.76                     | 0.42              |
| 2:H:28:HIS:HB2    | 14:H:828:CLA:O1A   | 2.20                     | 0.42              |
| 2:H:447:VAL:HG22  | 2:H:452:PRO:HA     | 2.01                     | 0.42              |
| 2:H:591:ASN:HB2   | 14:H:801:CLA:HBC2  | 2.01                     | 0.42              |
| 14:H:803:CLA:H52  | 14:H:803:CLA:CMB   | 2.50                     | 0.42              |
| 15:H:839:PQN:H111 | 15:H:839:PQN:H2M1  | 1.91                     | 0.42              |
| 10:U:57:PHE:CD2   | 14:U:1004:CLA:HBC3 | 2.54                     | 0.42              |
| 11:V:10:VAL:O     | 11:V:14:ILE:HG13   | 2.19                     | 0.42              |
| 1:Y:399:TRP:CE2   | 1:Y:740:ILE:HG23   | 2.55                     | 0.42              |
| 1:Y:405:VAL:HG13  | 17:Y:850:BCR:H343  | 2.01                     | 0.42              |
| 2:Z:381:ILE:O     | 2:Z:385:LEU:HG     | 2.20                     | 0.42              |
| 2:Z:386:MET:O     | 2:Z:389:ALA:HB3    | 2.20                     | 0.42              |
| 2:Z:561:TYR:O     | 2:Z:577:SER:OG     | 2.37                     | 0.42              |
| 14:Z:826:CLA:H202 | 17:Z:842:BCR:H352  | 2.02                     | 0.42              |
| 1:A:56:HIS:O      | 14:A:805:CLA:HMC3  | 2.20                     | 0.41              |
| 2:B:383:GLY:HA3   | 2:B:589:MET:CE     | 2.49                     | 0.41              |
| 6:F:60:ALA:O      | 6:F:64:LEU:HB2     | 2.20                     | 0.41              |
| 1:G:28:TRP:HE1    | 14:G:811:CLA:CHB   | 2.33                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:G:826:CLA:CAB   | 17:G:849:BCR:H311  | 2.49                     | 0.41              |
| 14:G:843:CLA:HMC3  | 18:G:852:LHG:O2    | 2.20                     | 0.41              |
| 2:H:543:GLY:HA3    | 2:H:581:ALA:CB     | 2.50                     | 0.41              |
| 2:H:602:TRP:CE2    | 2:H:629:TYR:HB2    | 2.55                     | 0.41              |
| 14:H:814:CLA:NB    | 17:H:840:BCR:HC32  | 2.35                     | 0.41              |
| 17:H:844:BCR:H371  | 17:H:844:BCR:H24C  | 1.81                     | 0.41              |
| 10:L:153:PHE:CG    | 10:U:68:LEU:HD22   | 2.54                     | 0.41              |
| 14:H:806:CLA:HBC1  | 11:V:11:ALA:O      | 2.20                     | 0.41              |
| 12:W:18:LEU:O      | 12:W:22:ILE:HG13   | 2.19                     | 0.41              |
| 1:Y:205:LEU:HD23   | 14:Y:819:CLA:HBC3  | 2.01                     | 0.41              |
| 1:Y:377:MET:HG2    | 1:Y:509:ALA:O      | 2.19                     | 0.41              |
| 14:Y:827:CLA:C7    | 21:Y:904:HOH:O     | 2.63                     | 0.41              |
| 2:Z:188:ALA:O      | 2:Z:192:HIS:N      | 2.51                     | 0.41              |
| 2:Z:690:ARG:HA     | 2:Z:690:ARG:HD3    | 1.88                     | 0.41              |
| 1:Y:684:ALA:C      | 14:Z:801:CLA:HAB   | 2.41                     | 0.41              |
| 14:Z:828:CLA:CAB   | 14:Z:837:CLA:HBB2  | 2.50                     | 0.41              |
| 1:A:17:ASP:OD1     | 1:A:186:LYS:NZ     | 2.52                     | 0.41              |
| 1:A:212:TRP:O      | 1:A:216:GLN:HB2    | 2.21                     | 0.41              |
| 1:A:376:ALA:HA     | 1:A:526:MET:HE1    | 2.03                     | 0.41              |
| 1:A:52:HIS:HB3     | 14:A:804:CLA:HBC3  | 2.02                     | 0.41              |
| 1:A:77:PHE:CE1     | 14:A:810:CLA:HBB1  | 2.56                     | 0.41              |
| 1:A:300:HIS:HB2    | 14:A:818:CLA:C1B   | 2.50                     | 0.41              |
| 14:A:840:CLA:H111  | 14:B:801:CLA:H141  | 2.02                     | 0.41              |
| 2:B:602:TRP:CH2    | 2:B:618:SER:HB2    | 2.55                     | 0.41              |
| 14:B:808:CLA:HMA1  | 14:B:809:CLA:C2B   | 2.50                     | 0.41              |
| 2:B:431:PHE:HA     | 14:B:832:CLA:O1D   | 2.20                     | 0.41              |
| 1:G:664:SER:HB2    | 1:G:669:LEU:HB2    | 2.01                     | 0.41              |
| 14:G:819:CLA:CAD   | 14:G:829:CLA:H41   | 2.50                     | 0.41              |
| 2:H:548:ARG:NH1    | 6:Q:141:ARG:OXT    | 2.53                     | 0.41              |
| 2:H:601:HIS:O      | 2:H:605:LEU:HG     | 2.20                     | 0.41              |
| 14:H:801:CLA:H141  | 14:S:1101:CLA:C19  | 2.46                     | 0.41              |
| 2:H:663:TRP:CZ3    | 14:H:802:CLA:HMA1  | 2.55                     | 0.41              |
| 14:H:824:CLA:HBA2  | 14:H:824:CLA:H3A   | 1.61                     | 0.41              |
| 17:H:842:BCR:H351  | 17:H:842:BCR:H15C  | 1.59                     | 0.41              |
| 10:L:33:ASN:HB3    | 14:L:205:CLA:HAC1  | 2.02                     | 0.41              |
| 14:L:205:CLA:CBB   | 14:L:205:CLA:HHC   | 2.50                     | 0.41              |
| 10:L:6:LYS:HG3     | 10:L:18:SER:CB     | 2.48                     | 0.41              |
| 8:S:18:TRP:HA      | 8:S:18:TRP:CE3     | 2.53                     | 0.41              |
| 14:U:1002:CLA:H3A  | 14:U:1002:CLA:HBA2 | 1.79                     | 0.41              |
| 17:U:1007:BCR:H351 | 17:U:1007:BCR:H15C | 1.85                     | 0.41              |
| 1:Y:537:MET:HE1    | 1:Y:644:ILE:HA     | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:Y:808:CLA:HBA2 | 14:Y:808:CLA:H3A  | 1.64                     | 0.41              |
| 1:Y:407:GLY:HA2   | 14:Y:830:CLA:C3C  | 2.49                     | 0.41              |
| 17:Z:845:BCR:H371 | 17:Z:845:BCR:H24C | 1.84                     | 0.41              |
| 1:A:202:ALA:HB2   | 1:A:312:GLY:HA3   | 2.01                     | 0.41              |
| 1:A:429:VAL:HG23  | 14:A:831:CLA:CMD  | 2.50                     | 0.41              |
| 1:A:475:PHE:HA    | 1:A:480:ILE:O     | 2.19                     | 0.41              |
| 1:A:599:LEU:HD13  | 18:A:850:LHG:H321 | 2.02                     | 0.41              |
| 1:A:388:PRO:HG3   | 1:A:752:ILE:HA    | 2.02                     | 0.41              |
| 14:A:803:CLA:C17  | 14:A:840:CLA:H161 | 2.51                     | 0.41              |
| 1:A:674:LEU:O     | 14:A:852:CLA:H62  | 2.20                     | 0.41              |
| 2:B:392:HIS:HA    | 2:B:395:ILE:HB    | 2.03                     | 0.41              |
| 1:A:442:SER:HB2   | 2:B:687:ALA:HB2   | 2.01                     | 0.41              |
| 1:A:684:ALA:HB1   | 14:B:801:CLA:HBB2 | 2.01                     | 0.41              |
| 14:B:807:CLA:H91  | 19:B:849:LMG:H402 | 2.02                     | 0.41              |
| 2:B:122:TRP:HZ2   | 14:B:813:CLA:H191 | 1.84                     | 0.41              |
| 14:G:804:CLA:HBC2 | 14:G:830:CLA:H51  | 2.03                     | 0.41              |
| 1:G:72:ILE:HD13   | 14:G:805:CLA:C3C  | 2.51                     | 0.41              |
| 14:G:817:CLA:CGA  | 14:G:817:CLA:C1A  | 2.97                     | 0.41              |
| 1:G:362:MET:CG    | 14:G:825:CLA:HMB2 | 2.48                     | 0.41              |
| 2:H:398:VAL:O     | 4:O:125:PRO:HG2   | 2.20                     | 0.41              |
| 2:H:622:LEU:HD12  | 14:H:801:CLA:H11  | 2.02                     | 0.41              |
| 14:H:804:CLA:O2A  | 14:H:812:CLA:O1A  | 2.38                     | 0.41              |
| 9:K:24:LEU:HA     | 9:K:27:ILE:HG22   | 2.02                     | 0.41              |
| 1:Y:272:TRP:CG    | 14:Y:817:CLA:HMB2 | 2.55                     | 0.41              |
| 1:Y:293:TRP:O     | 1:Y:296:ASP:HB2   | 2.20                     | 0.41              |
| 1:Y:315:TYR:CE1   | 1:Y:325:LEU:HD21  | 2.55                     | 0.41              |
| 1:Y:566:ILE:O     | 1:Y:569:LYS:HG3   | 2.20                     | 0.41              |
| 1:Y:639:PHE:O     | 1:Y:643:ALA:HB3   | 2.20                     | 0.41              |
| 1:Y:190:PHE:O     | 14:Y:825:CLA:H141 | 2.21                     | 0.41              |
| 14:Y:806:CLA:CMA  | 14:Y:830:CLA:CAB  | 2.98                     | 0.41              |
| 1:A:379:PRO:HG3   | 14:A:819:CLA:CBA  | 2.49                     | 0.41              |
| 1:A:722:LEU:HD13  | 1:A:730:VAL:HG21  | 2.01                     | 0.41              |
| 14:A:818:CLA:H3A  | 14:A:818:CLA:HBA2 | 1.80                     | 0.41              |
| 14:A:837:CLA:HMB2 | 14:A:838:CLA:C3D  | 2.49                     | 0.41              |
| 4:D:123:PRO:HB2   | 4:D:128:LEU:HD11  | 2.02                     | 0.41              |
| 4:D:38:VAL:O      | 4:D:75:ARG:NH1    | 2.48                     | 0.41              |
| 1:G:253:TYR:CD2   | 1:G:253:TYR:N     | 2.88                     | 0.41              |
| 14:G:819:CLA:H162 | 14:G:819:CLA:H193 | 1.92                     | 0.41              |
| 14:G:812:CLA:HBB1 | 14:G:820:CLA:HBC2 | 2.03                     | 0.41              |
| 2:H:20:ILE:HD11   | 7:R:34:ILE:HD12   | 2.01                     | 0.41              |
| 2:H:241:HIS:HB3   | 2:H:261:HIS:NE2   | 2.34                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:662:VAL:O     | 2:H:665:THR:N      | 2.52                     | 0.41              |
| 2:H:536:THR:HG21  | 14:H:824:CLA:HBC3  | 2.02                     | 0.41              |
| 8:J:26:LEU:HD22   | 17:J:103:BCR:HC7   | 2.01                     | 0.41              |
| 6:Q:74:ALA:O      | 6:Q:77:ILE:HB      | 2.19                     | 0.41              |
| 17:V:1202:BCR:HC7 | 17:V:1202:BCR:H331 | 1.81                     | 0.41              |
| 1:Y:337:THR:O     | 1:Y:432:ARG:HD2    | 2.20                     | 0.41              |
| 1:Y:482:LEU:H     | 1:Y:533:THR:HG23   | 1.84                     | 0.41              |
| 1:Y:448:CYS:HB3   | 1:Y:548:VAL:HG22   | 2.02                     | 0.41              |
| 17:Y:851:BCR:H15C | 17:Y:851:BCR:H351  | 1.75                     | 0.41              |
| 14:Y:855:CLA:O1D  | 17:Y:856:BCR:H391  | 2.20                     | 0.41              |
| 2:Z:29:ASP:OD2    | 2:Z:32:SER:OG      | 2.38                     | 0.41              |
| 2:Z:320:MET:HB2   | 2:Z:322:HIS:CE1    | 2.56                     | 0.41              |
| 1:A:66:GLU:O      | 1:A:69:SER:OG      | 2.28                     | 0.41              |
| 1:A:682:ILE:HD11  | 14:A:840:CLA:HMB1  | 2.01                     | 0.41              |
| 14:A:819:CLA:C4A  | 14:A:819:CLA:O1A   | 2.69                     | 0.41              |
| 14:A:830:CLA:H102 | 14:A:840:CLA:HAA2  | 2.02                     | 0.41              |
| 14:A:841:CLA:HBA2 | 14:A:841:CLA:C4A   | 2.50                     | 0.41              |
| 2:B:30:PHE:O      | 2:B:33:HIS:HB2     | 2.21                     | 0.41              |
| 2:B:383:GLY:O     | 2:B:589:MET:HG3    | 2.21                     | 0.41              |
| 1:A:445:ASN:OD1   | 14:B:804:CLA:HED3  | 2.20                     | 0.41              |
| 14:B:805:CLA:HED2 | 14:B:805:CLA:H2A   | 2.01                     | 0.41              |
| 14:B:808:CLA:H102 | 14:B:808:CLA:H61   | 1.89                     | 0.41              |
| 14:B:823:CLA:OBD  | 14:B:824:CLA:HAB   | 2.21                     | 0.41              |
| 17:B:845:BCR:C38  | 17:B:845:BCR:H23C  | 2.48                     | 0.41              |
| 17:B:847:BCR:H351 | 17:B:847:BCR:H15C  | 1.78                     | 0.41              |
| 4:D:30:THR:HG22   | 4:D:55:LEU:HD13    | 2.02                     | 0.41              |
| 6:F:101:ILE:HB    | 8:J:14:LEU:CD1     | 2.50                     | 0.41              |
| 2:H:176:HIS:HB3   | 14:H:812:CLA:CAB   | 2.50                     | 0.41              |
| 2:H:339:TRP:O     | 2:H:342:ALA:HB3    | 2.19                     | 0.41              |
| 14:H:802:CLA:H41  | 14:H:802:CLA:H62   | 1.73                     | 0.41              |
| 2:H:350:LEU:HD13  | 14:H:825:CLA:HAA1  | 2.02                     | 0.41              |
| 14:H:827:CLA:H3A  | 14:H:827:CLA:HBA2  | 1.68                     | 0.41              |
| 14:L:205:CLA:HMB2 | 17:L:209:BCR:C12   | 2.50                     | 0.41              |
| 17:L:209:BCR:C38  | 17:L:209:BCR:C23   | 2.98                     | 0.41              |
| 3:N:64:ILE:HG23   | 3:N:64:ILE:O       | 2.20                     | 0.41              |
| 14:Y:826:CLA:HBA1 | 14:Y:827:CLA:OBD   | 2.19                     | 0.41              |
| 2:Z:516:LEU:HD13  | 2:Z:603:LYS:HG2    | 2.02                     | 0.41              |
| 2:Z:667:PHE:HE1   | 2:Z:719:PHE:CD1    | 2.38                     | 0.41              |
| 14:Z:806:CLA:H3A  | 14:Z:807:CLA:HMB3  | 2.02                     | 0.41              |
| 1:A:394:PHE:CE1   | 1:A:613:PHE:HB2    | 2.56                     | 0.41              |
| 1:A:682:ILE:HD13  | 14:A:840:CLA:HMB3  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:604:ASN:OD1   | 13:A:801:CL0:H37  | 2.19                     | 0.41              |
| 1:A:14:VAL:HG21   | 14:A:810:CLA:HMA2 | 2.03                     | 0.41              |
| 14:A:821:CLA:HMB2 | 14:A:825:CLA:HMA3 | 2.02                     | 0.41              |
| 1:A:440:ILE:HG23  | 14:A:838:CLA:HBB2 | 2.03                     | 0.41              |
| 1:G:655:TRP:CD1   | 2:H:631:TRP:CD1   | 3.09                     | 0.41              |
| 1:G:90:MET:HE1    | 14:G:808:CLA:H2A  | 2.03                     | 0.41              |
| 14:G:808:CLA:H91  | 14:G:808:CLA:H121 | 2.02                     | 0.41              |
| 14:G:819:CLA:HBB1 | 14:G:819:CLA:HMB1 | 2.02                     | 0.41              |
| 17:G:847:BCR:H371 | 17:G:847:BCR:H24C | 1.85                     | 0.41              |
| 2:H:522:ASP:HB3   | 2:H:526:HIS:HD2   | 1.84                     | 0.41              |
| 2:H:713:LEU:HD22  | 19:H:846:LMG:H122 | 2.03                     | 0.41              |
| 14:H:824:CLA:HMB3 | 17:H:844:BCR:C17  | 2.50                     | 0.41              |
| 6:F:100:ILE:CG2   | 8:J:10:THR:HG22   | 2.50                     | 0.41              |
| 6:Q:16:LYS:O      | 6:Q:19:ALA:HB3    | 2.20                     | 0.41              |
| 1:Y:403:PHE:O     | 14:Y:830:CLA:HMC1 | 2.20                     | 0.41              |
| 1:Y:549:THR:HA    | 1:Y:552:ILE:HD12  | 2.01                     | 0.41              |
| 13:Y:801:CL0:H13  | 14:Y:854:CLA:OBD  | 2.20                     | 0.41              |
| 14:Y:818:CLA:HMD2 | 14:Y:819:CLA:H202 | 2.02                     | 0.41              |
| 2:Z:198:ILE:HD13  | 2:Z:202:ARG:NH1   | 2.35                     | 0.41              |
| 14:Z:832:CLA:H3A  | 14:Z:832:CLA:HBA1 | 1.77                     | 0.41              |
| 1:A:356:LEU:HD23  | 1:A:411:HIS:CE1   | 2.55                     | 0.41              |
| 1:A:529:ILE:HG12  | 1:A:621:VAL:CG2   | 2.51                     | 0.41              |
| 14:A:821:CLA:HED2 | 14:A:824:CLA:HED2 | 2.03                     | 0.41              |
| 14:A:826:CLA:H51  | 14:A:836:CLA:H12  | 2.02                     | 0.41              |
| 14:A:827:CLA:HED1 | 14:A:834:CLA:HAB  | 2.01                     | 0.41              |
| 2:B:278:ALA:HB2   | 14:B:817:CLA:HAB  | 2.01                     | 0.41              |
| 2:B:339:TRP:HE1   | 14:B:824:CLA:C3B  | 2.32                     | 0.41              |
| 2:B:450:GLY:C     | 2:B:452:PRO:HD3   | 2.41                     | 0.41              |
| 14:B:805:CLA:HHC  | 14:B:807:CLA:OBD  | 2.21                     | 0.41              |
| 1:G:504:ASN:HB2   | 14:G:835:CLA:HED2 | 2.03                     | 0.41              |
| 1:G:697:TRP:HZ3   | 14:G:802:CLA:O1D  | 2.04                     | 0.41              |
| 14:G:832:CLA:O1A  | 14:G:842:CLA:H11  | 2.21                     | 0.41              |
| 14:G:841:CLA:H3A  | 14:G:841:CLA:HBA2 | 1.69                     | 0.41              |
| 2:H:446:VAL:HG22  | 2:H:451:THR:OG1   | 2.21                     | 0.41              |
| 2:H:379:GLN:NE2   | 2:H:596:VAL:HG11  | 2.36                     | 0.41              |
| 14:G:803:CLA:H41  | 2:H:654:TRP:NE1   | 2.36                     | 0.41              |
| 14:H:805:CLA:H72  | 14:H:805:CLA:H151 | 2.03                     | 0.41              |
| 6:F:40:GLN:OE1    | 8:J:40:PRO:HB3    | 2.21                     | 0.41              |
| 11:M:12:LEU:HB3   | 17:M:101:BCR:C21  | 2.51                     | 0.41              |
| 1:Y:455:SER:OG    | 1:Y:456:PHE:N     | 2.53                     | 0.41              |
| 14:Y:802:CLA:H91  | 14:Y:855:CLA:H8   | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Z:154:LEU:O     | 2:Z:157:GLN:N     | 2.41                     | 0.41              |
| 2:Z:67:VAL:HA     | 2:Z:71:GLY:HA3    | 2.02                     | 0.41              |
| 14:Z:828:CLA:CAC  | 17:Z:844:BCR:H402 | 2.50                     | 0.41              |
| 1:A:434:LEU:O     | 1:A:437:ARG:HG2   | 2.21                     | 0.41              |
| 1:A:682:ILE:CD1   | 14:A:840:CLA:CMB  | 2.98                     | 0.41              |
| 17:A:846:BCR:HC8  | 17:A:846:BCR:H311 | 2.02                     | 0.41              |
| 17:A:849:BCR:C23  | 17:A:849:BCR:H403 | 2.47                     | 0.41              |
| 2:B:13:GLN:HB2    | 2:B:13:GLN:HE21   | 1.73                     | 0.41              |
| 2:B:185:SER:O     | 14:B:814:CLA:HBB2 | 2.20                     | 0.41              |
| 2:B:241:HIS:HA    | 2:B:247:GLN:O     | 2.20                     | 0.41              |
| 2:B:46:PHE:CE2    | 2:B:50:PHE:HE2    | 2.39                     | 0.41              |
| 2:B:588:TRP:O     | 2:B:591:ASN:N     | 2.53                     | 0.41              |
| 14:B:802:CLA:H141 | 14:B:802:CLA:H162 | 1.98                     | 0.41              |
| 17:B:847:BCR:H321 | 17:B:847:BCR:HC8  | 2.02                     | 0.41              |
| 1:G:213:ALA:O     | 1:G:217:ILE:HG13  | 2.21                     | 0.41              |
| 1:G:629:GLY:O     | 1:G:631:VAL:HG23  | 2.21                     | 0.41              |
| 1:G:466:ARG:HH22  | 1:G:645:THR:HG21  | 1.85                     | 0.41              |
| 1:G:73:PHE:O      | 1:G:76:HIS:HB2    | 2.21                     | 0.41              |
| 14:G:824:CLA:HAC1 | 17:G:848:BCR:H323 | 2.02                     | 0.41              |
| 2:H:60:VAL:CG1    | 2:H:141:LEU:HD13  | 2.46                     | 0.41              |
| 2:H:738:LYS:O     | 2:H:739:PHE:HB2   | 2.21                     | 0.41              |
| 9:K:69:LEU:HA     | 14:K:103:CLA:HBC2 | 2.01                     | 0.41              |
| 10:L:68:LEU:HD12  | 10:L:77:GLY:HA3   | 2.03                     | 0.41              |
| 4:O:50:ARG:H      | 4:O:54:ASN:HD21   | 1.68                     | 0.41              |
| 4:O:5:GLY:CA      | 4:O:53:GLU:HG2    | 2.51                     | 0.41              |
| 5:P:11:ARG:HB3    | 5:P:14:SER:HB2    | 2.03                     | 0.41              |
| 11:V:3:LEU:HD23   | 11:V:3:LEU:HA     | 1.92                     | 0.41              |
| 1:Y:221:LEU:HB3   | 1:Y:253:TYR:OH    | 2.21                     | 0.41              |
| 1:Y:372:GLN:O     | 1:Y:375:TYR:CE2   | 2.74                     | 0.41              |
| 1:Y:533:THR:O     | 1:Y:537:MET:HG3   | 2.20                     | 0.41              |
| 1:Y:60:THR:OG1    | 1:Y:61:HIS:CD2    | 2.74                     | 0.41              |
| 2:Z:391:ALA:O     | 2:Z:395:ILE:HG13  | 2.20                     | 0.41              |
| 2:Z:672:SER:C     | 2:Z:673:TRP:HD1   | 2.24                     | 0.41              |
| 14:Z:819:CLA:C3D  | 17:Z:841:BCR:H393 | 2.51                     | 0.41              |
| 1:A:615:TRP:O     | 1:A:615:TRP:CD1   | 2.73                     | 0.41              |
| 1:A:700:LEU:O     | 1:A:704:ILE:HG13  | 2.20                     | 0.41              |
| 17:A:848:BCR:H15C | 17:A:848:BCR:H351 | 1.88                     | 0.41              |
| 14:B:813:CLA:H192 | 14:B:828:CLA:H51  | 2.03                     | 0.41              |
| 2:B:458:ILE:HD11  | 17:B:851:BCR:C34  | 2.51                     | 0.41              |
| 1:G:387:TYR:HB3   | 1:G:751:ILE:CD1   | 2.50                     | 0.41              |
| 1:G:545:THR:O     | 1:G:549:THR:OG1   | 2.34                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:603:TYR:CE1    | 1:G:740:ILE:HG13   | 2.56                     | 0.41              |
| 1:G:348:LEU:CB     | 14:G:825:CLA:HBC3  | 2.51                     | 0.41              |
| 14:G:834:CLA:HBA1  | 14:G:834:CLA:H3A   | 1.79                     | 0.41              |
| 17:G:849:BCR:C38   | 17:G:849:BCR:C23   | 2.97                     | 0.41              |
| 17:G:849:BCR:C27   | 17:G:849:BCR:H393  | 2.51                     | 0.41              |
| 2:H:577:SER:OG     | 2:H:578:ALA:N      | 2.53                     | 0.41              |
| 9:T:66:GLY:HA2     | 9:T:69:LEU:CD2     | 2.50                     | 0.41              |
| 1:Y:128:GLY:O      | 1:Y:130:VAL:N      | 2.53                     | 0.41              |
| 1:Y:153:THR:HG21   | 1:Y:236:ILE:CD1    | 2.51                     | 0.41              |
| 1:Y:356:LEU:CD1    | 1:Y:360:LEU:HG     | 2.50                     | 0.41              |
| 14:Y:802:CLA:H93   | 14:Z:839:CLA:CBB   | 2.51                     | 0.41              |
| 14:Y:828:CLA:H193  | 14:Y:828:CLA:H161  | 1.89                     | 0.41              |
| 2:Z:86:ILE:CD1     | 2:Z:108:ALA:HB2    | 2.51                     | 0.41              |
| 2:Z:425:LEU:HD21   | 14:Z:837:CLA:C2B   | 2.50                     | 0.41              |
| 14:Z:838:CLA:H71   | 14:Z:838:CLA:H111  | 1.97                     | 0.41              |
| 1:A:407:GLY:O      | 1:A:410:ALA:HB3    | 2.20                     | 0.41              |
| 14:A:818:CLA:C6    | 14:A:835:CLA:HMA2  | 2.51                     | 0.41              |
| 2:B:353:GLN:O      | 2:B:356:TYR:CE1    | 2.74                     | 0.41              |
| 2:B:55:ILE:HD12    | 14:B:805:CLA:CBB   | 2.51                     | 0.41              |
| 2:B:254:LEU:HD11   | 14:B:815:CLA:HAC1  | 2.03                     | 0.41              |
| 14:B:834:CLA:HBA2  | 14:B:835:CLA:HMB3  | 2.02                     | 0.41              |
| 17:F:201:BCR:H403  | 17:F:201:BCR:H24C  | 1.85                     | 0.41              |
| 1:G:649:TRP:CE2    | 13:G:801:CL0:H56   | 2.55                     | 0.41              |
| 1:G:681:PHE:CZ     | 14:G:802:CLA:HMB1  | 2.56                     | 0.41              |
| 14:G:839:CLA:O1A   | 14:Q:201:CLA:HED2  | 2.20                     | 0.41              |
| 14:H:805:CLA:H43   | 19:H:846:LMG:H321  | 2.03                     | 0.41              |
| 14:L:206:CLA:HAC2  | 17:L:208:BCR:C38   | 2.51                     | 0.41              |
| 6:Q:108:LYS:HA     | 6:Q:108:LYS:HD2    | 1.86                     | 0.41              |
| 14:U:1006:CLA:HED1 | 17:U:1007:BCR:C6   | 2.50                     | 0.41              |
| 14:H:834:CLA:H41   | 14:W:1701:CLA:HED2 | 2.02                     | 0.41              |
| 1:Y:111:LYS:HD2    | 1:Y:130:VAL:O      | 2.20                     | 0.41              |
| 14:Y:810:CLA:H2A   | 14:Y:810:CLA:O2D   | 2.21                     | 0.41              |
| 14:Y:828:CLA:C2C   | 17:Y:851:BCR:HC42  | 2.50                     | 0.41              |
| 14:Y:833:CLA:H93   | 14:Z:838:CLA:H52   | 2.02                     | 0.41              |
| 2:Z:566:ASP:HB2    | 2:Z:573:THR:HG21   | 2.02                     | 0.41              |
| 2:Z:680:LEU:O      | 2:Z:683:THR:CG2    | 2.69                     | 0.41              |
| 2:Z:663:TRP:CE3    | 14:Z:802:CLA:HMA1  | 2.55                     | 0.41              |
| 2:Z:166:TRP:HH2    | 14:Z:809:CLA:HMB3  | 1.86                     | 0.41              |
| 14:A:818:CLA:HBB1  | 14:A:818:CLA:HMB1  | 2.02                     | 0.41              |
| 14:A:830:CLA:HMB1  | 14:A:830:CLA:HBB1  | 2.03                     | 0.41              |
| 1:A:432:ARG:NE     | 14:A:831:CLA:OBD   | 2.52                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:A:845:BCR:H351 | 17:A:845:BCR:H15C | 1.76                     | 0.41              |
| 2:B:186:SER:O     | 2:B:190:ALA:N     | 2.41                     | 0.41              |
| 2:B:21:TRP:HH2    | 15:B:842:PQN:H261 | 1.86                     | 0.41              |
| 2:B:369:THR:O     | 2:B:372:ALA:HB3   | 2.21                     | 0.41              |
| 4:D:9:LEU:HD12    | 4:D:48:VAL:HG21   | 2.02                     | 0.41              |
| 1:G:100:TYR:OH    | 1:G:152:ILE:O     | 2.28                     | 0.41              |
| 1:G:289:THR:HA    | 1:G:382:TYR:CZ    | 2.56                     | 0.41              |
| 1:G:53:ALA:HB1    | 18:G:851:LHG:O10  | 2.21                     | 0.41              |
| 1:G:398:MET:HB3   | 1:G:606:ILE:HG23  | 2.03                     | 0.41              |
| 14:G:802:CLA:HBA2 | 2:H:430:LEU:HD13  | 2.03                     | 0.41              |
| 14:G:818:CLA:O1D  | 14:G:819:CLA:HMA1 | 2.20                     | 0.41              |
| 14:G:821:CLA:H8   | 17:G:848:BCR:C10  | 2.51                     | 0.41              |
| 2:H:321:PRO:HG2   | 2:H:409:ASN:HA    | 2.03                     | 0.41              |
| 14:H:835:CLA:H171 | 14:Q:201:CLA:HBC1 | 2.03                     | 0.41              |
| 14:H:838:CLA:HMC1 | 14:H:838:CLA:HBC2 | 2.01                     | 0.41              |
| 10:L:11:ASP:OD2   | 10:L:14:VAL:HB    | 2.21                     | 0.41              |
| 10:L:35:PRO:O     | 10:L:46:ARG:HG2   | 2.21                     | 0.41              |
| 6:Q:48:LEU:HD23   | 6:Q:48:LEU:HA     | 1.97                     | 0.41              |
| 1:Y:120:ILE:O     | 1:Y:122:GLY:N     | 2.54                     | 0.41              |
| 1:Y:308:PHE:CE1   | 14:Y:821:CLA:HAB  | 2.56                     | 0.41              |
| 1:Y:35:ASP:OD1    | 1:Y:37:THR:OG1    | 2.37                     | 0.41              |
| 1:Y:319:TRP:HZ3   | 14:Y:812:CLA:HMA1 | 1.86                     | 0.41              |
| 14:Y:809:CLA:HBC2 | 14:Y:828:CLA:H151 | 2.02                     | 0.41              |
| 2:Z:67:VAL:CG1    | 2:Z:123:TRP:HZ3   | 2.24                     | 0.41              |
| 2:Z:509:SER:CB    | 2:Z:511:THR:HG22  | 2.50                     | 0.41              |
| 14:Z:823:CLA:HAA2 | 14:Z:824:CLA:OBD  | 2.21                     | 0.41              |
| 1:A:380:TYR:HA    | 1:A:381:PRO:HD3   | 1.96                     | 0.40              |
| 17:A:848:BCR:H331 | 17:A:848:BCR:C8   | 2.50                     | 0.40              |
| 2:B:500:LEU:N     | 2:B:501:PRO:CD    | 2.84                     | 0.40              |
| 14:B:809:CLA:H92  | 14:B:829:CLA:H202 | 2.02                     | 0.40              |
| 17:B:846:BCR:H24C | 17:B:846:BCR:H371 | 1.81                     | 0.40              |
| 17:B:848:BCR:H24C | 17:B:848:BCR:H371 | 1.87                     | 0.40              |
| 1:G:650:LEU:HD23  | 2:H:638:ILE:CD1   | 2.51                     | 0.40              |
| 1:G:75:ALA:HB1    | 14:G:805:CLA:HBB1 | 2.03                     | 0.40              |
| 2:H:470:HIS:HA    | 2:H:481:LEU:HD12  | 2.01                     | 0.40              |
| 1:G:698:GLN:HB3   | 2:H:552:LEU:HD22  | 2.02                     | 0.40              |
| 2:H:647:ASN:ND2   | 2:H:649:LEU:H     | 2.08                     | 0.40              |
| 14:H:802:CLA:HBA2 | 14:H:802:CLA:H3A  | 1.63                     | 0.40              |
| 14:H:807:CLA:H142 | 14:H:808:CLA:H41  | 2.02                     | 0.40              |
| 8:J:21:ILE:O      | 8:J:25:ILE:HG13   | 2.21                     | 0.40              |
| 14:L:207:CLA:H3A  | 14:L:207:CLA:HBA2 | 1.91                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:G:583:ARG:CG     | 3:N:48:VAL:HG13   | 2.49                     | 0.40              |
| 2:H:704:VAL:HG11   | 3:N:76:MET:HE2    | 2.03                     | 0.40              |
| 6:Q:113:GLY:O      | 6:Q:116:TRP:HD1   | 2.03                     | 0.40              |
| 14:U:1006:CLA:HAA2 | 14:U:1006:CLA:HBD | 2.02                     | 0.40              |
| 11:V:17:LEU:HD23   | 11:V:17:LEU:HA    | 1.91                     | 0.40              |
| 1:Y:184:ALA:HA     | 1:Y:185:PRO:HD3   | 1.94                     | 0.40              |
| 1:Y:461:HIS:CE1    | 14:Y:834:CLA:NA   | 2.89                     | 0.40              |
| 1:Y:647:ASN:OD1    | 2:Z:641:TYR:O     | 2.39                     | 0.40              |
| 2:Z:375:TYR:OH     | 14:Z:835:CLA:HMC3 | 2.21                     | 0.40              |
| 14:Z:808:CLA:H102  | 14:Z:825:CLA:H172 | 2.04                     | 0.40              |
| 1:A:682:ILE:HG23   | 1:A:734:HIS:CD2   | 2.56                     | 0.40              |
| 14:A:822:CLA:HBB1  | 14:A:822:CLA:HMB1 | 2.03                     | 0.40              |
| 15:A:843:PQN:H171  | 17:F:201:BCR:H382 | 2.03                     | 0.40              |
| 2:B:198:ILE:CG1    | 2:B:199:PRO:HD3   | 2.46                     | 0.40              |
| 2:B:497:ASN:O      | 2:B:499:TRP:CD2   | 2.74                     | 0.40              |
| 2:B:588:TRP:O      | 2:B:592:THR:HG23  | 2.21                     | 0.40              |
| 2:B:596:VAL:HG22   | 14:B:837:CLA:HBB2 | 2.03                     | 0.40              |
| 2:B:443:ASN:HB3    | 2:B:621:TYR:HB3   | 2.03                     | 0.40              |
| 14:B:827:CLA:H162  | 14:B:827:CLA:H203 | 1.86                     | 0.40              |
| 1:G:224:ASN:HB3    | 1:G:294:LEU:HD13  | 2.03                     | 0.40              |
| 1:G:738:GLY:O      | 1:G:742:THR:OG1   | 2.38                     | 0.40              |
| 1:G:744:TRP:HA     | 14:G:828:CLA:HBB1 | 2.02                     | 0.40              |
| 1:G:85:ILE:HD13    | 14:G:809:CLA:H201 | 2.02                     | 0.40              |
| 1:G:375:TYR:CE1    | 14:G:836:CLA:HBC3 | 2.57                     | 0.40              |
| 1:G:704:ILE:HD13   | 14:G:839:CLA:CMD  | 2.51                     | 0.40              |
| 14:G:839:CLA:H72   | 14:G:839:CLA:H111 | 1.96                     | 0.40              |
| 1:G:334:GLY:HA3    | 18:G:852:LHG:O4   | 2.21                     | 0.40              |
| 2:H:304:MET:HB3    | 2:H:322:HIS:O     | 2.21                     | 0.40              |
| 2:H:586:MET:HG2    | 2:H:716:LEU:HD11  | 2.04                     | 0.40              |
| 14:H:836:CLA:CBB   | 14:H:836:CLA:HHC  | 2.49                     | 0.40              |
| 14:H:837:CLA:HBD   | 14:H:837:CLA:HAA1 | 2.02                     | 0.40              |
| 6:Q:61:GLY:O       | 8:S:38:PHE:HB2    | 2.20                     | 0.40              |
| 12:X:13:THR:O      | 12:X:16:ALA:HB3   | 2.21                     | 0.40              |
| 1:Y:221:LEU:HD21   | 1:Y:295:SER:HA    | 2.03                     | 0.40              |
| 1:Y:25:PHE:O       | 1:Y:28:TRP:HB2    | 2.20                     | 0.40              |
| 1:Y:538:VAL:O      | 1:Y:541:ILE:HB    | 2.21                     | 0.40              |
| 1:Y:599:LEU:HD23   | 1:Y:599:LEU:HA    | 1.94                     | 0.40              |
| 14:Z:825:CLA:HBC3  | 19:Z:847:LMG:H422 | 2.02                     | 0.40              |
| 14:Z:830:CLA:OBD   | 14:Z:830:CLA:H93  | 2.21                     | 0.40              |
| 1:A:310:ILE:HD12   | 9:K:68:LEU:HD12   | 2.03                     | 0.40              |
| 1:A:553:LEU:HD21   | 1:A:598:GLY:HA3   | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:A:832:CLA:HBC2 | 14:A:832:CLA:HMC1  | 2.02                     | 0.40              |
| 17:A:849:BCR:H24C | 17:A:849:BCR:H371  | 1.91                     | 0.40              |
| 2:B:178:LEU:HD21  | 14:B:819:CLA:C3B   | 2.50                     | 0.40              |
| 14:B:808:CLA:HMB3 | 14:B:809:CLA:HHB   | 2.03                     | 0.40              |
| 14:B:825:CLA:H112 | 17:B:847:BCR:H312  | 2.04                     | 0.40              |
| 14:B:840:CLA:H201 | 7:I:20:TRP:HA      | 2.02                     | 0.40              |
| 6:F:76:TRP:O      | 6:F:80:VAL:HG13    | 2.22                     | 0.40              |
| 1:G:81:ALA:HA     | 1:G:169:ALA:HA     | 2.03                     | 0.40              |
| 1:G:74:SER:OG     | 1:G:180:TYR:HB2    | 2.21                     | 0.40              |
| 1:G:270:PHE:HD1   | 14:T:101:CLA:HMD2  | 1.87                     | 0.40              |
| 14:G:827:CLA:H143 | 14:G:827:CLA:H112  | 1.72                     | 0.40              |
| 14:G:830:CLA:HBA2 | 14:G:830:CLA:H3A   | 1.82                     | 0.40              |
| 2:H:220:GLY:O     | 2:H:222:ALA:N      | 2.54                     | 0.40              |
| 2:H:240:SER:OG    | 2:H:240:SER:O      | 2.33                     | 0.40              |
| 14:G:803:CLA:HAA1 | 2:H:661:LEU:HA     | 2.02                     | 0.40              |
| 1:G:121:VAL:CG1   | 14:H:830:CLA:HMD1  | 2.38                     | 0.40              |
| 9:K:22:CYS:SG     | 9:K:22:CYS:O       | 2.79                     | 0.40              |
| 3:N:23:ASP:OD1    | 3:N:43:ARG:NH2     | 2.55                     | 0.40              |
| 15:G:844:PQN:H193 | 17:Q:202:BCR:H382  | 2.02                     | 0.40              |
| 14:U:1002:CLA:C1B | 14:U:1003:CLA:HED1 | 2.52                     | 0.40              |
| 1:Y:529:ILE:HD13  | 1:Y:617:MET:SD     | 2.61                     | 0.40              |
| 1:Y:686:SER:HB3   | 1:Y:731:GLY:O      | 2.21                     | 0.40              |
| 14:Y:818:CLA:C2   | 14:Y:818:CLA:O1A   | 2.69                     | 0.40              |
| 1:Y:355:GLN:HG3   | 14:Y:825:CLA:H152  | 2.03                     | 0.40              |
| 14:Y:829:CLA:C2D  | 14:Y:829:CLA:H51   | 2.51                     | 0.40              |
| 2:Z:162:PRO:HG2   | 2:Z:167:PHE:CZ     | 2.57                     | 0.40              |
| 14:Z:823:CLA:HBA2 | 14:Z:823:CLA:H3A   | 1.89                     | 0.40              |
| 2:Z:89:ALA:O      | 2:Z:90:ILE:HG13    | 2.22                     | 0.40              |
| 1:A:100:TYR:CE1   | 1:A:104:LEU:HD21   | 2.57                     | 0.40              |
| 1:A:213:ALA:O     | 1:A:217:ILE:N      | 2.40                     | 0.40              |
| 1:A:397:HIS:O     | 1:A:401:GLY:N      | 2.35                     | 0.40              |
| 14:A:813:CLA:HBD  | 14:A:813:CLA:HAA2  | 2.03                     | 0.40              |
| 17:A:846:BCR:H15C | 17:A:846:BCR:H351  | 1.76                     | 0.40              |
| 2:B:129:ARG:HA    | 2:B:129:ARG:HD3    | 1.91                     | 0.40              |
| 2:B:275:HIS:CE1   | 2:B:279:ILE:HG13   | 2.57                     | 0.40              |
| 2:B:344:LEU:HD12  | 2:B:344:LEU:HA     | 1.90                     | 0.40              |
| 2:B:396:PHE:HD1   | 2:B:400:ASP:HB2    | 1.84                     | 0.40              |
| 14:B:803:CLA:H62  | 14:B:803:CLA:H41   | 1.85                     | 0.40              |
| 14:B:819:CLA:HMD1 | 14:B:821:CLA:HAB   | 2.03                     | 0.40              |
| 1:G:391:LEU:O     | 1:G:395:THR:HG23   | 2.21                     | 0.40              |
| 1:G:517:VAL:HG13  | 1:G:527:MET:HB3    | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:138:GLN:OE1   | 1:G:752:ILE:HG23   | 2.21                     | 0.40              |
| 14:G:821:CLA:H121 | 14:G:821:CLA:H162  | 1.94                     | 0.40              |
| 17:G:849:BCR:H371 | 17:G:849:BCR:H24C  | 1.76                     | 0.40              |
| 2:H:682:GLU:HG2   | 3:N:80:TYR:HE1     | 1.86                     | 0.40              |
| 2:H:187:LEU:HD21  | 17:H:840:BCR:H331  | 2.03                     | 0.40              |
| 4:O:106:ASN:ND2   | 4:O:107:LYS:O      | 2.54                     | 0.40              |
| 14:S:1101:CLA:C4B | 17:S:1104:BCR:H281 | 2.52                     | 0.40              |
| 10:U:111:LEU:O    | 10:U:117:TRP:HE3   | 2.04                     | 0.40              |
| 14:Y:803:CLA:O2A  | 14:Y:841:CLA:H43   | 2.21                     | 0.40              |
| 14:Y:830:CLA:H62  | 14:Y:830:CLA:H41   | 1.82                     | 0.40              |
| 14:Z:809:CLA:CMC  | 14:Z:812:CLA:H192  | 2.52                     | 0.40              |
| 1:A:216:GLN:HA    | 1:A:220:SER:HB3    | 2.03                     | 0.40              |
| 1:A:455:SER:HB2   | 1:A:541:ILE:HG12   | 2.04                     | 0.40              |
| 1:A:409:ALA:CB    | 1:A:553:LEU:HB3    | 2.51                     | 0.40              |
| 1:A:647:ASN:HD22  | 2:B:657:LEU:CD1    | 2.34                     | 0.40              |
| 1:A:695:GLY:O     | 1:A:699:GLU:HG3    | 2.22                     | 0.40              |
| 1:A:577:PRO:HA    | 1:A:728:ARG:NH1    | 2.36                     | 0.40              |
| 14:A:817:CLA:HBA2 | 14:A:817:CLA:H3A   | 1.95                     | 0.40              |
| 14:A:833:CLA:HAB  | 14:L:201:CLA:CHB   | 2.45                     | 0.40              |
| 2:B:255:THR:OG1   | 2:B:256:PHE:N      | 2.52                     | 0.40              |
| 2:B:703:PRO:HB3   | 14:B:840:CLA:C1C   | 2.52                     | 0.40              |
| 14:B:829:CLA:H142 | 19:B:849:LMG:H202  | 2.03                     | 0.40              |
| 17:B:845:BCR:H371 | 17:B:845:BCR:H24C  | 1.86                     | 0.40              |
| 17:B:851:BCR:H351 | 17:B:851:BCR:H15C  | 1.76                     | 0.40              |
| 3:C:61:PHE:CZ     | 3:C:65:ARG:NH1     | 2.89                     | 0.40              |
| 6:F:24:THR:HG22   | 6:F:24:THR:O       | 2.21                     | 0.40              |
| 1:G:221:LEU:N     | 1:G:222:PRO:CD     | 2.85                     | 0.40              |
| 1:G:675:LEU:HD23  | 1:G:675:LEU:HA     | 1.97                     | 0.40              |
| 14:G:810:CLA:HBB2 | 14:G:813:CLA:HED2  | 2.03                     | 0.40              |
| 14:G:834:CLA:HMD2 | 14:G:835:CLA:CAB   | 2.47                     | 0.40              |
| 17:G:847:BCR:H351 | 17:G:847:BCR:H15C  | 1.74                     | 0.40              |
| 2:H:215:MET:HE1   | 2:H:220:GLY:HA3    | 2.04                     | 0.40              |
| 2:H:38:GLU:O      | 2:H:41:LEU:HB3     | 2.22                     | 0.40              |
| 2:H:413:ARG:O     | 2:H:416:GLN:HB2    | 2.22                     | 0.40              |
| 2:H:626:LEU:O     | 2:H:631:TRP:N      | 2.39                     | 0.40              |
| 10:L:63:VAL:O     | 10:L:69:ARG:HB3    | 2.22                     | 0.40              |
| 1:Y:189:TRP:CZ2   | 14:Y:810:CLA:HMA1  | 2.57                     | 0.40              |
| 14:Y:855:CLA:CAB  | 2:Z:665:THR:CG2    | 2.99                     | 0.40              |
| 2:Z:340:HIS:CG    | 14:Z:822:CLA:HAA1  | 2.56                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



| Atom-1         | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|--------------------|--------------------------|-------------------|
| 5:c:28:GLN:OE1 | 6:d:1:ASP:N[2_545] | 2.13                     | 0.07              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 737/755 (98%)  | 634 (86%) | 89 (12%) | 14 (2%)  | 8           | 28  |
| 1   | G     | 737/755 (98%)  | 634 (86%) | 86 (12%) | 17 (2%)  | 6           | 23  |
| 1   | Y     | 737/755 (98%)  | 627 (85%) | 98 (13%) | 12 (2%)  | 9           | 32  |
| 2   | B     | 737/741 (100%) | 639 (87%) | 84 (11%) | 14 (2%)  | 8           | 28  |
| 2   | H     | 737/741 (100%) | 658 (89%) | 69 (9%)  | 10 (1%)  | 11          | 36  |
| 2   | Z     | 737/741 (100%) | 642 (87%) | 86 (12%) | 9 (1%)   | 13          | 40  |
| 3   | C     | 78/81 (96%)    | 72 (92%)  | 4 (5%)   | 2 (3%)   | 5           | 20  |
| 3   | N     | 78/81 (96%)    | 69 (88%)  | 8 (10%)  | 1 (1%)   | 12          | 37  |
| 3   | a     | 78/81 (96%)    | 64 (82%)  | 12 (15%) | 2 (3%)   | 5           | 20  |
| 4   | D     | 136/139 (98%)  | 119 (88%) | 14 (10%) | 3 (2%)   | 6           | 24  |
| 4   | O     | 136/139 (98%)  | 122 (90%) | 11 (8%)  | 3 (2%)   | 6           | 24  |
| 4   | b     | 136/139 (98%)  | 117 (86%) | 15 (11%) | 4 (3%)   | 4           | 18  |
| 5   | E     | 67/76 (88%)    | 58 (87%)  | 6 (9%)   | 3 (4%)   | 2           | 9   |
| 5   | P     | 67/76 (88%)    | 56 (84%)  | 6 (9%)   | 5 (8%)   | 1           | 2   |
| 5   | c     | 67/76 (88%)    | 56 (84%)  | 8 (12%)  | 3 (4%)   | 2           | 9   |
| 6   | F     | 139/164 (85%)  | 126 (91%) | 12 (9%)  | 1 (1%)   | 22          | 54  |
| 6   | Q     | 139/164 (85%)  | 124 (89%) | 14 (10%) | 1 (1%)   | 22          | 54  |
| 6   | d     | 139/164 (85%)  | 118 (85%) | 18 (13%) | 3 (2%)   | 6           | 24  |
| 7   | I     | 36/38 (95%)    | 30 (83%)  | 6 (17%)  | 0        | 100         | 100 |
| 7   | R     | 36/38 (95%)    | 31 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 7   | e     | 36/38 (95%)    | 31 (86%)  | 4 (11%)  | 1 (3%)   | 5           | 19  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 8   | J     | 39/41 (95%)     | 34 (87%)   | 5 (13%)   | 0        | 100         | 100 |
| 8   | S     | 39/41 (95%)     | 34 (87%)   | 5 (13%)   | 0        | 100         | 100 |
| 8   | f     | 39/41 (95%)     | 38 (97%)   | 0         | 1 (3%)   | 5           | 20  |
| 9   | K     | 40/83 (48%)     | 31 (78%)   | 7 (18%)   | 2 (5%)   | 2           | 7   |
| 9   | T     | 40/83 (48%)     | 33 (82%)   | 4 (10%)   | 3 (8%)   | 1           | 2   |
| 9   | g     | 40/83 (48%)     | 30 (75%)   | 8 (20%)   | 2 (5%)   | 2           | 7   |
| 10  | L     | 149/155 (96%)   | 124 (83%)  | 22 (15%)  | 3 (2%)   | 7           | 27  |
| 10  | U     | 149/155 (96%)   | 138 (93%)  | 11 (7%)   | 0        | 100         | 100 |
| 10  | h     | 149/155 (96%)   | 129 (87%)  | 17 (11%)  | 3 (2%)   | 7           | 27  |
| 11  | M     | 28/31 (90%)     | 26 (93%)   | 2 (7%)    | 0        | 100         | 100 |
| 11  | V     | 28/31 (90%)     | 26 (93%)   | 2 (7%)    | 0        | 100         | 100 |
| 11  | i     | 28/31 (90%)     | 28 (100%)  | 0         | 0        | 100         | 100 |
| 12  | W     | 24/39 (62%)     | 23 (96%)   | 1 (4%)    | 0        | 100         | 100 |
| 12  | X     | 24/39 (62%)     | 24 (100%)  | 0         | 0        | 100         | 100 |
| 12  | j     | 24/39 (62%)     | 23 (96%)   | 1 (4%)    | 0        | 100         | 100 |
| All | All   | 6630/7029 (94%) | 5768 (87%) | 740 (11%) | 122 (2%) | 8           | 29  |

All (122) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 121 | VAL  |
| 4   | D     | 95  | HIS  |
| 5   | E     | 55  | VAL  |
| 1   | G     | 320 | GLY  |
| 1   | G     | 508 | THR  |
| 2   | H     | 481 | LEU  |
| 9   | K     | 41  | PRO  |
| 3   | N     | 61  | PHE  |
| 9   | T     | 21  | LEU  |
| 9   | T     | 41  | PRO  |
| 1   | Y     | 121 | VAL  |
| 1   | Y     | 250 | ALA  |
| 1   | Y     | 261 | PHE  |
| 1   | Y     | 320 | GLY  |
| 2   | Z     | 247 | GLN  |
| 3   | a     | 61  | PHE  |
| 5   | c     | 55  | VAL  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | g     | 41  | PRO  |
| 1   | A     | 115 | GLN  |
| 1   | A     | 235 | ASP  |
| 1   | A     | 250 | ALA  |
| 1   | A     | 283 | GLY  |
| 2   | B     | 96  | GLY  |
| 2   | B     | 169 | ASN  |
| 2   | B     | 236 | PRO  |
| 2   | B     | 247 | GLN  |
| 2   | B     | 295 | GLY  |
| 5   | E     | 54  | GLY  |
| 6   | F     | 91  | SER  |
| 1   | G     | 182 | LYS  |
| 1   | G     | 232 | ALA  |
| 1   | G     | 428 | ASN  |
| 1   | G     | 526 | MET  |
| 2   | H     | 474 | LEU  |
| 2   | H     | 518 | ILE  |
| 10  | L     | 108 | SER  |
| 4   | O     | 44  | ALA  |
| 5   | P     | 3   | ARG  |
| 6   | Q     | 63  | PHE  |
| 9   | T     | 36  | SER  |
| 1   | Y     | 129 | ASP  |
| 1   | Y     | 152 | ILE  |
| 1   | Y     | 249 | MET  |
| 1   | Y     | 590 | SER  |
| 4   | b     | 132 | GLY  |
| 5   | c     | 3   | ARG  |
| 1   | A     | 13  | ARG  |
| 1   | A     | 234 | LYS  |
| 1   | A     | 526 | MET  |
| 2   | B     | 29  | ASP  |
| 2   | B     | 234 | GLN  |
| 2   | B     | 480 | LEU  |
| 2   | B     | 699 | TRP  |
| 3   | C     | 14  | THR  |
| 3   | C     | 61  | PHE  |
| 1   | G     | 115 | GLN  |
| 1   | G     | 410 | ALA  |
| 1   | G     | 427 | ASN  |
| 1   | G     | 630 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 723 | SER  |
| 2   | H     | 169 | ASN  |
| 2   | H     | 221 | LEU  |
| 2   | H     | 480 | LEU  |
| 2   | H     | 517 | THR  |
| 10  | L     | 106 | SER  |
| 5   | P     | 46  | THR  |
| 5   | P     | 55  | VAL  |
| 2   | Z     | 29  | ASP  |
| 2   | Z     | 234 | GLN  |
| 2   | Z     | 255 | THR  |
| 2   | Z     | 427 | TRP  |
| 2   | Z     | 565 | CYS  |
| 3   | a     | 23  | ASP  |
| 4   | b     | 9   | LEU  |
| 6   | d     | 63  | PHE  |
| 7   | e     | 6   | ALA  |
| 1   | A     | 114 | ALA  |
| 1   | A     | 260 | PHE  |
| 2   | B     | 216 | PRO  |
| 4   | D     | 36  | GLU  |
| 1   | G     | 317 | THR  |
| 1   | G     | 401 | GLY  |
| 1   | G     | 750 | ARG  |
| 2   | H     | 165 | SER  |
| 2   | H     | 438 | GLY  |
| 4   | O     | 31  | TRP  |
| 1   | Y     | 115 | GLN  |
| 1   | Y     | 621 | VAL  |
| 2   | Z     | 374 | LEU  |
| 5   | c     | 54  | GLY  |
| 9   | g     | 75  | SER  |
| 2   | B     | 265 | GLU  |
| 2   | B     | 409 | ASN  |
| 5   | E     | 46  | THR  |
| 1   | G     | 605 | CYS  |
| 1   | Y     | 258 | TRP  |
| 1   | Y     | 544 | PHE  |
| 2   | Z     | 78  | GLN  |
| 2   | Z     | 93  | PRO  |
| 10  | h     | 20  | PRO  |
| 10  | h     | 67  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 436 | HIS  |
| 2   | B     | 707 | SER  |
| 4   | O     | 95  | HIS  |
| 4   | b     | 44  | ALA  |
| 4   | b     | 95  | HIS  |
| 6   | d     | 49  | PRO  |
| 1   | A     | 503 | PRO  |
| 1   | A     | 717 | ILE  |
| 1   | G     | 121 | VAL  |
| 1   | G     | 500 | GLY  |
| 4   | D     | 132 | GLY  |
| 2   | H     | 180 | GLY  |
| 9   | K     | 56  | LEU  |
| 6   | d     | 53  | VAL  |
| 8   | f     | 24  | GLY  |
| 10  | h     | 55  | GLY  |
| 2   | B     | 708 | ILE  |
| 10  | L     | 151 | GLY  |
| 5   | P     | 35  | PRO  |
| 1   | A     | 310 | ILE  |
| 5   | P     | 68  | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 590/603 (98%)  | 574 (97%) | 16 (3%)  | 44          | 77 |
| 1   | G     | 590/603 (98%)  | 575 (98%) | 15 (2%)  | 47          | 78 |
| 1   | Y     | 590/603 (98%)  | 572 (97%) | 18 (3%)  | 40          | 74 |
| 2   | B     | 597/598 (100%) | 575 (96%) | 22 (4%)  | 34          | 68 |
| 2   | H     | 597/598 (100%) | 577 (97%) | 20 (3%)  | 37          | 71 |
| 2   | Z     | 597/598 (100%) | 573 (96%) | 24 (4%)  | 31          | 65 |
| 3   | C     | 67/68 (98%)    | 64 (96%)  | 3 (4%)   | 27          | 61 |
| 3   | N     | 67/68 (98%)    | 65 (97%)  | 2 (3%)   | 41          | 75 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 3   | a     | 67/68 (98%)     | 65 (97%)   | 2 (3%)   | 41          | 75  |
| 4   | D     | 115/116 (99%)   | 110 (96%)  | 5 (4%)   | 29          | 62  |
| 4   | O     | 115/116 (99%)   | 110 (96%)  | 5 (4%)   | 29          | 62  |
| 4   | b     | 115/116 (99%)   | 111 (96%)  | 4 (4%)   | 36          | 70  |
| 5   | E     | 59/65 (91%)     | 56 (95%)   | 3 (5%)   | 24          | 56  |
| 5   | P     | 59/65 (91%)     | 57 (97%)   | 2 (3%)   | 37          | 71  |
| 5   | c     | 59/65 (91%)     | 58 (98%)   | 1 (2%)   | 60          | 86  |
| 6   | F     | 109/128 (85%)   | 106 (97%)  | 3 (3%)   | 43          | 76  |
| 6   | Q     | 109/128 (85%)   | 106 (97%)  | 3 (3%)   | 43          | 76  |
| 6   | d     | 109/128 (85%)   | 108 (99%)  | 1 (1%)   | 78          | 93  |
| 7   | I     | 32/32 (100%)    | 32 (100%)  | 0        | 100         | 100 |
| 7   | R     | 32/32 (100%)    | 32 (100%)  | 0        | 100         | 100 |
| 7   | e     | 32/32 (100%)    | 31 (97%)   | 1 (3%)   | 40          | 74  |
| 8   | J     | 36/36 (100%)    | 36 (100%)  | 0        | 100         | 100 |
| 8   | S     | 36/36 (100%)    | 35 (97%)   | 1 (3%)   | 43          | 76  |
| 8   | f     | 36/36 (100%)    | 36 (100%)  | 0        | 100         | 100 |
| 9   | K     | 33/61 (54%)     | 32 (97%)   | 1 (3%)   | 41          | 75  |
| 9   | T     | 33/61 (54%)     | 31 (94%)   | 2 (6%)   | 18          | 48  |
| 9   | g     | 33/61 (54%)     | 30 (91%)   | 3 (9%)   | 9           | 28  |
| 10  | L     | 117/120 (98%)   | 112 (96%)  | 5 (4%)   | 29          | 62  |
| 10  | U     | 117/120 (98%)   | 113 (97%)  | 4 (3%)   | 37          | 71  |
| 10  | h     | 117/120 (98%)   | 109 (93%)  | 8 (7%)   | 16          | 42  |
| 11  | M     | 25/26 (96%)     | 25 (100%)  | 0        | 100         | 100 |
| 11  | V     | 25/26 (96%)     | 24 (96%)   | 1 (4%)   | 31          | 65  |
| 11  | i     | 25/26 (96%)     | 25 (100%)  | 0        | 100         | 100 |
| 12  | W     | 20/31 (64%)     | 20 (100%)  | 0        | 100         | 100 |
| 12  | X     | 20/31 (64%)     | 19 (95%)   | 1 (5%)   | 24          | 57  |
| 12  | j     | 20/31 (64%)     | 19 (95%)   | 1 (5%)   | 24          | 57  |
| All | All   | 5400/5652 (96%) | 5223 (97%) | 177 (3%) | 38          | 72  |

All (177) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 34  | PHE  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 59  | ASP  |
| 1   | A     | 84  | PHE  |
| 1   | A     | 106 | ASP  |
| 1   | A     | 209 | SER  |
| 1   | A     | 253 | TYR  |
| 1   | A     | 281 | PHE  |
| 1   | A     | 324 | SER  |
| 1   | A     | 375 | TYR  |
| 1   | A     | 468 | PHE  |
| 1   | A     | 510 | SER  |
| 1   | A     | 605 | CYS  |
| 1   | A     | 607 | SER  |
| 1   | A     | 625 | VAL  |
| 1   | A     | 661 | VAL  |
| 2   | B     | 3   | LYS  |
| 2   | B     | 4   | PHE  |
| 2   | B     | 18  | ARG  |
| 2   | B     | 112 | VAL  |
| 2   | B     | 159 | LYS  |
| 2   | B     | 165 | SER  |
| 2   | B     | 213 | SER  |
| 2   | B     | 256 | PHE  |
| 2   | B     | 271 | ASP  |
| 2   | B     | 318 | PHE  |
| 2   | B     | 340 | HIS  |
| 2   | B     | 357 | SER  |
| 2   | B     | 396 | PHE  |
| 2   | B     | 419 | GLU  |
| 2   | B     | 489 | SER  |
| 2   | B     | 494 | ASN  |
| 2   | B     | 522 | ASP  |
| 2   | B     | 551 | LYS  |
| 2   | B     | 574 | CYS  |
| 2   | B     | 583 | TYR  |
| 2   | B     | 589 | MET  |
| 2   | B     | 647 | ASN  |
| 3   | C     | 9   | THR  |
| 3   | C     | 50  | CYS  |
| 3   | C     | 61  | PHE  |
| 4   | D     | 13  | SER  |
| 4   | D     | 48  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 54  | ASN  |
| 4   | D     | 118 | SER  |
| 4   | D     | 136 | TYR  |
| 5   | E     | 22  | THR  |
| 5   | E     | 59  | ASN  |
| 5   | E     | 62  | LEU  |
| 6   | F     | 40  | GLN  |
| 6   | F     | 50  | HIS  |
| 6   | F     | 137 | THR  |
| 1   | G     | 46  | THR  |
| 1   | G     | 51  | LEU  |
| 1   | G     | 61  | HIS  |
| 1   | G     | 147 | TRP  |
| 1   | G     | 195 | SER  |
| 1   | G     | 209 | SER  |
| 1   | G     | 294 | LEU  |
| 1   | G     | 319 | TRP  |
| 1   | G     | 324 | SER  |
| 1   | G     | 333 | LYS  |
| 1   | G     | 355 | GLN  |
| 1   | G     | 365 | SER  |
| 1   | G     | 367 | SER  |
| 1   | G     | 463 | ASP  |
| 1   | G     | 465 | MET  |
| 2   | H     | 39  | GLU  |
| 2   | H     | 64  | LEU  |
| 2   | H     | 235 | ASN  |
| 2   | H     | 237 | ASP  |
| 2   | H     | 256 | PHE  |
| 2   | H     | 271 | ASP  |
| 2   | H     | 318 | PHE  |
| 2   | H     | 322 | HIS  |
| 2   | H     | 328 | THR  |
| 2   | H     | 340 | HIS  |
| 2   | H     | 429 | SER  |
| 2   | H     | 446 | VAL  |
| 2   | H     | 473 | LEU  |
| 2   | H     | 494 | ASN  |
| 2   | H     | 522 | ASP  |
| 2   | H     | 575 | ASP  |
| 2   | H     | 577 | SER  |
| 2   | H     | 582 | PHE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 583 | TYR  |
| 2   | H     | 647 | ASN  |
| 9   | K     | 64  | SER  |
| 10  | L     | 4   | LEU  |
| 10  | L     | 19  | THR  |
| 10  | L     | 29  | THR  |
| 10  | L     | 48  | LEU  |
| 10  | L     | 73  | VAL  |
| 3   | N     | 16  | CYS  |
| 3   | N     | 65  | ARG  |
| 4   | O     | 22  | ASP  |
| 4   | O     | 31  | TRP  |
| 4   | O     | 65  | LEU  |
| 4   | O     | 122 | ASN  |
| 4   | O     | 126 | SER  |
| 5   | P     | 36  | VAL  |
| 5   | P     | 68  | VAL  |
| 6   | Q     | 85  | LEU  |
| 6   | Q     | 90  | ASN  |
| 6   | Q     | 114 | PHE  |
| 8   | S     | 19  | MET  |
| 9   | T     | 22  | CYS  |
| 9   | T     | 69  | LEU  |
| 10  | U     | 19  | THR  |
| 10  | U     | 48  | LEU  |
| 10  | U     | 101 | PHE  |
| 10  | U     | 136 | PHE  |
| 11  | V     | 5   | ASP  |
| 12  | X     | 13  | THR  |
| 1   | Y     | 34  | PHE  |
| 1   | Y     | 40  | ARG  |
| 1   | Y     | 45  | THR  |
| 1   | Y     | 59  | ASP  |
| 1   | Y     | 73  | PHE  |
| 1   | Y     | 147 | TRP  |
| 1   | Y     | 219 | VAL  |
| 1   | Y     | 253 | TYR  |
| 1   | Y     | 261 | PHE  |
| 1   | Y     | 342 | LYS  |
| 1   | Y     | 350 | THR  |
| 1   | Y     | 442 | SER  |
| 1   | Y     | 465 | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 478 | THR  |
| 1   | Y     | 562 | SER  |
| 1   | Y     | 587 | CYS  |
| 1   | Y     | 605 | CYS  |
| 1   | Y     | 642 | SER  |
| 2   | Z     | 32  | SER  |
| 2   | Z     | 64  | LEU  |
| 2   | Z     | 66  | HIS  |
| 2   | Z     | 75  | GLN  |
| 2   | Z     | 159 | LYS  |
| 2   | Z     | 165 | SER  |
| 2   | Z     | 185 | SER  |
| 2   | Z     | 186 | SER  |
| 2   | Z     | 238 | THR  |
| 2   | Z     | 256 | PHE  |
| 2   | Z     | 349 | SER  |
| 2   | Z     | 411 | LEU  |
| 2   | Z     | 444 | ASP  |
| 2   | Z     | 494 | ASN  |
| 2   | Z     | 551 | LYS  |
| 2   | Z     | 574 | CYS  |
| 2   | Z     | 589 | MET  |
| 2   | Z     | 605 | LEU  |
| 2   | Z     | 632 | LEU  |
| 2   | Z     | 650 | SER  |
| 2   | Z     | 683 | THR  |
| 2   | Z     | 698 | ARG  |
| 2   | Z     | 707 | SER  |
| 2   | Z     | 731 | LEU  |
| 3   | a     | 15  | GLN  |
| 3   | a     | 61  | PHE  |
| 4   | b     | 33  | SER  |
| 4   | b     | 41  | MET  |
| 4   | b     | 88  | ASP  |
| 4   | b     | 134 | LYS  |
| 5   | c     | 53  | SER  |
| 6   | d     | 24  | THR  |
| 7   | e     | 2   | MET  |
| 9   | g     | 32  | TYR  |
| 9   | g     | 58  | GLU  |
| 9   | g     | 64  | SER  |
| 10  | h     | 19  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | h     | 48  | LEU  |
| 10  | h     | 70  | ASP  |
| 10  | h     | 71  | SER  |
| 10  | h     | 85  | LEU  |
| 10  | h     | 114 | SER  |
| 10  | h     | 118 | SER  |
| 10  | h     | 140 | GLU  |
| 12  | j     | 9   | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 215 | HIS  |
| 1   | A     | 218 | HIS  |
| 1   | A     | 224 | ASN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 301 | HIS  |
| 1   | A     | 373 | HIS  |
| 1   | A     | 504 | ASN  |
| 1   | A     | 542 | HIS  |
| 1   | A     | 718 | GLN  |
| 2   | B     | 9   | GLN  |
| 2   | B     | 13  | GLN  |
| 2   | B     | 33  | HIS  |
| 2   | B     | 52  | HIS  |
| 2   | B     | 82  | ASN  |
| 2   | B     | 94  | GLN  |
| 2   | B     | 136 | GLN  |
| 2   | B     | 241 | HIS  |
| 2   | B     | 298 | HIS  |
| 2   | B     | 417 | HIS  |
| 2   | B     | 443 | ASN  |
| 2   | B     | 455 | GLN  |
| 2   | B     | 494 | ASN  |
| 2   | B     | 497 | ASN  |
| 2   | B     | 527 | HIS  |
| 2   | B     | 639 | ASN  |
| 2   | B     | 647 | ASN  |
| 2   | B     | 688 | HIS  |
| 2   | B     | 710 | GLN  |
| 4   | D     | 70  | GLN  |
| 5   | E     | 63  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 32  | GLN  |
| 6   | F     | 134 | ASN  |
| 1   | G     | 43  | GLN  |
| 1   | G     | 61  | HIS  |
| 1   | G     | 123 | GLN  |
| 1   | G     | 192 | ASN  |
| 1   | G     | 198 | ASN  |
| 1   | G     | 282 | ASN  |
| 1   | G     | 301 | HIS  |
| 1   | G     | 323 | HIS  |
| 1   | G     | 332 | HIS  |
| 1   | G     | 355 | GLN  |
| 1   | G     | 359 | ASN  |
| 1   | G     | 390 | GLN  |
| 1   | G     | 426 | GLN  |
| 1   | G     | 547 | HIS  |
| 1   | G     | 618 | GLN  |
| 1   | G     | 641 | GLN  |
| 1   | G     | 718 | GLN  |
| 2   | H     | 52  | HIS  |
| 2   | H     | 78  | GLN  |
| 2   | H     | 110 | ASN  |
| 2   | H     | 131 | ASN  |
| 2   | H     | 155 | HIS  |
| 2   | H     | 192 | HIS  |
| 2   | H     | 205 | HIS  |
| 2   | H     | 234 | GLN  |
| 2   | H     | 331 | ASN  |
| 2   | H     | 340 | HIS  |
| 2   | H     | 378 | HIS  |
| 2   | H     | 455 | GLN  |
| 2   | H     | 494 | ASN  |
| 2   | H     | 497 | ASN  |
| 2   | H     | 601 | HIS  |
| 2   | H     | 633 | ASN  |
| 2   | H     | 647 | ASN  |
| 2   | H     | 648 | ASN  |
| 9   | K     | 35  | GLN  |
| 10  | L     | 16  | HIS  |
| 10  | L     | 75  | ASN  |
| 4   | O     | 54  | ASN  |
| 4   | O     | 63  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | O     | 106 | ASN  |
| 4   | O     | 122 | ASN  |
| 6   | Q     | 23  | ASN  |
| 9   | T     | 67  | HIS  |
| 10  | U     | 16  | HIS  |
| 10  | U     | 75  | ASN  |
| 10  | U     | 141 | ASN  |
| 12  | X     | 23  | ASN  |
| 1   | Y     | 123 | GLN  |
| 1   | Y     | 179 | HIS  |
| 1   | Y     | 198 | ASN  |
| 1   | Y     | 301 | HIS  |
| 1   | Y     | 359 | ASN  |
| 1   | Y     | 372 | GLN  |
| 1   | Y     | 461 | HIS  |
| 1   | Y     | 504 | ASN  |
| 1   | Y     | 547 | HIS  |
| 2   | Z     | 131 | ASN  |
| 2   | Z     | 136 | GLN  |
| 2   | Z     | 192 | HIS  |
| 2   | Z     | 241 | HIS  |
| 2   | Z     | 298 | HIS  |
| 2   | Z     | 353 | GLN  |
| 2   | Z     | 366 | GLN  |
| 2   | Z     | 378 | HIS  |
| 2   | Z     | 406 | ASN  |
| 2   | Z     | 455 | GLN  |
| 2   | Z     | 494 | ASN  |
| 2   | Z     | 639 | ASN  |
| 2   | Z     | 647 | ASN  |
| 2   | Z     | 710 | GLN  |
| 4   | b     | 95  | HIS  |
| 8   | f     | 39  | HIS  |
| 10  | h     | 75  | ASN  |
| 10  | h     | 119 | GLN  |
| 11  | i     | 7   | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 14  | CLA  | B     | 811  | -    | 49,63,73     | 2.35 | 14 (28%)    | 55,101,113  | 2.42 | 21 (38%)    |
| 14  | CLA  | B     | 817  | -    | 59,73,73     | 2.06 | 15 (25%)    | 67,113,113  | 2.13 | 18 (26%)    |
| 14  | CLA  | B     | 833  | -    | 49,63,73     | 2.37 | 15 (30%)    | 55,101,113  | 2.42 | 22 (40%)    |
| 14  | CLA  | H     | 820  | -    | 36,53,73     | 2.71 | 14 (38%)    | 39,89,113   | 2.54 | 16 (41%)    |
| 14  | CLA  | Y     | 810  | -    | 36,53,73     | 2.64 | 14 (38%)    | 39,89,113   | 2.47 | 12 (30%)    |
| 14  | CLA  | Y     | 827  | -    | 59,73,73     | 2.26 | 15 (25%)    | 67,113,113  | 2.33 | 19 (28%)    |
| 14  | CLA  | A     | 852  | -    | 59,73,73     | 2.18 | 15 (25%)    | 67,113,113  | 2.60 | 20 (29%)    |
| 14  | CLA  | A     | 826  | -    | 54,68,73     | 2.23 | 15 (27%)    | 61,107,113  | 2.22 | 16 (26%)    |
| 14  | CLA  | Y     | 835  | -    | 49,63,73     | 2.51 | 16 (32%)    | 55,101,113  | 2.36 | 16 (29%)    |
| 18  | LHG  | Y     | 852  | -    | 48,48,48     | 1.01 | 2 (4%)      | 51,54,54    | 1.00 | 2 (3%)      |
| 14  | CLA  | Z     | 808  | 2    | 59,73,73     | 2.11 | 15 (25%)    | 67,113,113  | 2.20 | 17 (25%)    |
| 14  | CLA  | B     | 841  | -    | 59,73,73     | 2.10 | 14 (23%)    | 67,113,113  | 2.46 | 23 (34%)    |
| 17  | BCR  | M     | 101  | -    | 41,41,41     | 2.80 | 6 (14%)     | 56,56,56    | 7.13 | 27 (48%)    |
| 14  | CLA  | H     | 817  | -    | 54,68,73     | 2.27 | 15 (27%)    | 61,107,113  | 2.21 | 15 (24%)    |
| 14  | CLA  | H     | 818  | -    | 54,68,73     | 2.34 | 16 (29%)    | 61,107,113  | 2.18 | 16 (26%)    |
| 14  | CLA  | H     | 831  | -    | 36,53,73     | 2.66 | 13 (36%)    | 39,89,113   | 2.64 | 15 (38%)    |
| 17  | BCR  | U     | 1005 | -    | 41,41,41     | 2.72 | 6 (14%)     | 56,56,56    | 6.90 | 21 (37%)    |
| 14  | CLA  | A     | 832  | -    | 59,73,73     | 2.18 | 14 (23%)    | 67,113,113  | 2.13 | 17 (25%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | G     | 846  | -    | 41,41,41     | 2.81 | 7 (17%)  | 56,56,56    | 7.22 | 30 (53%) |
| 14  | CLA  | G     | 824  | -    | 54,68,73     | 2.26 | 14 (25%) | 61,107,113  | 2.16 | 15 (24%) |
| 14  | CLA  | d     | 202  | -    | 36,53,73     | 2.67 | 14 (38%) | 39,89,113   | 2.45 | 14 (35%) |
| 14  | CLA  | B     | 802  | -    | 59,73,73     | 2.10 | 14 (23%) | 67,113,113  | 2.18 | 20 (29%) |
| 14  | CLA  | Z     | 831  | -    | 49,63,73     | 2.34 | 13 (26%) | 55,101,113  | 2.49 | 22 (40%) |
| 14  | CLA  | B     | 838  | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.25 | 17 (25%) |
| 14  | CLA  | H     | 804  | -    | 59,73,73     | 2.19 | 14 (23%) | 67,113,113  | 2.08 | 17 (25%) |
| 17  | BCR  | e     | 101  | -    | 41,41,41     | 2.73 | 6 (14%)  | 56,56,56    | 7.45 | 26 (46%) |
| 14  | CLA  | Y     | 855  | -    | 59,73,73     | 2.09 | 13 (22%) | 67,113,113  | 2.11 | 17 (25%) |
| 14  | CLA  | G     | 839  | -    | 59,73,73     | 2.14 | 15 (25%) | 67,113,113  | 2.42 | 21 (31%) |
| 14  | CLA  | H     | 813  | -    | 59,73,73     | 2.20 | 15 (25%) | 67,113,113  | 2.13 | 17 (25%) |
| 14  | CLA  | A     | 822  | -    | 59,73,73     | 2.25 | 16 (27%) | 67,113,113  | 2.34 | 19 (28%) |
| 14  | CLA  | H     | 837  | -    | 59,73,73     | 2.19 | 15 (25%) | 67,113,113  | 1.98 | 18 (26%) |
| 14  | CLA  | L     | 205  | 10   | 59,73,73     | 2.19 | 15 (25%) | 67,113,113  | 2.20 | 17 (25%) |
| 14  | CLA  | F     | 202  | -    | 36,53,73     | 2.64 | 13 (36%) | 39,89,113   | 2.40 | 14 (35%) |
| 14  | CLA  | Y     | 830  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.39 | 16 (23%) |
| 14  | CLA  | Y     | 825  | -    | 59,73,73     | 2.23 | 15 (25%) | 67,113,113  | 2.28 | 17 (25%) |
| 14  | CLA  | Y     | 809  | -    | 59,73,73     | 2.16 | 15 (25%) | 67,113,113  | 2.05 | 17 (25%) |
| 14  | CLA  | A     | 840  | -    | 59,73,73     | 2.18 | 15 (25%) | 67,113,113  | 2.00 | 16 (23%) |
| 14  | CLA  | G     | 813  | -    | 54,68,73     | 2.19 | 16 (29%) | 61,107,113  | 2.54 | 19 (31%) |
| 14  | CLA  | Y     | 840  | -    | 59,73,73     | 2.25 | 15 (25%) | 67,113,113  | 2.37 | 18 (26%) |
| 14  | CLA  | B     | 837  | -    | 54,68,73     | 2.28 | 13 (24%) | 61,107,113  | 2.45 | 17 (27%) |
| 14  | CLA  | U     | 1003 | -    | 59,73,73     | 2.22 | 15 (25%) | 67,113,113  | 2.26 | 18 (26%) |
| 17  | BCR  | H     | 845  | -    | 41,41,41     | 2.78 | 8 (19%)  | 56,56,56    | 7.11 | 28 (50%) |
| 14  | CLA  | B     | 834  | -    | 36,53,73     | 2.77 | 15 (41%) | 39,89,113   | 3.14 | 17 (43%) |
| 18  | LHG  | G     | 852  | 14   | 31,31,48     | 1.26 | 2 (6%)   | 34,37,54    | 1.31 | 4 (11%)  |
| 14  | CLA  | A     | 836  | -    | 44,58,73     | 2.61 | 15 (34%) | 49,95,113   | 2.28 | 15 (30%) |
| 17  | BCR  | J     | 103  | -    | 41,41,41     | 2.61 | 6 (14%)  | 56,56,56    | 6.88 | 28 (50%) |
| 14  | CLA  | U     | 1002 | 10   | 59,73,73     | 2.13 | 16 (27%) | 67,113,113  | 2.41 | 22 (32%) |
| 14  | CLA  | A     | 812  | -    | 48,62,73     | 2.40 | 15 (31%) | 53,99,113   | 2.26 | 18 (33%) |
| 17  | BCR  | A     | 847  | -    | 41,41,41     | 2.70 | 6 (14%)  | 56,56,56    | 7.09 | 26 (46%) |
| 17  | BCR  | G     | 854  | -    | 41,41,41     | 2.96 | 6 (14%)  | 56,56,56    | 7.14 | 27 (48%) |
| 14  | CLA  | H     | 805  | -    | 59,73,73     | 2.14 | 15 (25%) | 67,113,113  | 2.06 | 16 (23%) |
| 17  | BCR  | Y     | 846  | -    | 41,41,41     | 2.50 | 6 (14%)  | 56,56,56    | 7.20 | 24 (42%) |
| 18  | LHG  | A     | 850  | -    | 48,48,48     | 0.99 | 2 (4%)   | 51,54,54    | 1.05 | 3 (5%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | G     | 816  | -    | 44,58,73     | 2.57 | 15 (34%) | 49,95,113   | 2.64 | 15 (30%) |
| 14  | CLA  | G     | 836  | -    | 44,58,73     | 2.48 | 15 (34%) | 49,95,113   | 2.60 | 17 (34%) |
| 14  | CLA  | A     | 820  | -    | 54,68,73     | 2.27 | 16 (29%) | 61,107,113  | 2.33 | 18 (29%) |
| 17  | BCR  | d     | 203  | -    | 41,41,41     | 2.62 | 6 (14%)  | 56,56,56    | 7.01 | 27 (48%) |
| 14  | CLA  | G     | 817  | -    | 54,68,73     | 2.37 | 14 (25%) | 61,107,113  | 2.21 | 20 (32%) |
| 14  | CLA  | H     | 807  | -    | 59,73,73     | 2.28 | 16 (27%) | 67,113,113  | 2.45 | 23 (34%) |
| 14  | CLA  | Y     | 811  | 14   | 59,73,73     | 2.26 | 13 (22%) | 67,113,113  | 2.13 | 17 (25%) |
| 14  | CLA  | Y     | 838  | -    | 59,73,73     | 2.18 | 16 (27%) | 67,113,113  | 2.11 | 18 (26%) |
| 14  | CLA  | H     | 815  | -    | 49,63,73     | 2.36 | 14 (28%) | 55,101,113  | 2.44 | 19 (34%) |
| 14  | CLA  | B     | 825  | -    | 59,73,73     | 2.22 | 15 (25%) | 67,113,113  | 2.29 | 21 (31%) |
| 14  | CLA  | Y     | 812  | -    | 49,63,73     | 2.35 | 15 (30%) | 55,101,113  | 2.33 | 20 (36%) |
| 18  | LHG  | j     | 101  | -    | 27,27,48     | 1.28 | 2 (7%)   | 30,33,54    | 1.36 | 4 (13%)  |
| 14  | CLA  | Z     | 821  | -    | 54,68,73     | 2.34 | 15 (27%) | 61,107,113  | 2.10 | 19 (31%) |
| 14  | CLA  | J     | 102  | -    | 49,63,73     | 2.47 | 15 (30%) | 55,101,113  | 2.46 | 18 (32%) |
| 17  | BCR  | B     | 844  | -    | 41,41,41     | 2.78 | 6 (14%)  | 56,56,56    | 7.31 | 25 (44%) |
| 14  | CLA  | S     | 1102 | 8    | 36,53,73     | 2.62 | 13 (36%) | 39,89,113   | 2.31 | 11 (28%) |
| 17  | BCR  | H     | 841  | -    | 41,41,41     | 3.03 | 7 (17%)  | 56,56,56    | 6.95 | 26 (46%) |
| 17  | BCR  | A     | 845  | -    | 41,41,41     | 2.55 | 6 (14%)  | 56,56,56    | 7.14 | 28 (50%) |
| 14  | CLA  | A     | 807  | -    | 45,59,73     | 2.47 | 14 (31%) | 50,96,113   | 2.41 | 15 (30%) |
| 14  | CLA  | Z     | 815  | -    | 59,73,73     | 2.12 | 15 (25%) | 67,113,113  | 2.15 | 19 (28%) |
| 14  | CLA  | H     | 810  | -    | 49,63,73     | 2.28 | 14 (28%) | 55,101,113  | 2.35 | 16 (29%) |
| 18  | LHG  | A     | 851  | 14   | 31,31,48     | 1.19 | 2 (6%)   | 34,37,54    | 1.20 | 3 (8%)   |
| 14  | CLA  | H     | 802  | -    | 59,73,73     | 2.16 | 16 (27%) | 67,113,113  | 2.14 | 19 (28%) |
| 14  | CLA  | Y     | 820  | -    | 54,68,73     | 2.24 | 15 (27%) | 61,107,113  | 2.26 | 19 (31%) |
| 17  | BCR  | G     | 849  | -    | 41,41,41     | 2.83 | 7 (17%)  | 56,56,56    | 6.96 | 25 (44%) |
| 17  | BCR  | H     | 842  | -    | 41,41,41     | 2.74 | 6 (14%)  | 56,56,56    | 7.14 | 24 (42%) |
| 17  | BCR  | Y     | 851  | -    | 41,41,41     | 2.94 | 6 (14%)  | 56,56,56    | 7.30 | 29 (51%) |
| 14  | CLA  | T     | 101  | -    | 32,49,73     | 2.69 | 13 (40%) | 32,83,113   | 2.33 | 11 (34%) |
| 14  | CLA  | U     | 1006 | 2    | 59,73,73     | 2.22 | 14 (23%) | 67,113,113  | 2.26 | 23 (34%) |
| 14  | CLA  | Y     | 834  | -    | 59,73,73     | 2.18 | 13 (22%) | 67,113,113  | 2.04 | 20 (29%) |
| 14  | CLA  | Z     | 832  | -    | 36,53,73     | 2.76 | 14 (38%) | 39,89,113   | 2.53 | 15 (38%) |
| 14  | CLA  | Z     | 833  | -    | 36,53,73     | 2.74 | 13 (36%) | 39,89,113   | 2.42 | 11 (28%) |
| 17  | BCR  | A     | 849  | -    | 41,41,41     | 2.67 | 6 (14%)  | 56,56,56    | 7.34 | 26 (46%) |
| 17  | BCR  | Y     | 856  | -    | 41,41,41     | 2.71 | 7 (17%)  | 56,56,56    | 7.00 | 30 (53%) |
| 17  | BCR  | B     | 851  | -    | 41,41,41     | 2.77 | 6 (14%)  | 56,56,56    | 7.08 | 27 (48%) |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | H     | 821  | -    | 49,63,73     | 2.47 | 15 (30%) | 55,101,113  | 2.43 | 17 (30%) |
| 14  | CLA  | L     | 207  | -    | 59,73,73     | 2.20 | 15 (25%) | 67,113,113  | 2.11 | 17 (25%) |
| 14  | CLA  | B     | 819  | -    | 54,68,73     | 2.30 | 16 (29%) | 61,107,113  | 2.27 | 20 (32%) |
| 14  | CLA  | G     | 809  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.17 | 20 (29%) |
| 18  | LHG  | H     | 847  | -    | 36,36,48     | 1.10 | 2 (5%)   | 39,42,54    | 0.92 | 3 (7%)   |
| 17  | BCR  | B     | 848  | -    | 41,41,41     | 2.76 | 7 (17%)  | 56,56,56    | 6.90 | 27 (48%) |
| 16  | SF4  | a     | 101  | 3    | 0,12,12      | 0.00 | -        | -           |      |          |
| 14  | CLA  | A     | 841  | -    | 59,73,73     | 2.17 | 16 (27%) | 67,113,113  | 2.06 | 18 (26%) |
| 14  | CLA  | G     | 834  | -    | 49,63,73     | 2.43 | 15 (30%) | 55,101,113  | 2.16 | 17 (30%) |
| 14  | CLA  | A     | 816  | -    | 44,58,73     | 2.61 | 15 (34%) | 49,95,113   | 2.45 | 14 (28%) |
| 14  | CLA  | Z     | 837  | -    | 36,53,73     | 2.69 | 14 (38%) | 39,89,113   | 2.60 | 12 (30%) |
| 14  | CLA  | A     | 815  | -    | 44,58,73     | 2.53 | 14 (31%) | 49,95,113   | 2.73 | 19 (38%) |
| 14  | CLA  | H     | 823  | 2    | 49,63,73     | 2.50 | 16 (32%) | 55,101,113  | 2.59 | 20 (36%) |
| 14  | CLA  | B     | 801  | -    | 59,73,73     | 2.04 | 11 (18%) | 67,113,113  | 2.19 | 15 (22%) |
| 17  | BCR  | h     | 202  | -    | 41,41,41     | 2.53 | 8 (19%)  | 56,56,56    | 7.31 | 28 (50%) |
| 14  | CLA  | H     | 824  | -    | 59,73,73     | 2.16 | 16 (27%) | 67,113,113  | 2.52 | 24 (35%) |
| 14  | CLA  | Y     | 833  | -    | 59,73,73     | 2.18 | 13 (22%) | 67,113,113  | 2.26 | 18 (26%) |
| 14  | CLA  | H     | 835  | -    | 59,73,73     | 2.12 | 15 (25%) | 67,113,113  | 2.13 | 17 (25%) |
| 14  | CLA  | G     | 806  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.16 | 14 (20%) |
| 14  | CLA  | Z     | 814  | -    | 49,63,73     | 2.42 | 15 (30%) | 55,101,113  | 2.45 | 19 (34%) |
| 14  | CLA  | A     | 804  | 14   | 53,67,73     | 2.29 | 15 (28%) | 59,105,113  | 2.49 | 17 (28%) |
| 14  | CLA  | A     | 829  | -    | 59,73,73     | 2.15 | 15 (25%) | 67,113,113  | 1.98 | 16 (23%) |
| 14  | CLA  | G     | 812  | -    | 48,62,73     | 2.41 | 14 (29%) | 53,99,113   | 2.24 | 14 (26%) |
| 14  | CLA  | Y     | 808  | 1    | 59,73,73     | 2.16 | 14 (23%) | 67,113,113  | 2.32 | 20 (29%) |
| 14  | CLA  | H     | 832  | -    | 36,53,73     | 2.64 | 14 (38%) | 39,89,113   | 2.58 | 13 (33%) |
| 14  | CLA  | Z     | 801  | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.08 | 17 (25%) |
| 14  | CLA  | Z     | 807  | -    | 59,73,73     | 2.21 | 16 (27%) | 67,113,113  | 2.43 | 19 (28%) |
| 14  | CLA  | U     | 1004 | -    | 59,73,73     | 2.18 | 14 (23%) | 67,113,113  | 2.26 | 14 (20%) |
| 17  | BCR  | J     | 104  | -    | 41,41,41     | 2.91 | 7 (17%)  | 56,56,56    | 7.08 | 27 (48%) |
| 14  | CLA  | H     | 827  | -    | 59,73,73     | 2.16 | 15 (25%) | 67,113,113  | 2.13 | 19 (28%) |
| 17  | BCR  | Y     | 848  | -    | 41,41,41     | 2.60 | 6 (14%)  | 56,56,56    | 7.21 | 29 (51%) |
| 19  | LMG  | Z     | 847  | -    | 49,49,55     | 1.26 | 6 (12%)  | 57,57,63    | 1.24 | 5 (8%)   |
| 14  | CLA  | G     | 804  | -    | 53,67,73     | 2.24 | 15 (28%) | 59,105,113  | 2.34 | 14 (23%) |
| 14  | CLA  | Y     | 802  | -    | 59,73,73     | 2.05 | 14 (23%) | 67,113,113  | 2.32 | 17 (25%) |
| 14  | CLA  | G     | 811  | -    | 59,73,73     | 2.24 | 16 (27%) | 67,113,113  | 2.06 | 15 (22%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | H     | 808  | 2    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.32 | 21 (31%) |
| 14  | CLA  | H     | 838  | -    | 59,73,73     | 2.14 | 14 (23%) | 67,113,113  | 2.38 | 20 (29%) |
| 14  | CLA  | A     | 825  | -    | 59,73,73     | 2.21 | 16 (27%) | 67,113,113  | 2.33 | 18 (26%) |
| 17  | BCR  | L     | 203  | -    | 41,41,41     | 2.92 | 6 (14%)  | 56,56,56    | 6.97 | 29 (51%) |
| 13  | CL0  | G     | 801  | -    | 59,73,73     | 2.35 | 16 (27%) | 67,113,113  | 2.49 | 20 (29%) |
| 14  | CLA  | B     | 804  | -    | 59,73,73     | 2.12 | 16 (27%) | 67,113,113  | 2.09 | 16 (23%) |
| 17  | BCR  | f     | 103  | -    | 41,41,41     | 2.56 | 6 (14%)  | 56,56,56    | 7.19 | 28 (50%) |
| 14  | CLA  | Z     | 812  | -    | 59,73,73     | 2.38 | 14 (23%) | 67,113,113  | 2.00 | 15 (22%) |
| 14  | CLA  | j     | 102  | -    | 36,53,73     | 2.63 | 13 (36%) | 39,89,113   | 2.36 | 12 (30%) |
| 14  | CLA  | L     | 206  | -    | 59,73,73     | 2.22 | 16 (27%) | 67,113,113  | 2.23 | 16 (23%) |
| 18  | LHG  | Y     | 853  | 14   | 24,24,48     | 1.51 | 2 (8%)   | 27,30,54    | 1.60 | 4 (14%)  |
| 14  | CLA  | A     | 838  | -    | 44,58,73     | 2.43 | 14 (31%) | 49,95,113   | 2.41 | 17 (34%) |
| 14  | CLA  | Z     | 830  | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.07 | 14 (20%) |
| 16  | SF4  | N     | 102  | 3,21 | 0,12,12      | 0.00 | -        | -           | -    | -        |
| 14  | CLA  | B     | 832  | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.28 | 16 (23%) |
| 14  | CLA  | B     | 810  | 2    | 59,73,73     | 2.14 | 16 (27%) | 67,113,113  | 2.66 | 20 (29%) |
| 14  | CLA  | S     | 1103 | -    | 49,63,73     | 2.39 | 15 (30%) | 55,101,113  | 2.51 | 18 (32%) |
| 17  | BCR  | f     | 104  | -    | 41,41,41     | 2.95 | 6 (14%)  | 56,56,56    | 6.95 | 28 (50%) |
| 14  | CLA  | T     | 103  | -    | 36,53,73     | 2.74 | 15 (41%) | 39,89,113   | 2.26 | 11 (28%) |
| 14  | CLA  | H     | 833  | -    | 36,53,73     | 2.61 | 13 (36%) | 39,89,113   | 2.49 | 15 (38%) |
| 17  | BCR  | Y     | 850  | -    | 41,41,41     | 2.70 | 6 (14%)  | 56,56,56    | 7.10 | 24 (42%) |
| 17  | BCR  | R     | 101  | -    | 41,41,41     | 2.76 | 6 (14%)  | 56,56,56    | 7.47 | 24 (42%) |
| 14  | CLA  | H     | 809  | 2    | 59,73,73     | 2.14 | 14 (23%) | 67,113,113  | 2.31 | 21 (31%) |
| 14  | CLA  | Y     | 822  | -    | 59,73,73     | 2.24 | 15 (25%) | 67,113,113  | 2.23 | 15 (22%) |
| 14  | CLA  | H     | 803  | -    | 59,73,73     | 2.11 | 13 (22%) | 67,113,113  | 2.27 | 18 (26%) |
| 14  | CLA  | G     | 837  | -    | 59,73,73     | 2.16 | 15 (25%) | 67,113,113  | 2.20 | 20 (29%) |
| 14  | CLA  | J     | 101  | 8    | 36,53,73     | 2.62 | 13 (36%) | 39,89,113   | 2.45 | 13 (33%) |
| 15  | PQN  | G     | 844  | -    | 34,34,34     | 1.53 | 2 (5%)   | 42,45,45    | 1.24 | 6 (14%)  |
| 14  | CLA  | Y     | 832  | -    | 59,73,73     | 2.23 | 14 (23%) | 67,113,113  | 2.33 | 17 (25%) |
| 14  | CLA  | A     | 827  | -    | 59,73,73     | 2.12 | 15 (25%) | 67,113,113  | 2.04 | 17 (25%) |
| 14  | CLA  | H     | 830  | -    | 49,63,73     | 2.36 | 15 (30%) | 55,101,113  | 2.23 | 17 (30%) |
| 14  | CLA  | Y     | 818  | -    | 59,73,73     | 2.21 | 15 (25%) | 67,113,113  | 2.38 | 19 (28%) |
| 14  | CLA  | A     | 809  | 1    | 59,73,73     | 2.13 | 15 (25%) | 67,113,113  | 2.36 | 19 (28%) |
| 14  | CLA  | B     | 813  | -    | 59,73,73     | 2.14 | 15 (25%) | 67,113,113  | 2.31 | 19 (28%) |
| 14  | CLA  | G     | 840  | -    | 44,58,73     | 2.60 | 13 (29%) | 49,95,113   | 2.19 | 16 (32%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | Z     | 806 | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.19 | 17 (25%) |
| 14  | CLA  | Z     | 834 | -    | 36,53,73     | 2.65 | 16 (44%) | 39,89,113   | 2.74 | 16 (41%) |
| 14  | CLA  | B     | 806 | -    | 59,73,73     | 2.00 | 14 (23%) | 67,113,113  | 2.47 | 19 (28%) |
| 14  | CLA  | Z     | 809 | -    | 49,63,73     | 2.44 | 15 (30%) | 55,101,113  | 2.25 | 17 (30%) |
| 14  | CLA  | G     | 808 | 1    | 59,73,73     | 2.16 | 14 (23%) | 67,113,113  | 2.25 | 20 (29%) |
| 14  | CLA  | G     | 832 | -    | 59,73,73     | 2.08 | 14 (23%) | 67,113,113  | 2.17 | 19 (28%) |
| 14  | CLA  | H     | 801 | -    | 59,73,73     | 2.25 | 14 (23%) | 67,113,113  | 2.52 | 20 (29%) |
| 14  | CLA  | Y     | 821 | -    | 59,73,73     | 2.31 | 15 (25%) | 67,113,113  | 1.99 | 16 (23%) |
| 14  | CLA  | Z     | 828 | -    | 36,53,73     | 2.55 | 14 (38%) | 39,89,113   | 2.26 | 14 (35%) |
| 14  | CLA  | B     | 812 | -    | 44,58,73     | 2.48 | 15 (34%) | 49,95,113   | 2.45 | 18 (36%) |
| 14  | CLA  | H     | 806 | -    | 59,73,73     | 2.14 | 14 (23%) | 67,113,113  | 1.95 | 14 (20%) |
| 14  | CLA  | G     | 810 | -    | 36,53,73     | 2.64 | 14 (38%) | 39,89,113   | 2.44 | 13 (33%) |
| 17  | BCR  | A     | 848 | -    | 41,41,41     | 2.57 | 6 (14%)  | 56,56,56    | 7.07 | 22 (39%) |
| 14  | CLA  | G     | 841 | -    | 59,73,73     | 2.25 | 14 (23%) | 67,113,113  | 2.20 | 18 (26%) |
| 14  | CLA  | A     | 805 | -    | 59,73,73     | 2.07 | 15 (25%) | 67,113,113  | 2.15 | 16 (23%) |
| 14  | CLA  | Z     | 817 | -    | 54,68,73     | 2.34 | 14 (25%) | 61,107,113  | 2.17 | 18 (29%) |
| 14  | CLA  | Z     | 803 | -    | 48,62,73     | 2.48 | 15 (31%) | 53,99,113   | 2.69 | 18 (33%) |
| 14  | CLA  | Y     | 814 | -    | 49,63,73     | 2.44 | 15 (30%) | 55,101,113  | 2.38 | 16 (29%) |
| 14  | CLA  | h     | 201 | -    | 59,73,73     | 2.13 | 16 (27%) | 67,113,113  | 2.08 | 15 (22%) |
| 14  | CLA  | Z     | 819 | -    | 36,53,73     | 2.76 | 13 (36%) | 39,89,113   | 2.66 | 14 (35%) |
| 14  | CLA  | B     | 827 | -    | 59,73,73     | 2.10 | 15 (25%) | 67,113,113  | 2.17 | 18 (26%) |
| 17  | BCR  | B     | 847 | -    | 41,41,41     | 2.87 | 6 (14%)  | 56,56,56    | 7.00 | 24 (42%) |
| 17  | BCR  | G     | 847 | -    | 41,41,41     | 2.78 | 6 (14%)  | 56,56,56    | 6.97 | 26 (46%) |
| 14  | CLA  | Y     | 815 | -    | 44,58,73     | 2.62 | 15 (34%) | 49,95,113   | 2.64 | 17 (34%) |
| 14  | CLA  | B     | 803 | -    | 59,73,73     | 2.04 | 12 (20%) | 67,113,113  | 2.12 | 18 (26%) |
| 14  | CLA  | B     | 824 | 2    | 49,63,73     | 2.43 | 14 (28%) | 55,101,113  | 2.50 | 19 (34%) |
| 14  | CLA  | B     | 821 | -    | 36,53,73     | 2.64 | 14 (38%) | 39,89,113   | 2.55 | 15 (38%) |
| 17  | BCR  | Z     | 841 | -    | 41,41,41     | 2.90 | 6 (14%)  | 56,56,56    | 7.13 | 25 (44%) |
| 16  | SF4  | Y     | 845 | 1,2  | 0,12,12      | 0.00 | -        | -           | -    | -        |
| 14  | CLA  | Z     | 804 | -    | 59,73,73     | 2.11 | 16 (27%) | 67,113,113  | 2.35 | 21 (31%) |
| 14  | CLA  | H     | 812 | -    | 59,73,73     | 2.21 | 15 (25%) | 67,113,113  | 2.20 | 15 (22%) |
| 14  | CLA  | A     | 821 | -    | 59,73,73     | 2.19 | 14 (23%) | 67,113,113  | 2.01 | 16 (23%) |
| 14  | CLA  | G     | 830 | -    | 59,73,73     | 2.16 | 14 (23%) | 67,113,113  | 2.29 | 18 (26%) |
| 15  | PQN  | H     | 839 | -    | 34,34,34     | 1.61 | 2 (5%)   | 42,45,45    | 1.28 | 6 (14%)  |
| 14  | CLA  | A     | 842 | 18   | 44,58,73     | 2.55 | 14 (31%) | 49,95,113   | 2.75 | 14 (28%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 802  | -    | 59,73,73     | 2.08 | 16 (27%) | 67,113,113  | 2.47 | 23 (34%) |
| 18  | LHG  | B     | 850  | -    | 38,38,48     | 1.09 | 2 (5%)   | 41,44,54    | 1.28 | 4 (9%)   |
| 17  | BCR  | L     | 208  | -    | 41,41,41     | 3.06 | 7 (17%)  | 56,56,56    | 6.91 | 24 (42%) |
| 14  | CLA  | A     | 831  | -    | 44,58,73     | 2.44 | 14 (31%) | 49,95,113   | 2.50 | 18 (36%) |
| 14  | CLA  | Y     | 823  | -    | 44,58,73     | 2.61 | 14 (31%) | 49,95,113   | 2.38 | 18 (36%) |
| 17  | BCR  | f     | 105  | -    | 41,41,41     | 2.74 | 6 (14%)  | 56,56,56    | 7.07 | 26 (46%) |
| 17  | BCR  | Z     | 846  | -    | 41,41,41     | 2.70 | 7 (17%)  | 56,56,56    | 7.02 | 20 (35%) |
| 17  | BCR  | Y     | 847  | -    | 41,41,41     | 2.71 | 6 (14%)  | 56,56,56    | 7.10 | 29 (51%) |
| 14  | CLA  | A     | 839  | -    | 44,58,73     | 2.56 | 15 (34%) | 49,95,113   | 2.34 | 16 (32%) |
| 19  | LMG  | B     | 849  | -    | 52,52,55     | 1.29 | 7 (13%)  | 60,60,63    | 0.99 | 3 (5%)   |
| 17  | BCR  | Z     | 845  | -    | 41,41,41     | 2.59 | 8 (19%)  | 56,56,56    | 7.27 | 30 (53%) |
| 14  | CLA  | Y     | 839  | -    | 44,58,73     | 2.55 | 16 (36%) | 49,95,113   | 2.63 | 18 (36%) |
| 17  | BCR  | B     | 845  | -    | 41,41,41     | 2.72 | 7 (17%)  | 56,56,56    | 7.05 | 27 (48%) |
| 14  | CLA  | G     | 825  | -    | 59,73,73     | 2.16 | 15 (25%) | 67,113,113  | 2.22 | 20 (29%) |
| 14  | CLA  | Y     | 816  | -    | 44,58,73     | 2.43 | 14 (31%) | 49,95,113   | 2.49 | 16 (32%) |
| 14  | CLA  | Q     | 201  | -    | 59,73,73     | 2.06 | 14 (23%) | 67,113,113  | 2.26 | 16 (23%) |
| 17  | BCR  | G     | 850  | -    | 41,41,41     | 2.70 | 6 (14%)  | 56,56,56    | 7.31 | 27 (48%) |
| 14  | CLA  | K     | 101  | -    | 32,49,73     | 2.74 | 13 (40%) | 32,83,113   | 2.47 | 13 (40%) |
| 14  | CLA  | L     | 201  | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.22 | 20 (29%) |
| 14  | CLA  | A     | 833  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.28 | 22 (32%) |
| 14  | CLA  | H     | 829  | -    | 36,53,73     | 2.63 | 13 (36%) | 39,89,113   | 2.45 | 13 (33%) |
| 14  | CLA  | A     | 824  | -    | 54,68,73     | 2.33 | 14 (25%) | 61,107,113  | 2.14 | 17 (27%) |
| 14  | CLA  | L     | 202  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.35 | 21 (31%) |
| 14  | CLA  | G     | 820  | -    | 54,68,73     | 2.29 | 16 (29%) | 61,107,113  | 2.32 | 17 (27%) |
| 14  | CLA  | G     | 835  | 1    | 36,53,73     | 2.61 | 14 (38%) | 39,89,113   | 2.52 | 15 (38%) |
| 14  | CLA  | Y     | 826  | -    | 54,68,73     | 2.29 | 15 (27%) | 61,107,113  | 2.24 | 17 (27%) |
| 14  | CLA  | Y     | 804  | 14   | 53,67,73     | 2.29 | 15 (28%) | 59,105,113  | 2.52 | 19 (32%) |
| 14  | CLA  | d     | 201  | -    | 44,58,73     | 2.55 | 15 (34%) | 49,95,113   | 2.46 | 20 (40%) |
| 17  | BCR  | Q     | 204  | -    | 41,41,41     | 2.72 | 7 (17%)  | 56,56,56    | 7.13 | 28 (50%) |
| 17  | BCR  | V     | 1202 | -    | 41,41,41     | 2.74 | 7 (17%)  | 56,56,56    | 7.27 | 30 (53%) |
| 14  | CLA  | Z     | 825  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 1.91 | 14 (20%) |
| 14  | CLA  | Y     | 837  | -    | 44,58,73     | 2.51 | 15 (34%) | 49,95,113   | 2.48 | 17 (34%) |
| 14  | CLA  | Z     | 818  | -    | 36,53,73     | 2.67 | 12 (33%) | 39,89,113   | 2.47 | 14 (35%) |
| 14  | CLA  | A     | 814  | -    | 44,58,73     | 2.57 | 15 (34%) | 49,95,113   | 2.63 | 20 (40%) |
| 17  | BCR  | U     | 1008 | -    | 41,41,41     | 2.56 | 6 (14%)  | 56,56,56    | 7.17 | 25 (44%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | G     | 803  | -    | 59,73,73     | 2.13 | 14 (23%) | 67,113,113  | 2.39 | 21 (31%) |
| 14  | CLA  | Y     | 813  | -    | 54,68,73     | 2.20 | 15 (27%) | 61,107,113  | 2.03 | 17 (27%) |
| 14  | CLA  | S     | 1101 | -    | 59,73,73     | 2.13 | 15 (25%) | 67,113,113  | 2.28 | 16 (23%) |
| 17  | BCR  | F     | 203  | -    | 41,41,41     | 2.71 | 7 (17%)  | 56,56,56    | 7.14 | 29 (51%) |
| 14  | CLA  | B     | 820  | -    | 36,53,73     | 2.60 | 14 (38%) | 39,89,113   | 2.60 | 14 (35%) |
| 17  | BCR  | U     | 1007 | -    | 41,41,41     | 2.80 | 6 (14%)  | 56,56,56    | 7.10 | 21 (37%) |
| 14  | CLA  | G     | 833  | -    | 59,73,73     | 2.26 | 14 (23%) | 67,113,113  | 2.14 | 17 (25%) |
| 14  | CLA  | Z     | 838  | -    | 59,73,73     | 2.22 | 15 (25%) | 67,113,113  | 2.11 | 19 (28%) |
| 14  | CLA  | Z     | 811  | -    | 59,73,73     | 2.13 | 14 (23%) | 67,113,113  | 2.07 | 17 (25%) |
| 14  | CLA  | H     | 822  | -    | 54,68,73     | 2.19 | 14 (25%) | 61,107,113  | 2.32 | 20 (32%) |
| 17  | BCR  | G     | 848  | -    | 41,41,41     | 2.71 | 6 (14%)  | 56,56,56    | 7.23 | 31 (55%) |
| 14  | CLA  | G     | 829  | -    | 59,73,73     | 2.18 | 15 (25%) | 67,113,113  | 2.01 | 19 (28%) |
| 16  | SF4  | C     | 101  | 3,21 | 0,12,12      | 0.00 | -        | -           |      |          |
| 17  | BCR  | H     | 843  | -    | 25,25,41     | 2.03 | 2 (8%)   | 33,33,56    | 8.12 | 17 (51%) |
| 14  | CLA  | Y     | 806  | -    | 59,73,73     | 2.18 | 13 (22%) | 67,113,113  | 2.25 | 17 (25%) |
| 14  | CLA  | h     | 207  | -    | 59,73,73     | 2.21 | 15 (25%) | 67,113,113  | 2.21 | 19 (28%) |
| 14  | CLA  | Y     | 829  | -    | 59,73,73     | 2.20 | 15 (25%) | 67,113,113  | 2.12 | 15 (22%) |
| 14  | CLA  | G     | 853  | -    | 36,53,73     | 2.68 | 14 (38%) | 39,89,113   | 2.22 | 10 (25%) |
| 16  | SF4  | C     | 102  | 3    | 0,12,12      | 0.00 | -        | -           |      |          |
| 16  | SF4  | a     | 102  | 3    | 0,12,12      | 0.00 | -        | -           |      |          |
| 14  | CLA  | A     | 828  | -    | 59,73,73     | 2.12 | 15 (25%) | 67,113,113  | 2.13 | 15 (22%) |
| 17  | BCR  | A     | 846  | -    | 41,41,41     | 2.62 | 6 (14%)  | 56,56,56    | 7.05 | 26 (46%) |
| 14  | CLA  | A     | 803  | -    | 59,73,73     | 2.22 | 17 (28%) | 67,113,113  | 2.44 | 19 (28%) |
| 17  | BCR  | Z     | 843  | -    | 41,41,41     | 2.56 | 6 (14%)  | 56,56,56    | 7.31 | 29 (51%) |
| 14  | CLA  | B     | 830  | -    | 36,53,73     | 2.53 | 14 (38%) | 39,89,113   | 2.73 | 15 (38%) |
| 14  | CLA  | Z     | 820  | -    | 49,63,73     | 2.48 | 15 (30%) | 55,101,113  | 2.20 | 19 (34%) |
| 14  | CLA  | G     | 838  | -    | 44,58,73     | 2.53 | 15 (34%) | 49,95,113   | 2.48 | 19 (38%) |
| 14  | CLA  | Y     | 841  | -    | 59,73,73     | 2.11 | 15 (25%) | 67,113,113  | 1.93 | 15 (22%) |
| 17  | BCR  | B     | 843  | -    | 30,30,41     | 3.42 | 6 (20%)  | 39,39,56    | 8.21 | 19 (48%) |
| 14  | CLA  | Z     | 822  | 2    | 49,63,73     | 2.39 | 15 (30%) | 55,101,113  | 2.60 | 20 (36%) |
| 15  | PQN  | B     | 842  | -    | 34,34,34     | 1.53 | 3 (8%)   | 42,45,45    | 1.22 | 6 (14%)  |
| 14  | CLA  | Y     | 842  | -    | 59,73,73     | 2.14 | 14 (23%) | 67,113,113  | 2.15 | 19 (28%) |
| 14  | CLA  | A     | 819  | -    | 59,73,73     | 2.12 | 15 (25%) | 67,113,113  | 2.05 | 17 (25%) |
| 14  | CLA  | V     | 1201 | -    | 48,62,73     | 2.46 | 14 (29%) | 53,99,113   | 2.29 | 16 (30%) |
| 14  | CLA  | W     | 1701 | -    | 36,53,73     | 2.59 | 14 (38%) | 39,89,113   | 2.36 | 12 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | Z     | 802 | -    | 59,73,73     | 2.14 | 15 (25%) | 67,113,113  | 2.26 | 20 (29%) |
| 14  | CLA  | H     | 834 | -    | 54,68,73     | 2.22 | 14 (25%) | 61,107,113  | 2.07 | 18 (29%) |
| 16  | SF4  | A     | 844 | 1,2  | 0,12,12      | 0.00 | -        | -           |      |          |
| 14  | CLA  | B     | 814 | -    | 59,73,73     | 2.30 | 14 (23%) | 67,113,113  | 2.10 | 19 (28%) |
| 14  | CLA  | Y     | 805 | -    | 59,73,73     | 2.07 | 14 (23%) | 67,113,113  | 2.26 | 21 (31%) |
| 14  | CLA  | Q     | 203 | -    | 36,53,73     | 2.59 | 13 (36%) | 39,89,113   | 2.64 | 13 (33%) |
| 14  | CLA  | Y     | 854 | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.39 | 18 (26%) |
| 14  | CLA  | G     | 802 | -    | 59,73,73     | 2.18 | 14 (23%) | 67,113,113  | 2.20 | 15 (22%) |
| 16  | SF4  | N     | 101 | 3    | 0,12,12      | 0.00 | -        | -           |      |          |
| 14  | CLA  | A     | 830 | -    | 59,73,73     | 2.09 | 16 (27%) | 67,113,113  | 2.30 | 16 (23%) |
| 14  | CLA  | G     | 828 | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.21 | 21 (31%) |
| 14  | CLA  | H     | 836 | -    | 36,53,73     | 2.63 | 16 (44%) | 39,89,113   | 2.57 | 15 (38%) |
| 17  | BCR  | Z     | 842 | -    | 41,41,41     | 2.69 | 8 (19%)  | 56,56,56    | 7.04 | 26 (46%) |
| 14  | CLA  | B     | 808 | -    | 59,73,73     | 2.11 | 15 (25%) | 67,113,113  | 2.12 | 18 (26%) |
| 14  | CLA  | B     | 816 | -    | 49,63,73     | 2.48 | 14 (28%) | 55,101,113  | 2.28 | 18 (32%) |
| 14  | CLA  | Z     | 839 | -    | 59,73,73     | 2.26 | 16 (27%) | 67,113,113  | 2.29 | 19 (28%) |
| 14  | CLA  | G     | 826 | -    | 54,68,73     | 2.23 | 14 (25%) | 61,107,113  | 2.24 | 17 (27%) |
| 14  | CLA  | A     | 823 | -    | 44,58,73     | 2.56 | 15 (34%) | 49,95,113   | 2.47 | 18 (36%) |
| 17  | BCR  | h     | 203 | -    | 41,41,41     | 3.00 | 7 (17%)  | 56,56,56    | 7.05 | 27 (48%) |
| 14  | CLA  | G     | 821 | -    | 59,73,73     | 2.18 | 14 (23%) | 67,113,113  | 1.95 | 15 (22%) |
| 14  | CLA  | B     | 822 | -    | 49,63,73     | 2.42 | 14 (28%) | 55,101,113  | 2.37 | 19 (34%) |
| 14  | CLA  | Y     | 843 | 18   | 44,58,73     | 2.58 | 15 (34%) | 49,95,113   | 2.60 | 18 (36%) |
| 14  | CLA  | B     | 839 | -    | 36,53,73     | 2.61 | 13 (36%) | 39,89,113   | 2.24 | 9 (23%)  |
| 14  | CLA  | A     | 808 | 1    | 59,73,73     | 2.15 | 14 (23%) | 67,113,113  | 2.29 | 17 (25%) |
| 14  | CLA  | H     | 811 | -    | 36,53,73     | 2.58 | 13 (36%) | 39,89,113   | 2.23 | 13 (33%) |
| 14  | CLA  | B     | 823 | -    | 54,68,73     | 2.34 | 15 (27%) | 61,107,113  | 2.10 | 16 (26%) |
| 14  | CLA  | A     | 811 | 14   | 59,73,73     | 2.16 | 15 (25%) | 67,113,113  | 1.99 | 15 (22%) |
| 14  | CLA  | Z     | 810 | -    | 36,53,73     | 2.60 | 12 (33%) | 39,89,113   | 2.35 | 15 (38%) |
| 14  | CLA  | Y     | 803 | -    | 59,73,73     | 2.24 | 14 (23%) | 67,113,113  | 2.28 | 18 (26%) |
| 14  | CLA  | H     | 826 | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.10 | 18 (26%) |
| 14  | CLA  | B     | 807 | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.18 | 18 (26%) |
| 19  | LMG  | H     | 846 | -    | 49,49,55     | 1.36 | 6 (12%)  | 57,57,63    | 1.18 | 4 (7%)   |
| 14  | CLA  | Z     | 816 | -    | 54,68,73     | 2.30 | 15 (27%) | 61,107,113  | 2.21 | 19 (31%) |
| 14  | CLA  | B     | 836 | -    | 36,53,73     | 2.58 | 15 (41%) | 39,89,113   | 2.70 | 13 (33%) |
| 14  | CLA  | G     | 805 | -    | 59,73,73     | 2.09 | 14 (23%) | 67,113,113  | 2.19 | 18 (26%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | i     | 101  | -    | 41,41,41     | 2.84 | 7 (17%)  | 56,56,56    | 7.60 | 32 (57%) |
| 14  | CLA  | H     | 828  | -    | 59,73,73     | 2.20 | 15 (25%) | 67,113,113  | 2.50 | 17 (25%) |
| 14  | CLA  | B     | 831  | -    | 36,53,73     | 2.60 | 14 (38%) | 39,89,113   | 2.53 | 14 (35%) |
| 14  | CLA  | f     | 102  | -    | 49,63,73     | 2.46 | 15 (30%) | 55,101,113  | 2.35 | 19 (34%) |
| 14  | CLA  | Z     | 824  | -    | 59,73,73     | 2.10 | 13 (22%) | 67,113,113  | 2.07 | 19 (28%) |
| 14  | CLA  | Z     | 835  | -    | 54,68,73     | 2.23 | 17 (31%) | 61,107,113  | 2.08 | 15 (24%) |
| 14  | CLA  | B     | 826  | -    | 59,73,73     | 2.20 | 16 (27%) | 67,113,113  | 2.35 | 24 (35%) |
| 15  | PQN  | A     | 843  | -    | 34,34,34     | 1.61 | 2 (5%)   | 42,45,45    | 1.09 | 3 (7%)   |
| 14  | CLA  | A     | 835  | 1    | 36,53,73     | 2.62 | 14 (38%) | 39,89,113   | 2.35 | 13 (33%) |
| 17  | BCR  | L     | 209  | -    | 41,41,41     | 2.75 | 6 (14%)  | 56,56,56    | 7.10 | 26 (46%) |
| 14  | CLA  | B     | 815  | -    | 36,53,73     | 2.54 | 12 (33%) | 39,89,113   | 2.50 | 15 (38%) |
| 14  | CLA  | Z     | 813  | -    | 36,53,73     | 2.77 | 15 (41%) | 39,89,113   | 2.85 | 17 (43%) |
| 17  | BCR  | F     | 201  | -    | 41,41,41     | 2.76 | 6 (14%)  | 56,56,56    | 6.88 | 24 (42%) |
| 14  | CLA  | X     | 1701 | -    | 36,53,73     | 2.65 | 15 (41%) | 39,89,113   | 2.58 | 11 (28%) |
| 14  | CLA  | A     | 806  | -    | 59,73,73     | 2.17 | 16 (27%) | 67,113,113  | 2.10 | 16 (23%) |
| 14  | CLA  | B     | 829  | -    | 59,73,73     | 2.16 | 14 (23%) | 67,113,113  | 2.31 | 15 (22%) |
| 14  | CLA  | Y     | 828  | -    | 59,73,73     | 2.08 | 15 (25%) | 67,113,113  | 1.95 | 17 (25%) |
| 17  | BCR  | H     | 844  | -    | 41,41,41     | 2.75 | 6 (14%)  | 56,56,56    | 7.04 | 29 (51%) |
| 14  | CLA  | Z     | 826  | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.10 | 18 (26%) |
| 14  | CLA  | B     | 805  | -    | 48,62,73     | 2.40 | 16 (33%) | 53,99,113   | 2.68 | 18 (33%) |
| 14  | CLA  | G     | 815  | -    | 44,58,73     | 2.47 | 14 (31%) | 49,95,113   | 2.82 | 19 (38%) |
| 14  | CLA  | g     | 102  | -    | 36,53,73     | 2.70 | 13 (36%) | 39,89,113   | 2.41 | 12 (30%) |
| 14  | CLA  | G     | 831  | -    | 44,58,73     | 2.44 | 14 (31%) | 49,95,113   | 2.59 | 17 (34%) |
| 14  | CLA  | B     | 809  | -    | 59,73,73     | 2.13 | 14 (23%) | 67,113,113  | 2.55 | 18 (26%) |
| 17  | BCR  | H     | 840  | -    | 41,41,41     | 2.81 | 6 (14%)  | 56,56,56    | 7.12 | 21 (37%) |
| 14  | CLA  | G     | 823  | -    | 44,58,73     | 2.49 | 15 (34%) | 49,95,113   | 2.43 | 17 (34%) |
| 14  | CLA  | Y     | 807  | -    | 45,59,73     | 2.58 | 16 (35%) | 50,96,113   | 2.45 | 16 (32%) |
| 17  | BCR  | S     | 1104 | -    | 41,41,41     | 2.89 | 7 (17%)  | 56,56,56    | 7.21 | 27 (48%) |
| 14  | CLA  | K     | 103  | -    | 36,53,73     | 2.63 | 13 (36%) | 39,89,113   | 2.45 | 11 (28%) |
| 14  | CLA  | Z     | 829  | -    | 36,53,73     | 2.75 | 15 (41%) | 39,89,113   | 2.77 | 17 (43%) |
| 14  | CLA  | B     | 840  | -    | 59,73,73     | 2.20 | 16 (27%) | 67,113,113  | 2.09 | 21 (31%) |
| 14  | CLA  | G     | 822  | -    | 59,73,73     | 2.16 | 15 (25%) | 67,113,113  | 2.43 | 21 (31%) |
| 14  | CLA  | H     | 814  | -    | 36,53,73     | 2.66 | 15 (41%) | 39,89,113   | 2.59 | 17 (43%) |
| 14  | CLA  | Y     | 824  | -    | 54,68,73     | 2.35 | 15 (27%) | 61,107,113  | 2.22 | 16 (26%) |
| 14  | CLA  | A     | 837  | -    | 59,73,73     | 2.12 | 14 (23%) | 67,113,113  | 2.07 | 19 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | Q     | 202 | -    | 41,41,41     | 2.79 | 6 (14%)  | 56,56,56    | 6.74 | 27 (48%) |
| 14  | CLA  | H     | 819 | -    | 36,53,73     | 2.60 | 14 (38%) | 39,89,113   | 2.82 | 15 (38%) |
| 15  | PQN  | Y     | 844 | -    | 34,34,34     | 1.82 | 2 (5%)   | 42,45,45    | 0.83 | 1 (2%)   |
| 14  | CLA  | Z     | 823 | -    | 59,73,73     | 2.20 | 15 (25%) | 67,113,113  | 2.44 | 21 (31%) |
| 14  | CLA  | g     | 101 | -    | 32,49,73     | 2.73 | 12 (37%) | 32,83,113   | 2.31 | 11 (34%) |
| 14  | CLA  | B     | 818 | -    | 54,68,73     | 2.24 | 15 (27%) | 61,107,113  | 2.20 | 18 (29%) |
| 14  | CLA  | H     | 816 | -    | 59,73,73     | 2.11 | 15 (25%) | 67,113,113  | 2.38 | 23 (34%) |
| 17  | BCR  | T     | 102 | -    | 41,41,41     | 2.46 | 6 (14%)  | 56,56,56    | 7.40 | 24 (42%) |
| 17  | BCR  | B     | 846 | -    | 25,25,41     | 2.18 | 2 (8%)   | 33,33,56    | 8.00 | 15 (45%) |
| 14  | CLA  | G     | 818 | -    | 59,73,73     | 2.18 | 14 (23%) | 67,113,113  | 2.15 | 20 (29%) |
| 14  | CLA  | A     | 818 | -    | 59,73,73     | 2.18 | 15 (25%) | 67,113,113  | 2.25 | 19 (28%) |
| 14  | CLA  | Z     | 827 | -    | 59,73,73     | 2.05 | 15 (25%) | 67,113,113  | 2.36 | 17 (25%) |
| 13  | CL0  | A     | 801 | -    | 59,73,73     | 2.33 | 16 (27%) | 67,113,113  | 2.34 | 14 (20%) |
| 17  | BCR  | I     | 101 | -    | 41,41,41     | 2.59 | 7 (17%)  | 56,56,56    | 7.30 | 26 (46%) |
| 14  | CLA  | f     | 101 | 8    | 36,53,73     | 2.76 | 15 (41%) | 39,89,113   | 2.36 | 13 (33%) |
| 14  | CLA  | Y     | 817 | -    | 54,68,73     | 2.36 | 15 (27%) | 61,107,113  | 2.09 | 17 (27%) |
| 13  | CL0  | Y     | 801 | -    | 59,73,73     | 2.26 | 14 (23%) | 67,113,113  | 2.29 | 17 (25%) |
| 14  | CLA  | A     | 817 | -    | 54,68,73     | 2.25 | 15 (27%) | 61,107,113  | 2.26 | 20 (32%) |
| 14  | CLA  | Z     | 836 | -    | 59,73,73     | 2.11 | 14 (23%) | 67,113,113  | 2.11 | 16 (23%) |
| 18  | LHG  | G     | 851 | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.10 | 3 (5%)   |
| 14  | CLA  | G     | 814 | -    | 44,58,73     | 2.52 | 14 (31%) | 49,95,113   | 2.91 | 23 (46%) |
| 14  | CLA  | A     | 810 | -    | 36,53,73     | 2.65 | 14 (38%) | 39,89,113   | 2.36 | 10 (25%) |
| 14  | CLA  | h     | 205 | 10   | 59,73,73     | 2.20 | 14 (23%) | 67,113,113  | 2.30 | 18 (26%) |
| 14  | CLA  | Y     | 836 | 1    | 36,53,73     | 2.67 | 14 (38%) | 39,89,113   | 2.36 | 11 (28%) |
| 14  | CLA  | h     | 206 | -    | 59,73,73     | 2.20 | 15 (25%) | 67,113,113  | 2.50 | 23 (34%) |
| 14  | CLA  | H     | 825 | -    | 59,73,73     | 2.17 | 16 (27%) | 67,113,113  | 2.18 | 21 (31%) |
| 14  | CLA  | A     | 834 | -    | 49,63,73     | 2.37 | 15 (30%) | 55,101,113  | 2.20 | 17 (30%) |
| 14  | CLA  | Y     | 831 | -    | 44,58,73     | 2.47 | 15 (34%) | 49,95,113   | 2.59 | 18 (36%) |
| 14  | CLA  | Z     | 805 | -    | 59,73,73     | 2.18 | 16 (27%) | 67,113,113  | 2.28 | 21 (31%) |
| 15  | PQN  | Z     | 840 | -    | 34,34,34     | 1.66 | 2 (5%)   | 42,45,45    | 1.10 | 4 (9%)   |
| 17  | BCR  | R     | 102 | -    | 41,41,41     | 3.00 | 8 (19%)  | 56,56,56    | 6.94 | 23 (41%) |
| 14  | CLA  | G     | 807 | -    | 45,59,73     | 2.54 | 16 (35%) | 50,96,113   | 2.56 | 17 (34%) |
| 17  | BCR  | Z     | 844 | -    | 25,25,41     | 2.29 | 2 (8%)   | 33,33,56    | 7.89 | 20 (60%) |
| 14  | CLA  | B     | 828 | -    | 59,73,73     | 2.10 | 15 (25%) | 67,113,113  | 2.24 | 18 (26%) |
| 14  | CLA  | G     | 819 | -    | 59,73,73     | 2.25 | 15 (25%) | 67,113,113  | 2.35 | 18 (26%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | B     | 835 | -    | 36,53,73     | 2.66 | 16 (44%) | 39,89,113   | 2.58 | 14 (35%) |
| 17  | BCR  | H     | 848 | -    | 41,41,41     | 2.77 | 6 (14%)  | 56,56,56    | 7.05 | 28 (50%) |
| 14  | CLA  | G     | 842 | -    | 59,73,73     | 2.16 | 16 (27%) | 67,113,113  | 1.93 | 17 (25%) |
| 17  | BCR  | K     | 102 | -    | 41,41,41     | 2.78 | 6 (14%)  | 56,56,56    | 7.21 | 24 (42%) |
| 16  | SF4  | G     | 845 | 1,2  | 0,12,12      | 0.00 | -        | -           |      |          |
| 14  | CLA  | Y     | 819 | -    | 59,73,73     | 2.18 | 16 (27%) | 67,113,113  | 2.21 | 15 (22%) |
| 14  | CLA  | G     | 827 | -    | 59,73,73     | 2.17 | 15 (25%) | 67,113,113  | 1.92 | 17 (25%) |
| 14  | CLA  | A     | 813 | -    | 54,68,73     | 2.26 | 15 (27%) | 61,107,113  | 2.30 | 18 (29%) |
| 17  | BCR  | Y     | 849 | -    | 41,41,41     | 2.74 | 6 (14%)  | 56,56,56    | 7.20 | 24 (42%) |
| 14  | CLA  | G     | 843 | 18   | 44,58,73     | 2.54 | 16 (36%) | 49,95,113   | 2.46 | 18 (36%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | H     | 808  | 2    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | B     | 817  | -    | 3/3/20/25 | 9/37/135/135  | -       |
| 14  | CLA  | B     | 833  | -    | 3/3/18/25 | 10/25/123/135 | -       |
| 14  | CLA  | H     | 820  | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | Y     | 810  | -    | 3/3/16/25 | 7/11/111/135  | -       |
| 14  | CLA  | Y     | 827  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | A     | 852  | -    | 3/3/20/25 | 11/37/135/135 | -       |
| 14  | CLA  | A     | 826  | -    | 3/3/19/25 | 11/31/129/135 | -       |
| 14  | CLA  | Y     | 835  | -    | 3/3/18/25 | 9/25/123/135  | -       |
| 18  | LHG  | Y     | 852  | -    | -         | 27/53/53/53   | -       |
| 14  | CLA  | Z     | 808  | 2    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | B     | 841  | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 17  | BCR  | M     | 101  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | H     | 817  | -    | 3/3/19/25 | 13/31/129/135 | -       |
| 14  | CLA  | H     | 818  | -    | 3/3/19/25 | 16/31/129/135 | -       |
| 14  | CLA  | H     | 831  | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 17  | BCR  | U     | 1005 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 832  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 17  | BCR  | G     | 846  | -    | -         | 7/29/63/63    | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | G     | 824  | -    | 3/3/19/25 | 16/31/129/135 | -       |
| 14  | CLA  | d     | 202  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 14  | CLA  | B     | 802  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | Z     | 831  | -    | 3/3/18/25 | 12/25/123/135 | -       |
| 14  | CLA  | B     | 838  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | H     | 804  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 17  | BCR  | e     | 101  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | Y     | 855  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | G     | 839  | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | H     | 813  | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 17  | BCR  | Z     | 846  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 837  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | L     | 205  | 10   | 3/3/20/25 | 24/37/135/135 | -       |
| 14  | CLA  | F     | 202  | -    | 3/3/16/25 | 2/11/111/135  | -       |
| 15  | PQN  | Y     | 844  | -    | -         | 6/23/43/43    | 0/2/2/2 |
| 14  | CLA  | Y     | 830  | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | Y     | 825  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 17  | BCR  | Z     | 843  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | W     | 1701 | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 14  | CLA  | G     | 813  | -    | 3/3/19/25 | 10/31/129/135 | -       |
| 14  | CLA  | Y     | 840  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | B     | 837  | -    | 3/3/19/25 | 8/31/129/135  | -       |
| 14  | CLA  | U     | 1003 | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 17  | BCR  | H     | 845  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 834  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 18  | LHG  | G     | 852  | 14   | -         | 15/36/36/53   | -       |
| 14  | CLA  | A     | 836  | -    | 3/3/17/25 | 7/19/117/135  | -       |
| 17  | BCR  | J     | 103  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | U     | 1002 | 10   | 3/3/20/25 | 25/37/135/135 | -       |
| 14  | CLA  | A     | 812  | -    | 3/3/17/25 | 11/24/122/135 | -       |
| 17  | BCR  | A     | 847  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | BCR  | G     | 854  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | H     | 805  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 17  | BCR  | Y     | 846  | -    | -         | 9/29/63/63    | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 18  | LHG  | A     | 850  | -    | -         | 28/53/53/53   | -       |
| 14  | CLA  | G     | 816  | -    | 3/3/17/25 | 9/19/117/135  | -       |
| 14  | CLA  | G     | 836  | -    | 3/3/17/25 | 9/19/117/135  | -       |
| 14  | CLA  | A     | 820  | -    | 3/3/19/25 | 15/31/129/135 | -       |
| 17  | BCR  | d     | 203  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 817  | -    | 3/3/19/25 | 9/31/129/135  | -       |
| 16  | SF4  | N     | 102  | 3,21 | -         | -             | 0/6/5/5 |
| 14  | CLA  | H     | 807  | -    | 3/3/20/25 | 9/37/135/135  | -       |
| 14  | CLA  | Y     | 811  | 14   | 3/3/20/25 | 21/37/135/135 | -       |
| 14  | CLA  | Y     | 838  | -    | 3/3/20/25 | 22/37/135/135 | -       |
| 14  | CLA  | H     | 815  | -    | 3/3/18/25 | 11/25/123/135 | -       |
| 14  | CLA  | B     | 825  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | Y     | 812  | -    | 3/3/18/25 | 12/25/123/135 | -       |
| 18  | LHG  | j     | 101  | -    | -         | 16/32/32/53   | -       |
| 14  | CLA  | J     | 102  | -    | 3/3/18/25 | 14/25/123/135 | -       |
| 17  | BCR  | B     | 844  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | S     | 1102 | 8    | 3/3/16/25 | 6/11/111/135  | -       |
| 17  | BCR  | H     | 841  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 17  | BCR  | A     | 845  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 807  | -    | 3/3/17/25 | 9/21/119/135  | -       |
| 14  | CLA  | B     | 809  | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 18  | LHG  | A     | 851  | 14   | -         | 17/36/36/53   | -       |
| 14  | CLA  | H     | 802  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | Y     | 820  | -    | 3/3/19/25 | 14/31/129/135 | -       |
| 17  | BCR  | G     | 849  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 17  | BCR  | H     | 842  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 17  | BCR  | Y     | 851  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | T     | 101  | -    | 3/3/14/25 | 5/5/101/135   | -       |
| 14  | CLA  | U     | 1006 | 2    | 3/3/20/25 | 16/37/135/135 | -       |
| 14  | CLA  | Y     | 834  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | Z     | 832  | -    | 3/3/16/25 | 7/11/111/135  | -       |
| 14  | CLA  | Z     | 833  | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 17  | BCR  | A     | 849  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 825  | -    | 3/3/20/25 | 15/37/135/135 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17  | BCR  | Y     | 856  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 821  | -    | 3/3/18/25 | 9/25/123/135  | -       |
| 14  | CLA  | L     | 207  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | B     | 819  | -    | 3/3/19/25 | 19/31/129/135 | -       |
| 14  | CLA  | G     | 809  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 17  | BCR  | B     | 848  | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 16  | SF4  | a     | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | A     | 841  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | G     | 834  | -    | 3/3/18/25 | 8/25/123/135  | -       |
| 14  | CLA  | A     | 816  | -    | 3/3/17/25 | 10/19/117/135 | -       |
| 14  | CLA  | Z     | 837  | -    | 3/3/16/25 | 2/11/111/135  | -       |
| 14  | CLA  | A     | 815  | -    | 3/3/17/25 | 9/19/117/135  | -       |
| 14  | CLA  | H     | 823  | 2    | 3/3/18/25 | 10/25/123/135 | -       |
| 14  | CLA  | B     | 801  | -    | 3/3/20/25 | 21/37/135/135 | -       |
| 17  | BCR  | h     | 202  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | H     | 824  | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | Y     | 833  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | H     | 835  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 14  | CLA  | G     | 806  | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 14  | CLA  | Z     | 814  | -    | 3/3/18/25 | 12/25/123/135 | -       |
| 14  | CLA  | A     | 804  | 14   | 3/3/18/25 | 14/30/128/135 | -       |
| 14  | CLA  | A     | 829  | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | G     | 812  | -    | 3/3/17/25 | 12/24/122/135 | -       |
| 14  | CLA  | Y     | 808  | 1    | 3/3/20/25 | 21/37/135/135 | -       |
| 14  | CLA  | H     | 832  | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 14  | CLA  | G     | 822  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | Z     | 807  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | U     | 1004 | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 17  | BCR  | J     | 104  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 827  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 17  | BCR  | Y     | 848  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 19  | LMG  | Z     | 847  | -    | -         | 16/44/64/70   | 0/1/1/1 |
| 14  | CLA  | G     | 804  | -    | 3/3/18/25 | 12/30/128/135 | -       |
| 14  | CLA  | Y     | 802  | -    | 3/3/20/25 | 9/37/135/135  | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | G     | 811  | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | B     | 811  | -    | 3/3/18/25 | 15/25/123/135 | -       |
| 14  | CLA  | H     | 838  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 17  | BCR  | L     | 203  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 13  | CL0  | G     | 801  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | B     | 804  | -    | 3/3/20/25 | 8/37/135/135  | -       |
| 17  | BCR  | f     | 103  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | Z     | 812  | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | j     | 102  | -    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | L     | 206  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 18  | LHG  | Y     | 853  | 14   | -         | 20/28/28/53   | -       |
| 14  | CLA  | A     | 838  | -    | 3/3/17/25 | 9/19/117/135  | -       |
| 14  | CLA  | Z     | 830  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 18  | LHG  | H     | 847  | -    | -         | 18/41/41/53   | -       |
| 14  | CLA  | B     | 832  | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 14  | CLA  | H     | 809  | 2    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | S     | 1103 | -    | 3/3/18/25 | 14/25/123/135 | -       |
| 17  | BCR  | f     | 104  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | T     | 103  | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | H     | 833  | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 17  | BCR  | Y     | 850  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | BCR  | R     | 101  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | B     | 810  | 2    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | Y     | 822  | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | H     | 803  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 17  | BCR  | B     | 851  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 837  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | J     | 101  | 8    | 3/3/16/25 | 5/11/111/135  | -       |
| 15  | PQN  | G     | 844  | -    | -         | 10/23/43/43   | 0/2/2/2 |
| 14  | CLA  | Y     | 832  | -    | 3/3/20/25 | 22/37/135/135 | -       |
| 14  | CLA  | A     | 827  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | H     | 830  | -    | 3/3/18/25 | 12/25/123/135 | -       |
| 14  | CLA  | Y     | 818  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 14  | CLA  | A     | 809  | 1    | 3/3/20/25 | 17/37/135/135 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | B     | 813 | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | G     | 840 | -    | 3/3/17/25 | 4/19/117/135  | -       |
| 14  | CLA  | Z     | 806 | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | Z     | 834 | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 14  | CLA  | B     | 806 | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | Z     | 809 | -    | 3/3/18/25 | 10/25/123/135 | -       |
| 14  | CLA  | G     | 808 | 1    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | G     | 832 | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | B     | 818 | -    | 3/3/19/25 | 10/31/129/135 | -       |
| 14  | CLA  | Y     | 821 | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | Z     | 828 | -    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | B     | 812 | -    | 3/3/17/25 | 9/19/117/135  | -       |
| 14  | CLA  | H     | 806 | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | G     | 810 | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 14  | CLA  | A     | 830 | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | G     | 841 | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | A     | 805 | -    | 3/3/20/25 | 22/37/135/135 | -       |
| 14  | CLA  | Z     | 817 | -    | 3/3/19/25 | 15/31/129/135 | -       |
| 14  | CLA  | G     | 820 | -    | 3/3/19/25 | 15/31/129/135 | -       |
| 14  | CLA  | Y     | 814 | -    | 3/3/18/25 | 11/25/123/135 | -       |
| 14  | CLA  | h     | 201 | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | Z     | 819 | -    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | B     | 827 | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 17  | BCR  | B     | 847 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 17  | BCR  | G     | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | Y     | 815 | -    | 3/3/17/25 | 10/19/117/135 | -       |
| 14  | CLA  | B     | 803 | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 14  | CLA  | B     | 824 | 2    | 3/3/18/25 | 10/25/123/135 | -       |
| 14  | CLA  | B     | 821 | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 17  | BCR  | Z     | 841 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 842 | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | Z     | 804 | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | H     | 812 | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | A     | 821 | -    | 3/3/20/25 | 16/37/135/135 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | G     | 830  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 15  | PQN  | H     | 839  | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 13  | CL0  | A     | 801  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | A     | 802  | -    | 3/3/20/25 | 11/37/135/135 | -       |
| 18  | LHG  | B     | 850  | -    | -         | 24/43/43/53   | -       |
| 17  | BCR  | L     | 208  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 831  | -    | 3/3/17/25 | 5/19/117/135  | -       |
| 14  | CLA  | Y     | 823  | -    | 3/3/17/25 | 6/19/117/135  | -       |
| 17  | BCR  | f     | 105  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 822  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 17  | BCR  | Y     | 847  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 839  | -    | 3/3/17/25 | 4/19/117/135  | -       |
| 19  | LMG  | B     | 849  | -    | -         | 14/47/67/70   | 0/1/1/1 |
| 17  | BCR  | Z     | 845  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | Y     | 839  | -    | 3/3/17/25 | 11/19/117/135 | -       |
| 17  | BCR  | B     | 845  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 825  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | Y     | 816  | -    | 3/3/17/25 | 5/19/117/135  | -       |
| 14  | CLA  | Q     | 201  | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 17  | BCR  | G     | 850  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | K     | 101  | -    | 3/3/14/25 | 5/5/101/135   | -       |
| 14  | CLA  | L     | 201  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | A     | 833  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | H     | 829  | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | A     | 824  | -    | 3/3/19/25 | 17/31/129/135 | -       |
| 14  | CLA  | L     | 202  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 14  | CLA  | Z     | 803  | -    | 3/3/17/25 | 9/24/122/135  | -       |
| 14  | CLA  | G     | 835  | 1    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | Y     | 826  | -    | 3/3/19/25 | 7/31/129/135  | -       |
| 14  | CLA  | Y     | 804  | 14   | 3/3/18/25 | 15/30/128/135 | -       |
| 14  | CLA  | d     | 201  | -    | 3/3/17/25 | 4/19/117/135  | -       |
| 17  | BCR  | Q     | 204  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | BCR  | V     | 1202 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | Z     | 825  | -    | 3/3/20/25 | 15/37/135/135 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | Y     | 837  | -    | 3/3/17/25 | 7/19/117/135  | -       |
| 14  | CLA  | Z     | 818  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 14  | CLA  | A     | 814  | -    | 3/3/17/25 | 9/19/117/135  | -       |
| 17  | BCR  | U     | 1008 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 803  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | Y     | 813  | -    | 3/3/19/25 | 10/31/129/135 | -       |
| 14  | CLA  | S     | 1101 | -    | 3/3/20/25 | 23/37/135/135 | -       |
| 17  | BCR  | F     | 203  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 820  | -    | 3/3/16/25 | 2/11/111/135  | -       |
| 17  | BCR  | U     | 1007 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 833  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | Z     | 838  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | Z     | 811  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | H     | 822  | -    | 3/3/19/25 | 13/31/129/135 | -       |
| 17  | BCR  | G     | 848  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 829  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 16  | SF4  | C     | 101  | 3,21 | -         | -             | 0/6/5/5 |
| 17  | BCR  | H     | 843  | -    | -         | 7/18/35/63    | 0/1/1/2 |
| 14  | CLA  | Y     | 806  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | h     | 207  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | Y     | 829  | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | G     | 853  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 16  | SF4  | C     | 102  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | Z     | 823  | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | h     | 205  | 10   | 3/3/20/25 | 23/37/135/135 | -       |
| 17  | BCR  | A     | 846  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 803  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | Y     | 809  | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | B     | 830  | -    | 3/3/16/25 | 6/11/111/135  | -       |
| 14  | CLA  | Z     | 820  | -    | 3/3/18/25 | 8/25/123/135  | -       |
| 14  | CLA  | G     | 838  | -    | 3/3/17/25 | 3/19/117/135  | -       |
| 14  | CLA  | Y     | 841  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 17  | BCR  | B     | 843  | -    | -         | 3/24/41/63    | 0/1/1/2 |
| 14  | CLA  | Z     | 822  | 2    | 3/3/18/25 | 10/25/123/135 | -       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 15  | PQN  | B     | 842  | -    | -         | 12/23/43/43   | 0/2/2/2 |
| 14  | CLA  | Y     | 842  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | A     | 819  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | V     | 1201 | -    | 3/3/17/25 | 9/24/122/135  | -       |
| 14  | CLA  | A     | 840  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | G     | 821  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 14  | CLA  | H     | 834  | -    | 3/3/19/25 | 11/31/129/135 | -       |
| 16  | SF4  | A     | 844  | 1,2  | -         | -             | 0/6/5/5 |
| 14  | CLA  | B     | 814  | -    | 3/3/20/25 | 22/37/135/135 | -       |
| 14  | CLA  | Y     | 805  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | Q     | 203  | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | Y     | 854  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | Z     | 821  | -    | 3/3/19/25 | 14/31/129/135 | -       |
| 16  | SF4  | N     | 101  | 3    | -         | -             | 0/6/5/5 |
| 17  | BCR  | A     | 848  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 828  | -    | 3/3/20/25 | 11/37/135/135 | -       |
| 14  | CLA  | H     | 836  | -    | 3/3/16/25 | 1/11/111/135  | -       |
| 17  | BCR  | Z     | 842  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 808  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | B     | 816  | -    | 3/3/18/25 | 9/25/123/135  | -       |
| 14  | CLA  | Z     | 839  | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | G     | 826  | -    | 3/3/19/25 | 16/31/129/135 | -       |
| 14  | CLA  | A     | 823  | -    | 3/3/17/25 | 8/19/117/135  | -       |
| 17  | BCR  | h     | 203  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | Z     | 802  | -    | 3/3/20/25 | 22/37/135/135 | -       |
| 14  | CLA  | B     | 822  | -    | 3/3/18/25 | 9/25/123/135  | -       |
| 14  | CLA  | Y     | 843  | 18   | 3/3/17/25 | 11/19/117/135 | -       |
| 14  | CLA  | B     | 839  | -    | 3/3/16/25 | 1/11/111/135  | -       |
| 14  | CLA  | A     | 808  | 1    | 3/3/20/25 | 23/37/135/135 | -       |
| 14  | CLA  | H     | 811  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 14  | CLA  | B     | 823  | -    | 3/3/19/25 | 15/31/129/135 | -       |
| 14  | CLA  | A     | 811  | 14   | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | Z     | 810  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 14  | CLA  | Y     | 803  | -    | 3/3/20/25 | 18/37/135/135 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | H     | 826  | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | B     | 807  | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 19  | LMG  | H     | 846  | -    | -         | 11/44/64/70   | 0/1/1/1 |
| 14  | CLA  | Z     | 816  | -    | 3/3/19/25 | 13/31/129/135 | -       |
| 14  | CLA  | B     | 836  | -    | 3/3/16/25 | 2/11/111/135  | -       |
| 14  | CLA  | G     | 805  | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 17  | BCR  | i     | 101  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | H     | 828  | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | B     | 831  | -    | 3/3/16/25 | 8/11/111/135  | -       |
| 14  | CLA  | f     | 102  | -    | 3/3/18/25 | 15/25/123/135 | -       |
| 14  | CLA  | Z     | 824  | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | Z     | 835  | -    | 3/3/19/25 | 11/31/129/135 | -       |
| 14  | CLA  | B     | 826  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 15  | PQN  | A     | 843  | -    | -         | 5/23/43/43    | 0/2/2/2 |
| 14  | CLA  | A     | 835  | 1    | 3/3/16/25 | 4/11/111/135  | -       |
| 17  | BCR  | L     | 209  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 815  | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | Z     | 813  | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 17  | BCR  | F     | 201  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 14  | CLA  | X     | 1701 | -    | 3/3/16/25 | 3/11/111/135  | -       |
| 14  | CLA  | A     | 806  | -    | 3/3/20/25 | 21/37/135/135 | -       |
| 14  | CLA  | B     | 829  | -    | 3/3/20/25 | 11/37/135/135 | -       |
| 14  | CLA  | Y     | 828  | -    | 3/3/20/25 | 16/37/135/135 | -       |
| 17  | BCR  | H     | 844  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | Z     | 826  | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | B     | 805  | -    | 3/3/17/25 | 10/24/122/135 | -       |
| 14  | CLA  | G     | 815  | -    | 3/3/17/25 | 6/19/117/135  | -       |
| 14  | CLA  | g     | 102  | -    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | G     | 831  | -    | 3/3/17/25 | 8/19/117/135  | -       |
| 14  | CLA  | H     | 810  | -    | 3/3/18/25 | 13/25/123/135 | -       |
| 17  | BCR  | H     | 840  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 823  | -    | 3/3/17/25 | 6/19/117/135  | -       |
| 14  | CLA  | Y     | 807  | -    | 3/3/17/25 | 11/21/119/135 | -       |
| 17  | BCR  | S     | 1104 | -    | -         | 11/29/63/63   | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | K     | 103 | -    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | Z     | 829 | -    | 3/3/16/25 | 7/11/111/135  | -       |
| 14  | CLA  | B     | 840 | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 14  | CLA  | Z     | 801 | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 14  | CLA  | H     | 814 | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | Y     | 824 | -    | 3/3/19/25 | 20/31/129/135 | -       |
| 14  | CLA  | A     | 837 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 17  | BCR  | Q     | 202 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | H     | 819 | -    | 3/3/16/25 | 7/11/111/135  | -       |
| 14  | CLA  | Z     | 815 | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 16  | SF4  | a     | 102 | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | g     | 101 | -    | 3/3/14/25 | 3/5/101/135   | -       |
| 14  | CLA  | H     | 801 | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | H     | 816 | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 17  | BCR  | T     | 102 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 17  | BCR  | B     | 846 | -    | -         | 3/18/35/63    | 0/1/1/2 |
| 14  | CLA  | G     | 802 | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 14  | CLA  | G     | 818 | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 14  | CLA  | A     | 818 | -    | 3/3/20/25 | 23/37/135/135 | -       |
| 14  | CLA  | Z     | 827 | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | A     | 842 | 18   | 3/3/17/25 | 10/19/117/135 | -       |
| 17  | BCR  | I     | 101 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | f     | 101 | 8    | 3/3/16/25 | 5/11/111/135  | -       |
| 14  | CLA  | Y     | 817 | -    | 3/3/19/25 | 9/31/129/135  | -       |
| 13  | CL0  | Y     | 801 | -    | 3/3/20/25 | 14/37/135/135 | -       |
| 14  | CLA  | A     | 817 | -    | 3/3/19/25 | 15/31/129/135 | -       |
| 14  | CLA  | Z     | 836 | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 18  | LHG  | G     | 851 | -    | -         | 28/53/53/53   | -       |
| 14  | CLA  | G     | 814 | -    | 3/3/17/25 | 3/19/117/135  | -       |
| 14  | CLA  | A     | 810 | -    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | A     | 828 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | Y     | 836 | 1    | 3/3/16/25 | 4/11/111/135  | -       |
| 14  | CLA  | h     | 206 | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 14  | CLA  | H     | 825 | -    | 3/3/20/25 | 11/37/135/135 | -       |

*Continued on next page...*

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | A     | 834 | -    | 3/3/18/25 | 9/25/123/135  | -       |
| 14  | CLA  | Y     | 831 | -    | 3/3/17/25 | 3/19/117/135  | -       |
| 14  | CLA  | Z     | 805 | -    | 3/3/20/25 | 19/37/135/135 | -       |
| 15  | PQN  | Z     | 840 | -    | -         | 10/23/43/43   | 0/2/2/2 |
| 17  | BCR  | R     | 102 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 807 | -    | 3/3/17/25 | 10/21/119/135 | -       |
| 17  | BCR  | Z     | 844 | -    | -         | 8/18/35/63    | 0/1/1/2 |
| 14  | CLA  | B     | 828 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | G     | 819 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 14  | CLA  | B     | 835 | -    | 3/3/16/25 | 2/11/111/135  | -       |
| 17  | BCR  | H     | 848 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 16  | SF4  | Y     | 845 | 1,2  | -         | -             | 0/6/5/5 |
| 17  | BCR  | K     | 102 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 16  | SF4  | G     | 845 | 1,2  | -         | -             | 0/6/5/5 |
| 14  | CLA  | Y     | 819 | -    | 3/3/20/25 | 20/37/135/135 | -       |
| 14  | CLA  | G     | 827 | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 14  | CLA  | A     | 813 | -    | 3/3/19/25 | 10/31/129/135 | -       |
| 17  | BCR  | Y     | 849 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 843 | 18   | 3/3/17/25 | 8/19/117/135  | -       |

All (4609) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | A     | 801 | CL0  | MG-NA   | 9.56  | 2.29        | 2.06     |
| 13  | G     | 801 | CL0  | MG-NA   | 9.35  | 2.28        | 2.06     |
| 17  | G     | 854 | BCR  | C10-C9  | -8.86 | 1.24        | 1.35     |
| 15  | Y     | 844 | PQN  | C3-C2   | 8.79  | 1.51        | 1.35     |
| 17  | L     | 208 | BCR  | C10-C9  | -8.72 | 1.24        | 1.35     |
| 17  | H     | 841 | BCR  | C11-C10 | -8.66 | 1.16        | 1.43     |
| 17  | G     | 854 | BCR  | C11-C10 | -8.61 | 1.16        | 1.43     |
| 13  | Y     | 801 | CL0  | MG-NA   | 8.54  | 2.26        | 2.06     |
| 17  | f     | 104 | BCR  | C8-C9   | -8.51 | 1.27        | 1.45     |
| 17  | B     | 843 | BCR  | C11-C10 | -8.50 | 1.17        | 1.43     |
| 17  | Y     | 851 | BCR  | C11-C10 | -8.50 | 1.17        | 1.43     |
| 17  | L     | 203 | BCR  | C8-C9   | -8.48 | 1.27        | 1.45     |
| 17  | H     | 841 | BCR  | C10-C9  | -8.47 | 1.24        | 1.35     |
| 17  | i     | 101 | BCR  | C11-C10 | -8.47 | 1.17        | 1.43     |
| 17  | f     | 104 | BCR  | C10-C9  | -8.47 | 1.24        | 1.35     |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | R     | 102  | BCR  | C11-C10 | -8.43 | 1.17        | 1.43     |
| 17  | G     | 854  | BCR  | C8-C9   | -8.39 | 1.27        | 1.45     |
| 17  | B     | 843  | BCR  | C10-C9  | -8.38 | 1.24        | 1.35     |
| 17  | B     | 847  | BCR  | C11-C10 | -8.37 | 1.17        | 1.43     |
| 17  | L     | 208  | BCR  | C8-C9   | -8.32 | 1.28        | 1.45     |
| 17  | f     | 104  | BCR  | C11-C10 | -8.29 | 1.17        | 1.43     |
| 17  | h     | 203  | BCR  | C20-C21 | -8.29 | 1.17        | 1.43     |
| 17  | G     | 846  | BCR  | C20-C21 | -8.26 | 1.17        | 1.43     |
| 17  | H     | 844  | BCR  | C11-C10 | -8.26 | 1.17        | 1.43     |
| 17  | L     | 208  | BCR  | C11-C10 | -8.25 | 1.17        | 1.43     |
| 17  | Y     | 856  | BCR  | C8-C9   | -8.24 | 1.28        | 1.45     |
| 17  | U     | 1007 | BCR  | C11-C10 | -8.22 | 1.18        | 1.43     |
| 17  | Y     | 851  | BCR  | C8-C9   | -8.21 | 1.28        | 1.45     |
| 17  | h     | 203  | BCR  | C11-C10 | -8.20 | 1.18        | 1.43     |
| 17  | L     | 208  | BCR  | C20-C21 | -8.20 | 1.18        | 1.43     |
| 17  | M     | 101  | BCR  | C11-C10 | -8.19 | 1.18        | 1.43     |
| 17  | J     | 104  | BCR  | C11-C10 | -8.19 | 1.18        | 1.43     |
| 17  | Q     | 202  | BCR  | C11-C10 | -8.19 | 1.18        | 1.43     |
| 17  | B     | 847  | BCR  | C10-C9  | -8.19 | 1.24        | 1.35     |
| 17  | H     | 840  | BCR  | C11-C10 | -8.18 | 1.18        | 1.43     |
| 17  | R     | 102  | BCR  | C10-C9  | -8.16 | 1.25        | 1.35     |
| 17  | R     | 102  | BCR  | C20-C21 | -8.16 | 1.18        | 1.43     |
| 17  | Z     | 841  | BCR  | C8-C9   | -8.14 | 1.28        | 1.45     |
| 17  | B     | 843  | BCR  | C8-C9   | -8.11 | 1.28        | 1.45     |
| 17  | Y     | 849  | BCR  | C11-C10 | -8.10 | 1.18        | 1.43     |
| 17  | A     | 847  | BCR  | C11-C10 | -8.09 | 1.18        | 1.43     |
| 17  | V     | 1202 | BCR  | C8-C9   | -8.08 | 1.28        | 1.45     |
| 17  | Z     | 841  | BCR  | C11-C10 | -8.08 | 1.18        | 1.43     |
| 17  | Q     | 202  | BCR  | C10-C9  | -8.07 | 1.25        | 1.35     |
| 17  | H     | 845  | BCR  | C20-C21 | -8.07 | 1.18        | 1.43     |
| 17  | h     | 203  | BCR  | C16-C17 | -8.07 | 1.18        | 1.43     |
| 17  | H     | 841  | BCR  | C8-C9   | -8.06 | 1.28        | 1.45     |
| 17  | H     | 848  | BCR  | C11-C10 | -8.06 | 1.18        | 1.43     |
| 17  | S     | 1104 | BCR  | C11-C10 | -8.05 | 1.18        | 1.43     |
| 17  | Y     | 851  | BCR  | C10-C9  | -8.04 | 1.25        | 1.35     |
| 17  | B     | 848  | BCR  | C8-C9   | -8.04 | 1.28        | 1.45     |
| 17  | h     | 203  | BCR  | C10-C9  | -8.04 | 1.25        | 1.35     |
| 17  | L     | 209  | BCR  | C11-C10 | -8.04 | 1.18        | 1.43     |
| 17  | B     | 844  | BCR  | C11-C10 | -8.04 | 1.18        | 1.43     |
| 17  | R     | 101  | BCR  | C10-C9  | -8.04 | 1.25        | 1.35     |
| 17  | S     | 1104 | BCR  | C10-C9  | -8.04 | 1.25        | 1.35     |
| 17  | B     | 851  | BCR  | C11-C10 | -8.02 | 1.18        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | G     | 847  | BCR  | C11-C10 | -8.00 | 1.18        | 1.43     |
| 17  | R     | 102  | BCR  | C16-C17 | -8.00 | 1.18        | 1.43     |
| 17  | H     | 841  | BCR  | C20-C21 | -7.99 | 1.18        | 1.43     |
| 17  | V     | 1202 | BCR  | C11-C10 | -7.98 | 1.18        | 1.43     |
| 14  | B     | 835  | CLA  | MG-NA   | 7.98  | 2.25        | 2.06     |
| 17  | Z     | 842  | BCR  | C20-C21 | -7.98 | 1.18        | 1.43     |
| 17  | G     | 849  | BCR  | C10-C9  | -7.98 | 1.25        | 1.35     |
| 14  | Y     | 833  | CLA  | MG-NA   | 7.95  | 2.25        | 2.06     |
| 17  | H     | 842  | BCR  | C20-C21 | -7.95 | 1.18        | 1.43     |
| 17  | J     | 104  | BCR  | C10-C9  | -7.94 | 1.25        | 1.35     |
| 17  | Q     | 202  | BCR  | C8-C9   | -7.93 | 1.28        | 1.45     |
| 14  | G     | 838  | CLA  | MG-NA   | 7.92  | 2.25        | 2.06     |
| 14  | G     | 817  | CLA  | MG-NA   | 7.91  | 2.25        | 2.06     |
| 17  | Q     | 204  | BCR  | C11-C10 | -7.90 | 1.19        | 1.43     |
| 17  | Y     | 856  | BCR  | C20-C21 | -7.89 | 1.19        | 1.43     |
| 17  | Z     | 844  | BCR  | C20-C21 | -7.89 | 1.19        | 1.43     |
| 17  | J     | 104  | BCR  | C8-C9   | -7.89 | 1.29        | 1.45     |
| 14  | Y     | 822  | CLA  | MG-NA   | 7.88  | 2.25        | 2.06     |
| 17  | Y     | 850  | BCR  | C11-C10 | -7.88 | 1.19        | 1.43     |
| 17  | L     | 203  | BCR  | C10-C9  | -7.87 | 1.25        | 1.35     |
| 17  | L     | 203  | BCR  | C20-C21 | -7.87 | 1.19        | 1.43     |
| 17  | J     | 104  | BCR  | C20-C21 | -7.86 | 1.19        | 1.43     |
| 17  | M     | 101  | BCR  | C8-C9   | -7.85 | 1.29        | 1.45     |
| 17  | F     | 201  | BCR  | C20-C21 | -7.85 | 1.19        | 1.43     |
| 17  | Y     | 851  | BCR  | C20-C21 | -7.85 | 1.19        | 1.43     |
| 14  | B     | 810  | CLA  | MG-NA   | 7.85  | 2.24        | 2.06     |
| 17  | i     | 101  | BCR  | C10-C9  | -7.84 | 1.25        | 1.35     |
| 17  | H     | 845  | BCR  | C8-C9   | -7.84 | 1.29        | 1.45     |
| 17  | e     | 101  | BCR  | C20-C21 | -7.83 | 1.19        | 1.43     |
| 14  | G     | 827  | CLA  | MG-NA   | 7.83  | 2.24        | 2.06     |
| 17  | H     | 840  | BCR  | C8-C9   | -7.82 | 1.29        | 1.45     |
| 14  | Y     | 817  | CLA  | MG-NA   | 7.82  | 2.24        | 2.06     |
| 17  | K     | 102  | BCR  | C11-C10 | -7.82 | 1.19        | 1.43     |
| 17  | L     | 203  | BCR  | C11-C10 | -7.82 | 1.19        | 1.43     |
| 17  | F     | 203  | BCR  | C11-C10 | -7.81 | 1.19        | 1.43     |
| 17  | R     | 101  | BCR  | C11-C10 | -7.81 | 1.19        | 1.43     |
| 17  | U     | 1005 | BCR  | C20-C21 | -7.80 | 1.19        | 1.43     |
| 17  | B     | 851  | BCR  | C8-C9   | -7.80 | 1.29        | 1.45     |
| 17  | B     | 847  | BCR  | C8-C9   | -7.80 | 1.29        | 1.45     |
| 14  | Y     | 825  | CLA  | MG-NA   | 7.80  | 2.24        | 2.06     |
| 14  | h     | 207  | CLA  | MG-NA   | 7.80  | 2.24        | 2.06     |
| 17  | h     | 203  | BCR  | C8-C9   | -7.79 | 1.29        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 829  | CLA  | MG-NA   | 7.79  | 2.24        | 2.06     |
| 14  | B     | 808  | CLA  | MG-NA   | 7.79  | 2.24        | 2.06     |
| 14  | H     | 818  | CLA  | MG-NA   | 7.78  | 2.24        | 2.06     |
| 14  | G     | 823  | CLA  | MG-NA   | 7.78  | 2.24        | 2.06     |
| 17  | G     | 848  | BCR  | C8-C9   | -7.78 | 1.29        | 1.45     |
| 17  | H     | 842  | BCR  | C11-C10 | -7.78 | 1.19        | 1.43     |
| 17  | H     | 841  | BCR  | C16-C17 | -7.77 | 1.19        | 1.43     |
| 17  | Z     | 841  | BCR  | C20-C21 | -7.77 | 1.19        | 1.43     |
| 17  | f     | 105  | BCR  | C8-C9   | -7.77 | 1.29        | 1.45     |
| 14  | T     | 103  | CLA  | MG-NA   | 7.77  | 2.24        | 2.06     |
| 17  | i     | 101  | BCR  | C8-C9   | -7.77 | 1.29        | 1.45     |
| 17  | G     | 849  | BCR  | C20-C21 | -7.77 | 1.19        | 1.43     |
| 14  | Y     | 803  | CLA  | MG-NA   | 7.77  | 2.24        | 2.06     |
| 17  | B     | 848  | BCR  | C20-C21 | -7.76 | 1.19        | 1.43     |
| 14  | G     | 822  | CLA  | MG-NA   | 7.76  | 2.24        | 2.06     |
| 17  | B     | 844  | BCR  | C20-C21 | -7.76 | 1.19        | 1.43     |
| 17  | U     | 1007 | BCR  | C8-C9   | -7.76 | 1.29        | 1.45     |
| 17  | U     | 1005 | BCR  | C11-C10 | -7.75 | 1.19        | 1.43     |
| 17  | J     | 104  | BCR  | C16-C17 | -7.75 | 1.19        | 1.43     |
| 14  | g     | 101  | CLA  | MG-NA   | 7.75  | 2.24        | 2.06     |
| 17  | Y     | 850  | BCR  | C20-C21 | -7.75 | 1.19        | 1.43     |
| 17  | B     | 845  | BCR  | C8-C9   | -7.74 | 1.29        | 1.45     |
| 14  | G     | 811  | CLA  | MG-NA   | 7.74  | 2.24        | 2.06     |
| 17  | Y     | 847  | BCR  | C11-C10 | -7.74 | 1.19        | 1.43     |
| 17  | G     | 849  | BCR  | C11-C10 | -7.74 | 1.19        | 1.43     |
| 17  | L     | 208  | BCR  | C16-C17 | -7.73 | 1.19        | 1.43     |
| 14  | X     | 1701 | CLA  | MG-NA   | 7.73  | 2.24        | 2.06     |
| 17  | f     | 105  | BCR  | C11-C10 | -7.73 | 1.19        | 1.43     |
| 14  | Y     | 823  | CLA  | MG-NA   | 7.73  | 2.24        | 2.06     |
| 17  | S     | 1104 | BCR  | C16-C17 | -7.73 | 1.19        | 1.43     |
| 14  | A     | 824  | CLA  | MG-NA   | 7.72  | 2.24        | 2.06     |
| 14  | G     | 807  | CLA  | MG-NA   | 7.72  | 2.24        | 2.06     |
| 14  | Y     | 827  | CLA  | MG-NA   | 7.72  | 2.24        | 2.06     |
| 17  | G     | 850  | BCR  | C20-C21 | -7.71 | 1.19        | 1.43     |
| 14  | B     | 837  | CLA  | MG-NA   | 7.71  | 2.24        | 2.06     |
| 17  | B     | 843  | BCR  | C16-C17 | -7.70 | 1.19        | 1.43     |
| 17  | S     | 1104 | BCR  | C20-C21 | -7.70 | 1.19        | 1.43     |
| 17  | L     | 203  | BCR  | C16-C17 | -7.70 | 1.19        | 1.43     |
| 14  | Y     | 831  | CLA  | MG-NA   | 7.69  | 2.24        | 2.06     |
| 17  | A     | 849  | BCR  | C8-C9   | -7.69 | 1.29        | 1.45     |
| 17  | F     | 201  | BCR  | C8-C9   | -7.69 | 1.29        | 1.45     |
| 17  | G     | 846  | BCR  | C11-C10 | -7.69 | 1.19        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | Z     | 840  | PQN  | C3-C2   | 7.68  | 1.49        | 1.35     |
| 17  | H     | 848  | BCR  | C20-C21 | -7.68 | 1.19        | 1.43     |
| 17  | G     | 850  | BCR  | C8-C9   | -7.68 | 1.29        | 1.45     |
| 17  | M     | 101  | BCR  | C20-C21 | -7.68 | 1.19        | 1.43     |
| 14  | B     | 839  | CLA  | MG-NA   | 7.67  | 2.24        | 2.06     |
| 14  | Z     | 820  | CLA  | MG-NA   | 7.67  | 2.24        | 2.06     |
| 14  | f     | 102  | CLA  | MG-NA   | 7.67  | 2.24        | 2.06     |
| 17  | G     | 847  | BCR  | C8-C9   | -7.67 | 1.29        | 1.45     |
| 17  | L     | 209  | BCR  | C20-C21 | -7.66 | 1.19        | 1.43     |
| 17  | H     | 840  | BCR  | C16-C17 | -7.66 | 1.19        | 1.43     |
| 14  | H     | 832  | CLA  | MG-NA   | 7.66  | 2.24        | 2.06     |
| 17  | f     | 104  | BCR  | C20-C21 | -7.65 | 1.19        | 1.43     |
| 17  | S     | 1104 | BCR  | C8-C9   | -7.65 | 1.29        | 1.45     |
| 17  | f     | 103  | BCR  | C11-C10 | -7.65 | 1.19        | 1.43     |
| 14  | B     | 831  | CLA  | MG-NA   | 7.65  | 2.24        | 2.06     |
| 17  | B     | 845  | BCR  | C11-C10 | -7.65 | 1.19        | 1.43     |
| 17  | e     | 101  | BCR  | C11-C10 | -7.64 | 1.19        | 1.43     |
| 14  | H     | 804  | CLA  | MG-NA   | 7.64  | 2.24        | 2.06     |
| 14  | L     | 205  | CLA  | MG-NA   | 7.64  | 2.24        | 2.06     |
| 14  | Z     | 817  | CLA  | MG-NA   | 7.64  | 2.24        | 2.06     |
| 14  | B     | 822  | CLA  | MG-NA   | 7.64  | 2.24        | 2.06     |
| 17  | R     | 101  | BCR  | C8-C9   | -7.64 | 1.29        | 1.45     |
| 17  | B     | 845  | BCR  | C20-C21 | -7.64 | 1.19        | 1.43     |
| 17  | Z     | 846  | BCR  | C11-C10 | -7.63 | 1.19        | 1.43     |
| 14  | F     | 202  | CLA  | MG-NA   | 7.63  | 2.24        | 2.06     |
| 17  | K     | 102  | BCR  | C20-C21 | -7.63 | 1.19        | 1.43     |
| 14  | H     | 833  | CLA  | MG-NA   | 7.63  | 2.24        | 2.06     |
| 17  | Z     | 845  | BCR  | C8-C9   | -7.62 | 1.29        | 1.45     |
| 17  | G     | 849  | BCR  | C16-C17 | -7.62 | 1.19        | 1.43     |
| 17  | F     | 201  | BCR  | C16-C17 | -7.62 | 1.19        | 1.43     |
| 14  | A     | 822  | CLA  | MG-NA   | 7.62  | 2.24        | 2.06     |
| 14  | Z     | 807  | CLA  | MG-NA   | 7.62  | 2.24        | 2.06     |
| 14  | S     | 1102 | CLA  | MG-NA   | 7.62  | 2.24        | 2.06     |
| 17  | H     | 848  | BCR  | C16-C17 | -7.62 | 1.19        | 1.43     |
| 17  | Z     | 841  | BCR  | C16-C17 | -7.61 | 1.19        | 1.43     |
| 14  | Y     | 843  | CLA  | MG-NA   | 7.61  | 2.24        | 2.06     |
| 14  | Y     | 835  | CLA  | MG-NA   | 7.60  | 2.24        | 2.06     |
| 14  | A     | 833  | CLA  | MG-NA   | 7.60  | 2.24        | 2.06     |
| 17  | G     | 846  | BCR  | C16-C17 | -7.60 | 1.19        | 1.43     |
| 14  | B     | 823  | CLA  | MG-NA   | 7.60  | 2.24        | 2.06     |
| 14  | A     | 812  | CLA  | MG-NA   | 7.59  | 2.24        | 2.06     |
| 14  | B     | 826  | CLA  | MG-NA   | 7.59  | 2.24        | 2.06     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | B     | 843  | BCR  | C20-C21 | -7.59 | 1.19        | 1.43     |
| 17  | K     | 102  | BCR  | C16-C17 | -7.59 | 1.19        | 1.43     |
| 14  | Y     | 806  | CLA  | MG-NA   | 7.59  | 2.24        | 2.06     |
| 14  | h     | 201  | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | Z     | 838  | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | K     | 101  | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | B     | 813  | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 14  | G     | 841  | CLA  | MG-NA   | 7.58  | 2.24        | 2.06     |
| 17  | Z     | 841  | BCR  | C10-C9  | -7.57 | 1.25        | 1.35     |
| 14  | W     | 1701 | CLA  | MG-NA   | 7.57  | 2.24        | 2.06     |
| 14  | Z     | 812  | CLA  | MG-NA   | 7.57  | 2.24        | 2.06     |
| 14  | Y     | 813  | CLA  | MG-NA   | 7.56  | 2.24        | 2.06     |
| 14  | Y     | 807  | CLA  | MG-NA   | 7.56  | 2.24        | 2.06     |
| 14  | Z     | 818  | CLA  | MG-NA   | 7.56  | 2.24        | 2.06     |
| 14  | Z     | 821  | CLA  | MG-NA   | 7.56  | 2.24        | 2.06     |
| 17  | A     | 847  | BCR  | C8-C9   | -7.56 | 1.29        | 1.45     |
| 14  | Z     | 839  | CLA  | MG-NA   | 7.56  | 2.24        | 2.06     |
| 14  | G     | 816  | CLA  | MG-NA   | 7.56  | 2.24        | 2.06     |
| 14  | A     | 838  | CLA  | MG-NA   | 7.55  | 2.24        | 2.06     |
| 17  | G     | 850  | BCR  | C11-C10 | -7.55 | 1.20        | 1.43     |
| 14  | Z     | 825  | CLA  | MG-NA   | 7.55  | 2.24        | 2.06     |
| 17  | G     | 848  | BCR  | C11-C10 | -7.55 | 1.20        | 1.43     |
| 17  | H     | 840  | BCR  | C20-C21 | -7.55 | 1.20        | 1.43     |
| 17  | d     | 203  | BCR  | C8-C9   | -7.55 | 1.29        | 1.45     |
| 17  | G     | 847  | BCR  | C16-C17 | -7.54 | 1.20        | 1.43     |
| 17  | G     | 847  | BCR  | C20-C21 | -7.54 | 1.20        | 1.43     |
| 15  | A     | 843  | PQN  | C3-C2   | 7.54  | 1.49        | 1.35     |
| 14  | Y     | 829  | CLA  | MG-NA   | 7.54  | 2.24        | 2.06     |
| 14  | G     | 836  | CLA  | MG-NA   | 7.54  | 2.24        | 2.06     |
| 17  | Z     | 846  | BCR  | C8-C9   | -7.53 | 1.29        | 1.45     |
| 17  | H     | 844  | BCR  | C8-C9   | -7.53 | 1.29        | 1.45     |
| 14  | Z     | 822  | CLA  | MG-NA   | 7.53  | 2.24        | 2.06     |
| 14  | L     | 207  | CLA  | MG-NA   | 7.53  | 2.24        | 2.06     |
| 14  | H     | 812  | CLA  | MG-NA   | 7.53  | 2.24        | 2.06     |
| 14  | G     | 812  | CLA  | MG-NA   | 7.53  | 2.24        | 2.06     |
| 17  | Y     | 850  | BCR  | C16-C17 | -7.53 | 1.20        | 1.43     |
| 17  | J     | 103  | BCR  | C8-C9   | -7.53 | 1.29        | 1.45     |
| 17  | H     | 845  | BCR  | C11-C10 | -7.53 | 1.20        | 1.43     |
| 14  | B     | 814  | CLA  | MG-NA   | 7.52  | 2.24        | 2.06     |
| 17  | Y     | 847  | BCR  | C20-C21 | -7.52 | 1.20        | 1.43     |
| 17  | U     | 1007 | BCR  | C20-C21 | -7.52 | 1.20        | 1.43     |
| 14  | H     | 821  | CLA  | MG-NA   | 7.52  | 2.24        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 808  | CLA  | MG-NA   | 7.51  | 2.24        | 2.06     |
| 17  | B     | 847  | BCR  | C20-C21 | -7.51 | 1.20        | 1.43     |
| 14  | H     | 807  | CLA  | MG-NA   | 7.51  | 2.24        | 2.06     |
| 17  | B     | 851  | BCR  | C10-C9  | -7.51 | 1.25        | 1.35     |
| 14  | J     | 101  | CLA  | MG-NA   | 7.50  | 2.24        | 2.06     |
| 14  | J     | 102  | CLA  | MG-NA   | 7.50  | 2.24        | 2.06     |
| 14  | Y     | 814  | CLA  | MG-NA   | 7.50  | 2.24        | 2.06     |
| 14  | A     | 835  | CLA  | MG-NA   | 7.50  | 2.24        | 2.06     |
| 14  | h     | 205  | CLA  | MG-NA   | 7.50  | 2.24        | 2.06     |
| 17  | A     | 846  | BCR  | C8-C9   | -7.50 | 1.29        | 1.45     |
| 17  | e     | 101  | BCR  | C8-C9   | -7.49 | 1.29        | 1.45     |
| 14  | j     | 102  | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 14  | A     | 840  | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 14  | Z     | 833  | CLA  | MG-NA   | 7.49  | 2.24        | 2.06     |
| 15  | H     | 839  | PQN  | C3-C2   | 7.49  | 1.48        | 1.35     |
| 14  | f     | 101  | CLA  | MG-NA   | 7.48  | 2.24        | 2.06     |
| 17  | Z     | 845  | BCR  | C11-C10 | -7.48 | 1.20        | 1.43     |
| 17  | L     | 209  | BCR  | C10-C9  | -7.47 | 1.25        | 1.35     |
| 14  | g     | 102  | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 14  | A     | 832  | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 14  | Y     | 812  | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 14  | H     | 814  | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 14  | d     | 201  | CLA  | MG-NA   | 7.47  | 2.24        | 2.06     |
| 17  | Z     | 843  | BCR  | C11-C10 | -7.46 | 1.20        | 1.43     |
| 17  | R     | 102  | BCR  | C8-C9   | -7.46 | 1.29        | 1.45     |
| 17  | V     | 1202 | BCR  | C10-C9  | -7.46 | 1.25        | 1.35     |
| 17  | Y     | 848  | BCR  | C11-C10 | -7.46 | 1.20        | 1.43     |
| 14  | Z     | 824  | CLA  | MG-NA   | 7.46  | 2.24        | 2.06     |
| 17  | i     | 101  | BCR  | C16-C17 | -7.45 | 1.20        | 1.43     |
| 14  | G     | 814  | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 14  | A     | 825  | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 17  | Z     | 842  | BCR  | C11-C10 | -7.45 | 1.20        | 1.43     |
| 14  | A     | 831  | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 17  | A     | 846  | BCR  | C11-C10 | -7.45 | 1.20        | 1.43     |
| 14  | H     | 819  | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 14  | A     | 807  | CLA  | MG-NA   | 7.45  | 2.24        | 2.06     |
| 17  | f     | 104  | BCR  | C16-C17 | -7.44 | 1.20        | 1.43     |
| 14  | U     | 1006 | CLA  | MG-NA   | 7.44  | 2.23        | 2.06     |
| 17  | K     | 102  | BCR  | C8-C9   | -7.44 | 1.30        | 1.45     |
| 14  | S     | 1103 | CLA  | MG-NA   | 7.44  | 2.23        | 2.06     |
| 17  | Y     | 851  | BCR  | C16-C17 | -7.43 | 1.20        | 1.43     |
| 17  | A     | 849  | BCR  | C11-C10 | -7.43 | 1.20        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 801  | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | Y     | 819  | CLA  | MG-NA   | 7.43  | 2.23        | 2.06     |
| 14  | G     | 837  | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | Z     | 834  | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 17  | U     | 1005 | BCR  | C16-C17 | -7.42 | 1.20        | 1.43     |
| 17  | H     | 848  | BCR  | C10-C9  | -7.42 | 1.25        | 1.35     |
| 14  | Z     | 809  | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 14  | A     | 803  | CLA  | MG-NA   | 7.42  | 2.23        | 2.06     |
| 17  | d     | 203  | BCR  | C11-C10 | -7.41 | 1.20        | 1.43     |
| 17  | H     | 842  | BCR  | C16-C17 | -7.41 | 1.20        | 1.43     |
| 14  | G     | 818  | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 14  | H     | 837  | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 14  | Z     | 823  | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 14  | G     | 853  | CLA  | MG-NA   | 7.41  | 2.23        | 2.06     |
| 17  | G     | 846  | BCR  | C8-C9   | -7.40 | 1.30        | 1.45     |
| 14  | Y     | 810  | CLA  | MG-NA   | 7.40  | 2.23        | 2.06     |
| 14  | A     | 814  | CLA  | MG-NA   | 7.40  | 2.23        | 2.06     |
| 14  | Y     | 815  | CLA  | MG-NA   | 7.40  | 2.23        | 2.06     |
| 17  | T     | 102  | BCR  | C11-C10 | -7.40 | 1.20        | 1.43     |
| 17  | G     | 847  | BCR  | C10-C9  | -7.39 | 1.26        | 1.35     |
| 17  | Y     | 849  | BCR  | C8-C9   | -7.39 | 1.30        | 1.45     |
| 17  | Y     | 849  | BCR  | C10-C9  | -7.39 | 1.26        | 1.35     |
| 14  | H     | 823  | CLA  | MG-NA   | 7.39  | 2.23        | 2.06     |
| 14  | A     | 842  | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 14  | Z     | 832  | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 14  | B     | 818  | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 17  | B     | 846  | BCR  | C16-C17 | -7.38 | 1.20        | 1.43     |
| 17  | A     | 849  | BCR  | C16-C17 | -7.38 | 1.20        | 1.43     |
| 14  | A     | 808  | CLA  | MG-NA   | 7.37  | 2.23        | 2.06     |
| 14  | Z     | 819  | CLA  | MG-NA   | 7.37  | 2.23        | 2.06     |
| 14  | H     | 836  | CLA  | MG-NA   | 7.37  | 2.23        | 2.06     |
| 14  | Q     | 203  | CLA  | MG-NA   | 7.37  | 2.23        | 2.06     |
| 17  | B     | 847  | BCR  | C16-C17 | -7.37 | 1.20        | 1.43     |
| 17  | F     | 201  | BCR  | C11-C10 | -7.36 | 1.20        | 1.43     |
| 17  | H     | 845  | BCR  | C16-C17 | -7.36 | 1.20        | 1.43     |
| 17  | K     | 102  | BCR  | C10-C9  | -7.36 | 1.26        | 1.35     |
| 14  | Z     | 806  | CLA  | MG-NA   | 7.35  | 2.23        | 2.06     |
| 14  | Z     | 814  | CLA  | MG-NA   | 7.35  | 2.23        | 2.06     |
| 17  | d     | 203  | BCR  | C16-C17 | -7.35 | 1.20        | 1.43     |
| 17  | B     | 844  | BCR  | C16-C17 | -7.35 | 1.20        | 1.43     |
| 17  | U     | 1008 | BCR  | C20-C21 | -7.34 | 1.20        | 1.43     |
| 17  | Z     | 844  | BCR  | C16-C17 | -7.34 | 1.20        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Y     | 826  | CLA  | MG-NA   | 7.34  | 2.23        | 2.06     |
| 17  | I     | 101  | BCR  | C8-C9   | -7.34 | 1.30        | 1.45     |
| 17  | B     | 844  | BCR  | C8-C9   | -7.34 | 1.30        | 1.45     |
| 17  | Q     | 204  | BCR  | C8-C9   | -7.34 | 1.30        | 1.45     |
| 14  | Y     | 842  | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 17  | U     | 1007 | BCR  | C16-C17 | -7.33 | 1.20        | 1.43     |
| 14  | B     | 824  | CLA  | MG-NA   | 7.33  | 2.23        | 2.06     |
| 17  | B     | 851  | BCR  | C16-C17 | -7.32 | 1.20        | 1.43     |
| 17  | A     | 845  | BCR  | C20-C21 | -7.32 | 1.20        | 1.43     |
| 14  | H     | 802  | CLA  | MG-NA   | 7.32  | 2.23        | 2.06     |
| 17  | B     | 848  | BCR  | C16-C17 | -7.32 | 1.20        | 1.43     |
| 14  | H     | 806  | CLA  | MG-NA   | 7.32  | 2.23        | 2.06     |
| 17  | Z     | 843  | BCR  | C20-C21 | -7.32 | 1.20        | 1.43     |
| 17  | G     | 848  | BCR  | C20-C21 | -7.32 | 1.20        | 1.43     |
| 15  | G     | 844  | PQN  | C3-C2   | 7.32  | 1.48        | 1.35     |
| 14  | A     | 836  | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |
| 17  | B     | 845  | BCR  | C16-C17 | -7.31 | 1.20        | 1.43     |
| 17  | Z     | 846  | BCR  | C20-C21 | -7.31 | 1.20        | 1.43     |
| 17  | Y     | 847  | BCR  | C10-C9  | -7.31 | 1.26        | 1.35     |
| 14  | U     | 1002 | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |
| 17  | A     | 849  | BCR  | C20-C21 | -7.31 | 1.20        | 1.43     |
| 14  | B     | 816  | CLA  | MG-NA   | 7.31  | 2.23        | 2.06     |
| 17  | h     | 202  | BCR  | C11-C10 | -7.30 | 1.20        | 1.43     |
| 14  | H     | 820  | CLA  | MG-NA   | 7.30  | 2.23        | 2.06     |
| 17  | d     | 203  | BCR  | C20-C21 | -7.29 | 1.20        | 1.43     |
| 14  | G     | 840  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 17  | H     | 844  | BCR  | C20-C21 | -7.29 | 1.20        | 1.43     |
| 14  | B     | 825  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | Z     | 816  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | Y     | 821  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | A     | 813  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 14  | Y     | 824  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 17  | J     | 103  | BCR  | C11-C10 | -7.29 | 1.20        | 1.43     |
| 14  | B     | 840  | CLA  | MG-NA   | 7.29  | 2.23        | 2.06     |
| 17  | f     | 105  | BCR  | C20-C21 | -7.29 | 1.20        | 1.43     |
| 14  | G     | 820  | CLA  | MG-NA   | 7.28  | 2.23        | 2.06     |
| 17  | M     | 101  | BCR  | C16-C17 | -7.28 | 1.20        | 1.43     |
| 17  | F     | 201  | BCR  | C10-C9  | -7.28 | 1.26        | 1.35     |
| 17  | A     | 848  | BCR  | C11-C10 | -7.28 | 1.20        | 1.43     |
| 14  | H     | 815  | CLA  | MG-NA   | 7.28  | 2.23        | 2.06     |
| 17  | G     | 854  | BCR  | C16-C17 | -7.28 | 1.20        | 1.43     |
| 17  | f     | 105  | BCR  | C16-C17 | -7.28 | 1.20        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 819  | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 14  | G     | 825  | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 14  | S     | 1101 | CLA  | MG-NA   | 7.27  | 2.23        | 2.06     |
| 17  | A     | 845  | BCR  | C8-C9   | -7.27 | 1.30        | 1.45     |
| 17  | H     | 844  | BCR  | C10-C9  | -7.26 | 1.26        | 1.35     |
| 14  | H     | 811  | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 14  | H     | 825  | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 17  | L     | 209  | BCR  | C8-C9   | -7.26 | 1.30        | 1.45     |
| 17  | f     | 103  | BCR  | C20-C21 | -7.26 | 1.20        | 1.43     |
| 14  | A     | 810  | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 14  | B     | 815  | CLA  | MG-NA   | 7.26  | 2.23        | 2.06     |
| 17  | Y     | 849  | BCR  | C16-C17 | -7.26 | 1.21        | 1.43     |
| 14  | B     | 834  | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 17  | Y     | 847  | BCR  | C8-C9   | -7.25 | 1.30        | 1.45     |
| 14  | Z     | 811  | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 14  | G     | 842  | CLA  | MG-NA   | 7.25  | 2.23        | 2.06     |
| 14  | A     | 828  | CLA  | MG-NA   | 7.24  | 2.23        | 2.06     |
| 14  | A     | 811  | CLA  | MG-NA   | 7.24  | 2.23        | 2.06     |
| 14  | Z     | 813  | CLA  | MG-NA   | 7.24  | 2.23        | 2.06     |
| 14  | Y     | 839  | CLA  | MG-NA   | 7.24  | 2.23        | 2.06     |
| 17  | Y     | 848  | BCR  | C8-C9   | -7.24 | 1.30        | 1.45     |
| 17  | Y     | 849  | BCR  | C20-C21 | -7.24 | 1.21        | 1.43     |
| 17  | Q     | 204  | BCR  | C20-C21 | -7.24 | 1.21        | 1.43     |
| 14  | d     | 202  | CLA  | MG-NA   | 7.23  | 2.23        | 2.06     |
| 17  | F     | 203  | BCR  | C8-C9   | -7.23 | 1.30        | 1.45     |
| 17  | R     | 101  | BCR  | C20-C21 | -7.23 | 1.21        | 1.43     |
| 14  | B     | 833  | CLA  | MG-NA   | 7.23  | 2.23        | 2.06     |
| 14  | H     | 830  | CLA  | MG-NA   | 7.23  | 2.23        | 2.06     |
| 17  | F     | 203  | BCR  | C10-C9  | -7.23 | 1.26        | 1.35     |
| 14  | G     | 831  | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 17  | Q     | 202  | BCR  | C20-C21 | -7.22 | 1.21        | 1.43     |
| 14  | Z     | 826  | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 17  | Z     | 846  | BCR  | C16-C17 | -7.22 | 1.21        | 1.43     |
| 17  | A     | 845  | BCR  | C11-C10 | -7.22 | 1.21        | 1.43     |
| 17  | B     | 846  | BCR  | C20-C21 | -7.22 | 1.21        | 1.43     |
| 14  | A     | 852  | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 14  | B     | 821  | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 17  | U     | 1008 | BCR  | C8-C9   | -7.22 | 1.30        | 1.45     |
| 14  | A     | 821  | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |
| 14  | A     | 820  | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |
| 17  | F     | 203  | BCR  | C16-C17 | -7.21 | 1.21        | 1.43     |
| 14  | H     | 822  | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | H     | 844  | BCR  | C16-C17 | -7.21 | 1.21        | 1.43     |
| 14  | G     | 824  | CLA  | MG-NA   | 7.20  | 2.23        | 2.06     |
| 17  | M     | 101  | BCR  | C10-C9  | -7.20 | 1.26        | 1.35     |
| 17  | A     | 847  | BCR  | C20-C21 | -7.20 | 1.21        | 1.43     |
| 17  | I     | 101  | BCR  | C16-C17 | -7.20 | 1.21        | 1.43     |
| 17  | H     | 840  | BCR  | C10-C9  | -7.20 | 1.26        | 1.35     |
| 14  | L     | 201  | CLA  | MG-NA   | 7.20  | 2.23        | 2.06     |
| 17  | G     | 848  | BCR  | C16-C17 | -7.20 | 1.21        | 1.43     |
| 14  | Z     | 829  | CLA  | MG-NA   | 7.20  | 2.23        | 2.06     |
| 17  | H     | 848  | BCR  | C8-C9   | -7.19 | 1.30        | 1.45     |
| 17  | B     | 851  | BCR  | C20-C21 | -7.18 | 1.21        | 1.43     |
| 17  | I     | 101  | BCR  | C11-C10 | -7.18 | 1.21        | 1.43     |
| 14  | Y     | 811  | CLA  | MG-NA   | 7.18  | 2.23        | 2.06     |
| 17  | G     | 848  | BCR  | C10-C9  | -7.18 | 1.26        | 1.35     |
| 17  | A     | 846  | BCR  | C20-C21 | -7.17 | 1.21        | 1.43     |
| 17  | H     | 842  | BCR  | C8-C9   | -7.17 | 1.30        | 1.45     |
| 14  | A     | 816  | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 14  | Y     | 832  | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 14  | H     | 826  | CLA  | MG-NA   | 7.17  | 2.23        | 2.06     |
| 17  | Y     | 856  | BCR  | C16-C17 | -7.16 | 1.21        | 1.43     |
| 14  | Z     | 835  | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 17  | Z     | 842  | BCR  | C8-C9   | -7.16 | 1.30        | 1.45     |
| 17  | B     | 848  | BCR  | C11-C10 | -7.16 | 1.21        | 1.43     |
| 14  | G     | 813  | CLA  | MG-NA   | 7.16  | 2.23        | 2.06     |
| 17  | Z     | 846  | BCR  | C10-C9  | -7.15 | 1.26        | 1.35     |
| 14  | G     | 835  | CLA  | MG-NA   | 7.15  | 2.23        | 2.06     |
| 17  | Z     | 845  | BCR  | C20-C21 | -7.15 | 1.21        | 1.43     |
| 17  | U     | 1008 | BCR  | C11-C10 | -7.15 | 1.21        | 1.43     |
| 14  | Z     | 810  | CLA  | MG-NA   | 7.15  | 2.23        | 2.06     |
| 14  | Y     | 838  | CLA  | MG-NA   | 7.15  | 2.23        | 2.06     |
| 17  | Y     | 848  | BCR  | C20-C21 | -7.14 | 1.21        | 1.43     |
| 17  | G     | 846  | BCR  | C10-C9  | -7.14 | 1.26        | 1.35     |
| 17  | A     | 847  | BCR  | C10-C9  | -7.14 | 1.26        | 1.35     |
| 14  | G     | 843  | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 14  | Y     | 809  | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 14  | Y     | 854  | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 14  | Z     | 808  | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 14  | B     | 809  | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 14  | H     | 816  | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 14  | A     | 815  | CLA  | MG-NA   | 7.13  | 2.23        | 2.06     |
| 14  | Z     | 837  | CLA  | MG-NA   | 7.13  | 2.23        | 2.06     |
| 17  | Y     | 856  | BCR  | C11-C10 | -7.13 | 1.21        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 826  | CLA  | MG-NA   | 7.13  | 2.23        | 2.06     |
| 17  | G     | 849  | BCR  | C8-C9   | -7.12 | 1.30        | 1.45     |
| 17  | A     | 848  | BCR  | C20-C21 | -7.12 | 1.21        | 1.43     |
| 17  | f     | 105  | BCR  | C10-C9  | -7.12 | 1.26        | 1.35     |
| 14  | Y     | 816  | CLA  | MG-NA   | 7.12  | 2.23        | 2.06     |
| 14  | U     | 1004 | CLA  | MG-NA   | 7.12  | 2.23        | 2.06     |
| 17  | B     | 844  | BCR  | C10-C9  | -7.11 | 1.26        | 1.35     |
| 14  | A     | 819  | CLA  | MG-NA   | 7.11  | 2.23        | 2.06     |
| 14  | G     | 819  | CLA  | MG-NA   | 7.11  | 2.23        | 2.06     |
| 17  | Y     | 847  | BCR  | C16-C17 | -7.11 | 1.21        | 1.43     |
| 14  | Y     | 836  | CLA  | MG-NA   | 7.10  | 2.23        | 2.06     |
| 17  | J     | 103  | BCR  | C16-C17 | -7.10 | 1.21        | 1.43     |
| 14  | L     | 202  | CLA  | MG-NA   | 7.10  | 2.23        | 2.06     |
| 14  | H     | 805  | CLA  | MG-NA   | 7.10  | 2.23        | 2.06     |
| 14  | H     | 831  | CLA  | MG-NA   | 7.10  | 2.23        | 2.06     |
| 14  | Y     | 840  | CLA  | MG-NA   | 7.10  | 2.23        | 2.06     |
| 17  | J     | 103  | BCR  | C20-C21 | -7.10 | 1.21        | 1.43     |
| 14  | B     | 832  | CLA  | MG-NA   | 7.09  | 2.23        | 2.06     |
| 14  | B     | 827  | CLA  | MG-NA   | 7.09  | 2.23        | 2.06     |
| 17  | e     | 101  | BCR  | C16-C17 | -7.08 | 1.21        | 1.43     |
| 17  | Y     | 846  | BCR  | C8-C9   | -7.08 | 1.30        | 1.45     |
| 17  | Q     | 204  | BCR  | C16-C17 | -7.08 | 1.21        | 1.43     |
| 14  | G     | 830  | CLA  | MG-NA   | 7.08  | 2.23        | 2.06     |
| 14  | Z     | 815  | CLA  | MG-NA   | 7.08  | 2.23        | 2.06     |
| 17  | G     | 850  | BCR  | C16-C17 | -7.08 | 1.21        | 1.43     |
| 17  | I     | 101  | BCR  | C20-C21 | -7.07 | 1.21        | 1.43     |
| 14  | H     | 829  | CLA  | MG-NA   | 7.07  | 2.23        | 2.06     |
| 17  | Q     | 204  | BCR  | C10-C9  | -7.07 | 1.26        | 1.35     |
| 14  | H     | 824  | CLA  | MG-NA   | 7.06  | 2.23        | 2.06     |
| 17  | Z     | 842  | BCR  | C16-C17 | -7.06 | 1.21        | 1.43     |
| 17  | G     | 854  | BCR  | C20-C21 | -7.06 | 1.21        | 1.43     |
| 14  | G     | 810  | CLA  | MG-NA   | 7.06  | 2.23        | 2.06     |
| 17  | G     | 850  | BCR  | C10-C9  | -7.06 | 1.26        | 1.35     |
| 14  | B     | 807  | CLA  | MG-NA   | 7.06  | 2.23        | 2.06     |
| 17  | B     | 848  | BCR  | C10-C9  | -7.05 | 1.26        | 1.35     |
| 14  | B     | 828  | CLA  | MG-NA   | 7.05  | 2.23        | 2.06     |
| 17  | A     | 846  | BCR  | C16-C17 | -7.05 | 1.21        | 1.43     |
| 14  | Z     | 830  | CLA  | MG-NA   | 7.05  | 2.23        | 2.06     |
| 17  | U     | 1008 | BCR  | C16-C17 | -7.05 | 1.21        | 1.43     |
| 17  | Y     | 846  | BCR  | C16-C17 | -7.04 | 1.21        | 1.43     |
| 17  | Y     | 846  | BCR  | C20-C21 | -7.04 | 1.21        | 1.43     |
| 14  | Y     | 804  | CLA  | MG-NA   | 7.04  | 2.23        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 817  | CLA  | MG-NA   | 7.04  | 2.23        | 2.06     |
| 14  | B     | 802  | CLA  | MG-NA   | 7.04  | 2.23        | 2.06     |
| 14  | G     | 832  | CLA  | MG-NA   | 7.04  | 2.23        | 2.06     |
| 14  | A     | 837  | CLA  | MG-NA   | 7.04  | 2.23        | 2.06     |
| 17  | V     | 1202 | BCR  | C16-C17 | -7.04 | 1.21        | 1.43     |
| 14  | K     | 103  | CLA  | MG-NA   | 7.03  | 2.23        | 2.06     |
| 14  | B     | 804  | CLA  | MG-NA   | 7.03  | 2.23        | 2.06     |
| 14  | V     | 1201 | CLA  | MG-NA   | 7.03  | 2.23        | 2.06     |
| 14  | B     | 820  | CLA  | MG-NA   | 7.03  | 2.23        | 2.06     |
| 14  | Y     | 841  | CLA  | MG-NA   | 7.03  | 2.23        | 2.06     |
| 14  | G     | 828  | CLA  | MG-NA   | 7.02  | 2.22        | 2.06     |
| 14  | B     | 811  | CLA  | MG-NA   | 7.02  | 2.22        | 2.06     |
| 14  | Z     | 802  | CLA  | MG-NA   | 7.02  | 2.22        | 2.06     |
| 14  | Z     | 836  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 17  | U     | 1007 | BCR  | C10-C9  | -7.01 | 1.26        | 1.35     |
| 14  | A     | 806  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 14  | A     | 827  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 14  | A     | 839  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 17  | F     | 203  | BCR  | C20-C21 | -7.01 | 1.21        | 1.43     |
| 17  | e     | 101  | BCR  | C10-C9  | -7.01 | 1.26        | 1.35     |
| 17  | A     | 848  | BCR  | C16-C17 | -7.01 | 1.21        | 1.43     |
| 14  | G     | 808  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 14  | A     | 834  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 15  | B     | 842  | PQN  | C3-C2   | 7.00  | 1.48        | 1.35     |
| 14  | T     | 101  | CLA  | MG-NA   | 7.00  | 2.22        | 2.06     |
| 17  | Y     | 846  | BCR  | C11-C10 | -6.99 | 1.21        | 1.43     |
| 14  | G     | 834  | CLA  | MG-NA   | 6.99  | 2.22        | 2.06     |
| 14  | H     | 834  | CLA  | MG-NA   | 6.99  | 2.22        | 2.06     |
| 14  | A     | 802  | CLA  | MG-NA   | 6.99  | 2.22        | 2.06     |
| 14  | B     | 836  | CLA  | MG-NA   | 6.99  | 2.22        | 2.06     |
| 17  | Z     | 843  | BCR  | C16-C17 | -6.98 | 1.21        | 1.43     |
| 14  | B     | 812  | CLA  | MG-NA   | 6.98  | 2.22        | 2.06     |
| 14  | G     | 803  | CLA  | MG-NA   | 6.98  | 2.22        | 2.06     |
| 14  | Z     | 828  | CLA  | MG-NA   | 6.98  | 2.22        | 2.06     |
| 14  | A     | 817  | CLA  | MG-NA   | 6.97  | 2.22        | 2.06     |
| 14  | Z     | 804  | CLA  | MG-NA   | 6.97  | 2.22        | 2.06     |
| 14  | A     | 826  | CLA  | MG-NA   | 6.97  | 2.22        | 2.06     |
| 14  | B     | 805  | CLA  | MG-NA   | 6.96  | 2.22        | 2.06     |
| 17  | Z     | 843  | BCR  | C8-C9   | -6.96 | 1.31        | 1.45     |
| 14  | G     | 833  | CLA  | MG-NA   | 6.96  | 2.22        | 2.06     |
| 14  | Y     | 837  | CLA  | MG-NA   | 6.95  | 2.22        | 2.06     |
| 17  | Y     | 848  | BCR  | C10-C9  | -6.95 | 1.26        | 1.35     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | U     | 1005 | BCR  | C8-C9   | -6.95 | 1.31        | 1.45     |
| 14  | A     | 823  | CLA  | MG-NA   | 6.94  | 2.22        | 2.06     |
| 17  | V     | 1202 | BCR  | C20-C21 | -6.93 | 1.22        | 1.43     |
| 14  | Y     | 830  | CLA  | MG-NA   | 6.93  | 2.22        | 2.06     |
| 14  | A     | 829  | CLA  | MG-NA   | 6.92  | 2.22        | 2.06     |
| 14  | B     | 829  | CLA  | MG-NA   | 6.92  | 2.22        | 2.06     |
| 17  | L     | 209  | BCR  | C16-C17 | -6.91 | 1.22        | 1.43     |
| 14  | B     | 838  | CLA  | MG-NA   | 6.91  | 2.22        | 2.06     |
| 14  | B     | 803  | CLA  | MG-NA   | 6.91  | 2.22        | 2.06     |
| 14  | Y     | 820  | CLA  | MG-NA   | 6.90  | 2.22        | 2.06     |
| 17  | Z     | 845  | BCR  | C16-C17 | -6.90 | 1.22        | 1.43     |
| 17  | U     | 1005 | BCR  | C10-C9  | -6.90 | 1.26        | 1.35     |
| 14  | H     | 828  | CLA  | MG-NA   | 6.90  | 2.22        | 2.06     |
| 14  | A     | 841  | CLA  | MG-NA   | 6.88  | 2.22        | 2.06     |
| 14  | H     | 838  | CLA  | MG-NA   | 6.88  | 2.22        | 2.06     |
| 14  | G     | 815  | CLA  | MG-NA   | 6.87  | 2.22        | 2.06     |
| 17  | f     | 103  | BCR  | C16-C17 | -6.87 | 1.22        | 1.43     |
| 17  | H     | 842  | BCR  | C10-C9  | -6.87 | 1.26        | 1.35     |
| 14  | G     | 805  | CLA  | MG-NA   | 6.87  | 2.22        | 2.06     |
| 14  | Y     | 808  | CLA  | MG-NA   | 6.86  | 2.22        | 2.06     |
| 14  | G     | 809  | CLA  | MG-NA   | 6.86  | 2.22        | 2.06     |
| 17  | R     | 101  | BCR  | C16-C17 | -6.85 | 1.22        | 1.43     |
| 14  | Z     | 831  | CLA  | MG-NA   | 6.84  | 2.22        | 2.06     |
| 14  | Z     | 805  | CLA  | MG-NA   | 6.84  | 2.22        | 2.06     |
| 14  | Y     | 818  | CLA  | MG-NA   | 6.84  | 2.22        | 2.06     |
| 17  | h     | 202  | BCR  | C8-C9   | -6.84 | 1.31        | 1.45     |
| 14  | U     | 1003 | CLA  | MG-NA   | 6.83  | 2.22        | 2.06     |
| 14  | G     | 821  | CLA  | MG-NA   | 6.82  | 2.22        | 2.06     |
| 17  | T     | 102  | BCR  | C20-C21 | -6.82 | 1.22        | 1.43     |
| 17  | Q     | 202  | BCR  | C16-C17 | -6.82 | 1.22        | 1.43     |
| 17  | A     | 845  | BCR  | C16-C17 | -6.81 | 1.22        | 1.43     |
| 17  | A     | 847  | BCR  | C16-C17 | -6.81 | 1.22        | 1.43     |
| 17  | Y     | 848  | BCR  | C16-C17 | -6.81 | 1.22        | 1.43     |
| 14  | H     | 835  | CLA  | MG-NA   | 6.81  | 2.22        | 2.06     |
| 14  | Z     | 803  | CLA  | MG-NA   | 6.80  | 2.22        | 2.06     |
| 17  | h     | 202  | BCR  | C20-C21 | -6.80 | 1.22        | 1.43     |
| 14  | G     | 839  | CLA  | MG-NA   | 6.80  | 2.22        | 2.06     |
| 14  | G     | 804  | CLA  | MG-NA   | 6.79  | 2.22        | 2.06     |
| 17  | A     | 848  | BCR  | C8-C9   | -6.78 | 1.31        | 1.45     |
| 14  | Z     | 801  | CLA  | MG-NA   | 6.78  | 2.22        | 2.06     |
| 17  | A     | 849  | BCR  | C10-C9  | -6.77 | 1.26        | 1.35     |
| 17  | Y     | 850  | BCR  | C8-C9   | -6.77 | 1.31        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 809  | CLA  | MG-NA   | 6.76  | 2.22        | 2.06     |
| 14  | H     | 813  | CLA  | MG-NA   | 6.76  | 2.22        | 2.06     |
| 14  | Y     | 834  | CLA  | MG-NA   | 6.74  | 2.22        | 2.06     |
| 17  | Y     | 850  | BCR  | C10-C9  | -6.74 | 1.26        | 1.35     |
| 14  | Y     | 828  | CLA  | MG-NA   | 6.72  | 2.22        | 2.06     |
| 17  | T     | 102  | BCR  | C16-C17 | -6.69 | 1.22        | 1.43     |
| 17  | H     | 843  | BCR  | C20-C21 | -6.68 | 1.22        | 1.43     |
| 14  | A     | 804  | CLA  | MG-NA   | 6.67  | 2.22        | 2.06     |
| 17  | A     | 848  | BCR  | C10-C9  | -6.67 | 1.26        | 1.35     |
| 17  | T     | 102  | BCR  | C8-C9   | -6.66 | 1.31        | 1.45     |
| 14  | H     | 810  | CLA  | MG-NA   | 6.66  | 2.22        | 2.06     |
| 14  | G     | 806  | CLA  | MG-NA   | 6.65  | 2.22        | 2.06     |
| 14  | A     | 809  | CLA  | MG-NA   | 6.63  | 2.22        | 2.06     |
| 17  | B     | 845  | BCR  | C10-C9  | -6.63 | 1.27        | 1.35     |
| 14  | A     | 830  | CLA  | MG-NA   | 6.62  | 2.22        | 2.06     |
| 17  | H     | 845  | BCR  | C10-C9  | -6.61 | 1.27        | 1.35     |
| 14  | A     | 818  | CLA  | MG-NA   | 6.60  | 2.22        | 2.06     |
| 14  | Y     | 802  | CLA  | MG-NA   | 6.60  | 2.21        | 2.06     |
| 17  | A     | 846  | BCR  | C10-C9  | -6.59 | 1.27        | 1.35     |
| 17  | f     | 103  | BCR  | C8-C9   | -6.58 | 1.31        | 1.45     |
| 14  | H     | 827  | CLA  | MG-NA   | 6.57  | 2.21        | 2.06     |
| 17  | h     | 202  | BCR  | C16-C17 | -6.55 | 1.23        | 1.43     |
| 14  | Q     | 201  | CLA  | MG-NA   | 6.55  | 2.21        | 2.06     |
| 14  | L     | 206  | CLA  | MG-NA   | 6.53  | 2.21        | 2.06     |
| 14  | h     | 206  | CLA  | MG-NA   | 6.52  | 2.21        | 2.06     |
| 17  | H     | 843  | BCR  | C16-C17 | -6.51 | 1.23        | 1.43     |
| 14  | H     | 817  | CLA  | MG-NA   | 6.51  | 2.21        | 2.06     |
| 17  | i     | 101  | BCR  | C20-C21 | -6.49 | 1.23        | 1.43     |
| 17  | J     | 103  | BCR  | C10-C9  | -6.47 | 1.27        | 1.35     |
| 14  | A     | 805  | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 17  | h     | 202  | BCR  | C10-C9  | -6.38 | 1.27        | 1.35     |
| 14  | B     | 830  | CLA  | MG-NA   | 6.37  | 2.21        | 2.06     |
| 17  | Z     | 842  | BCR  | C10-C9  | -6.37 | 1.27        | 1.35     |
| 14  | B     | 801  | CLA  | MG-NA   | 6.35  | 2.21        | 2.06     |
| 17  | Y     | 856  | BCR  | C10-C9  | -6.32 | 1.27        | 1.35     |
| 14  | Y     | 805  | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 17  | f     | 103  | BCR  | C10-C9  | -6.31 | 1.27        | 1.35     |
| 14  | B     | 841  | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 14  | H     | 823  | CLA  | C3B-C2B | 6.30  | 1.49        | 1.40     |
| 14  | U     | 1004 | CLA  | OBD-CAD | 6.26  | 1.31        | 1.22     |
| 14  | G     | 802  | CLA  | MG-NA   | 6.25  | 2.21        | 2.06     |
| 17  | d     | 203  | BCR  | C10-C9  | -6.23 | 1.27        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | U     | 1006 | CLA  | O2D-CGD | 6.23  | 1.48        | 1.33     |
| 14  | A     | 852  | CLA  | OBD-CAD | 6.21  | 1.31        | 1.22     |
| 17  | A     | 845  | BCR  | C10-C9  | -6.19 | 1.27        | 1.35     |
| 14  | Y     | 855  | CLA  | MG-NA   | 6.17  | 2.20        | 2.06     |
| 14  | Z     | 827  | CLA  | MG-NA   | 6.12  | 2.20        | 2.06     |
| 14  | h     | 205  | CLA  | O2A-C1  | 6.12  | 1.63        | 1.46     |
| 14  | B     | 834  | CLA  | C3B-C2B | 6.10  | 1.48        | 1.40     |
| 17  | I     | 101  | BCR  | C10-C9  | -6.09 | 1.27        | 1.35     |
| 14  | B     | 806  | CLA  | MG-NA   | 6.06  | 2.20        | 2.06     |
| 14  | A     | 837  | CLA  | CHC-C1C | 6.04  | 1.50        | 1.35     |
| 14  | Z     | 819  | CLA  | O2D-CGD | 6.02  | 1.47        | 1.33     |
| 14  | Z     | 812  | CLA  | O2A-C1  | 6.02  | 1.63        | 1.46     |
| 14  | Z     | 837  | CLA  | O2D-CGD | 6.02  | 1.47        | 1.33     |
| 14  | H     | 820  | CLA  | O2D-CGD | 5.99  | 1.47        | 1.33     |
| 14  | A     | 842  | CLA  | O2A-C1  | 5.98  | 1.63        | 1.46     |
| 14  | G     | 841  | CLA  | OBD-CAD | 5.97  | 1.30        | 1.22     |
| 14  | H     | 807  | CLA  | O2D-CGD | 5.97  | 1.47        | 1.33     |
| 14  | G     | 840  | CLA  | CHC-C1C | 5.88  | 1.50        | 1.35     |
| 17  | U     | 1008 | BCR  | C10-C9  | -5.88 | 1.28        | 1.35     |
| 14  | Y     | 838  | CLA  | CHC-C1C | 5.87  | 1.50        | 1.35     |
| 14  | h     | 205  | CLA  | O2D-CGD | 5.85  | 1.47        | 1.33     |
| 14  | Z     | 803  | CLA  | O2A-C1  | 5.84  | 1.62        | 1.46     |
| 14  | Z     | 829  | CLA  | C3B-C2B | 5.83  | 1.48        | 1.40     |
| 14  | G     | 830  | CLA  | O2A-C1  | 5.83  | 1.62        | 1.46     |
| 14  | H     | 828  | CLA  | O2A-C1  | 5.83  | 1.62        | 1.46     |
| 14  | V     | 1201 | CLA  | OBD-CAD | 5.82  | 1.30        | 1.22     |
| 14  | G     | 819  | CLA  | OBD-CAD | 5.82  | 1.30        | 1.22     |
| 14  | A     | 818  | CLA  | O2A-C1  | 5.81  | 1.62        | 1.46     |
| 14  | G     | 827  | CLA  | CHC-C1C | 5.81  | 1.49        | 1.35     |
| 14  | Z     | 819  | CLA  | C3B-C2B | 5.81  | 1.48        | 1.40     |
| 17  | Z     | 845  | BCR  | C10-C9  | -5.80 | 1.28        | 1.35     |
| 14  | H     | 821  | CLA  | C3B-C2B | 5.80  | 1.48        | 1.40     |
| 14  | Y     | 854  | CLA  | OBD-CAD | 5.78  | 1.30        | 1.22     |
| 14  | A     | 809  | CLA  | O2A-C1  | 5.78  | 1.62        | 1.46     |
| 14  | Z     | 806  | CLA  | O2D-CGD | 5.76  | 1.47        | 1.33     |
| 14  | A     | 824  | CLA  | CHC-C1C | 5.76  | 1.49        | 1.35     |
| 14  | Y     | 821  | CLA  | CHC-C1C | 5.74  | 1.49        | 1.35     |
| 14  | Z     | 816  | CLA  | O2A-C1  | 5.74  | 1.62        | 1.46     |
| 14  | G     | 817  | CLA  | C3B-C2B | 5.73  | 1.48        | 1.40     |
| 14  | Y     | 828  | CLA  | CHC-C1C | 5.73  | 1.49        | 1.35     |
| 14  | H     | 838  | CLA  | CHC-C1C | 5.73  | 1.49        | 1.35     |
| 14  | B     | 834  | CLA  | OBD-CAD | 5.73  | 1.30        | 1.22     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 833  | CLA  | OBD-CAD | 5.73  | 1.30        | 1.22     |
| 14  | Y     | 832  | CLA  | C3B-C2B | 5.72  | 1.48        | 1.40     |
| 14  | h     | 206  | CLA  | CHC-C1C | 5.71  | 1.49        | 1.35     |
| 14  | B     | 824  | CLA  | C3B-C2B | 5.70  | 1.48        | 1.40     |
| 14  | H     | 836  | CLA  | O2D-CGD | 5.70  | 1.47        | 1.33     |
| 14  | Z     | 839  | CLA  | OBD-CAD | 5.70  | 1.30        | 1.22     |
| 14  | Z     | 819  | CLA  | OBD-CAD | 5.68  | 1.30        | 1.22     |
| 14  | B     | 821  | CLA  | O2D-CGD | 5.67  | 1.47        | 1.33     |
| 14  | Z     | 811  | CLA  | CHC-C1C | 5.67  | 1.49        | 1.35     |
| 14  | Y     | 827  | CLA  | O2A-C1  | 5.67  | 1.62        | 1.46     |
| 14  | V     | 1201 | CLA  | CHC-C1C | 5.66  | 1.49        | 1.35     |
| 17  | Z     | 843  | BCR  | C10-C9  | -5.66 | 1.28        | 1.35     |
| 14  | Y     | 805  | CLA  | OBD-CAD | 5.66  | 1.30        | 1.22     |
| 14  | Z     | 812  | CLA  | CHC-C1C | 5.66  | 1.49        | 1.35     |
| 14  | Y     | 814  | CLA  | CHC-C1C | 5.66  | 1.49        | 1.35     |
| 14  | Y     | 843  | CLA  | O2A-C1  | 5.66  | 1.62        | 1.46     |
| 14  | Y     | 834  | CLA  | CHC-C1C | 5.66  | 1.49        | 1.35     |
| 14  | G     | 811  | CLA  | O2A-C1  | 5.65  | 1.62        | 1.46     |
| 14  | Y     | 826  | CLA  | CHC-C1C | 5.64  | 1.49        | 1.35     |
| 14  | g     | 102  | CLA  | O2D-CGD | 5.64  | 1.47        | 1.33     |
| 14  | H     | 813  | CLA  | O2A-C1  | 5.64  | 1.62        | 1.46     |
| 14  | Y     | 836  | CLA  | CHC-C1C | 5.64  | 1.49        | 1.35     |
| 14  | h     | 206  | CLA  | O2A-C1  | 5.64  | 1.62        | 1.46     |
| 14  | Y     | 830  | CLA  | CHC-C1C | 5.64  | 1.49        | 1.35     |
| 14  | Z     | 803  | CLA  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 14  | A     | 814  | CLA  | OBD-CAD | 5.63  | 1.30        | 1.22     |
| 14  | B     | 826  | CLA  | OBD-CAD | 5.63  | 1.30        | 1.22     |
| 14  | A     | 833  | CLA  | O2D-CGD | 5.63  | 1.46        | 1.33     |
| 14  | G     | 818  | CLA  | O2A-C1  | 5.63  | 1.62        | 1.46     |
| 14  | A     | 823  | CLA  | O2D-CGD | 5.62  | 1.46        | 1.33     |
| 14  | A     | 808  | CLA  | CHC-C1C | 5.62  | 1.49        | 1.35     |
| 14  | G     | 802  | CLA  | CHC-C1C | 5.62  | 1.49        | 1.35     |
| 14  | A     | 816  | CLA  | O2A-C1  | 5.62  | 1.62        | 1.46     |
| 14  | A     | 818  | CLA  | CHC-C1C | 5.62  | 1.49        | 1.35     |
| 14  | Z     | 801  | CLA  | O2D-CGD | 5.62  | 1.46        | 1.33     |
| 14  | G     | 802  | CLA  | O2A-C1  | 5.62  | 1.62        | 1.46     |
| 14  | A     | 822  | CLA  | O2D-CGD | 5.61  | 1.46        | 1.33     |
| 14  | Z     | 832  | CLA  | O2D-CGD | 5.61  | 1.46        | 1.33     |
| 14  | B     | 805  | CLA  | O2A-C1  | 5.61  | 1.61        | 1.46     |
| 14  | B     | 837  | CLA  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 14  | Z     | 803  | CLA  | OBD-CAD | 5.61  | 1.30        | 1.22     |
| 14  | G     | 834  | CLA  | CHC-C1C | 5.61  | 1.49        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 820  | CLA  | C3D-C2D | 5.60  | 1.49        | 1.39     |
| 14  | H     | 803  | CLA  | MG-NA   | 5.60  | 2.19        | 2.06     |
| 14  | L     | 205  | CLA  | O2A-C1  | 5.60  | 1.61        | 1.46     |
| 14  | G     | 802  | CLA  | O2D-CGD | 5.60  | 1.46        | 1.33     |
| 14  | A     | 840  | CLA  | O2A-C1  | 5.60  | 1.61        | 1.46     |
| 14  | Z     | 839  | CLA  | CHC-C1C | 5.60  | 1.49        | 1.35     |
| 14  | H     | 801  | CLA  | OBD-CAD | 5.59  | 1.30        | 1.22     |
| 14  | G     | 830  | CLA  | C3D-C2D | 5.59  | 1.49        | 1.39     |
| 14  | B     | 838  | CLA  | O2A-C1  | 5.59  | 1.61        | 1.46     |
| 14  | Y     | 831  | CLA  | O2D-CGD | 5.59  | 1.46        | 1.33     |
| 14  | G     | 804  | CLA  | O2A-C1  | 5.59  | 1.61        | 1.46     |
| 14  | B     | 830  | CLA  | O2D-CGD | 5.58  | 1.46        | 1.33     |
| 14  | f     | 101  | CLA  | CHC-C1C | 5.58  | 1.49        | 1.35     |
| 14  | Y     | 818  | CLA  | O2D-CGD | 5.58  | 1.46        | 1.33     |
| 14  | Y     | 822  | CLA  | O2A-C1  | 5.58  | 1.61        | 1.46     |
| 14  | Z     | 821  | CLA  | O2D-CGD | 5.58  | 1.46        | 1.33     |
| 14  | L     | 202  | CLA  | O2D-CGD | 5.58  | 1.46        | 1.33     |
| 14  | B     | 823  | CLA  | O2D-CGD | 5.57  | 1.46        | 1.33     |
| 14  | U     | 1003 | CLA  | OBD-CAD | 5.57  | 1.30        | 1.22     |
| 14  | Y     | 817  | CLA  | CHC-C1C | 5.57  | 1.49        | 1.35     |
| 17  | Y     | 846  | BCR  | C10-C9  | -5.57 | 1.28        | 1.35     |
| 14  | B     | 835  | CLA  | CHC-C1C | 5.57  | 1.49        | 1.35     |
| 14  | B     | 819  | CLA  | OBD-CAD | 5.57  | 1.30        | 1.22     |
| 14  | G     | 821  | CLA  | CHC-C1C | 5.56  | 1.49        | 1.35     |
| 14  | h     | 207  | CLA  | CHC-C1C | 5.56  | 1.49        | 1.35     |
| 14  | Y     | 811  | CLA  | O2A-C1  | 5.56  | 1.61        | 1.46     |
| 14  | H     | 811  | CLA  | O2D-CGD | 5.56  | 1.46        | 1.33     |
| 14  | G     | 830  | CLA  | O2D-CGD | 5.55  | 1.46        | 1.33     |
| 14  | G     | 818  | CLA  | O2D-CGD | 5.54  | 1.46        | 1.33     |
| 14  | B     | 822  | CLA  | O2D-CGD | 5.54  | 1.46        | 1.33     |
| 14  | B     | 829  | CLA  | O2D-CGD | 5.54  | 1.46        | 1.33     |
| 14  | A     | 818  | CLA  | O2D-CGD | 5.54  | 1.46        | 1.33     |
| 14  | Y     | 832  | CLA  | O2A-C1  | 5.54  | 1.61        | 1.46     |
| 14  | Q     | 201  | CLA  | O2D-CGD | 5.54  | 1.46        | 1.33     |
| 14  | B     | 825  | CLA  | O2A-C1  | 5.53  | 1.61        | 1.46     |
| 14  | B     | 810  | CLA  | O2A-C1  | 5.53  | 1.61        | 1.46     |
| 14  | L     | 207  | CLA  | C3B-C2B | 5.53  | 1.48        | 1.40     |
| 14  | B     | 840  | CLA  | CHC-C1C | 5.53  | 1.49        | 1.35     |
| 14  | Y     | 837  | CLA  | O2D-CGD | 5.52  | 1.46        | 1.33     |
| 14  | G     | 813  | CLA  | CHC-C1C | 5.52  | 1.49        | 1.35     |
| 14  | B     | 805  | CLA  | C3B-C2B | 5.52  | 1.48        | 1.40     |
| 14  | B     | 814  | CLA  | C3B-C2B | 5.52  | 1.48        | 1.40     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 834  | CLA  | O2D-CGD | 5.52 | 1.46        | 1.33     |
| 14  | H     | 809  | CLA  | O2A-C1  | 5.52 | 1.61        | 1.46     |
| 14  | H     | 815  | CLA  | O2D-CGD | 5.51 | 1.46        | 1.33     |
| 14  | Y     | 811  | CLA  | C3B-C2B | 5.51 | 1.48        | 1.40     |
| 14  | Y     | 837  | CLA  | O2A-C1  | 5.51 | 1.61        | 1.46     |
| 14  | d     | 201  | CLA  | O2A-C1  | 5.51 | 1.61        | 1.46     |
| 14  | H     | 807  | CLA  | C3D-C2D | 5.51 | 1.49        | 1.39     |
| 14  | Y     | 807  | CLA  | CHC-C1C | 5.51 | 1.49        | 1.35     |
| 14  | B     | 819  | CLA  | O2D-CGD | 5.50 | 1.46        | 1.33     |
| 14  | h     | 206  | CLA  | OBD-CAD | 5.50 | 1.30        | 1.22     |
| 14  | A     | 806  | CLA  | CHC-C1C | 5.50 | 1.49        | 1.35     |
| 14  | Y     | 823  | CLA  | CHC-C1C | 5.50 | 1.49        | 1.35     |
| 14  | Z     | 805  | CLA  | O2D-CGD | 5.50 | 1.46        | 1.33     |
| 14  | A     | 828  | CLA  | O2D-CGD | 5.50 | 1.46        | 1.33     |
| 14  | B     | 839  | CLA  | O2D-CGD | 5.50 | 1.46        | 1.33     |
| 14  | A     | 821  | CLA  | O2A-C1  | 5.50 | 1.61        | 1.46     |
| 14  | Z     | 832  | CLA  | OBD-CAD | 5.50 | 1.30        | 1.22     |
| 14  | H     | 816  | CLA  | O2A-C1  | 5.49 | 1.61        | 1.46     |
| 14  | G     | 808  | CLA  | CHC-C1C | 5.49 | 1.49        | 1.35     |
| 14  | Y     | 835  | CLA  | O2D-CGD | 5.48 | 1.46        | 1.33     |
| 14  | Y     | 822  | CLA  | O2D-CGD | 5.48 | 1.46        | 1.33     |
| 14  | H     | 823  | CLA  | O2D-CGD | 5.48 | 1.46        | 1.33     |
| 14  | U     | 1002 | CLA  | O2A-C1  | 5.48 | 1.61        | 1.46     |
| 14  | A     | 836  | CLA  | O2D-CGD | 5.48 | 1.46        | 1.33     |
| 14  | L     | 206  | CLA  | CHC-C1C | 5.48 | 1.49        | 1.35     |
| 14  | B     | 840  | CLA  | OBD-CAD | 5.48 | 1.30        | 1.22     |
| 14  | A     | 832  | CLA  | C3B-C2B | 5.48 | 1.48        | 1.40     |
| 14  | L     | 201  | CLA  | CHC-C1C | 5.48 | 1.49        | 1.35     |
| 14  | B     | 827  | CLA  | O2A-C1  | 5.48 | 1.61        | 1.46     |
| 14  | B     | 814  | CLA  | CHC-C1C | 5.48 | 1.49        | 1.35     |
| 14  | Z     | 823  | CLA  | O2A-C1  | 5.48 | 1.61        | 1.46     |
| 14  | A     | 836  | CLA  | OBD-CAD | 5.47 | 1.30        | 1.22     |
| 14  | Z     | 820  | CLA  | O2D-CGD | 5.47 | 1.46        | 1.33     |
| 14  | H     | 803  | CLA  | O2D-CGD | 5.47 | 1.46        | 1.33     |
| 14  | G     | 820  | CLA  | O2A-C1  | 5.47 | 1.61        | 1.46     |
| 14  | A     | 827  | CLA  | CHC-C1C | 5.47 | 1.49        | 1.35     |
| 14  | d     | 202  | CLA  | O2D-CGD | 5.47 | 1.46        | 1.33     |
| 14  | Z     | 818  | CLA  | CHC-C1C | 5.47 | 1.49        | 1.35     |
| 14  | Y     | 815  | CLA  | OBD-CAD | 5.47 | 1.29        | 1.22     |
| 14  | h     | 201  | CLA  | C3B-C2B | 5.46 | 1.47        | 1.40     |
| 14  | G     | 819  | CLA  | C3B-C2B | 5.46 | 1.47        | 1.40     |
| 14  | Z     | 821  | CLA  | CHC-C1C | 5.46 | 1.49        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | G     | 814 | CLA  | CHC-C1C | 5.46 | 1.49        | 1.35     |
| 14  | Z     | 810 | CLA  | O2D-CGD | 5.46 | 1.46        | 1.33     |
| 14  | Y     | 823 | CLA  | O2A-C1  | 5.45 | 1.61        | 1.46     |
| 14  | B     | 824 | CLA  | O2A-C1  | 5.45 | 1.61        | 1.46     |
| 14  | G     | 817 | CLA  | CHC-C1C | 5.45 | 1.48        | 1.35     |
| 14  | Y     | 841 | CLA  | CHC-C1C | 5.45 | 1.48        | 1.35     |
| 14  | Z     | 833 | CLA  | O2D-CGD | 5.45 | 1.46        | 1.33     |
| 14  | G     | 821 | CLA  | O2A-C1  | 5.45 | 1.61        | 1.46     |
| 14  | B     | 831 | CLA  | O2D-CGD | 5.45 | 1.46        | 1.33     |
| 14  | Y     | 840 | CLA  | C3B-C2B | 5.45 | 1.47        | 1.40     |
| 14  | Z     | 830 | CLA  | O2D-CGD | 5.45 | 1.46        | 1.33     |
| 14  | A     | 837 | CLA  | O2D-CGD | 5.45 | 1.46        | 1.33     |
| 14  | Z     | 816 | CLA  | O2D-CGD | 5.45 | 1.46        | 1.33     |
| 14  | T     | 101 | CLA  | CHC-C1C | 5.45 | 1.48        | 1.35     |
| 14  | A     | 820 | CLA  | CHC-C1C | 5.44 | 1.48        | 1.35     |
| 14  | Z     | 815 | CLA  | CHC-C1C | 5.44 | 1.48        | 1.35     |
| 14  | A     | 842 | CLA  | CHC-C1C | 5.44 | 1.48        | 1.35     |
| 14  | B     | 818 | CLA  | C3B-C2B | 5.44 | 1.47        | 1.40     |
| 14  | Y     | 804 | CLA  | OBD-CAD | 5.43 | 1.29        | 1.22     |
| 14  | G     | 808 | CLA  | O2D-CGD | 5.43 | 1.46        | 1.33     |
| 14  | H     | 822 | CLA  | CHC-C1C | 5.43 | 1.48        | 1.35     |
| 14  | Y     | 816 | CLA  | CHC-C1C | 5.43 | 1.48        | 1.35     |
| 14  | H     | 809 | CLA  | O2D-CGD | 5.43 | 1.46        | 1.33     |
| 14  | G     | 841 | CLA  | CHC-C1C | 5.43 | 1.48        | 1.35     |
| 14  | A     | 817 | CLA  | O2D-CGD | 5.43 | 1.46        | 1.33     |
| 14  | A     | 834 | CLA  | O2A-C1  | 5.43 | 1.61        | 1.46     |
| 14  | A     | 839 | CLA  | O2A-C1  | 5.43 | 1.61        | 1.46     |
| 14  | H     | 814 | CLA  | O2D-CGD | 5.43 | 1.46        | 1.33     |
| 14  | Z     | 814 | CLA  | CHC-C1C | 5.43 | 1.48        | 1.35     |
| 14  | H     | 809 | CLA  | CHC-C1C | 5.42 | 1.48        | 1.35     |
| 14  | A     | 828 | CLA  | CHC-C1C | 5.42 | 1.48        | 1.35     |
| 14  | f     | 102 | CLA  | CHC-C1C | 5.42 | 1.48        | 1.35     |
| 14  | J     | 102 | CLA  | CHC-C1C | 5.41 | 1.48        | 1.35     |
| 14  | G     | 843 | CLA  | O2D-CGD | 5.41 | 1.46        | 1.33     |
| 14  | G     | 841 | CLA  | O2A-C1  | 5.41 | 1.61        | 1.46     |
| 14  | L     | 207 | CLA  | CHC-C1C | 5.41 | 1.48        | 1.35     |
| 14  | L     | 206 | CLA  | O2D-CGD | 5.41 | 1.46        | 1.33     |
| 14  | A     | 815 | CLA  | O2A-C1  | 5.41 | 1.61        | 1.46     |
| 14  | A     | 821 | CLA  | CHC-C1C | 5.41 | 1.48        | 1.35     |
| 14  | H     | 813 | CLA  | CHC-C1C | 5.41 | 1.48        | 1.35     |
| 14  | A     | 834 | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | Z     | 829 | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | Y     | 805  | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | B     | 825  | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | Y     | 843  | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | Z     | 833  | CLA  | OBD-CAD | 5.40 | 1.29        | 1.22     |
| 14  | G     | 837  | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | Y     | 820  | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | Y     | 834  | CLA  | O2D-CGD | 5.40 | 1.46        | 1.33     |
| 14  | Z     | 809  | CLA  | O2D-CGD | 5.40 | 1.46        | 1.33     |
| 14  | J     | 101  | CLA  | CHC-C1C | 5.40 | 1.48        | 1.35     |
| 14  | H     | 817  | CLA  | CHC-C1C | 5.39 | 1.48        | 1.35     |
| 14  | B     | 839  | CLA  | CHC-C1C | 5.39 | 1.48        | 1.35     |
| 14  | Y     | 855  | CLA  | CHC-C1C | 5.39 | 1.48        | 1.35     |
| 14  | Z     | 830  | CLA  | CHC-C1C | 5.39 | 1.48        | 1.35     |
| 14  | A     | 825  | CLA  | O2D-CGD | 5.39 | 1.46        | 1.33     |
| 14  | B     | 814  | CLA  | O2A-C1  | 5.39 | 1.61        | 1.46     |
| 14  | U     | 1002 | CLA  | CHC-C1C | 5.39 | 1.48        | 1.35     |
| 14  | Z     | 839  | CLA  | O2A-C1  | 5.38 | 1.61        | 1.46     |
| 14  | H     | 829  | CLA  | CHC-C1C | 5.38 | 1.48        | 1.35     |
| 14  | Y     | 824  | CLA  | O2D-CGD | 5.38 | 1.46        | 1.33     |
| 14  | L     | 201  | CLA  | O2A-C1  | 5.38 | 1.61        | 1.46     |
| 14  | Y     | 819  | CLA  | CHC-C1C | 5.38 | 1.48        | 1.35     |
| 14  | Y     | 855  | CLA  | O2D-CGD | 5.38 | 1.46        | 1.33     |
| 14  | G     | 839  | CLA  | O2D-CGD | 5.38 | 1.46        | 1.33     |
| 14  | H     | 828  | CLA  | O2D-CGD | 5.38 | 1.46        | 1.33     |
| 14  | Z     | 834  | CLA  | CHC-C1C | 5.38 | 1.48        | 1.35     |
| 14  | H     | 812  | CLA  | O2D-CGD | 5.38 | 1.46        | 1.33     |
| 14  | K     | 103  | CLA  | O2D-CGD | 5.38 | 1.46        | 1.33     |
| 14  | Y     | 815  | CLA  | CHC-C1C | 5.37 | 1.48        | 1.35     |
| 14  | Y     | 812  | CLA  | O2D-CGD | 5.37 | 1.46        | 1.33     |
| 14  | L     | 202  | CLA  | O2A-C1  | 5.37 | 1.61        | 1.46     |
| 14  | B     | 815  | CLA  | CHC-C1C | 5.37 | 1.48        | 1.35     |
| 14  | G     | 817  | CLA  | O2D-CGD | 5.37 | 1.46        | 1.33     |
| 14  | T     | 103  | CLA  | O2D-CGD | 5.37 | 1.46        | 1.33     |
| 14  | A     | 803  | CLA  | CHC-C1C | 5.37 | 1.48        | 1.35     |
| 14  | A     | 810  | CLA  | O2D-CGD | 5.36 | 1.46        | 1.33     |
| 14  | A     | 817  | CLA  | CHC-C1C | 5.36 | 1.48        | 1.35     |
| 14  | A     | 822  | CLA  | OBD-CAD | 5.36 | 1.29        | 1.22     |
| 14  | G     | 810  | CLA  | O2D-CGD | 5.36 | 1.46        | 1.33     |
| 14  | Y     | 807  | CLA  | O2D-CGD | 5.36 | 1.46        | 1.33     |
| 14  | G     | 833  | CLA  | O2A-C1  | 5.36 | 1.61        | 1.46     |
| 14  | Z     | 832  | CLA  | CHC-C1C | 5.35 | 1.48        | 1.35     |
| 14  | A     | 804  | CLA  | C3B-C2B | 5.35 | 1.47        | 1.40     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 836 | CLA  | OBD-CAD | 5.35  | 1.29        | 1.22     |
| 14  | Y     | 809 | CLA  | CHC-C1C | 5.35  | 1.48        | 1.35     |
| 14  | Y     | 827 | CLA  | CHC-C1C | 5.35  | 1.48        | 1.35     |
| 14  | H     | 801 | CLA  | CHC-C1C | 5.35  | 1.48        | 1.35     |
| 14  | H     | 806 | CLA  | CHC-C1C | 5.35  | 1.48        | 1.35     |
| 14  | A     | 842 | CLA  | O2D-CGD | 5.35  | 1.46        | 1.33     |
| 14  | Y     | 835 | CLA  | CHC-C1C | 5.35  | 1.48        | 1.35     |
| 14  | Y     | 825 | CLA  | O2A-C1  | 5.34  | 1.61        | 1.46     |
| 14  | G     | 804 | CLA  | OBD-CAD | 5.34  | 1.29        | 1.22     |
| 14  | A     | 836 | CLA  | CHC-C1C | 5.34  | 1.48        | 1.35     |
| 14  | H     | 803 | CLA  | OBD-CAD | 5.34  | 1.29        | 1.22     |
| 14  | K     | 103 | CLA  | OBD-CAD | 5.34  | 1.29        | 1.22     |
| 14  | Y     | 814 | CLA  | O2A-C1  | 5.34  | 1.61        | 1.46     |
| 14  | B     | 829 | CLA  | O2A-C1  | 5.34  | 1.61        | 1.46     |
| 14  | G     | 806 | CLA  | CHC-C1C | 5.34  | 1.48        | 1.35     |
| 14  | Z     | 817 | CLA  | CHC-C1C | 5.34  | 1.48        | 1.35     |
| 14  | B     | 832 | CLA  | O2D-CGD | 5.34  | 1.46        | 1.33     |
| 14  | Y     | 824 | CLA  | CHC-C1C | 5.34  | 1.48        | 1.35     |
| 14  | H     | 824 | CLA  | OBD-CAD | 5.34  | 1.29        | 1.22     |
| 14  | G     | 840 | CLA  | OBD-CAD | 5.34  | 1.29        | 1.22     |
| 14  | G     | 832 | CLA  | O2D-CGD | 5.33  | 1.46        | 1.33     |
| 17  | T     | 102 | BCR  | C10-C9  | -5.33 | 1.28        | 1.35     |
| 14  | Z     | 827 | CLA  | O2A-C1  | 5.33  | 1.61        | 1.46     |
| 14  | G     | 831 | CLA  | CHC-C1C | 5.33  | 1.48        | 1.35     |
| 14  | B     | 840 | CLA  | O2D-CGD | 5.33  | 1.46        | 1.33     |
| 14  | Z     | 807 | CLA  | O2A-C1  | 5.33  | 1.61        | 1.46     |
| 14  | G     | 810 | CLA  | C3C-C2C | 5.33  | 1.48        | 1.36     |
| 14  | G     | 828 | CLA  | O2D-CGD | 5.33  | 1.46        | 1.33     |
| 14  | Z     | 838 | CLA  | O2A-C1  | 5.33  | 1.61        | 1.46     |
| 14  | B     | 811 | CLA  | CHC-C1C | 5.32  | 1.48        | 1.35     |
| 14  | Z     | 818 | CLA  | C3B-C2B | 5.32  | 1.47        | 1.40     |
| 14  | G     | 832 | CLA  | O2A-C1  | 5.32  | 1.61        | 1.46     |
| 14  | G     | 811 | CLA  | CHC-C1C | 5.32  | 1.48        | 1.35     |
| 14  | J     | 101 | CLA  | O2D-CGD | 5.32  | 1.46        | 1.33     |
| 14  | Y     | 818 | CLA  | CHC-C1C | 5.32  | 1.48        | 1.35     |
| 14  | Y     | 821 | CLA  | O2A-C1  | 5.32  | 1.61        | 1.46     |
| 14  | B     | 822 | CLA  | CHC-C1C | 5.32  | 1.48        | 1.35     |
| 14  | T     | 101 | CLA  | OBD-CAD | 5.31  | 1.30        | 1.22     |
| 14  | A     | 826 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |
| 14  | G     | 816 | CLA  | O2A-C1  | 5.31  | 1.61        | 1.46     |
| 14  | Z     | 838 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |
| 14  | g     | 101 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 824  | CLA  | O2A-C1  | 5.31 | 1.61        | 1.46     |
| 14  | H     | 824  | CLA  | O2A-C1  | 5.31 | 1.61        | 1.46     |
| 14  | H     | 815  | CLA  | CHC-C1C | 5.31 | 1.48        | 1.35     |
| 14  | Y     | 826  | CLA  | O2D-CGD | 5.31 | 1.46        | 1.33     |
| 14  | H     | 804  | CLA  | O2A-C1  | 5.31 | 1.61        | 1.46     |
| 14  | G     | 810  | CLA  | CHC-C1C | 5.30 | 1.48        | 1.35     |
| 14  | B     | 809  | CLA  | O2D-CGD | 5.30 | 1.46        | 1.33     |
| 14  | G     | 807  | CLA  | O2D-CGD | 5.30 | 1.46        | 1.33     |
| 14  | Y     | 840  | CLA  | CHC-C1C | 5.30 | 1.48        | 1.35     |
| 14  | d     | 202  | CLA  | C3B-C2B | 5.30 | 1.47        | 1.40     |
| 14  | Y     | 834  | CLA  | O2A-C1  | 5.30 | 1.61        | 1.46     |
| 14  | G     | 812  | CLA  | CHC-C1C | 5.30 | 1.48        | 1.35     |
| 14  | G     | 823  | CLA  | O2A-C1  | 5.30 | 1.61        | 1.46     |
| 14  | H     | 825  | CLA  | O2D-CGD | 5.30 | 1.46        | 1.33     |
| 14  | Y     | 813  | CLA  | O2A-C1  | 5.30 | 1.61        | 1.46     |
| 14  | A     | 833  | CLA  | O2A-C1  | 5.29 | 1.61        | 1.46     |
| 14  | H     | 835  | CLA  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 14  | Y     | 824  | CLA  | O2A-C1  | 5.29 | 1.61        | 1.46     |
| 14  | G     | 842  | CLA  | C3D-C2D | 5.29 | 1.48        | 1.39     |
| 14  | B     | 834  | CLA  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 14  | B     | 812  | CLA  | O2A-C1  | 5.29 | 1.61        | 1.46     |
| 14  | L     | 206  | CLA  | OBD-CAD | 5.29 | 1.29        | 1.22     |
| 14  | H     | 829  | CLA  | C3D-C2D | 5.29 | 1.48        | 1.39     |
| 14  | S     | 1103 | CLA  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 14  | H     | 805  | CLA  | O2D-CGD | 5.29 | 1.46        | 1.33     |
| 14  | Y     | 821  | CLA  | OBD-CAD | 5.29 | 1.29        | 1.22     |
| 14  | Y     | 811  | CLA  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 14  | f     | 101  | CLA  | O2D-CGD | 5.29 | 1.46        | 1.33     |
| 14  | Y     | 840  | CLA  | O2A-C1  | 5.28 | 1.61        | 1.46     |
| 14  | Y     | 837  | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 14  | B     | 806  | CLA  | O2A-C1  | 5.28 | 1.61        | 1.46     |
| 14  | F     | 202  | CLA  | O2D-CGD | 5.28 | 1.46        | 1.33     |
| 14  | G     | 815  | CLA  | O2A-C1  | 5.28 | 1.61        | 1.46     |
| 14  | G     | 805  | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 14  | Y     | 840  | CLA  | O2D-CGD | 5.28 | 1.46        | 1.33     |
| 14  | Y     | 843  | CLA  | O2D-CGD | 5.28 | 1.46        | 1.33     |
| 14  | X     | 1701 | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 14  | G     | 807  | CLA  | O2A-C1  | 5.28 | 1.61        | 1.46     |
| 14  | G     | 807  | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 14  | G     | 835  | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 14  | G     | 828  | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 14  | G     | 818  | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 816  | CLA  | OBD-CAD | 5.27 | 1.29        | 1.22     |
| 14  | H     | 830  | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 14  | Z     | 828  | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 14  | A     | 825  | CLA  | O2A-C1  | 5.27 | 1.61        | 1.46     |
| 14  | B     | 834  | CLA  | O2D-CGD | 5.27 | 1.46        | 1.33     |
| 14  | Y     | 808  | CLA  | O2D-CGD | 5.27 | 1.46        | 1.33     |
| 14  | Z     | 813  | CLA  | OBD-CAD | 5.27 | 1.29        | 1.22     |
| 14  | f     | 102  | CLA  | O2A-C1  | 5.27 | 1.61        | 1.46     |
| 14  | U     | 1003 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 14  | H     | 837  | CLA  | CHC-C1C | 5.26 | 1.48        | 1.35     |
| 14  | B     | 823  | CLA  | CHC-C1C | 5.26 | 1.48        | 1.35     |
| 14  | G     | 839  | CLA  | CHC-C1C | 5.26 | 1.48        | 1.35     |
| 14  | Z     | 821  | CLA  | O2A-C1  | 5.26 | 1.61        | 1.46     |
| 14  | Y     | 821  | CLA  | C3B-C2B | 5.26 | 1.47        | 1.40     |
| 14  | Y     | 833  | CLA  | O2D-CGD | 5.26 | 1.46        | 1.33     |
| 14  | G     | 834  | CLA  | O2D-CGD | 5.26 | 1.46        | 1.33     |
| 14  | G     | 802  | CLA  | OBD-CAD | 5.26 | 1.29        | 1.22     |
| 14  | J     | 102  | CLA  | O2A-C1  | 5.26 | 1.61        | 1.46     |
| 14  | G     | 808  | CLA  | O2A-C1  | 5.26 | 1.61        | 1.46     |
| 14  | Z     | 829  | CLA  | O2D-CGD | 5.26 | 1.46        | 1.33     |
| 14  | Y     | 835  | CLA  | O2A-C1  | 5.26 | 1.61        | 1.46     |
| 14  | B     | 825  | CLA  | O2D-CGD | 5.25 | 1.46        | 1.33     |
| 14  | Y     | 803  | CLA  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 14  | H     | 823  | CLA  | O2A-C1  | 5.25 | 1.60        | 1.46     |
| 14  | H     | 813  | CLA  | O2D-CGD | 5.25 | 1.46        | 1.33     |
| 14  | Z     | 802  | CLA  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 14  | Y     | 823  | CLA  | O2D-CGD | 5.25 | 1.46        | 1.33     |
| 14  | Y     | 832  | CLA  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 14  | G     | 809  | CLA  | OBD-CAD | 5.25 | 1.29        | 1.22     |
| 14  | A     | 838  | CLA  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 14  | H     | 811  | CLA  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 14  | J     | 102  | CLA  | O2D-CGD | 5.25 | 1.46        | 1.33     |
| 14  | B     | 841  | CLA  | O2D-CGD | 5.25 | 1.46        | 1.33     |
| 14  | Y     | 804  | CLA  | O2A-C1  | 5.24 | 1.60        | 1.46     |
| 14  | Z     | 835  | CLA  | CHC-C1C | 5.24 | 1.48        | 1.35     |
| 14  | Y     | 842  | CLA  | O2D-CGD | 5.24 | 1.46        | 1.33     |
| 14  | B     | 802  | CLA  | CHC-C1C | 5.24 | 1.48        | 1.35     |
| 14  | B     | 821  | CLA  | OBD-CAD | 5.24 | 1.29        | 1.22     |
| 14  | H     | 831  | CLA  | OBD-CAD | 5.24 | 1.29        | 1.22     |
| 14  | Y     | 818  | CLA  | O2A-C1  | 5.24 | 1.60        | 1.46     |
| 14  | G     | 835  | CLA  | OBD-CAD | 5.24 | 1.29        | 1.22     |
| 14  | V     | 1201 | CLA  | O2D-CGD | 5.24 | 1.46        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | Z     | 826  | CLA  | O2A-C1  | 5.24 | 1.60        | 1.46     |
| 14  | f     | 101  | CLA  | OBD-CAD | 5.24 | 1.29        | 1.22     |
| 14  | G     | 835  | CLA  | O2D-CGD | 5.24 | 1.46        | 1.33     |
| 14  | X     | 1701 | CLA  | O2D-CGD | 5.24 | 1.46        | 1.33     |
| 14  | Y     | 809  | CLA  | OBD-CAD | 5.24 | 1.29        | 1.22     |
| 14  | H     | 809  | CLA  | C3B-C2B | 5.24 | 1.47        | 1.40     |
| 14  | H     | 801  | CLA  | C3C-C2C | 5.24 | 1.47        | 1.36     |
| 13  | Y     | 801  | CL0  | O2A-C1  | 5.24 | 1.60        | 1.46     |
| 14  | G     | 833  | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 14  | Z     | 817  | CLA  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 14  | G     | 838  | CLA  | O2A-C1  | 5.23 | 1.60        | 1.46     |
| 14  | G     | 838  | CLA  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 14  | Z     | 807  | CLA  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 14  | Y     | 803  | CLA  | O2A-C1  | 5.23 | 1.60        | 1.46     |
| 14  | L     | 206  | CLA  | O2A-C1  | 5.23 | 1.60        | 1.46     |
| 14  | H     | 804  | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 14  | A     | 830  | CLA  | O2A-C1  | 5.23 | 1.60        | 1.46     |
| 14  | G     | 829  | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 14  | A     | 852  | CLA  | O2A-C1  | 5.23 | 1.60        | 1.46     |
| 14  | Z     | 810  | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 14  | G     | 841  | CLA  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 14  | A     | 803  | CLA  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 14  | Z     | 838  | CLA  | OBD-CAD | 5.23 | 1.29        | 1.22     |
| 14  | H     | 818  | CLA  | O2A-C1  | 5.22 | 1.60        | 1.46     |
| 14  | Z     | 815  | CLA  | O2A-C1  | 5.22 | 1.60        | 1.46     |
| 14  | Y     | 840  | CLA  | OBD-CAD | 5.22 | 1.29        | 1.22     |
| 14  | Y     | 810  | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 14  | A     | 829  | CLA  | O2D-CGD | 5.22 | 1.45        | 1.33     |
| 14  | Y     | 811  | CLA  | O2D-CGD | 5.22 | 1.45        | 1.33     |
| 14  | Z     | 812  | CLA  | O2D-CGD | 5.22 | 1.45        | 1.33     |
| 14  | K     | 101  | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 18  | Y     | 853  | LHG  | O7-C7   | 5.22 | 1.47        | 1.35     |
| 14  | H     | 810  | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 14  | A     | 815  | CLA  | C3B-C2B | 5.22 | 1.47        | 1.40     |
| 14  | Y     | 817  | CLA  | O2A-C1  | 5.22 | 1.60        | 1.46     |
| 14  | Y     | 813  | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 14  | G     | 803  | CLA  | O2D-CGD | 5.21 | 1.45        | 1.33     |
| 14  | Y     | 831  | CLA  | O2A-C1  | 5.21 | 1.60        | 1.46     |
| 14  | Y     | 806  | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 14  | Y     | 829  | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 14  | Z     | 820  | CLA  | OBD-CAD | 5.21 | 1.29        | 1.22     |
| 14  | Y     | 814  | CLA  | OBD-CAD | 5.21 | 1.29        | 1.22     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 816  | CLA  | O2D-CGD | 5.21 | 1.45        | 1.33     |
| 14  | A     | 841  | CLA  | O2A-C1  | 5.21 | 1.60        | 1.46     |
| 14  | Y     | 818  | CLA  | C3C-C2C | 5.20 | 1.47        | 1.36     |
| 14  | G     | 816  | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 15  | Z     | 840  | PQN  | C10-C5  | 5.20 | 1.49        | 1.40     |
| 14  | g     | 101  | CLA  | OBD-CAD | 5.20 | 1.30        | 1.22     |
| 14  | G     | 803  | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 14  | A     | 827  | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 14  | A     | 815  | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 14  | Z     | 811  | CLA  | C3B-C2B | 5.20 | 1.47        | 1.40     |
| 14  | Z     | 825  | CLA  | O2A-C1  | 5.20 | 1.60        | 1.46     |
| 14  | G     | 832  | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 14  | Z     | 802  | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 14  | H     | 805  | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 14  | A     | 839  | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 14  | H     | 834  | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 14  | Z     | 802  | CLA  | OBD-CAD | 5.19 | 1.29        | 1.22     |
| 14  | f     | 102  | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | A     | 832  | CLA  | O2A-C1  | 5.19 | 1.60        | 1.46     |
| 14  | B     | 824  | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | H     | 804  | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | Z     | 808  | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | V     | 1201 | CLA  | C3B-C2B | 5.19 | 1.47        | 1.40     |
| 14  | G     | 804  | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 14  | Z     | 817  | CLA  | O2A-C1  | 5.19 | 1.60        | 1.46     |
| 14  | Y     | 803  | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | G     | 824  | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 14  | G     | 840  | CLA  | C3C-C2C | 5.19 | 1.47        | 1.36     |
| 14  | H     | 827  | CLA  | OBD-CAD | 5.18 | 1.29        | 1.22     |
| 14  | d     | 202  | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 14  | H     | 815  | CLA  | O2A-C1  | 5.18 | 1.60        | 1.46     |
| 14  | Y     | 808  | CLA  | OBD-CAD | 5.18 | 1.29        | 1.22     |
| 14  | A     | 823  | CLA  | O2A-C1  | 5.18 | 1.60        | 1.46     |
| 14  | H     | 827  | CLA  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 14  | B     | 810  | CLA  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 14  | H     | 826  | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 14  | W     | 1701 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 14  | G     | 829  | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 14  | H     | 824  | CLA  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 13  | G     | 801  | CL0  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 14  | G     | 817  | CLA  | O2A-C1  | 5.17 | 1.60        | 1.46     |
| 14  | Y     | 815  | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 803  | CLA  | OBD-CAD | 5.17 | 1.29        | 1.22     |
| 14  | A     | 804  | CLA  | OBD-CAD | 5.17 | 1.29        | 1.22     |
| 14  | H     | 835  | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 14  | H     | 827  | CLA  | O2A-C1  | 5.17 | 1.60        | 1.46     |
| 14  | Y     | 854  | CLA  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 14  | B     | 817  | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 14  | A     | 811  | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 14  | A     | 805  | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 14  | Z     | 831  | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 14  | S     | 1102 | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 14  | Z     | 801  | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 14  | A     | 831  | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 14  | J     | 102  | CLA  | OBD-CAD | 5.16 | 1.29        | 1.22     |
| 14  | G     | 821  | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 14  | G     | 839  | CLA  | OBD-CAD | 5.16 | 1.29        | 1.22     |
| 14  | Y     | 807  | CLA  | O2A-C1  | 5.16 | 1.60        | 1.46     |
| 14  | A     | 823  | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 14  | Y     | 825  | CLA  | C3B-C2B | 5.16 | 1.47        | 1.40     |
| 14  | G     | 803  | CLA  | O2A-C1  | 5.16 | 1.60        | 1.46     |
| 14  | Z     | 822  | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 14  | G     | 826  | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 14  | A     | 835  | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 14  | H     | 830  | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 14  | H     | 819  | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 14  | B     | 836  | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 13  | A     | 801  | CL0  | OBD-CAD | 5.15 | 1.29        | 1.22     |
| 13  | Y     | 801  | CL0  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 14  | L     | 201  | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 14  | Y     | 815  | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 13  | G     | 801  | CL0  | O2A-C1  | 5.15 | 1.60        | 1.46     |
| 14  | Z     | 820  | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 14  | H     | 831  | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 14  | Y     | 820  | CLA  | O2A-C1  | 5.14 | 1.60        | 1.46     |
| 14  | Z     | 804  | CLA  | OBD-CAD | 5.14 | 1.29        | 1.22     |
| 14  | A     | 841  | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 14  | B     | 816  | CLA  | OBD-CAD | 5.13 | 1.29        | 1.22     |
| 14  | G     | 834  | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 14  | H     | 813  | CLA  | OBD-CAD | 5.13 | 1.29        | 1.22     |
| 14  | Z     | 813  | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 14  | B     | 816  | CLA  | C3D-C2D | 5.13 | 1.48        | 1.39     |
| 14  | H     | 812  | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 14  | G     | 853  | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | Y     | 843  | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 14  | Z     | 839  | CLA  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 14  | Z     | 813  | CLA  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 14  | G     | 827  | CLA  | O2A-C1  | 5.12 | 1.60        | 1.46     |
| 14  | Y     | 831  | CLA  | CHC-C1C | 5.12 | 1.48        | 1.35     |
| 14  | Z     | 809  | CLA  | CHC-C1C | 5.12 | 1.48        | 1.35     |
| 14  | A     | 821  | CLA  | C3B-C2B | 5.12 | 1.47        | 1.40     |
| 14  | B     | 816  | CLA  | O2A-C1  | 5.12 | 1.60        | 1.46     |
| 14  | G     | 833  | CLA  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 14  | Q     | 203  | CLA  | C3B-C2B | 5.12 | 1.47        | 1.40     |
| 14  | A     | 809  | CLA  | CHC-C1C | 5.12 | 1.48        | 1.35     |
| 14  | H     | 825  | CLA  | CHC-C1C | 5.12 | 1.48        | 1.35     |
| 14  | g     | 102  | CLA  | C3B-C2B | 5.12 | 1.47        | 1.40     |
| 14  | H     | 817  | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 14  | G     | 809  | CLA  | CHC-C1C | 5.12 | 1.48        | 1.35     |
| 14  | A     | 824  | CLA  | O2A-C1  | 5.12 | 1.60        | 1.46     |
| 14  | Y     | 815  | CLA  | O2A-C1  | 5.12 | 1.60        | 1.46     |
| 14  | A     | 808  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | G     | 814  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | L     | 207  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | Z     | 817  | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 14  | G     | 826  | CLA  | OBD-CAD | 5.11 | 1.29        | 1.22     |
| 14  | Y     | 804  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | Y     | 812  | CLA  | CHC-C1C | 5.11 | 1.48        | 1.35     |
| 14  | A     | 811  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | B     | 802  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | Y     | 809  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | G     | 822  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | Z     | 828  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | A     | 817  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | U     | 1002 | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | A     | 806  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | G     | 819  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | A     | 812  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | Z     | 831  | CLA  | C3D-C2D | 5.11 | 1.48        | 1.39     |
| 14  | Y     | 816  | CLA  | O2A-C1  | 5.11 | 1.60        | 1.46     |
| 14  | Z     | 803  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | Z     | 836  | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 14  | A     | 819  | CLA  | CHC-C1C | 5.11 | 1.48        | 1.35     |
| 14  | H     | 838  | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | H     | 801  | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | Z     | 803  | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 816  | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 14  | G     | 806  | CLA  | OBD-CAD | 5.10 | 1.29        | 1.22     |
| 14  | H     | 806  | CLA  | OBD-CAD | 5.10 | 1.29        | 1.22     |
| 14  | B     | 803  | CLA  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 14  | A     | 807  | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | Z     | 818  | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | B     | 820  | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | S     | 1103 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 14  | Z     | 831  | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 14  | G     | 811  | CLA  | C3B-C2B | 5.10 | 1.47        | 1.40     |
| 14  | Z     | 805  | CLA  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 14  | B     | 822  | CLA  | O2A-C1  | 5.10 | 1.60        | 1.46     |
| 14  | G     | 811  | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 14  | T     | 103  | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 14  | Z     | 834  | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 14  | G     | 806  | CLA  | C3B-C2B | 5.09 | 1.47        | 1.40     |
| 14  | G     | 815  | CLA  | C3B-C2B | 5.09 | 1.47        | 1.40     |
| 14  | S     | 1103 | CLA  | O2A-C1  | 5.09 | 1.60        | 1.46     |
| 14  | A     | 841  | CLA  | C3C-C2C | 5.09 | 1.47        | 1.36     |
| 14  | H     | 820  | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 14  | H     | 828  | CLA  | C3B-C2B | 5.08 | 1.47        | 1.40     |
| 14  | H     | 821  | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 14  | G     | 814  | CLA  | OBD-CAD | 5.08 | 1.29        | 1.22     |
| 13  | A     | 801  | CL0  | O2A-C1  | 5.08 | 1.60        | 1.46     |
| 14  | B     | 838  | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 14  | Y     | 832  | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 14  | Z     | 822  | CLA  | C3B-C2B | 5.08 | 1.47        | 1.40     |
| 14  | B     | 813  | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 14  | Y     | 802  | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 14  | Y     | 807  | CLA  | OBD-CAD | 5.08 | 1.29        | 1.22     |
| 14  | Y     | 821  | CLA  | C3D-C2D | 5.08 | 1.48        | 1.39     |
| 14  | B     | 820  | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 14  | Z     | 825  | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 14  | Z     | 812  | CLA  | OBD-CAD | 5.08 | 1.29        | 1.22     |
| 14  | B     | 816  | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 14  | A     | 804  | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 14  | G     | 836  | CLA  | O2A-C1  | 5.08 | 1.60        | 1.46     |
| 14  | A     | 831  | CLA  | O2A-C1  | 5.08 | 1.60        | 1.46     |
| 14  | Z     | 822  | CLA  | O2A-C1  | 5.08 | 1.60        | 1.46     |
| 14  | A     | 814  | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 14  | A     | 824  | CLA  | OBD-CAD | 5.08 | 1.29        | 1.22     |
| 14  | U     | 1006 | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 812  | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 14  | G     | 843  | CLA  | OBD-CAD | 5.07 | 1.29        | 1.22     |
| 14  | A     | 835  | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 14  | G     | 825  | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 14  | H     | 833  | CLA  | CHC-C1C | 5.07 | 1.48        | 1.35     |
| 14  | A     | 836  | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 14  | A     | 806  | CLA  | C3B-C2B | 5.07 | 1.47        | 1.40     |
| 14  | H     | 817  | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 14  | Y     | 839  | CLA  | CHC-C1C | 5.07 | 1.48        | 1.35     |
| 14  | Y     | 806  | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 14  | B     | 816  | CLA  | C3B-C2B | 5.07 | 1.47        | 1.40     |
| 14  | A     | 810  | CLA  | CHC-C1C | 5.07 | 1.48        | 1.35     |
| 14  | Z     | 813  | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 14  | A     | 820  | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 14  | H     | 810  | CLA  | O2A-C1  | 5.07 | 1.60        | 1.46     |
| 14  | A     | 806  | CLA  | O2A-C1  | 5.07 | 1.60        | 1.46     |
| 14  | B     | 835  | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 14  | j     | 102  | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 14  | Z     | 816  | CLA  | CHC-C1C | 5.06 | 1.48        | 1.35     |
| 14  | Y     | 841  | CLA  | O2A-C1  | 5.06 | 1.60        | 1.46     |
| 14  | A     | 804  | CLA  | O2A-C1  | 5.06 | 1.60        | 1.46     |
| 14  | Y     | 825  | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 14  | B     | 836  | CLA  | CHC-C1C | 5.06 | 1.47        | 1.35     |
| 14  | H     | 837  | CLA  | OBD-CAD | 5.06 | 1.29        | 1.22     |
| 14  | G     | 836  | CLA  | CHC-C1C | 5.06 | 1.47        | 1.35     |
| 14  | Z     | 833  | CLA  | CHC-C1C | 5.06 | 1.47        | 1.35     |
| 14  | B     | 811  | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 14  | U     | 1003 | CLA  | O2A-C1  | 5.06 | 1.60        | 1.46     |
| 14  | Y     | 854  | CLA  | O2A-C1  | 5.06 | 1.60        | 1.46     |
| 14  | Z     | 814  | CLA  | O2A-C1  | 5.06 | 1.60        | 1.46     |
| 14  | H     | 822  | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 14  | Y     | 806  | CLA  | O2A-C1  | 5.06 | 1.60        | 1.46     |
| 14  | Y     | 817  | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 14  | B     | 841  | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 14  | h     | 205  | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 14  | H     | 812  | CLA  | O2A-C1  | 5.05 | 1.60        | 1.46     |
| 14  | B     | 833  | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 14  | Y     | 836  | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 14  | Z     | 808  | CLA  | OBD-CAD | 5.05 | 1.29        | 1.22     |
| 14  | A     | 815  | CLA  | OBD-CAD | 5.05 | 1.29        | 1.22     |
| 14  | A     | 835  | CLA  | OBD-CAD | 5.05 | 1.29        | 1.22     |
| 14  | H     | 826  | CLA  | O2A-C1  | 5.05 | 1.60        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | d     | 201  | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 14  | B     | 801  | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 14  | B     | 840  | CLA  | O2A-C1  | 5.04 | 1.60        | 1.46     |
| 14  | G     | 816  | CLA  | CHC-C1C | 5.04 | 1.47        | 1.35     |
| 14  | H     | 836  | CLA  | CHC-C1C | 5.04 | 1.47        | 1.35     |
| 14  | Y     | 830  | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 14  | G     | 805  | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 14  | B     | 823  | CLA  | O2A-C1  | 5.04 | 1.60        | 1.46     |
| 14  | G     | 828  | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 14  | A     | 813  | CLA  | O2A-C1  | 5.04 | 1.60        | 1.46     |
| 14  | G     | 831  | CLA  | OBD-CAD | 5.04 | 1.29        | 1.22     |
| 14  | A     | 826  | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 14  | G     | 833  | CLA  | C3D-C2D | 5.04 | 1.48        | 1.39     |
| 14  | G     | 843  | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 14  | G     | 825  | CLA  | OBD-CAD | 5.03 | 1.29        | 1.22     |
| 14  | B     | 832  | CLA  | C3B-C2B | 5.03 | 1.47        | 1.40     |
| 14  | S     | 1103 | CLA  | OBD-CAD | 5.03 | 1.29        | 1.22     |
| 14  | Z     | 804  | CLA  | O2A-C1  | 5.03 | 1.60        | 1.46     |
| 14  | A     | 812  | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 14  | Y     | 836  | CLA  | OBD-CAD | 5.03 | 1.29        | 1.22     |
| 14  | Z     | 812  | CLA  | C3D-C2D | 5.03 | 1.48        | 1.39     |
| 14  | Y     | 819  | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 14  | H     | 816  | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 14  | G     | 843  | CLA  | O2A-C1  | 5.03 | 1.60        | 1.46     |
| 14  | A     | 839  | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 14  | G     | 809  | CLA  | O2A-C1  | 5.03 | 1.60        | 1.46     |
| 14  | H     | 835  | CLA  | OBD-CAD | 5.03 | 1.29        | 1.22     |
| 14  | H     | 814  | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 14  | H     | 823  | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 14  | H     | 838  | CLA  | O2A-C1  | 5.03 | 1.60        | 1.46     |
| 14  | B     | 804  | CLA  | O2A-C1  | 5.03 | 1.60        | 1.46     |
| 14  | H     | 812  | CLA  | C3B-C2B | 5.02 | 1.47        | 1.40     |
| 14  | B     | 804  | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 14  | g     | 102  | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 14  | A     | 825  | CLA  | OBD-CAD | 5.02 | 1.29        | 1.22     |
| 14  | Y     | 822  | CLA  | OBD-CAD | 5.02 | 1.29        | 1.22     |
| 14  | Z     | 813  | CLA  | C3D-C2D | 5.02 | 1.48        | 1.39     |
| 14  | H     | 819  | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 14  | H     | 801  | CLA  | C3D-C2D | 5.02 | 1.48        | 1.39     |
| 14  | B     | 801  | CLA  | O2A-C1  | 5.02 | 1.60        | 1.46     |
| 14  | H     | 804  | CLA  | OBD-CAD | 5.02 | 1.29        | 1.22     |
| 14  | Y     | 834  | CLA  | OBD-CAD | 5.02 | 1.29        | 1.22     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | L     | 202  | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 14  | G     | 820  | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 14  | Y     | 830  | CLA  | O2A-C1  | 5.02 | 1.60        | 1.46     |
| 14  | L     | 205  | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 14  | Z     | 803  | CLA  | C3D-C2D | 5.02 | 1.48        | 1.39     |
| 14  | G     | 820  | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 14  | H     | 818  | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 14  | H     | 818  | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 14  | B     | 833  | CLA  | OBD-CAD | 5.02 | 1.29        | 1.22     |
| 14  | B     | 824  | CLA  | CHC-C1C | 5.01 | 1.47        | 1.35     |
| 14  | G     | 812  | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 14  | Z     | 812  | CLA  | C3B-C2B | 5.01 | 1.47        | 1.40     |
| 14  | U     | 1003 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 14  | H     | 821  | CLA  | OBD-CAD | 5.01 | 1.29        | 1.22     |
| 14  | B     | 809  | CLA  | CHC-C1C | 5.01 | 1.47        | 1.35     |
| 14  | Z     | 813  | CLA  | CHC-C1C | 5.01 | 1.47        | 1.35     |
| 14  | Z     | 823  | CLA  | OBD-CAD | 5.01 | 1.29        | 1.22     |
| 14  | G     | 836  | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 14  | A     | 821  | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 14  | G     | 831  | CLA  | O2A-C1  | 5.00 | 1.60        | 1.46     |
| 14  | d     | 201  | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 14  | Z     | 830  | CLA  | O2A-C1  | 5.00 | 1.60        | 1.46     |
| 14  | Z     | 837  | CLA  | OBD-CAD | 5.00 | 1.29        | 1.22     |
| 14  | A     | 822  | CLA  | O2A-C1  | 5.00 | 1.60        | 1.46     |
| 14  | d     | 201  | CLA  | CHC-C1C | 5.00 | 1.47        | 1.35     |
| 14  | Z     | 811  | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 14  | K     | 101  | CLA  | C3B-C2B | 4.99 | 1.47        | 1.40     |
| 14  | A     | 839  | CLA  | C3B-C2B | 4.99 | 1.47        | 1.40     |
| 14  | H     | 832  | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 14  | Y     | 808  | CLA  | O2A-C1  | 4.99 | 1.60        | 1.46     |
| 14  | G     | 840  | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 14  | B     | 837  | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 14  | H     | 802  | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 14  | Z     | 808  | CLA  | C3D-C2D | 4.99 | 1.48        | 1.39     |
| 14  | Y     | 829  | CLA  | O2A-C1  | 4.99 | 1.60        | 1.46     |
| 14  | G     | 853  | CLA  | C3C-C2C | 4.99 | 1.47        | 1.36     |
| 14  | Y     | 855  | CLA  | C3D-C2D | 4.99 | 1.48        | 1.39     |
| 14  | A     | 808  | CLA  | O2A-C1  | 4.99 | 1.60        | 1.46     |
| 14  | B     | 807  | CLA  | CHC-C1C | 4.99 | 1.47        | 1.35     |
| 14  | G     | 838  | CLA  | C3B-C2B | 4.99 | 1.47        | 1.40     |
| 14  | H     | 808  | CLA  | O2A-C1  | 4.99 | 1.60        | 1.46     |
| 14  | B     | 812  | CLA  | CHC-C1C | 4.99 | 1.47        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | A     | 830 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 14  | Y     | 819 | CLA  | OBD-CAD | 4.99 | 1.29        | 1.22     |
| 14  | H     | 805 | CLA  | O2A-C1  | 4.98 | 1.60        | 1.46     |
| 14  | H     | 825 | CLA  | O2A-C1  | 4.98 | 1.60        | 1.46     |
| 14  | A     | 815 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 14  | H     | 827 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 14  | B     | 841 | CLA  | OBD-CAD | 4.98 | 1.29        | 1.22     |
| 14  | B     | 806 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 14  | Z     | 835 | CLA  | OBD-CAD | 4.98 | 1.29        | 1.22     |
| 14  | G     | 825 | CLA  | O2A-C1  | 4.98 | 1.60        | 1.46     |
| 14  | G     | 809 | CLA  | C3B-C2B | 4.98 | 1.47        | 1.40     |
| 14  | B     | 807 | CLA  | O2A-C1  | 4.98 | 1.60        | 1.46     |
| 14  | Q     | 203 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 14  | B     | 819 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 14  | B     | 803 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 14  | Y     | 838 | CLA  | OBD-CAD | 4.98 | 1.29        | 1.22     |
| 14  | B     | 814 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | Y     | 827 | CLA  | C3B-C2B | 4.97 | 1.47        | 1.40     |
| 14  | A     | 809 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | Y     | 837 | CLA  | C3B-C2B | 4.97 | 1.47        | 1.40     |
| 14  | f     | 102 | CLA  | OBD-CAD | 4.97 | 1.29        | 1.22     |
| 14  | Z     | 819 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | G     | 827 | CLA  | C3B-C2B | 4.97 | 1.47        | 1.40     |
| 14  | B     | 827 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 14  | A     | 820 | CLA  | O2A-C1  | 4.97 | 1.60        | 1.46     |
| 14  | B     | 826 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | Y     | 821 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | L     | 205 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 14  | Y     | 823 | CLA  | C3B-C2B | 4.96 | 1.47        | 1.40     |
| 14  | G     | 818 | CLA  | C3B-C2B | 4.96 | 1.47        | 1.40     |
| 14  | Y     | 808 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | B     | 811 | CLA  | OBD-CAD | 4.96 | 1.29        | 1.22     |
| 14  | H     | 808 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 14  | Z     | 807 | CLA  | OBD-CAD | 4.96 | 1.29        | 1.22     |
| 14  | B     | 829 | CLA  | C3D-C2D | 4.96 | 1.48        | 1.39     |
| 14  | B     | 816 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 14  | L     | 201 | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 14  | Y     | 833 | CLA  | O2A-C1  | 4.96 | 1.60        | 1.46     |
| 14  | B     | 815 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 14  | A     | 823 | CLA  | C3C-C2C | 4.95 | 1.47        | 1.36     |
| 14  | A     | 813 | CLA  | OBD-CAD | 4.95 | 1.29        | 1.22     |
| 14  | B     | 837 | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 814  | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |
| 14  | Y     | 838  | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |
| 14  | Y     | 839  | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 14  | Y     | 839  | CLA  | C3B-C2B | 4.95 | 1.47        | 1.40     |
| 14  | H     | 829  | CLA  | OBD-CAD | 4.95 | 1.29        | 1.22     |
| 14  | B     | 828  | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |
| 14  | G     | 811  | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 14  | H     | 835  | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |
| 14  | G     | 812  | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |
| 14  | j     | 102  | CLA  | CHC-C1C | 4.95 | 1.47        | 1.35     |
| 14  | G     | 826  | CLA  | O2A-C1  | 4.95 | 1.60        | 1.46     |
| 14  | Y     | 839  | CLA  | O2A-C1  | 4.94 | 1.60        | 1.46     |
| 14  | K     | 103  | CLA  | CHC-C1C | 4.94 | 1.47        | 1.35     |
| 14  | A     | 823  | CLA  | OBD-CAD | 4.94 | 1.29        | 1.22     |
| 14  | U     | 1004 | CLA  | C3D-C2D | 4.94 | 1.48        | 1.39     |
| 14  | Z     | 836  | CLA  | O2A-C1  | 4.94 | 1.60        | 1.46     |
| 14  | Y     | 809  | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 14  | G     | 809  | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 14  | Z     | 816  | CLA  | OBD-CAD | 4.94 | 1.29        | 1.22     |
| 14  | B     | 832  | CLA  | CHC-C1C | 4.94 | 1.47        | 1.35     |
| 14  | Y     | 810  | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 14  | G     | 804  | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 14  | H     | 807  | CLA  | O2A-C1  | 4.94 | 1.60        | 1.46     |
| 14  | T     | 103  | CLA  | OBD-CAD | 4.94 | 1.29        | 1.22     |
| 14  | G     | 820  | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 14  | Z     | 805  | CLA  | C3D-C2D | 4.94 | 1.48        | 1.39     |
| 14  | Y     | 804  | CLA  | CHC-C1C | 4.94 | 1.47        | 1.35     |
| 14  | A     | 820  | CLA  | OBD-CAD | 4.93 | 1.29        | 1.22     |
| 14  | A     | 830  | CLA  | CHC-C1C | 4.93 | 1.47        | 1.35     |
| 14  | U     | 1006 | CLA  | O2A-C1  | 4.93 | 1.60        | 1.46     |
| 14  | Z     | 826  | CLA  | CHC-C1C | 4.93 | 1.47        | 1.35     |
| 14  | G     | 824  | CLA  | CHC-C1C | 4.93 | 1.47        | 1.35     |
| 14  | B     | 826  | CLA  | CHC-C1C | 4.93 | 1.47        | 1.35     |
| 14  | G     | 816  | CLA  | OBD-CAD | 4.93 | 1.29        | 1.22     |
| 14  | Z     | 830  | CLA  | OBD-CAD | 4.93 | 1.29        | 1.22     |
| 14  | B     | 826  | CLA  | C3B-C2B | 4.93 | 1.47        | 1.40     |
| 14  | X     | 1701 | CLA  | OBD-CAD | 4.93 | 1.29        | 1.22     |
| 14  | H     | 834  | CLA  | C3B-C2B | 4.93 | 1.47        | 1.40     |
| 14  | Z     | 809  | CLA  | O2A-C1  | 4.93 | 1.60        | 1.46     |
| 14  | A     | 814  | CLA  | C3B-C2B | 4.93 | 1.47        | 1.40     |
| 14  | T     | 103  | CLA  | C3D-C2D | 4.93 | 1.48        | 1.39     |
| 14  | A     | 836  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 839  | CLA  | OBD-CAD | 4.92 | 1.29        | 1.22     |
| 14  | G     | 834  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |
| 14  | Y     | 810  | CLA  | C3B-C2B | 4.92 | 1.47        | 1.40     |
| 14  | A     | 826  | CLA  | C3B-C2B | 4.92 | 1.47        | 1.40     |
| 14  | H     | 803  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |
| 14  | G     | 843  | CLA  | C3C-C2C | 4.92 | 1.47        | 1.36     |
| 14  | A     | 810  | CLA  | OBD-CAD | 4.92 | 1.29        | 1.22     |
| 14  | A     | 827  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |
| 14  | Y     | 805  | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 14  | G     | 826  | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 14  | G     | 806  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |
| 14  | B     | 820  | CLA  | CHC-C1C | 4.92 | 1.47        | 1.35     |
| 14  | H     | 802  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |
| 14  | Z     | 816  | CLA  | C3D-C2D | 4.92 | 1.48        | 1.39     |
| 14  | Y     | 824  | CLA  | C3C-C2C | 4.92 | 1.47        | 1.36     |
| 14  | Z     | 820  | CLA  | O2A-C1  | 4.92 | 1.60        | 1.46     |
| 14  | A     | 807  | CLA  | O2A-C1  | 4.91 | 1.60        | 1.46     |
| 14  | Y     | 820  | CLA  | C3D-C2D | 4.91 | 1.48        | 1.39     |
| 14  | G     | 813  | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 14  | B     | 826  | CLA  | O2A-C1  | 4.91 | 1.60        | 1.46     |
| 14  | B     | 822  | CLA  | OBD-CAD | 4.91 | 1.29        | 1.22     |
| 14  | Z     | 823  | CLA  | CHC-C1C | 4.91 | 1.47        | 1.35     |
| 14  | B     | 817  | CLA  | CHC-C1C | 4.91 | 1.47        | 1.35     |
| 14  | Q     | 203  | CLA  | CHC-C1C | 4.91 | 1.47        | 1.35     |
| 13  | A     | 801  | CL0  | CHC-C1C | 4.91 | 1.47        | 1.35     |
| 14  | G     | 823  | CLA  | CHC-C1C | 4.91 | 1.47        | 1.35     |
| 14  | T     | 101  | CLA  | C3B-C2B | 4.90 | 1.47        | 1.40     |
| 14  | Z     | 806  | CLA  | O2A-C1  | 4.90 | 1.60        | 1.46     |
| 14  | S     | 1102 | CLA  | CHC-C1C | 4.90 | 1.47        | 1.35     |
| 14  | H     | 833  | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 14  | G     | 825  | CLA  | CHC-C1C | 4.90 | 1.47        | 1.35     |
| 14  | H     | 821  | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 14  | Y     | 833  | CLA  | CHC-C1C | 4.90 | 1.47        | 1.35     |
| 14  | B     | 840  | CLA  | C3D-C2D | 4.90 | 1.48        | 1.39     |
| 14  | G     | 816  | CLA  | C3D-C2D | 4.90 | 1.48        | 1.39     |
| 14  | Z     | 805  | CLA  | OBD-CAD | 4.90 | 1.29        | 1.22     |
| 14  | B     | 828  | CLA  | CHC-C1C | 4.90 | 1.47        | 1.35     |
| 14  | A     | 832  | CLA  | CHC-C1C | 4.90 | 1.47        | 1.35     |
| 14  | B     | 809  | CLA  | O2A-C1  | 4.90 | 1.59        | 1.46     |
| 14  | A     | 829  | CLA  | O2A-C1  | 4.90 | 1.59        | 1.46     |
| 14  | B     | 829  | CLA  | OBD-CAD | 4.90 | 1.29        | 1.22     |
| 14  | G     | 853  | CLA  | C3D-C2D | 4.90 | 1.48        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 815  | CLA  | OBD-CAD | 4.90 | 1.29        | 1.22     |
| 14  | A     | 812  | CLA  | CHC-C1C | 4.89 | 1.47        | 1.35     |
| 14  | Y     | 842  | CLA  | CHC-C1C | 4.89 | 1.47        | 1.35     |
| 14  | G     | 819  | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 14  | g     | 102  | CLA  | OBD-CAD | 4.89 | 1.29        | 1.22     |
| 14  | A     | 824  | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 14  | Z     | 806  | CLA  | CHC-C1C | 4.89 | 1.47        | 1.35     |
| 14  | B     | 831  | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 14  | A     | 833  | CLA  | CHC-C1C | 4.89 | 1.47        | 1.35     |
| 14  | G     | 834  | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 14  | B     | 816  | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 14  | A     | 807  | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 14  | G     | 824  | CLA  | OBD-CAD | 4.89 | 1.29        | 1.22     |
| 14  | A     | 838  | CLA  | C3D-C2D | 4.89 | 1.48        | 1.39     |
| 14  | B     | 808  | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 14  | B     | 812  | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 14  | G     | 815  | CLA  | CHC-C1C | 4.89 | 1.47        | 1.35     |
| 14  | H     | 823  | CLA  | OBD-CAD | 4.89 | 1.29        | 1.22     |
| 14  | H     | 837  | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 14  | f     | 102  | CLA  | C3C-C2C | 4.88 | 1.47        | 1.36     |
| 14  | H     | 828  | CLA  | OBD-CAD | 4.88 | 1.29        | 1.22     |
| 14  | B     | 833  | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 14  | A     | 840  | CLA  | CHC-C1C | 4.88 | 1.47        | 1.35     |
| 14  | S     | 1101 | CLA  | CHC-C1C | 4.88 | 1.47        | 1.35     |
| 14  | H     | 832  | CLA  | OBD-CAD | 4.88 | 1.29        | 1.22     |
| 14  | B     | 812  | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 14  | Z     | 825  | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 14  | H     | 801  | CLA  | O2A-C1  | 4.88 | 1.59        | 1.46     |
| 14  | Z     | 822  | CLA  | CHC-C1C | 4.88 | 1.47        | 1.35     |
| 18  | G     | 852  | LHG  | O7-C7   | 4.88 | 1.48        | 1.34     |
| 14  | G     | 842  | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 14  | S     | 1101 | CLA  | O2A-C1  | 4.88 | 1.59        | 1.46     |
| 14  | B     | 825  | CLA  | C3B-C2B | 4.88 | 1.47        | 1.40     |
| 14  | H     | 834  | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 14  | H     | 829  | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 14  | B     | 804  | CLA  | OBD-CAD | 4.87 | 1.29        | 1.22     |
| 14  | Z     | 821  | CLA  | C3C-C2C | 4.87 | 1.47        | 1.36     |
| 14  | H     | 816  | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 14  | Z     | 839  | CLA  | C3B-C2B | 4.87 | 1.47        | 1.40     |
| 14  | H     | 817  | CLA  | O2A-C1  | 4.87 | 1.59        | 1.46     |
| 14  | Y     | 802  | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 14  | Y     | 817  | CLA  | C3D-C2D | 4.87 | 1.48        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 805  | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 14  | Z     | 804  | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 14  | H     | 837  | CLA  | O2A-C1  | 4.86 | 1.59        | 1.46     |
| 14  | Y     | 820  | CLA  | C3B-C2B | 4.86 | 1.47        | 1.40     |
| 14  | Z     | 829  | CLA  | C3C-C2C | 4.86 | 1.47        | 1.36     |
| 14  | G     | 842  | CLA  | O2A-C1  | 4.86 | 1.59        | 1.46     |
| 14  | Y     | 829  | CLA  | C3C-C2C | 4.86 | 1.47        | 1.36     |
| 14  | G     | 840  | CLA  | O2A-C1  | 4.86 | 1.59        | 1.46     |
| 14  | H     | 819  | CLA  | C3B-C2B | 4.86 | 1.47        | 1.40     |
| 14  | B     | 837  | CLA  | CHC-C1C | 4.86 | 1.47        | 1.35     |
| 14  | Z     | 837  | CLA  | CHC-C1C | 4.86 | 1.47        | 1.35     |
| 14  | A     | 814  | CLA  | C3C-C2C | 4.86 | 1.47        | 1.36     |
| 14  | Y     | 823  | CLA  | OBD-CAD | 4.86 | 1.29        | 1.22     |
| 14  | G     | 831  | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 14  | Z     | 833  | CLA  | C3D-C2D | 4.86 | 1.48        | 1.39     |
| 14  | Z     | 814  | CLA  | OBD-CAD | 4.85 | 1.29        | 1.22     |
| 14  | H     | 821  | CLA  | O2A-C1  | 4.85 | 1.59        | 1.46     |
| 14  | G     | 815  | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 14  | U     | 1004 | CLA  | O2A-C1  | 4.85 | 1.59        | 1.46     |
| 14  | A     | 829  | CLA  | C3D-C2D | 4.85 | 1.48        | 1.39     |
| 14  | H     | 830  | CLA  | C3D-C2D | 4.85 | 1.48        | 1.39     |
| 14  | H     | 807  | CLA  | CHC-C1C | 4.85 | 1.47        | 1.35     |
| 14  | Z     | 809  | CLA  | C3D-C2D | 4.85 | 1.48        | 1.39     |
| 14  | A     | 826  | CLA  | O2A-C1  | 4.85 | 1.59        | 1.46     |
| 14  | B     | 818  | CLA  | CHC-C1C | 4.84 | 1.47        | 1.35     |
| 14  | h     | 207  | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 14  | G     | 813  | CLA  | C3B-C2B | 4.84 | 1.47        | 1.40     |
| 14  | H     | 802  | CLA  | CHC-C1C | 4.84 | 1.47        | 1.35     |
| 14  | Z     | 838  | CLA  | C3D-C2D | 4.84 | 1.48        | 1.39     |
| 14  | Z     | 823  | CLA  | C3C-C2C | 4.84 | 1.47        | 1.36     |
| 14  | G     | 837  | CLA  | C3B-C2B | 4.84 | 1.47        | 1.40     |
| 14  | Y     | 803  | CLA  | C3B-C2B | 4.84 | 1.47        | 1.40     |
| 14  | Y     | 825  | CLA  | CHC-C1C | 4.84 | 1.47        | 1.35     |
| 14  | Y     | 824  | CLA  | C3D-C2D | 4.84 | 1.48        | 1.39     |
| 14  | G     | 839  | CLA  | O2A-C1  | 4.84 | 1.59        | 1.46     |
| 14  | A     | 804  | CLA  | CHC-C1C | 4.84 | 1.47        | 1.35     |
| 14  | B     | 841  | CLA  | O2A-C1  | 4.84 | 1.59        | 1.46     |
| 14  | h     | 207  | CLA  | O2A-C1  | 4.83 | 1.59        | 1.46     |
| 14  | B     | 841  | CLA  | C3C-C2C | 4.83 | 1.47        | 1.36     |
| 14  | S     | 1101 | CLA  | C3C-C2C | 4.83 | 1.47        | 1.36     |
| 14  | Y     | 834  | CLA  | C3D-C2D | 4.83 | 1.48        | 1.39     |
| 14  | G     | 827  | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | B     | 811 | CLA  | C3C-C2C | 4.83 | 1.47        | 1.36     |
| 14  | H     | 809 | CLA  | OBD-CAD | 4.83 | 1.29        | 1.22     |
| 14  | Z     | 822 | CLA  | C3C-C2C | 4.83 | 1.47        | 1.36     |
| 14  | A     | 837 | CLA  | OBD-CAD | 4.83 | 1.29        | 1.22     |
| 14  | H     | 827 | CLA  | C3B-C2B | 4.83 | 1.47        | 1.40     |
| 14  | Z     | 826 | CLA  | C3D-C2D | 4.83 | 1.48        | 1.39     |
| 14  | Z     | 814 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 14  | h     | 206 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 14  | B     | 805 | CLA  | OBD-CAD | 4.82 | 1.29        | 1.22     |
| 14  | G     | 803 | CLA  | OBD-CAD | 4.82 | 1.29        | 1.22     |
| 14  | G     | 829 | CLA  | C3B-C2B | 4.82 | 1.47        | 1.40     |
| 14  | A     | 811 | CLA  | CHC-C1C | 4.82 | 1.47        | 1.35     |
| 14  | A     | 821 | CLA  | C3C-C2C | 4.82 | 1.47        | 1.36     |
| 14  | Y     | 802 | CLA  | O2A-C1  | 4.82 | 1.59        | 1.46     |
| 14  | Z     | 831 | CLA  | OBD-CAD | 4.82 | 1.29        | 1.22     |
| 14  | d     | 201 | CLA  | OBD-CAD | 4.81 | 1.29        | 1.22     |
| 14  | B     | 825 | CLA  | C3C-C2C | 4.81 | 1.47        | 1.36     |
| 14  | j     | 102 | CLA  | OBD-CAD | 4.81 | 1.29        | 1.22     |
| 14  | Z     | 824 | CLA  | CHC-C1C | 4.81 | 1.47        | 1.35     |
| 14  | B     | 820 | CLA  | C3B-C2B | 4.81 | 1.47        | 1.40     |
| 14  | F     | 202 | CLA  | C3D-C2D | 4.81 | 1.48        | 1.39     |
| 14  | h     | 206 | CLA  | C3C-C2C | 4.81 | 1.46        | 1.36     |
| 14  | A     | 813 | CLA  | C3B-C2B | 4.81 | 1.47        | 1.40     |
| 14  | h     | 201 | CLA  | O2D-CGD | 4.81 | 1.44        | 1.33     |
| 14  | A     | 852 | CLA  | CHC-C1C | 4.81 | 1.47        | 1.35     |
| 14  | G     | 815 | CLA  | C3C-C2C | 4.80 | 1.46        | 1.36     |
| 14  | Z     | 824 | CLA  | O2A-C1  | 4.80 | 1.59        | 1.46     |
| 14  | Y     | 814 | CLA  | C3C-C2C | 4.80 | 1.46        | 1.36     |
| 14  | G     | 836 | CLA  | C3C-C2C | 4.80 | 1.46        | 1.36     |
| 14  | H     | 831 | CLA  | O2D-CGD | 4.80 | 1.44        | 1.33     |
| 14  | H     | 821 | CLA  | CHC-C1C | 4.80 | 1.47        | 1.35     |
| 14  | G     | 829 | CLA  | O2A-C1  | 4.80 | 1.59        | 1.46     |
| 14  | Z     | 829 | CLA  | OBD-CAD | 4.80 | 1.29        | 1.22     |
| 14  | Y     | 826 | CLA  | C3B-C2B | 4.80 | 1.47        | 1.40     |
| 14  | G     | 812 | CLA  | C3C-C2C | 4.79 | 1.46        | 1.36     |
| 14  | Z     | 837 | CLA  | C3D-C2D | 4.79 | 1.48        | 1.39     |
| 14  | H     | 826 | CLA  | O2D-CGD | 4.79 | 1.44        | 1.33     |
| 14  | H     | 837 | CLA  | C3D-C2D | 4.79 | 1.48        | 1.39     |
| 14  | G     | 833 | CLA  | C3C-C2C | 4.79 | 1.46        | 1.36     |
| 14  | B     | 838 | CLA  | O2D-CGD | 4.79 | 1.44        | 1.33     |
| 14  | H     | 824 | CLA  | O2D-CGD | 4.79 | 1.44        | 1.33     |
| 14  | F     | 202 | CLA  | CHC-C1C | 4.79 | 1.47        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 13  | G     | 801  | CL0  | C3C-C2C | 4.79 | 1.46        | 1.36     |
| 14  | Z     | 834  | CLA  | C3C-C2C | 4.79 | 1.46        | 1.36     |
| 14  | A     | 838  | CLA  | C3B-C2B | 4.79 | 1.47        | 1.40     |
| 14  | Y     | 829  | CLA  | C3B-C2B | 4.79 | 1.47        | 1.40     |
| 14  | Z     | 814  | CLA  | C3B-C2B | 4.79 | 1.47        | 1.40     |
| 14  | Z     | 807  | CLA  | CHC-C1C | 4.79 | 1.47        | 1.35     |
| 14  | Y     | 828  | CLA  | O2D-CGD | 4.78 | 1.44        | 1.33     |
| 14  | A     | 805  | CLA  | O2A-C1  | 4.78 | 1.59        | 1.46     |
| 14  | h     | 201  | CLA  | CHC-C1C | 4.78 | 1.47        | 1.35     |
| 14  | A     | 832  | CLA  | C3C-C2C | 4.78 | 1.46        | 1.36     |
| 14  | G     | 814  | CLA  | O2D-CGD | 4.78 | 1.44        | 1.33     |
| 14  | H     | 813  | CLA  | C3C-C2C | 4.78 | 1.46        | 1.36     |
| 14  | S     | 1101 | CLA  | O2D-CGD | 4.78 | 1.44        | 1.33     |
| 14  | f     | 101  | CLA  | C3C-C2C | 4.78 | 1.46        | 1.36     |
| 14  | A     | 840  | CLA  | O2D-CGD | 4.78 | 1.44        | 1.33     |
| 14  | Z     | 818  | CLA  | C3C-C2C | 4.77 | 1.46        | 1.36     |
| 14  | H     | 820  | CLA  | OBD-CAD | 4.77 | 1.29        | 1.22     |
| 14  | Y     | 802  | CLA  | OBD-CAD | 4.77 | 1.29        | 1.22     |
| 14  | B     | 807  | CLA  | O2D-CGD | 4.77 | 1.44        | 1.33     |
| 14  | Z     | 817  | CLA  | OBD-CAD | 4.77 | 1.29        | 1.22     |
| 14  | A     | 816  | CLA  | C3C-C2C | 4.77 | 1.46        | 1.36     |
| 14  | Y     | 855  | CLA  | O2A-C1  | 4.77 | 1.59        | 1.46     |
| 14  | f     | 102  | CLA  | C3D-C2D | 4.77 | 1.48        | 1.39     |
| 14  | G     | 806  | CLA  | O2D-CGD | 4.77 | 1.44        | 1.33     |
| 14  | G     | 842  | CLA  | CHC-C1C | 4.77 | 1.47        | 1.35     |
| 14  | B     | 818  | CLA  | O2A-C1  | 4.77 | 1.59        | 1.46     |
| 14  | H     | 818  | CLA  | C3C-C2C | 4.77 | 1.46        | 1.36     |
| 14  | B     | 807  | CLA  | C3B-C2B | 4.77 | 1.47        | 1.40     |
| 14  | B     | 810  | CLA  | CHC-C1C | 4.77 | 1.47        | 1.35     |
| 14  | Y     | 827  | CLA  | O2D-CGD | 4.77 | 1.44        | 1.33     |
| 14  | A     | 803  | CLA  | O2A-C1  | 4.77 | 1.59        | 1.46     |
| 14  | J     | 101  | CLA  | C3C-C2C | 4.77 | 1.46        | 1.36     |
| 14  | V     | 1201 | CLA  | O2A-C1  | 4.76 | 1.59        | 1.46     |
| 14  | A     | 829  | CLA  | CHC-C1C | 4.76 | 1.47        | 1.35     |
| 14  | B     | 823  | CLA  | C3B-C2B | 4.76 | 1.47        | 1.40     |
| 13  | G     | 801  | CL0  | C3B-C2B | 4.76 | 1.47        | 1.40     |
| 14  | Z     | 831  | CLA  | O2A-C1  | 4.76 | 1.59        | 1.46     |
| 14  | A     | 818  | CLA  | OBD-CAD | 4.76 | 1.29        | 1.22     |
| 14  | H     | 825  | CLA  | OBD-CAD | 4.76 | 1.29        | 1.22     |
| 14  | B     | 825  | CLA  | OBD-CAD | 4.76 | 1.29        | 1.22     |
| 14  | G     | 838  | CLA  | CHC-C1C | 4.76 | 1.47        | 1.35     |
| 14  | B     | 805  | CLA  | CHC-C1C | 4.76 | 1.47        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | H     | 820  | CLA  | C3B-C2B | 4.76 | 1.47        | 1.40     |
| 13  | Y     | 801  | CL0  | C3D-C2D | 4.76 | 1.48        | 1.39     |
| 14  | Z     | 826  | CLA  | O2D-CGD | 4.75 | 1.44        | 1.33     |
| 14  | B     | 837  | CLA  | C3D-C2D | 4.75 | 1.48        | 1.39     |
| 14  | A     | 819  | CLA  | O2A-C1  | 4.75 | 1.59        | 1.46     |
| 14  | Y     | 840  | CLA  | C3C-C2C | 4.75 | 1.46        | 1.36     |
| 14  | f     | 101  | CLA  | C3D-C2D | 4.75 | 1.48        | 1.39     |
| 14  | G     | 807  | CLA  | C3B-C2B | 4.75 | 1.47        | 1.40     |
| 14  | A     | 852  | CLA  | O2D-CGD | 4.75 | 1.44        | 1.33     |
| 14  | G     | 822  | CLA  | CHC-C1C | 4.75 | 1.47        | 1.35     |
| 14  | Z     | 827  | CLA  | OBD-CAD | 4.75 | 1.28        | 1.22     |
| 14  | Q     | 201  | CLA  | O2A-C1  | 4.75 | 1.59        | 1.46     |
| 14  | U     | 1006 | CLA  | OBD-CAD | 4.75 | 1.28        | 1.22     |
| 14  | B     | 814  | CLA  | OBD-CAD | 4.75 | 1.28        | 1.22     |
| 14  | G     | 819  | CLA  | CHC-C1C | 4.75 | 1.47        | 1.35     |
| 14  | A     | 803  | CLA  | C3B-C2B | 4.75 | 1.47        | 1.40     |
| 14  | L     | 205  | CLA  | C3B-C2B | 4.75 | 1.47        | 1.40     |
| 14  | A     | 807  | CLA  | CHC-C1C | 4.75 | 1.47        | 1.35     |
| 14  | G     | 825  | CLA  | C3B-C2B | 4.75 | 1.47        | 1.40     |
| 14  | Z     | 836  | CLA  | CHC-C1C | 4.75 | 1.47        | 1.35     |
| 14  | Z     | 807  | CLA  | C3D-C2D | 4.74 | 1.47        | 1.39     |
| 14  | W     | 1701 | CLA  | O2D-CGD | 4.74 | 1.44        | 1.33     |
| 14  | Y     | 822  | CLA  | CHC-C1C | 4.74 | 1.47        | 1.35     |
| 14  | S     | 1101 | CLA  | C3B-C2B | 4.74 | 1.46        | 1.40     |
| 14  | B     | 809  | CLA  | C3C-C2C | 4.74 | 1.46        | 1.36     |
| 14  | B     | 819  | CLA  | O2A-C1  | 4.74 | 1.59        | 1.46     |
| 15  | H     | 839  | PQN  | C10-C5  | 4.74 | 1.48        | 1.40     |
| 14  | H     | 806  | CLA  | O2A-C1  | 4.74 | 1.59        | 1.46     |
| 14  | A     | 841  | CLA  | OBD-CAD | 4.74 | 1.28        | 1.22     |
| 14  | G     | 820  | CLA  | C3B-C2B | 4.74 | 1.46        | 1.40     |
| 14  | h     | 207  | CLA  | OBD-CAD | 4.74 | 1.28        | 1.22     |
| 14  | G     | 822  | CLA  | C3B-C2B | 4.74 | 1.46        | 1.40     |
| 14  | W     | 1701 | CLA  | OBD-CAD | 4.74 | 1.28        | 1.22     |
| 14  | Y     | 818  | CLA  | OBD-CAD | 4.73 | 1.28        | 1.22     |
| 14  | B     | 831  | CLA  | CHC-C1C | 4.73 | 1.47        | 1.35     |
| 14  | A     | 818  | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 14  | S     | 1102 | CLA  | OBD-CAD | 4.73 | 1.28        | 1.22     |
| 14  | Z     | 802  | CLA  | O2A-C1  | 4.73 | 1.59        | 1.46     |
| 14  | B     | 833  | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 14  | h     | 206  | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 14  | H     | 802  | CLA  | OBD-CAD | 4.72 | 1.28        | 1.22     |
| 14  | Z     | 824  | CLA  | C3D-C2D | 4.72 | 1.47        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | Z     | 814  | CLA  | C3C-C2C | 4.72 | 1.46        | 1.36     |
| 14  | Y     | 817  | CLA  | C3C-C2C | 4.72 | 1.46        | 1.36     |
| 14  | F     | 202  | CLA  | OBD-CAD | 4.72 | 1.28        | 1.22     |
| 13  | G     | 801  | CL0  | O2D-CGD | 4.72 | 1.44        | 1.33     |
| 14  | Y     | 836  | CLA  | C3D-C2D | 4.72 | 1.47        | 1.39     |
| 14  | Z     | 808  | CLA  | O2A-C1  | 4.72 | 1.59        | 1.46     |
| 14  | g     | 101  | CLA  | C3B-C2B | 4.72 | 1.46        | 1.40     |
| 14  | G     | 842  | CLA  | C3C-C2C | 4.72 | 1.46        | 1.36     |
| 14  | B     | 811  | CLA  | O2A-C1  | 4.72 | 1.59        | 1.46     |
| 14  | Z     | 809  | CLA  | OBD-CAD | 4.72 | 1.28        | 1.22     |
| 14  | H     | 819  | CLA  | OBD-CAD | 4.72 | 1.28        | 1.22     |
| 14  | B     | 803  | CLA  | O2D-CGD | 4.72 | 1.44        | 1.33     |
| 14  | A     | 829  | CLA  | C3C-C2C | 4.71 | 1.46        | 1.36     |
| 14  | H     | 830  | CLA  | C3C-C2C | 4.71 | 1.46        | 1.36     |
| 14  | W     | 1701 | CLA  | C3C-C2C | 4.71 | 1.46        | 1.36     |
| 14  | B     | 833  | CLA  | C3D-C2D | 4.71 | 1.47        | 1.39     |
| 14  | B     | 818  | CLA  | O2D-CGD | 4.71 | 1.44        | 1.33     |
| 14  | G     | 840  | CLA  | C3B-C2B | 4.71 | 1.46        | 1.40     |
| 14  | G     | 823  | CLA  | O2D-CGD | 4.71 | 1.44        | 1.33     |
| 14  | A     | 813  | CLA  | CHC-C1C | 4.71 | 1.47        | 1.35     |
| 14  | H     | 818  | CLA  | C3B-C2B | 4.71 | 1.46        | 1.40     |
| 14  | K     | 101  | CLA  | OBD-CAD | 4.70 | 1.29        | 1.22     |
| 14  | G     | 810  | CLA  | C3B-C2B | 4.70 | 1.46        | 1.40     |
| 14  | Z     | 812  | CLA  | C3C-C2C | 4.70 | 1.46        | 1.36     |
| 14  | A     | 811  | CLA  | C3C-C2C | 4.70 | 1.46        | 1.36     |
| 14  | Z     | 824  | CLA  | O2D-CGD | 4.70 | 1.44        | 1.33     |
| 14  | A     | 841  | CLA  | O2D-CGD | 4.70 | 1.44        | 1.33     |
| 14  | G     | 802  | CLA  | C3D-C2D | 4.70 | 1.47        | 1.39     |
| 13  | Y     | 801  | CL0  | C3C-C2C | 4.70 | 1.46        | 1.36     |
| 14  | B     | 808  | CLA  | CHC-C1C | 4.69 | 1.47        | 1.35     |
| 14  | Z     | 805  | CLA  | C3C-C2C | 4.69 | 1.46        | 1.36     |
| 14  | H     | 830  | CLA  | OBD-CAD | 4.69 | 1.28        | 1.22     |
| 14  | B     | 809  | CLA  | C3B-C2B | 4.69 | 1.46        | 1.40     |
| 14  | L     | 202  | CLA  | OBD-CAD | 4.69 | 1.28        | 1.22     |
| 14  | Y     | 816  | CLA  | O2D-CGD | 4.69 | 1.44        | 1.33     |
| 14  | B     | 813  | CLA  | O2A-C1  | 4.69 | 1.59        | 1.46     |
| 14  | B     | 821  | CLA  | CHC-C1C | 4.69 | 1.47        | 1.35     |
| 14  | Z     | 809  | CLA  | C3B-C2B | 4.69 | 1.46        | 1.40     |
| 14  | H     | 832  | CLA  | CHC-C1C | 4.69 | 1.47        | 1.35     |
| 14  | H     | 803  | CLA  | C3C-C2C | 4.69 | 1.46        | 1.36     |
| 14  | H     | 812  | CLA  | OBD-CAD | 4.69 | 1.28        | 1.22     |
| 14  | Y     | 837  | CLA  | C3C-C2C | 4.69 | 1.46        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 837  | CLA  | C3C-C2C | 4.69 | 1.46        | 1.36     |
| 14  | Y     | 828  | CLA  | O2A-C1  | 4.69 | 1.59        | 1.46     |
| 14  | A     | 825  | CLA  | CHC-C1C | 4.68 | 1.47        | 1.35     |
| 14  | G     | 837  | CLA  | O2D-CGD | 4.68 | 1.44        | 1.33     |
| 14  | B     | 802  | CLA  | OBD-CAD | 4.68 | 1.28        | 1.22     |
| 14  | A     | 829  | CLA  | OBD-CAD | 4.68 | 1.28        | 1.22     |
| 14  | Y     | 817  | CLA  | OBD-CAD | 4.68 | 1.28        | 1.22     |
| 14  | B     | 830  | CLA  | CHC-C1C | 4.68 | 1.47        | 1.35     |
| 14  | B     | 833  | CLA  | O2A-C1  | 4.68 | 1.59        | 1.46     |
| 14  | H     | 823  | CLA  | C3C-C2C | 4.68 | 1.46        | 1.36     |
| 14  | Z     | 804  | CLA  | CHC-C1C | 4.68 | 1.47        | 1.35     |
| 14  | B     | 822  | CLA  | C3B-C2B | 4.67 | 1.46        | 1.40     |
| 14  | A     | 827  | CLA  | C3B-C2B | 4.67 | 1.46        | 1.40     |
| 14  | A     | 842  | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 14  | U     | 1003 | CLA  | C3B-C2B | 4.67 | 1.46        | 1.40     |
| 14  | Z     | 804  | CLA  | C3B-C2B | 4.67 | 1.46        | 1.40     |
| 14  | A     | 811  | CLA  | C3B-C2B | 4.67 | 1.46        | 1.40     |
| 14  | Y     | 839  | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 14  | A     | 822  | CLA  | CHC-C1C | 4.67 | 1.46        | 1.35     |
| 14  | A     | 804  | CLA  | C3D-C2D | 4.67 | 1.47        | 1.39     |
| 14  | Y     | 813  | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 14  | H     | 830  | CLA  | O2A-C1  | 4.67 | 1.59        | 1.46     |
| 14  | Y     | 826  | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 13  | A     | 801  | CL0  | O2D-CGD | 4.66 | 1.44        | 1.33     |
| 14  | B     | 803  | CLA  | C3C-C2C | 4.66 | 1.46        | 1.36     |
| 14  | G     | 853  | CLA  | O2D-CGD | 4.66 | 1.44        | 1.33     |
| 14  | B     | 813  | CLA  | CHC-C1C | 4.66 | 1.46        | 1.35     |
| 14  | A     | 802  | CLA  | O2D-CGD | 4.66 | 1.44        | 1.33     |
| 14  | Y     | 835  | CLA  | C3B-C2B | 4.66 | 1.46        | 1.40     |
| 14  | Q     | 201  | CLA  | CHC-C1C | 4.66 | 1.46        | 1.35     |
| 14  | L     | 207  | CLA  | O2A-C1  | 4.66 | 1.59        | 1.46     |
| 14  | A     | 834  | CLA  | C3C-C2C | 4.66 | 1.46        | 1.36     |
| 14  | Y     | 812  | CLA  | O2A-C1  | 4.65 | 1.59        | 1.46     |
| 14  | T     | 103  | CLA  | C3C-C2C | 4.65 | 1.46        | 1.36     |
| 14  | Y     | 817  | CLA  | C3B-C2B | 4.65 | 1.46        | 1.40     |
| 14  | B     | 815  | CLA  | C3C-C2C | 4.65 | 1.46        | 1.36     |
| 14  | Z     | 802  | CLA  | C3C-C2C | 4.65 | 1.46        | 1.36     |
| 14  | H     | 838  | CLA  | OBD-CAD | 4.65 | 1.28        | 1.22     |
| 14  | H     | 816  | CLA  | C3B-C2B | 4.65 | 1.46        | 1.40     |
| 18  | Y     | 852  | LHG  | O8-C23  | 4.65 | 1.46        | 1.33     |
| 14  | h     | 201  | CLA  | O2A-C1  | 4.65 | 1.59        | 1.46     |
| 14  | G     | 828  | CLA  | OBD-CAD | 4.65 | 1.28        | 1.22     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 833  | CLA  | C3B-C2B | 4.65 | 1.46        | 1.40     |
| 14  | Z     | 821  | CLA  | OBD-CAD | 4.64 | 1.28        | 1.22     |
| 14  | B     | 829  | CLA  | CHC-C1C | 4.64 | 1.46        | 1.35     |
| 14  | G     | 827  | CLA  | C3D-C2D | 4.64 | 1.47        | 1.39     |
| 14  | G     | 842  | CLA  | OBD-CAD | 4.64 | 1.28        | 1.22     |
| 14  | Z     | 823  | CLA  | O2D-CGD | 4.64 | 1.44        | 1.33     |
| 14  | A     | 805  | CLA  | O2D-CGD | 4.64 | 1.44        | 1.33     |
| 14  | A     | 820  | CLA  | C3B-C2B | 4.64 | 1.46        | 1.40     |
| 14  | Y     | 826  | CLA  | O2A-C1  | 4.64 | 1.59        | 1.46     |
| 14  | Z     | 839  | CLA  | C3C-C2C | 4.64 | 1.46        | 1.36     |
| 14  | H     | 803  | CLA  | C3D-C2D | 4.64 | 1.47        | 1.39     |
| 14  | H     | 834  | CLA  | C3D-C2D | 4.63 | 1.47        | 1.39     |
| 14  | Y     | 811  | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 14  | j     | 102  | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 13  | Y     | 801  | CL0  | C3B-C2B | 4.63 | 1.46        | 1.40     |
| 14  | G     | 814  | CLA  | C3B-C2B | 4.63 | 1.46        | 1.40     |
| 14  | Y     | 835  | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 14  | A     | 831  | CLA  | OBD-CAD | 4.63 | 1.28        | 1.22     |
| 14  | K     | 103  | CLA  | C3D-C2D | 4.63 | 1.47        | 1.39     |
| 14  | A     | 840  | CLA  | C3B-C2B | 4.63 | 1.46        | 1.40     |
| 14  | Y     | 806  | CLA  | C3B-C2B | 4.63 | 1.46        | 1.40     |
| 14  | U     | 1004 | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 14  | H     | 819  | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 13  | A     | 801  | CL0  | C3D-C2D | 4.62 | 1.47        | 1.39     |
| 14  | Y     | 825  | CLA  | OBD-CAD | 4.62 | 1.28        | 1.22     |
| 14  | Z     | 815  | CLA  | O2D-CGD | 4.62 | 1.44        | 1.33     |
| 14  | H     | 825  | CLA  | C3D-C2D | 4.62 | 1.47        | 1.39     |
| 14  | Z     | 801  | CLA  | O2A-C1  | 4.62 | 1.59        | 1.46     |
| 14  | Z     | 810  | CLA  | C3D-C2D | 4.62 | 1.47        | 1.39     |
| 14  | G     | 817  | CLA  | C3D-C2D | 4.62 | 1.47        | 1.39     |
| 14  | A     | 819  | CLA  | C3D-C2D | 4.62 | 1.47        | 1.39     |
| 14  | H     | 807  | CLA  | C3B-C2B | 4.62 | 1.46        | 1.40     |
| 14  | G     | 853  | CLA  | C3B-C2B | 4.62 | 1.46        | 1.40     |
| 14  | H     | 806  | CLA  | O2D-CGD | 4.61 | 1.44        | 1.33     |
| 14  | J     | 101  | CLA  | OBD-CAD | 4.61 | 1.28        | 1.22     |
| 14  | Y     | 807  | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 14  | Y     | 819  | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 14  | A     | 816  | CLA  | C3D-C2D | 4.61 | 1.47        | 1.39     |
| 14  | Z     | 836  | CLA  | C3D-C2D | 4.61 | 1.47        | 1.39     |
| 14  | H     | 818  | CLA  | OBD-CAD | 4.61 | 1.28        | 1.22     |
| 14  | B     | 801  | CLA  | CHC-C1C | 4.61 | 1.46        | 1.35     |
| 14  | H     | 810  | CLA  | O2D-CGD | 4.61 | 1.44        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | Z     | 835  | CLA  | O2D-CGD | 4.61 | 1.44        | 1.33     |
| 14  | A     | 837  | CLA  | O2A-C1  | 4.61 | 1.59        | 1.46     |
| 14  | H     | 803  | CLA  | CHC-C1C | 4.61 | 1.46        | 1.35     |
| 14  | j     | 102  | CLA  | C3B-C2B | 4.61 | 1.46        | 1.40     |
| 14  | H     | 826  | CLA  | C3B-C2B | 4.61 | 1.46        | 1.40     |
| 14  | Y     | 805  | CLA  | O2A-C1  | 4.61 | 1.59        | 1.46     |
| 14  | H     | 815  | CLA  | C3B-C2B | 4.60 | 1.46        | 1.40     |
| 14  | A     | 802  | CLA  | CHC-C1C | 4.60 | 1.46        | 1.35     |
| 14  | Y     | 854  | CLA  | O2D-CGD | 4.60 | 1.44        | 1.33     |
| 14  | B     | 830  | CLA  | OBD-CAD | 4.60 | 1.28        | 1.22     |
| 14  | A     | 828  | CLA  | O2A-C1  | 4.60 | 1.59        | 1.46     |
| 14  | H     | 838  | CLA  | C3C-C2C | 4.60 | 1.46        | 1.36     |
| 14  | L     | 206  | CLA  | C3D-C2D | 4.60 | 1.47        | 1.39     |
| 13  | G     | 801  | CL0  | OBD-CAD | 4.60 | 1.28        | 1.22     |
| 14  | A     | 826  | CLA  | C3C-C2C | 4.60 | 1.46        | 1.36     |
| 15  | A     | 843  | PQN  | C10-C5  | 4.60 | 1.48        | 1.40     |
| 14  | G     | 825  | CLA  | C3C-C2C | 4.60 | 1.46        | 1.36     |
| 14  | U     | 1004 | CLA  | CHC-C1C | 4.60 | 1.46        | 1.35     |
| 14  | Z     | 837  | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |
| 14  | Y     | 820  | CLA  | O2D-CGD | 4.59 | 1.44        | 1.33     |
| 14  | Y     | 824  | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |
| 14  | Y     | 842  | CLA  | O2A-C1  | 4.59 | 1.59        | 1.46     |
| 14  | Z     | 834  | CLA  | OBD-CAD | 4.59 | 1.28        | 1.22     |
| 14  | Y     | 822  | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |
| 14  | Y     | 815  | CLA  | C3D-C2D | 4.59 | 1.47        | 1.39     |
| 14  | B     | 830  | CLA  | C3D-C2D | 4.59 | 1.47        | 1.39     |
| 14  | B     | 822  | CLA  | C3C-C2C | 4.59 | 1.46        | 1.36     |
| 14  | B     | 823  | CLA  | C3D-C2D | 4.59 | 1.47        | 1.39     |
| 14  | Y     | 838  | CLA  | C3D-C2D | 4.59 | 1.47        | 1.39     |
| 14  | H     | 832  | CLA  | C3C-C2C | 4.59 | 1.46        | 1.36     |
| 14  | G     | 808  | CLA  | C3D-C2D | 4.59 | 1.47        | 1.39     |
| 14  | H     | 801  | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |
| 14  | Y     | 840  | CLA  | C3D-C2D | 4.59 | 1.47        | 1.39     |
| 14  | A     | 838  | CLA  | O2A-C1  | 4.59 | 1.59        | 1.46     |
| 14  | Y     | 833  | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |
| 14  | H     | 810  | CLA  | OBD-CAD | 4.59 | 1.28        | 1.22     |
| 14  | Y     | 804  | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 14  | A     | 808  | CLA  | C3D-C2D | 4.58 | 1.47        | 1.39     |
| 14  | B     | 814  | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 14  | Y     | 828  | CLA  | C3B-C2B | 4.58 | 1.46        | 1.40     |
| 14  | B     | 837  | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 14  | Z     | 828  | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | B     | 808  | CLA  | OBD-CAD | 4.58 | 1.28        | 1.22     |
| 14  | H     | 814  | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 14  | A     | 813  | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 13  | A     | 801  | CL0  | C3C-C2C | 4.57 | 1.46        | 1.36     |
| 14  | A     | 832  | CLA  | OBD-CAD | 4.57 | 1.28        | 1.22     |
| 14  | A     | 810  | CLA  | C3B-C2B | 4.57 | 1.46        | 1.40     |
| 14  | H     | 827  | CLA  | C3C-C2C | 4.57 | 1.46        | 1.36     |
| 14  | B     | 801  | CLA  | OBD-CAD | 4.57 | 1.28        | 1.22     |
| 14  | B     | 805  | CLA  | O2D-CGD | 4.57 | 1.44        | 1.33     |
| 14  | H     | 825  | CLA  | C3B-C2B | 4.57 | 1.46        | 1.40     |
| 14  | G     | 838  | CLA  | OBD-CAD | 4.57 | 1.28        | 1.22     |
| 14  | U     | 1003 | CLA  | C3C-C2C | 4.57 | 1.46        | 1.36     |
| 14  | Z     | 817  | CLA  | C3B-C2B | 4.57 | 1.46        | 1.40     |
| 14  | H     | 808  | CLA  | OBD-CAD | 4.57 | 1.28        | 1.22     |
| 14  | B     | 828  | CLA  | O2D-CGD | 4.57 | 1.44        | 1.33     |
| 14  | A     | 817  | CLA  | OBD-CAD | 4.57 | 1.28        | 1.22     |
| 14  | Y     | 836  | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 14  | A     | 814  | CLA  | C3D-C2D | 4.56 | 1.47        | 1.39     |
| 14  | Y     | 815  | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 14  | B     | 823  | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 14  | A     | 804  | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 14  | g     | 102  | CLA  | C3D-C2D | 4.56 | 1.47        | 1.39     |
| 14  | G     | 834  | CLA  | OBD-CAD | 4.56 | 1.28        | 1.22     |
| 14  | H     | 822  | CLA  | O2A-C1  | 4.56 | 1.59        | 1.46     |
| 14  | d     | 202  | CLA  | C3D-C2D | 4.56 | 1.47        | 1.39     |
| 14  | A     | 817  | CLA  | C3B-C2B | 4.56 | 1.46        | 1.40     |
| 14  | H     | 814  | CLA  | OBD-CAD | 4.56 | 1.28        | 1.22     |
| 14  | L     | 206  | CLA  | C3B-C2B | 4.56 | 1.46        | 1.40     |
| 14  | B     | 824  | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 14  | Z     | 820  | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 14  | A     | 819  | CLA  | C3B-C2B | 4.56 | 1.46        | 1.40     |
| 14  | A     | 822  | CLA  | C3D-C2D | 4.56 | 1.47        | 1.39     |
| 14  | Y     | 855  | CLA  | OBD-CAD | 4.55 | 1.28        | 1.22     |
| 14  | Y     | 843  | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 14  | Q     | 203  | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 14  | Y     | 839  | CLA  | OBD-CAD | 4.55 | 1.28        | 1.22     |
| 14  | B     | 817  | CLA  | O2A-C1  | 4.55 | 1.59        | 1.46     |
| 14  | Y     | 854  | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 14  | Y     | 827  | CLA  | OBD-CAD | 4.55 | 1.28        | 1.22     |
| 14  | Y     | 811  | CLA  | C3D-C2D | 4.55 | 1.47        | 1.39     |
| 14  | F     | 202  | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 14  | G     | 834  | CLA  | C3D-C2D | 4.55 | 1.47        | 1.39     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 812  | CLA  | C3B-C2B | 4.55 | 1.46        | 1.40     |
| 14  | Z     | 827  | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 14  | A     | 802  | CLA  | OBD-CAD | 4.54 | 1.28        | 1.22     |
| 14  | G     | 823  | CLA  | C3B-C2B | 4.54 | 1.46        | 1.40     |
| 14  | G     | 821  | CLA  | C3C-C2C | 4.54 | 1.46        | 1.36     |
| 14  | A     | 802  | CLA  | C3D-C2D | 4.54 | 1.47        | 1.39     |
| 14  | B     | 806  | CLA  | O2D-CGD | 4.54 | 1.44        | 1.33     |
| 14  | Y     | 814  | CLA  | O2D-CGD | 4.54 | 1.44        | 1.33     |
| 14  | Z     | 817  | CLA  | C3D-C2D | 4.54 | 1.47        | 1.39     |
| 14  | B     | 838  | CLA  | OBD-CAD | 4.54 | 1.28        | 1.22     |
| 14  | H     | 808  | CLA  | CHC-C1C | 4.54 | 1.46        | 1.35     |
| 14  | A     | 830  | CLA  | C3D-C2D | 4.54 | 1.47        | 1.39     |
| 14  | A     | 824  | CLA  | C3C-C2C | 4.54 | 1.46        | 1.36     |
| 14  | B     | 827  | CLA  | O2D-CGD | 4.54 | 1.44        | 1.33     |
| 14  | B     | 824  | CLA  | OBD-CAD | 4.54 | 1.28        | 1.22     |
| 14  | H     | 817  | CLA  | C3D-C2D | 4.54 | 1.47        | 1.39     |
| 14  | A     | 802  | CLA  | O2A-C1  | 4.53 | 1.58        | 1.46     |
| 14  | H     | 805  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | Z     | 822  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | A     | 840  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | H     | 806  | CLA  | C3D-C2D | 4.53 | 1.47        | 1.39     |
| 14  | Y     | 824  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | Y     | 819  | CLA  | O2A-C1  | 4.53 | 1.58        | 1.46     |
| 14  | G     | 828  | CLA  | O2A-C1  | 4.53 | 1.58        | 1.46     |
| 14  | Z     | 836  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | S     | 1102 | CLA  | C3B-C2B | 4.53 | 1.46        | 1.40     |
| 14  | Z     | 823  | CLA  | C3B-C2B | 4.53 | 1.46        | 1.40     |
| 14  | Z     | 835  | CLA  | O2A-C1  | 4.53 | 1.58        | 1.46     |
| 14  | A     | 805  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | B     | 834  | CLA  | C3C-C2C | 4.53 | 1.46        | 1.36     |
| 14  | H     | 834  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | T     | 103  | CLA  | C3B-C2B | 4.53 | 1.46        | 1.40     |
| 14  | Y     | 841  | CLA  | C3B-C2B | 4.53 | 1.46        | 1.40     |
| 14  | Y     | 828  | CLA  | C3C-C2C | 4.53 | 1.46        | 1.36     |
| 14  | H     | 834  | CLA  | O2A-C1  | 4.53 | 1.58        | 1.46     |
| 14  | Y     | 810  | CLA  | OBD-CAD | 4.53 | 1.28        | 1.22     |
| 14  | H     | 815  | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 14  | A     | 822  | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 14  | H     | 835  | CLA  | C3D-C2D | 4.52 | 1.47        | 1.39     |
| 14  | H     | 802  | CLA  | C3D-C2D | 4.52 | 1.47        | 1.39     |
| 14  | Y     | 833  | CLA  | C3D-C2D | 4.52 | 1.47        | 1.39     |
| 14  | B     | 838  | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | U     | 1006 | CLA  | C3D-C2D | 4.52 | 1.47        | 1.39     |
| 14  | B     | 809  | CLA  | OBD-CAD | 4.52 | 1.28        | 1.22     |
| 14  | Z     | 801  | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 14  | A     | 826  | CLA  | OBD-CAD | 4.52 | 1.28        | 1.22     |
| 14  | S     | 1102 | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 14  | G     | 821  | CLA  | OBD-CAD | 4.52 | 1.28        | 1.22     |
| 14  | Y     | 854  | CLA  | C3D-C2D | 4.51 | 1.47        | 1.39     |
| 14  | A     | 839  | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 14  | H     | 834  | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 14  | H     | 836  | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 14  | B     | 805  | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 14  | Y     | 843  | CLA  | OBD-CAD | 4.51 | 1.28        | 1.22     |
| 14  | A     | 819  | CLA  | OBD-CAD | 4.51 | 1.28        | 1.22     |
| 14  | L     | 207  | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 14  | A     | 852  | CLA  | C3D-C2D | 4.50 | 1.47        | 1.39     |
| 14  | G     | 807  | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 14  | H     | 826  | CLA  | OBD-CAD | 4.50 | 1.28        | 1.22     |
| 14  | K     | 101  | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 14  | H     | 811  | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 14  | H     | 831  | CLA  | C3D-C2D | 4.50 | 1.47        | 1.39     |
| 14  | A     | 832  | CLA  | O2D-CGD | 4.50 | 1.44        | 1.33     |
| 14  | G     | 822  | CLA  | O2D-CGD | 4.50 | 1.44        | 1.33     |
| 14  | J     | 102  | CLA  | C3D-C2D | 4.50 | 1.47        | 1.39     |
| 14  | Y     | 842  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | B     | 802  | CLA  | C3B-C2B | 4.49 | 1.46        | 1.40     |
| 14  | B     | 812  | CLA  | C3B-C2B | 4.49 | 1.46        | 1.40     |
| 14  | Y     | 823  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | K     | 103  | CLA  | C3B-C2B | 4.49 | 1.46        | 1.40     |
| 14  | H     | 813  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | B     | 826  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | B     | 812  | CLA  | OBD-CAD | 4.49 | 1.28        | 1.22     |
| 14  | H     | 810  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | G     | 840  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | G     | 830  | CLA  | CHC-C1C | 4.49 | 1.46        | 1.35     |
| 15  | Y     | 844  | PQN  | C10-C5  | 4.49 | 1.48        | 1.40     |
| 14  | Z     | 808  | CLA  | CHC-C1C | 4.49 | 1.46        | 1.35     |
| 14  | B     | 828  | CLA  | C3C-C2C | 4.49 | 1.46        | 1.36     |
| 14  | G     | 803  | CLA  | C3D-C2D | 4.49 | 1.47        | 1.39     |
| 14  | G     | 824  | CLA  | C3B-C2B | 4.49 | 1.46        | 1.40     |
| 13  | Y     | 801  | CL0  | OBD-CAD | 4.48 | 1.28        | 1.22     |
| 14  | B     | 821  | CLA  | C3B-C2B | 4.48 | 1.46        | 1.40     |
| 14  | G     | 837  | CLA  | O2A-C1  | 4.48 | 1.58        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | L     | 207 | CLA  | OBD-CAD | 4.48 | 1.28        | 1.22     |
| 14  | G     | 810 | CLA  | OBD-CAD | 4.48 | 1.28        | 1.22     |
| 14  | Z     | 807 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 13  | Y     | 801 | CL0  | CHC-C1C | 4.47 | 1.46        | 1.35     |
| 14  | h     | 207 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 18  | A     | 850 | LHG  | O7-C7   | 4.47 | 1.46        | 1.34     |
| 14  | Y     | 834 | CLA  | C3B-C2B | 4.47 | 1.46        | 1.40     |
| 14  | Z     | 806 | CLA  | OBD-CAD | 4.47 | 1.28        | 1.22     |
| 14  | B     | 833 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 14  | Y     | 841 | CLA  | O2D-CGD | 4.47 | 1.44        | 1.33     |
| 14  | Y     | 841 | CLA  | OBD-CAD | 4.47 | 1.28        | 1.22     |
| 15  | G     | 844 | PQN  | C10-C5  | 4.47 | 1.48        | 1.40     |
| 14  | Z     | 832 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 14  | B     | 807 | CLA  | OBD-CAD | 4.47 | 1.28        | 1.22     |
| 14  | G     | 813 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 14  | B     | 803 | CLA  | OBD-CAD | 4.47 | 1.28        | 1.22     |
| 14  | G     | 818 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 14  | Y     | 808 | CLA  | C3B-C2B | 4.47 | 1.46        | 1.40     |
| 14  | Y     | 835 | CLA  | C3D-C2D | 4.47 | 1.47        | 1.39     |
| 14  | G     | 819 | CLA  | C3D-C2D | 4.47 | 1.47        | 1.39     |
| 14  | Z     | 838 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 14  | G     | 827 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 14  | A     | 812 | CLA  | C3B-C2B | 4.47 | 1.46        | 1.40     |
| 14  | Y     | 832 | CLA  | OBD-CAD | 4.46 | 1.28        | 1.22     |
| 14  | h     | 207 | CLA  | C3D-C2D | 4.46 | 1.47        | 1.39     |
| 18  | Y     | 853 | LHG  | O8-C23  | 4.46 | 1.46        | 1.33     |
| 18  | A     | 851 | LHG  | O8-C23  | 4.46 | 1.46        | 1.33     |
| 14  | H     | 812 | CLA  | C3D-C2D | 4.46 | 1.47        | 1.39     |
| 14  | G     | 805 | CLA  | OBD-CAD | 4.46 | 1.28        | 1.22     |
| 14  | Q     | 201 | CLA  | OBD-CAD | 4.46 | 1.28        | 1.22     |
| 14  | Y     | 810 | CLA  | C3D-C2D | 4.46 | 1.47        | 1.39     |
| 14  | H     | 817 | CLA  | OBD-CAD | 4.46 | 1.28        | 1.22     |
| 14  | G     | 823 | CLA  | C3C-C2C | 4.46 | 1.46        | 1.36     |
| 14  | Z     | 801 | CLA  | C3D-C2D | 4.45 | 1.47        | 1.39     |
| 14  | Y     | 816 | CLA  | OBD-CAD | 4.45 | 1.28        | 1.22     |
| 14  | G     | 841 | CLA  | C3B-C2B | 4.45 | 1.46        | 1.40     |
| 14  | B     | 814 | CLA  | C3D-C2D | 4.45 | 1.47        | 1.39     |
| 14  | G     | 822 | CLA  | OBD-CAD | 4.45 | 1.28        | 1.22     |
| 14  | A     | 815 | CLA  | C3C-C2C | 4.45 | 1.46        | 1.36     |
| 14  | Z     | 830 | CLA  | C3B-C2B | 4.45 | 1.46        | 1.40     |
| 14  | H     | 833 | CLA  | OBD-CAD | 4.45 | 1.28        | 1.22     |
| 14  | H     | 828 | CLA  | C3D-C2D | 4.45 | 1.47        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | Y     | 820  | CLA  | OBD-CAD | 4.44 | 1.28        | 1.22     |
| 14  | Z     | 805  | CLA  | CHC-C1C | 4.44 | 1.46        | 1.35     |
| 14  | A     | 807  | CLA  | OBD-CAD | 4.44 | 1.28        | 1.22     |
| 14  | A     | 816  | CLA  | C3B-C2B | 4.44 | 1.46        | 1.40     |
| 14  | B     | 836  | CLA  | C3C-C2C | 4.44 | 1.46        | 1.36     |
| 14  | Z     | 821  | CLA  | C3B-C2B | 4.44 | 1.46        | 1.40     |
| 14  | Y     | 806  | CLA  | OBD-CAD | 4.44 | 1.28        | 1.22     |
| 14  | Y     | 825  | CLA  | C3C-C2C | 4.44 | 1.46        | 1.36     |
| 14  | f     | 101  | CLA  | C3B-C2B | 4.44 | 1.46        | 1.40     |
| 14  | A     | 809  | CLA  | C3C-C2C | 4.44 | 1.46        | 1.36     |
| 14  | A     | 838  | CLA  | O2D-CGD | 4.44 | 1.44        | 1.33     |
| 14  | A     | 839  | CLA  | C3D-C2D | 4.44 | 1.47        | 1.39     |
| 14  | H     | 828  | CLA  | CHC-C1C | 4.43 | 1.46        | 1.35     |
| 14  | S     | 1103 | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 14  | g     | 102  | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 14  | A     | 810  | CLA  | C3D-C2D | 4.43 | 1.47        | 1.39     |
| 14  | Y     | 806  | CLA  | C3D-C2D | 4.43 | 1.47        | 1.39     |
| 14  | A     | 828  | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 14  | Y     | 834  | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 14  | A     | 825  | CLA  | C3B-C2B | 4.43 | 1.46        | 1.40     |
| 14  | B     | 828  | CLA  | OBD-CAD | 4.43 | 1.28        | 1.22     |
| 14  | Y     | 806  | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 18  | B     | 850  | LHG  | O8-C23  | 4.42 | 1.46        | 1.33     |
| 19  | H     | 846  | LMG  | O8-C28  | 4.42 | 1.46        | 1.33     |
| 14  | Y     | 808  | CLA  | C3C-C2C | 4.42 | 1.46        | 1.36     |
| 14  | G     | 837  | CLA  | C3D-C2D | 4.42 | 1.47        | 1.39     |
| 14  | B     | 802  | CLA  | O2D-CGD | 4.42 | 1.44        | 1.33     |
| 14  | Q     | 201  | CLA  | C3C-C2C | 4.41 | 1.46        | 1.36     |
| 14  | B     | 804  | CLA  | O2D-CGD | 4.41 | 1.44        | 1.33     |
| 14  | B     | 819  | CLA  | C3D-C2D | 4.41 | 1.47        | 1.39     |
| 14  | U     | 1004 | CLA  | C3B-C2B | 4.41 | 1.46        | 1.40     |
| 14  | Y     | 835  | CLA  | OBD-CAD | 4.41 | 1.28        | 1.22     |
| 14  | A     | 806  | CLA  | C3C-C2C | 4.41 | 1.46        | 1.36     |
| 14  | h     | 207  | CLA  | C3B-C2B | 4.41 | 1.46        | 1.40     |
| 14  | B     | 801  | CLA  | C3D-C2D | 4.41 | 1.47        | 1.39     |
| 14  | d     | 202  | CLA  | OBD-CAD | 4.41 | 1.28        | 1.22     |
| 14  | Y     | 830  | CLA  | OBD-CAD | 4.41 | 1.28        | 1.22     |
| 14  | Z     | 836  | CLA  | C3C-C2C | 4.41 | 1.46        | 1.36     |
| 14  | Z     | 835  | CLA  | C3B-C2B | 4.41 | 1.46        | 1.40     |
| 14  | Z     | 810  | CLA  | OBD-CAD | 4.41 | 1.28        | 1.22     |
| 14  | Y     | 842  | CLA  | C3C-C2C | 4.41 | 1.46        | 1.36     |
| 14  | K     | 101  | CLA  | C3D-C2D | 4.41 | 1.47        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | Z     | 811 | CLA  | O2A-C1  | 4.41 | 1.58        | 1.46     |
| 14  | A     | 824 | CLA  | C3D-C2D | 4.41 | 1.47        | 1.39     |
| 14  | Z     | 831 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 14  | G     | 841 | CLA  | C3D-C2D | 4.40 | 1.47        | 1.39     |
| 14  | A     | 811 | CLA  | OBD-CAD | 4.40 | 1.28        | 1.22     |
| 14  | B     | 830 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 14  | G     | 811 | CLA  | OBD-CAD | 4.40 | 1.28        | 1.22     |
| 14  | Z     | 833 | CLA  | C3B-C2B | 4.40 | 1.46        | 1.40     |
| 14  | B     | 823 | CLA  | OBD-CAD | 4.40 | 1.28        | 1.22     |
| 14  | Y     | 816 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 14  | A     | 831 | CLA  | O2D-CGD | 4.40 | 1.43        | 1.33     |
| 14  | T     | 101 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 14  | H     | 833 | CLA  | C3B-C2B | 4.40 | 1.46        | 1.40     |
| 14  | A     | 836 | CLA  | C3D-C2D | 4.40 | 1.47        | 1.39     |
| 14  | G     | 803 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 14  | g     | 101 | CLA  | C3D-C2D | 4.40 | 1.47        | 1.39     |
| 14  | Z     | 810 | CLA  | C3B-C2B | 4.39 | 1.46        | 1.40     |
| 14  | d     | 202 | CLA  | C3C-C2C | 4.39 | 1.46        | 1.36     |
| 14  | Y     | 826 | CLA  | OBD-CAD | 4.39 | 1.28        | 1.22     |
| 14  | B     | 824 | CLA  | C3D-C2D | 4.39 | 1.47        | 1.39     |
| 14  | Y     | 826 | CLA  | C3D-C2D | 4.39 | 1.47        | 1.39     |
| 14  | Q     | 203 | CLA  | C3D-C2D | 4.39 | 1.47        | 1.39     |
| 14  | G     | 836 | CLA  | C3B-C2B | 4.39 | 1.46        | 1.40     |
| 14  | Z     | 815 | CLA  | C3B-C2B | 4.39 | 1.46        | 1.40     |
| 14  | H     | 836 | CLA  | OBD-CAD | 4.39 | 1.28        | 1.22     |
| 14  | Y     | 803 | CLA  | C3D-C2D | 4.39 | 1.47        | 1.39     |
| 14  | H     | 833 | CLA  | C3D-C2D | 4.38 | 1.47        | 1.39     |
| 14  | Y     | 827 | CLA  | C3C-C2C | 4.38 | 1.46        | 1.36     |
| 14  | Y     | 836 | CLA  | C3B-C2B | 4.38 | 1.46        | 1.40     |
| 14  | Z     | 801 | CLA  | OBD-CAD | 4.38 | 1.28        | 1.22     |
| 14  | B     | 827 | CLA  | C3B-C2B | 4.38 | 1.46        | 1.40     |
| 14  | Z     | 816 | CLA  | C3C-C2C | 4.38 | 1.46        | 1.36     |
| 14  | A     | 823 | CLA  | C3D-C2D | 4.38 | 1.47        | 1.39     |
| 14  | Y     | 813 | CLA  | O2D-CGD | 4.38 | 1.43        | 1.33     |
| 14  | G     | 816 | CLA  | C3C-C2C | 4.38 | 1.46        | 1.36     |
| 14  | B     | 819 | CLA  | C3B-C2B | 4.38 | 1.46        | 1.40     |
| 14  | A     | 827 | CLA  | OBD-CAD | 4.38 | 1.28        | 1.22     |
| 14  | Y     | 809 | CLA  | C3B-C2B | 4.38 | 1.46        | 1.40     |
| 14  | A     | 813 | CLA  | C3D-C2D | 4.38 | 1.47        | 1.39     |
| 14  | Z     | 826 | CLA  | C3C-C2C | 4.38 | 1.46        | 1.36     |
| 14  | G     | 839 | CLA  | C3C-C2C | 4.38 | 1.46        | 1.36     |
| 14  | G     | 806 | CLA  | C3C-C2C | 4.38 | 1.46        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 805  | CLA  | O2A-C1  | 4.38 | 1.58        | 1.46     |
| 14  | H     | 805  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | Y     | 803  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | H     | 818  | CLA  | C3D-C2D | 4.37 | 1.47        | 1.39     |
| 14  | H     | 831  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | Y     | 809  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | A     | 829  | CLA  | C3B-C2B | 4.37 | 1.46        | 1.40     |
| 14  | Y     | 855  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | Z     | 824  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 19  | H     | 846  | LMG  | O7-C10  | 4.37 | 1.46        | 1.34     |
| 14  | Y     | 811  | CLA  | OBD-CAD | 4.37 | 1.28        | 1.22     |
| 14  | X     | 1701 | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | G     | 837  | CLA  | C3C-C2C | 4.37 | 1.46        | 1.36     |
| 14  | Y     | 830  | CLA  | C3B-C2B | 4.36 | 1.46        | 1.40     |
| 14  | Y     | 814  | CLA  | C3D-C2D | 4.36 | 1.47        | 1.39     |
| 14  | G     | 822  | CLA  | C3C-C2C | 4.36 | 1.46        | 1.36     |
| 14  | S     | 1102 | CLA  | C3D-C2D | 4.36 | 1.47        | 1.39     |
| 14  | Y     | 812  | CLA  | C3B-C2B | 4.36 | 1.46        | 1.40     |
| 14  | Z     | 838  | CLA  | O2D-CGD | 4.36 | 1.43        | 1.33     |
| 14  | H     | 822  | CLA  | C3C-C2C | 4.36 | 1.46        | 1.36     |
| 14  | B     | 808  | CLA  | O2A-C1  | 4.36 | 1.58        | 1.46     |
| 14  | B     | 827  | CLA  | OBD-CAD | 4.36 | 1.28        | 1.22     |
| 14  | B     | 826  | CLA  | C3C-C2C | 4.36 | 1.46        | 1.36     |
| 14  | J     | 102  | CLA  | C3C-C2C | 4.36 | 1.46        | 1.36     |
| 14  | G     | 829  | CLA  | C3C-C2C | 4.35 | 1.46        | 1.36     |
| 14  | Y     | 823  | CLA  | C3C-C2C | 4.35 | 1.46        | 1.36     |
| 14  | Y     | 812  | CLA  | OBD-CAD | 4.35 | 1.28        | 1.22     |
| 14  | G     | 818  | CLA  | C3D-C2D | 4.35 | 1.47        | 1.39     |
| 14  | G     | 835  | CLA  | C3C-C2C | 4.35 | 1.46        | 1.36     |
| 14  | A     | 827  | CLA  | C3C-C2C | 4.35 | 1.46        | 1.36     |
| 14  | A     | 828  | CLA  | C3B-C2B | 4.35 | 1.46        | 1.40     |
| 14  | Y     | 812  | CLA  | C3C-C2C | 4.35 | 1.46        | 1.36     |
| 14  | B     | 802  | CLA  | C3C-C2C | 4.34 | 1.46        | 1.36     |
| 14  | Y     | 803  | CLA  | OBD-CAD | 4.34 | 1.28        | 1.22     |
| 14  | B     | 835  | CLA  | OBD-CAD | 4.34 | 1.28        | 1.22     |
| 14  | Y     | 827  | CLA  | C3D-C2D | 4.34 | 1.47        | 1.39     |
| 14  | Y     | 838  | CLA  | O2D-CGD | 4.34 | 1.43        | 1.33     |
| 14  | A     | 822  | CLA  | C3B-C2B | 4.34 | 1.46        | 1.40     |
| 14  | A     | 817  | CLA  | C3C-C2C | 4.34 | 1.45        | 1.36     |
| 14  | Y     | 810  | CLA  | C3C-C2C | 4.34 | 1.45        | 1.36     |
| 14  | A     | 810  | CLA  | C3C-C2C | 4.34 | 1.45        | 1.36     |
| 14  | Z     | 819  | CLA  | C3D-C2D | 4.34 | 1.47        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | B     | 804  | CLA  | C3C-C2C | 4.34 | 1.45        | 1.36     |
| 14  | Y     | 842  | CLA  | OBD-CAD | 4.34 | 1.28        | 1.22     |
| 14  | g     | 101  | CLA  | C3C-C2C | 4.34 | 1.45        | 1.36     |
| 14  | Y     | 831  | CLA  | C3C-C2C | 4.34 | 1.45        | 1.36     |
| 14  | B     | 808  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | G     | 805  | CLA  | C3D-C2D | 4.33 | 1.47        | 1.39     |
| 15  | B     | 842  | PQN  | C10-C5  | 4.33 | 1.47        | 1.40     |
| 14  | G     | 821  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | G     | 832  | CLA  | C3C-C2C | 4.33 | 1.45        | 1.36     |
| 14  | B     | 832  | CLA  | O2A-C1  | 4.33 | 1.58        | 1.46     |
| 14  | H     | 836  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | B     | 813  | CLA  | C3C-C2C | 4.33 | 1.45        | 1.36     |
| 14  | H     | 822  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | U     | 1002 | CLA  | OBD-CAD | 4.33 | 1.28        | 1.22     |
| 14  | H     | 813  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | A     | 842  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | Z     | 811  | CLA  | OBD-CAD | 4.33 | 1.28        | 1.22     |
| 14  | H     | 817  | CLA  | C3B-C2B | 4.33 | 1.46        | 1.40     |
| 14  | G     | 826  | CLA  | C3C-C2C | 4.33 | 1.45        | 1.36     |
| 14  | Z     | 811  | CLA  | C3C-C2C | 4.32 | 1.45        | 1.36     |
| 14  | Z     | 827  | CLA  | O2D-CGD | 4.32 | 1.43        | 1.33     |
| 14  | G     | 831  | CLA  | C3B-C2B | 4.32 | 1.46        | 1.40     |
| 14  | U     | 1004 | CLA  | O2D-CGD | 4.32 | 1.43        | 1.33     |
| 14  | S     | 1103 | CLA  | C3B-C2B | 4.31 | 1.46        | 1.40     |
| 14  | H     | 814  | CLA  | C3D-C2D | 4.31 | 1.47        | 1.39     |
| 14  | Y     | 807  | CLA  | C3D-C2D | 4.31 | 1.47        | 1.39     |
| 14  | G     | 824  | CLA  | C3C-C2C | 4.31 | 1.45        | 1.36     |
| 14  | Z     | 833  | CLA  | C3C-C2C | 4.31 | 1.45        | 1.36     |
| 14  | Z     | 815  | CLA  | C3D-C2D | 4.31 | 1.47        | 1.39     |
| 14  | Y     | 802  | CLA  | C3D-C2D | 4.31 | 1.47        | 1.39     |
| 14  | B     | 818  | CLA  | C3C-C2C | 4.30 | 1.45        | 1.36     |
| 14  | A     | 820  | CLA  | C3C-C2C | 4.30 | 1.45        | 1.36     |
| 14  | Y     | 833  | CLA  | C3C-C2C | 4.30 | 1.45        | 1.36     |
| 14  | Z     | 810  | CLA  | C3C-C2C | 4.30 | 1.45        | 1.36     |
| 14  | H     | 824  | CLA  | C3B-C2B | 4.30 | 1.46        | 1.40     |
| 14  | B     | 811  | CLA  | C3B-C2B | 4.30 | 1.46        | 1.40     |
| 14  | A     | 817  | CLA  | C3D-C2D | 4.30 | 1.47        | 1.39     |
| 14  | H     | 808  | CLA  | C3B-C2B | 4.30 | 1.46        | 1.40     |
| 14  | Y     | 804  | CLA  | C3B-C2B | 4.30 | 1.46        | 1.40     |
| 14  | X     | 1701 | CLA  | C3B-C2B | 4.30 | 1.46        | 1.40     |
| 14  | G     | 841  | CLA  | C3C-C2C | 4.30 | 1.45        | 1.36     |
| 14  | G     | 813  | CLA  | O2A-C1  | 4.30 | 1.58        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | B     | 810  | CLA  | OBD-CAD | 4.30 | 1.28        | 1.22     |
| 18  | G     | 851  | LHG  | O8-C23  | 4.29 | 1.45        | 1.33     |
| 18  | Y     | 852  | LHG  | O7-C7   | 4.29 | 1.46        | 1.34     |
| 18  | j     | 101  | LHG  | O8-C23  | 4.29 | 1.45        | 1.33     |
| 14  | U     | 1003 | CLA  | C3D-C2D | 4.29 | 1.47        | 1.39     |
| 14  | B     | 811  | CLA  | C3D-C2D | 4.29 | 1.47        | 1.39     |
| 14  | T     | 101  | CLA  | C3D-C2D | 4.29 | 1.47        | 1.39     |
| 14  | B     | 819  | CLA  | C3C-C2C | 4.29 | 1.45        | 1.36     |
| 14  | U     | 1006 | CLA  | C3B-C2B | 4.29 | 1.46        | 1.40     |
| 14  | A     | 831  | CLA  | C3B-C2B | 4.29 | 1.46        | 1.40     |
| 14  | A     | 809  | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 14  | A     | 835  | CLA  | C3D-C2D | 4.28 | 1.47        | 1.39     |
| 14  | A     | 842  | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 14  | A     | 840  | CLA  | C3C-C2C | 4.28 | 1.45        | 1.36     |
| 14  | Y     | 829  | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 14  | H     | 810  | CLA  | C3C-C2C | 4.28 | 1.45        | 1.36     |
| 14  | h     | 205  | CLA  | C3D-C2D | 4.28 | 1.47        | 1.39     |
| 14  | B     | 832  | CLA  | C3D-C2D | 4.28 | 1.47        | 1.39     |
| 18  | A     | 850  | LHG  | O8-C23  | 4.28 | 1.45        | 1.33     |
| 14  | L     | 206  | CLA  | C3C-C2C | 4.28 | 1.45        | 1.36     |
| 14  | Y     | 832  | CLA  | C3C-C2C | 4.28 | 1.45        | 1.36     |
| 14  | Y     | 808  | CLA  | C3D-C2D | 4.28 | 1.47        | 1.39     |
| 14  | B     | 827  | CLA  | C3C-C2C | 4.28 | 1.45        | 1.36     |
| 14  | Y     | 839  | CLA  | C3D-C2D | 4.28 | 1.47        | 1.39     |
| 14  | B     | 832  | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 14  | H     | 820  | CLA  | C3D-C2D | 4.27 | 1.47        | 1.39     |
| 14  | A     | 819  | CLA  | C3C-C2C | 4.27 | 1.45        | 1.36     |
| 14  | A     | 805  | CLA  | C3D-C2D | 4.27 | 1.47        | 1.39     |
| 14  | A     | 807  | CLA  | C3B-C2B | 4.27 | 1.46        | 1.40     |
| 14  | L     | 207  | CLA  | C3D-C2D | 4.27 | 1.47        | 1.39     |
| 14  | B     | 813  | CLA  | C3B-C2B | 4.27 | 1.46        | 1.40     |
| 14  | A     | 806  | CLA  | OBD-CAD | 4.26 | 1.28        | 1.22     |
| 14  | G     | 820  | CLA  | C3D-C2D | 4.26 | 1.47        | 1.39     |
| 14  | B     | 831  | CLA  | C3B-C2B | 4.26 | 1.46        | 1.40     |
| 14  | Z     | 831  | CLA  | C3B-C2B | 4.26 | 1.46        | 1.40     |
| 14  | Z     | 809  | CLA  | C3C-C2C | 4.26 | 1.45        | 1.36     |
| 14  | Y     | 829  | CLA  | O2D-CGD | 4.26 | 1.43        | 1.33     |
| 14  | Y     | 813  | CLA  | C3B-C2B | 4.26 | 1.46        | 1.40     |
| 14  | B     | 821  | CLA  | C3C-C2C | 4.26 | 1.45        | 1.36     |
| 14  | L     | 201  | CLA  | C3B-C2B | 4.26 | 1.46        | 1.40     |
| 14  | Y     | 832  | CLA  | C3D-C2D | 4.26 | 1.47        | 1.39     |
| 14  | Y     | 825  | CLA  | C3D-C2D | 4.25 | 1.47        | 1.39     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 835  | CLA  | C3C-C2C | 4.25  | 1.45        | 1.36     |
| 14  | Y     | 838  | CLA  | C3C-C2C | 4.25  | 1.45        | 1.36     |
| 17  | H     | 841  | BCR  | C11-C12 | -4.25 | 1.23        | 1.34     |
| 14  | H     | 827  | CLA  | C3D-C2D | 4.25  | 1.47        | 1.39     |
| 14  | G     | 819  | CLA  | C3C-C2C | 4.25  | 1.45        | 1.36     |
| 14  | B     | 815  | CLA  | OBD-CAD | 4.25  | 1.28        | 1.22     |
| 14  | Z     | 832  | CLA  | C3D-C2D | 4.25  | 1.47        | 1.39     |
| 14  | B     | 801  | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | Z     | 818  | CLA  | C3D-C2D | 4.24  | 1.47        | 1.39     |
| 14  | V     | 1201 | CLA  | C3D-C2D | 4.24  | 1.47        | 1.39     |
| 14  | H     | 805  | CLA  | C3D-C2D | 4.24  | 1.47        | 1.39     |
| 18  | H     | 847  | LHG  | O7-C7   | 4.24  | 1.46        | 1.34     |
| 14  | Z     | 828  | CLA  | C3D-C2D | 4.24  | 1.47        | 1.39     |
| 14  | G     | 802  | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 14  | B     | 820  | CLA  | OBD-CAD | 4.23  | 1.28        | 1.22     |
| 14  | G     | 817  | CLA  | OBD-CAD | 4.23  | 1.28        | 1.22     |
| 14  | H     | 830  | CLA  | C3B-C2B | 4.23  | 1.46        | 1.40     |
| 14  | Y     | 814  | CLA  | C3B-C2B | 4.23  | 1.46        | 1.40     |
| 18  | j     | 101  | LHG  | O7-C7   | 4.23  | 1.46        | 1.34     |
| 14  | Y     | 829  | CLA  | C3D-C2D | 4.23  | 1.47        | 1.39     |
| 14  | Y     | 828  | CLA  | C3D-C2D | 4.22  | 1.47        | 1.39     |
| 14  | G     | 817  | CLA  | C3C-C2C | 4.22  | 1.45        | 1.36     |
| 14  | Z     | 821  | CLA  | C3D-C2D | 4.22  | 1.47        | 1.39     |
| 14  | A     | 825  | CLA  | C3C-C2C | 4.22  | 1.45        | 1.36     |
| 14  | Z     | 815  | CLA  | C3C-C2C | 4.22  | 1.45        | 1.36     |
| 14  | Y     | 819  | CLA  | C3D-C2D | 4.22  | 1.47        | 1.39     |
| 14  | G     | 807  | CLA  | OBD-CAD | 4.22  | 1.28        | 1.22     |
| 14  | G     | 808  | CLA  | OBD-CAD | 4.22  | 1.28        | 1.22     |
| 14  | A     | 830  | CLA  | OBD-CAD | 4.22  | 1.28        | 1.22     |
| 14  | H     | 838  | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | Z     | 827  | CLA  | CHC-C1C | 4.21  | 1.45        | 1.35     |
| 14  | H     | 814  | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | A     | 834  | CLA  | OBD-CAD | 4.21  | 1.28        | 1.22     |
| 14  | G     | 853  | CLA  | OBD-CAD | 4.21  | 1.28        | 1.22     |
| 14  | A     | 836  | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | B     | 825  | CLA  | C3D-C2D | 4.21  | 1.47        | 1.39     |
| 14  | A     | 819  | CLA  | O2D-CGD | 4.21  | 1.43        | 1.33     |
| 14  | A     | 852  | CLA  | C3B-C2B | 4.21  | 1.46        | 1.40     |
| 14  | H     | 820  | CLA  | C1D-C2D | 4.20  | 1.52        | 1.42     |
| 14  | B     | 828  | CLA  | C3D-C2D | 4.20  | 1.47        | 1.39     |
| 14  | H     | 820  | CLA  | C3C-C2C | 4.20  | 1.45        | 1.36     |
| 14  | Y     | 822  | CLA  | C3C-C2C | 4.20  | 1.45        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | G     | 812 | CLA  | OBD-CAD | 4.20 | 1.28        | 1.22     |
| 14  | Y     | 805 | CLA  | C3D-C2D | 4.20 | 1.47        | 1.39     |
| 14  | A     | 824 | CLA  | C3B-C2B | 4.20 | 1.46        | 1.40     |
| 14  | Y     | 821 | CLA  | C3C-C2C | 4.20 | 1.45        | 1.36     |
| 14  | L     | 205 | CLA  | C3D-C2D | 4.19 | 1.46        | 1.39     |
| 14  | B     | 807 | CLA  | C3C-C2C | 4.19 | 1.45        | 1.36     |
| 14  | Z     | 806 | CLA  | C3B-C2B | 4.18 | 1.46        | 1.40     |
| 14  | A     | 814 | CLA  | O2D-CGD | 4.18 | 1.43        | 1.33     |
| 14  | F     | 202 | CLA  | C3B-C2B | 4.18 | 1.46        | 1.40     |
| 14  | A     | 813 | CLA  | O2D-CGD | 4.18 | 1.43        | 1.33     |
| 14  | G     | 825 | CLA  | C3D-C2D | 4.18 | 1.46        | 1.39     |
| 14  | B     | 835 | CLA  | C3B-C2B | 4.17 | 1.46        | 1.40     |
| 14  | H     | 804 | CLA  | C3D-C2D | 4.17 | 1.46        | 1.39     |
| 14  | H     | 819 | CLA  | C3D-C2D | 4.17 | 1.46        | 1.39     |
| 14  | Y     | 833 | CLA  | OBD-CAD | 4.17 | 1.28        | 1.22     |
| 14  | A     | 818 | CLA  | C3C-C2C | 4.17 | 1.45        | 1.36     |
| 14  | B     | 804 | CLA  | C3D-C2D | 4.17 | 1.46        | 1.39     |
| 14  | Y     | 841 | CLA  | C3D-C2D | 4.17 | 1.46        | 1.39     |
| 14  | Z     | 824 | CLA  | C3B-C2B | 4.16 | 1.46        | 1.40     |
| 14  | H     | 804 | CLA  | C3C-C2C | 4.16 | 1.45        | 1.36     |
| 14  | Y     | 837 | CLA  | OBD-CAD | 4.16 | 1.28        | 1.22     |
| 14  | Z     | 834 | CLA  | C3B-C2B | 4.16 | 1.46        | 1.40     |
| 14  | B     | 841 | CLA  | C3D-C2D | 4.16 | 1.46        | 1.39     |
| 14  | G     | 839 | CLA  | C3B-C2B | 4.16 | 1.46        | 1.40     |
| 14  | Y     | 807 | CLA  | C3B-C2B | 4.16 | 1.46        | 1.40     |
| 14  | A     | 803 | CLA  | C3D-C2D | 4.15 | 1.46        | 1.39     |
| 14  | d     | 201 | CLA  | C3B-C2B | 4.15 | 1.46        | 1.40     |
| 14  | Y     | 831 | CLA  | C3B-C2B | 4.15 | 1.46        | 1.40     |
| 14  | A     | 833 | CLA  | C3B-C2B | 4.15 | 1.46        | 1.40     |
| 14  | B     | 840 | CLA  | C3C-C2C | 4.15 | 1.45        | 1.36     |
| 14  | H     | 824 | CLA  | C3C-C2C | 4.15 | 1.45        | 1.36     |
| 14  | G     | 843 | CLA  | C3D-C2D | 4.15 | 1.46        | 1.39     |
| 14  | B     | 817 | CLA  | C3D-C2D | 4.15 | 1.46        | 1.39     |
| 14  | A     | 809 | CLA  | C3D-C2D | 4.15 | 1.46        | 1.39     |
| 14  | G     | 804 | CLA  | C3C-C2C | 4.14 | 1.45        | 1.36     |
| 14  | A     | 833 | CLA  | C3C-C2C | 4.14 | 1.45        | 1.36     |
| 18  | G     | 852 | LHG  | O8-C23  | 4.14 | 1.45        | 1.33     |
| 14  | B     | 804 | CLA  | C3B-C2B | 4.13 | 1.46        | 1.40     |
| 14  | A     | 802 | CLA  | C3C-C2C | 4.13 | 1.45        | 1.36     |
| 14  | A     | 803 | CLA  | C3C-C2C | 4.13 | 1.45        | 1.36     |
| 14  | B     | 835 | CLA  | C3C-C2C | 4.13 | 1.45        | 1.36     |
| 14  | A     | 830 | CLA  | C3C-C2C | 4.13 | 1.45        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 838  | CLA  | C3D-C2D | 4.12  | 1.46        | 1.39     |
| 14  | B     | 806  | CLA  | C3C-C2C | 4.12  | 1.45        | 1.36     |
| 14  | Z     | 830  | CLA  | C3C-C2C | 4.12  | 1.45        | 1.36     |
| 14  | G     | 828  | CLA  | C3C-C2C | 4.12  | 1.45        | 1.36     |
| 14  | Y     | 818  | CLA  | C3B-C2B | 4.12  | 1.46        | 1.40     |
| 14  | H     | 807  | CLA  | OBD-CAD | 4.12  | 1.28        | 1.22     |
| 14  | Z     | 801  | CLA  | C3B-C2B | 4.12  | 1.46        | 1.40     |
| 14  | G     | 808  | CLA  | C3B-C2B | 4.12  | 1.46        | 1.40     |
| 17  | Y     | 851  | BCR  | C11-C12 | -4.11 | 1.24        | 1.34     |
| 14  | B     | 818  | CLA  | C3D-C2D | 4.11  | 1.46        | 1.39     |
| 14  | L     | 205  | CLA  | OBD-CAD | 4.11  | 1.28        | 1.22     |
| 14  | A     | 823  | CLA  | C3B-C2B | 4.11  | 1.46        | 1.40     |
| 14  | Z     | 836  | CLA  | C3B-C2B | 4.11  | 1.46        | 1.40     |
| 14  | Y     | 819  | CLA  | C3B-C2B | 4.11  | 1.46        | 1.40     |
| 14  | Y     | 841  | CLA  | C3C-C2C | 4.11  | 1.45        | 1.36     |
| 14  | G     | 838  | CLA  | C3C-C2C | 4.10  | 1.45        | 1.36     |
| 14  | H     | 811  | CLA  | C3D-C2D | 4.10  | 1.46        | 1.39     |
| 14  | G     | 837  | CLA  | OBD-CAD | 4.10  | 1.28        | 1.22     |
| 14  | B     | 817  | CLA  | C3B-C2B | 4.10  | 1.46        | 1.40     |
| 14  | A     | 811  | CLA  | C3D-C2D | 4.10  | 1.46        | 1.39     |
| 14  | B     | 832  | CLA  | C3C-C2C | 4.10  | 1.45        | 1.36     |
| 14  | G     | 804  | CLA  | C3D-C2D | 4.10  | 1.46        | 1.39     |
| 19  | B     | 849  | LMG  | O7-C10  | 4.10  | 1.45        | 1.34     |
| 14  | A     | 807  | CLA  | C3D-C2D | 4.09  | 1.46        | 1.39     |
| 14  | G     | 816  | CLA  | C3B-C2B | 4.09  | 1.46        | 1.40     |
| 14  | Y     | 804  | CLA  | C3D-C2D | 4.09  | 1.46        | 1.39     |
| 14  | G     | 807  | CLA  | C3D-C2D | 4.09  | 1.46        | 1.39     |
| 14  | Y     | 855  | CLA  | C3B-C2B | 4.09  | 1.46        | 1.40     |
| 14  | U     | 1006 | CLA  | C3C-C2C | 4.09  | 1.45        | 1.36     |
| 14  | G     | 814  | CLA  | C3C-C2C | 4.09  | 1.45        | 1.36     |
| 14  | J     | 101  | CLA  | C3B-C2B | 4.09  | 1.46        | 1.40     |
| 14  | B     | 813  | CLA  | C3D-C2D | 4.08  | 1.46        | 1.39     |
| 14  | H     | 836  | CLA  | C3D-C2D | 4.08  | 1.46        | 1.39     |
| 14  | Z     | 820  | CLA  | C3B-C2B | 4.08  | 1.46        | 1.40     |
| 14  | H     | 829  | CLA  | C3C-C2C | 4.08  | 1.45        | 1.36     |
| 14  | G     | 809  | CLA  | C3C-C2C | 4.08  | 1.45        | 1.36     |
| 14  | B     | 829  | CLA  | C3B-C2B | 4.08  | 1.46        | 1.40     |
| 14  | H     | 837  | CLA  | C3C-C2C | 4.08  | 1.45        | 1.36     |
| 14  | Q     | 201  | CLA  | C3D-C2D | 4.08  | 1.46        | 1.39     |
| 17  | G     | 854  | BCR  | C11-C12 | -4.08 | 1.24        | 1.34     |
| 14  | h     | 205  | CLA  | OBD-CAD | 4.07  | 1.28        | 1.22     |
| 14  | H     | 821  | CLA  | C3D-C2D | 4.07  | 1.46        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Y     | 805  | CLA  | C3B-C2B | 4.07  | 1.46        | 1.40     |
| 14  | Z     | 819  | CLA  | C3C-C2C | 4.07  | 1.45        | 1.36     |
| 14  | G     | 808  | CLA  | C3C-C2C | 4.06  | 1.45        | 1.36     |
| 17  | L     | 208  | BCR  | C11-C12 | -4.06 | 1.24        | 1.34     |
| 14  | B     | 839  | CLA  | C3C-C2C | 4.06  | 1.45        | 1.36     |
| 14  | Z     | 815  | CLA  | OBD-CAD | 4.06  | 1.28        | 1.22     |
| 14  | h     | 205  | CLA  | C3B-C2B | 4.06  | 1.46        | 1.40     |
| 14  | A     | 808  | CLA  | C3B-C2B | 4.06  | 1.46        | 1.40     |
| 18  | A     | 851  | LHG  | O7-C7   | 4.05  | 1.45        | 1.34     |
| 14  | G     | 802  | CLA  | C3B-C2B | 4.05  | 1.46        | 1.40     |
| 14  | G     | 820  | CLA  | OBD-CAD | 4.05  | 1.28        | 1.22     |
| 14  | Z     | 838  | CLA  | C3B-C2B | 4.05  | 1.46        | 1.40     |
| 14  | Y     | 837  | CLA  | C3D-C2D | 4.04  | 1.46        | 1.39     |
| 14  | B     | 839  | CLA  | C3B-C2B | 4.04  | 1.46        | 1.40     |
| 14  | Z     | 825  | CLA  | OBD-CAD | 4.04  | 1.28        | 1.22     |
| 14  | Y     | 820  | CLA  | C3C-C2C | 4.04  | 1.45        | 1.36     |
| 14  | h     | 201  | CLA  | C3D-C2D | 4.04  | 1.46        | 1.39     |
| 14  | U     | 1002 | CLA  | C3C-C2C | 4.04  | 1.45        | 1.36     |
| 14  | A     | 834  | CLA  | C3D-C2D | 4.04  | 1.46        | 1.39     |
| 14  | L     | 205  | CLA  | C3C-C2C | 4.04  | 1.45        | 1.36     |
| 14  | Z     | 832  | CLA  | C3B-C2B | 4.04  | 1.46        | 1.40     |
| 14  | Z     | 828  | CLA  | OBD-CAD | 4.03  | 1.27        | 1.22     |
| 14  | A     | 841  | CLA  | C3D-C2D | 4.03  | 1.46        | 1.39     |
| 14  | B     | 839  | CLA  | C3D-C2D | 4.03  | 1.46        | 1.39     |
| 14  | S     | 1103 | CLA  | C3D-C2D | 4.03  | 1.46        | 1.39     |
| 14  | Z     | 803  | CLA  | C3C-C2C | 4.03  | 1.45        | 1.36     |
| 14  | A     | 820  | CLA  | C3D-C2D | 4.03  | 1.46        | 1.39     |
| 14  | Z     | 825  | CLA  | C3D-C2D | 4.03  | 1.46        | 1.39     |
| 14  | H     | 831  | CLA  | C3B-C2B | 4.03  | 1.46        | 1.40     |
| 14  | B     | 815  | CLA  | C3D-C2D | 4.02  | 1.46        | 1.39     |
| 14  | X     | 1701 | CLA  | C3D-C2D | 4.02  | 1.46        | 1.39     |
| 14  | Z     | 818  | CLA  | OBD-CAD | 4.02  | 1.27        | 1.22     |
| 14  | H     | 823  | CLA  | C3D-C2D | 4.02  | 1.46        | 1.39     |
| 14  | Y     | 822  | CLA  | C3D-C2D | 4.02  | 1.46        | 1.39     |
| 17  | i     | 101  | BCR  | C11-C12 | -4.02 | 1.24        | 1.34     |
| 14  | G     | 826  | CLA  | C3B-C2B | 4.02  | 1.45        | 1.40     |
| 14  | H     | 816  | CLA  | C3D-C2D | 4.02  | 1.46        | 1.39     |
| 14  | B     | 821  | CLA  | C3D-C2D | 4.01  | 1.46        | 1.39     |
| 14  | Q     | 203  | CLA  | OBD-CAD | 4.01  | 1.27        | 1.22     |
| 14  | Z     | 811  | CLA  | C3D-C2D | 4.01  | 1.46        | 1.39     |
| 14  | Z     | 824  | CLA  | OBD-CAD | 4.01  | 1.27        | 1.22     |
| 14  | B     | 817  | CLA  | C3C-C2C | 4.01  | 1.45        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | Z     | 835 | CLA  | C3D-C2D | 4.01 | 1.46        | 1.39     |
| 14  | Y     | 830 | CLA  | C3C-C2C | 4.01 | 1.45        | 1.36     |
| 14  | H     | 808 | CLA  | C3C-C2C | 4.01 | 1.45        | 1.36     |
| 14  | Z     | 827 | CLA  | C3D-C2D | 4.01 | 1.46        | 1.39     |
| 14  | G     | 831 | CLA  | C3C-C2C | 4.00 | 1.45        | 1.36     |
| 14  | Z     | 826 | CLA  | C3B-C2B | 4.00 | 1.45        | 1.40     |
| 14  | B     | 817 | CLA  | OBD-CAD | 4.00 | 1.27        | 1.22     |
| 14  | B     | 829 | CLA  | C3C-C2C | 3.99 | 1.45        | 1.36     |
| 14  | G     | 814 | CLA  | C3D-C2D | 3.99 | 1.46        | 1.39     |
| 14  | A     | 805 | CLA  | C3B-C2B | 3.99 | 1.45        | 1.40     |
| 14  | H     | 826 | CLA  | C3C-C2C | 3.99 | 1.45        | 1.36     |
| 14  | G     | 811 | CLA  | C3D-C2D | 3.99 | 1.46        | 1.39     |
| 14  | A     | 808 | CLA  | C3C-C2C | 3.99 | 1.45        | 1.36     |
| 14  | B     | 815 | CLA  | C3B-C2B | 3.98 | 1.45        | 1.40     |
| 14  | d     | 201 | CLA  | C3D-C2D | 3.98 | 1.46        | 1.39     |
| 14  | G     | 823 | CLA  | C3D-C2D | 3.98 | 1.46        | 1.39     |
| 14  | H     | 832 | CLA  | C3D-C2D | 3.98 | 1.46        | 1.39     |
| 14  | Z     | 830 | CLA  | C3D-C2D | 3.98 | 1.46        | 1.39     |
| 14  | K     | 103 | CLA  | C3C-C2C | 3.98 | 1.45        | 1.36     |
| 14  | H     | 815 | CLA  | OBD-CAD | 3.98 | 1.27        | 1.22     |
| 14  | H     | 833 | CLA  | C3C-C2C | 3.98 | 1.45        | 1.36     |
| 14  | H     | 822 | CLA  | OBD-CAD | 3.97 | 1.27        | 1.22     |
| 14  | G     | 823 | CLA  | OBD-CAD | 3.97 | 1.27        | 1.22     |
| 14  | G     | 810 | CLA  | C3D-C2D | 3.97 | 1.46        | 1.39     |
| 14  | Z     | 825 | CLA  | C3C-C2C | 3.97 | 1.45        | 1.36     |
| 14  | B     | 837 | CLA  | OBD-CAD | 3.97 | 1.27        | 1.22     |
| 14  | H     | 825 | CLA  | C3C-C2C | 3.97 | 1.45        | 1.36     |
| 14  | Z     | 802 | CLA  | C3B-C2B | 3.97 | 1.45        | 1.40     |
| 14  | A     | 828 | CLA  | C3D-C2D | 3.96 | 1.46        | 1.39     |
| 14  | H     | 811 | CLA  | OBD-CAD | 3.96 | 1.27        | 1.22     |
| 14  | H     | 828 | CLA  | C3C-C2C | 3.96 | 1.45        | 1.36     |
| 14  | G     | 832 | CLA  | C3B-C2B | 3.96 | 1.45        | 1.40     |
| 14  | A     | 806 | CLA  | C3D-C2D | 3.96 | 1.46        | 1.39     |
| 14  | h     | 205 | CLA  | C3C-C2C | 3.96 | 1.45        | 1.36     |
| 14  | B     | 831 | CLA  | C3D-C2D | 3.95 | 1.46        | 1.39     |
| 14  | A     | 808 | CLA  | OBD-CAD | 3.95 | 1.27        | 1.22     |
| 14  | A     | 812 | CLA  | OBD-CAD | 3.95 | 1.27        | 1.22     |
| 14  | A     | 835 | CLA  | C3C-C2C | 3.95 | 1.45        | 1.36     |
| 14  | B     | 813 | CLA  | OBD-CAD | 3.95 | 1.27        | 1.22     |
| 14  | Z     | 834 | CLA  | C3D-C2D | 3.95 | 1.46        | 1.39     |
| 14  | G     | 829 | CLA  | C3D-C2D | 3.95 | 1.46        | 1.39     |
| 14  | Y     | 818 | CLA  | C1D-C2D | 3.95 | 1.51        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 808  | CLA  | C3D-C2D | 3.94  | 1.46        | 1.39     |
| 14  | G     | 826  | CLA  | C3D-C2D | 3.94  | 1.46        | 1.39     |
| 14  | H     | 804  | CLA  | C3B-C2B | 3.94  | 1.45        | 1.40     |
| 14  | H     | 807  | CLA  | C3C-C2C | 3.94  | 1.45        | 1.36     |
| 14  | A     | 821  | CLA  | OBD-CAD | 3.94  | 1.27        | 1.22     |
| 14  | G     | 824  | CLA  | C3D-C2D | 3.94  | 1.46        | 1.39     |
| 14  | Z     | 805  | CLA  | C3B-C2B | 3.94  | 1.45        | 1.40     |
| 14  | H     | 816  | CLA  | OBD-CAD | 3.93  | 1.27        | 1.22     |
| 17  | R     | 102  | BCR  | C11-C12 | -3.93 | 1.24        | 1.34     |
| 18  | H     | 847  | LHG  | O8-C23  | 3.93  | 1.44        | 1.33     |
| 14  | H     | 831  | CLA  | C1D-C2D | 3.93  | 1.51        | 1.42     |
| 14  | Z     | 808  | CLA  | C3C-C2C | 3.93  | 1.45        | 1.36     |
| 14  | B     | 803  | CLA  | C3D-C2D | 3.93  | 1.46        | 1.39     |
| 14  | G     | 821  | CLA  | C3D-C2D | 3.93  | 1.46        | 1.39     |
| 14  | Y     | 843  | CLA  | C3D-C2D | 3.93  | 1.46        | 1.39     |
| 14  | A     | 805  | CLA  | C3C-C2C | 3.93  | 1.45        | 1.36     |
| 14  | A     | 841  | CLA  | C1D-C2D | 3.93  | 1.51        | 1.42     |
| 14  | S     | 1101 | CLA  | OBD-CAD | 3.92  | 1.27        | 1.22     |
| 14  | A     | 852  | CLA  | C3C-C2C | 3.92  | 1.45        | 1.36     |
| 14  | V     | 1201 | CLA  | C3C-C2C | 3.92  | 1.45        | 1.36     |
| 14  | A     | 833  | CLA  | OBD-CAD | 3.92  | 1.27        | 1.22     |
| 14  | Z     | 822  | CLA  | C3D-C2D | 3.92  | 1.46        | 1.39     |
| 18  | B     | 850  | LHG  | O7-C7   | 3.92  | 1.45        | 1.34     |
| 14  | G     | 853  | CLA  | C1D-C2D | 3.92  | 1.51        | 1.42     |
| 14  | H     | 808  | CLA  | C3D-C2D | 3.91  | 1.46        | 1.39     |
| 14  | J     | 101  | CLA  | C3D-C2D | 3.91  | 1.46        | 1.39     |
| 14  | B     | 835  | CLA  | C3D-C2D | 3.91  | 1.46        | 1.39     |
| 14  | H     | 806  | CLA  | C3C-C2C | 3.91  | 1.45        | 1.36     |
| 14  | H     | 809  | CLA  | C3D-C2D | 3.91  | 1.46        | 1.39     |
| 14  | A     | 812  | CLA  | C3D-C2D | 3.91  | 1.46        | 1.39     |
| 14  | G     | 829  | CLA  | OBD-CAD | 3.91  | 1.27        | 1.22     |
| 14  | B     | 818  | CLA  | OBD-CAD | 3.91  | 1.27        | 1.22     |
| 14  | Y     | 802  | CLA  | C3C-C2C | 3.91  | 1.45        | 1.36     |
| 14  | Y     | 842  | CLA  | C3B-C2B | 3.90  | 1.45        | 1.40     |
| 14  | Y     | 818  | CLA  | C3D-C2D | 3.90  | 1.46        | 1.39     |
| 14  | G     | 823  | CLA  | C1D-C2D | 3.90  | 1.51        | 1.42     |
| 13  | G     | 801  | CL0  | C3D-C2D | 3.90  | 1.46        | 1.39     |
| 14  | Z     | 814  | CLA  | C3D-C2D | 3.90  | 1.46        | 1.39     |
| 14  | Y     | 813  | CLA  | C3D-C2D | 3.89  | 1.46        | 1.39     |
| 14  | U     | 1002 | CLA  | C3D-C2D | 3.89  | 1.46        | 1.39     |
| 14  | Y     | 842  | CLA  | C1D-C2D | 3.88  | 1.51        | 1.42     |
| 14  | A     | 809  | CLA  | C3B-C2B | 3.88  | 1.45        | 1.40     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 822  | CLA  | C3D-C2D | 3.88  | 1.46        | 1.39     |
| 14  | G     | 830  | CLA  | C3C-C2C | 3.87  | 1.45        | 1.36     |
| 14  | G     | 826  | CLA  | C1D-C2D | 3.87  | 1.51        | 1.42     |
| 14  | H     | 802  | CLA  | C3C-C2C | 3.87  | 1.44        | 1.36     |
| 14  | W     | 1701 | CLA  | C3B-C2B | 3.87  | 1.45        | 1.40     |
| 14  | A     | 831  | CLA  | C3C-C2C | 3.86  | 1.44        | 1.36     |
| 14  | Y     | 838  | CLA  | C3B-C2B | 3.86  | 1.45        | 1.40     |
| 14  | H     | 815  | CLA  | C3D-C2D | 3.86  | 1.46        | 1.39     |
| 14  | Y     | 831  | CLA  | OBD-CAD | 3.86  | 1.27        | 1.22     |
| 14  | Y     | 812  | CLA  | C3D-C2D | 3.86  | 1.46        | 1.39     |
| 14  | Z     | 826  | CLA  | OBD-CAD | 3.86  | 1.27        | 1.22     |
| 14  | G     | 812  | CLA  | C3D-C2D | 3.85  | 1.46        | 1.39     |
| 14  | Z     | 828  | CLA  | C3B-C2B | 3.85  | 1.45        | 1.40     |
| 14  | G     | 828  | CLA  | C3D-C2D | 3.85  | 1.46        | 1.39     |
| 14  | H     | 821  | CLA  | C1D-C2D | 3.85  | 1.51        | 1.42     |
| 14  | G     | 835  | CLA  | C3B-C2B | 3.85  | 1.45        | 1.40     |
| 14  | L     | 202  | CLA  | C1C-NC  | -3.84 | 1.32        | 1.37     |
| 14  | h     | 201  | CLA  | C3C-C2C | 3.84  | 1.44        | 1.36     |
| 14  | Y     | 816  | CLA  | C3D-C2D | 3.83  | 1.46        | 1.39     |
| 14  | S     | 1101 | CLA  | C3D-C2D | 3.83  | 1.46        | 1.39     |
| 14  | G     | 843  | CLA  | C3B-C2B | 3.83  | 1.45        | 1.40     |
| 17  | h     | 203  | BCR  | C11-C12 | -3.83 | 1.24        | 1.34     |
| 14  | G     | 822  | CLA  | C3D-C2D | 3.83  | 1.46        | 1.39     |
| 17  | H     | 844  | BCR  | C11-C12 | -3.83 | 1.24        | 1.34     |
| 14  | H     | 812  | CLA  | C3C-C2C | 3.83  | 1.44        | 1.36     |
| 17  | B     | 843  | BCR  | C11-C12 | -3.82 | 1.24        | 1.34     |
| 17  | B     | 847  | BCR  | C11-C12 | -3.82 | 1.24        | 1.34     |
| 14  | A     | 840  | CLA  | C3D-C2D | 3.82  | 1.46        | 1.39     |
| 14  | Z     | 837  | CLA  | C3C-C2C | 3.82  | 1.44        | 1.36     |
| 14  | G     | 835  | CLA  | C3D-C2D | 3.82  | 1.46        | 1.39     |
| 14  | H     | 826  | CLA  | C3D-C2D | 3.82  | 1.46        | 1.39     |
| 14  | Z     | 806  | CLA  | C3C-C2C | 3.81  | 1.44        | 1.36     |
| 14  | B     | 806  | CLA  | OBD-CAD | 3.81  | 1.27        | 1.22     |
| 14  | G     | 819  | CLA  | C1D-C2D | 3.81  | 1.51        | 1.42     |
| 19  | Z     | 847  | LMG  | O8-C28  | 3.81  | 1.44        | 1.33     |
| 14  | f     | 102  | CLA  | C1D-C2D | 3.81  | 1.51        | 1.42     |
| 14  | B     | 836  | CLA  | C3D-C2D | 3.81  | 1.46        | 1.39     |
| 14  | Y     | 807  | CLA  | C1D-C2D | 3.81  | 1.51        | 1.42     |
| 14  | Z     | 807  | CLA  | C3B-C2B | 3.81  | 1.45        | 1.40     |
| 14  | H     | 835  | CLA  | C3C-C2C | 3.80  | 1.44        | 1.36     |
| 17  | U     | 1007 | BCR  | C11-C12 | -3.80 | 1.24        | 1.34     |
| 14  | H     | 805  | CLA  | C3B-C2B | 3.79  | 1.45        | 1.40     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | j     | 102  | CLA  | C3D-C2D | 3.79  | 1.46        | 1.39     |
| 14  | J     | 102  | CLA  | C1D-C2D | 3.79  | 1.51        | 1.42     |
| 14  | B     | 808  | CLA  | C3C-C2C | 3.79  | 1.44        | 1.36     |
| 14  | H     | 811  | CLA  | C3B-C2B | 3.78  | 1.45        | 1.40     |
| 14  | G     | 804  | CLA  | C3B-C2B | 3.78  | 1.45        | 1.40     |
| 14  | H     | 832  | CLA  | C3B-C2B | 3.78  | 1.45        | 1.40     |
| 14  | Y     | 806  | CLA  | C1D-C2D | 3.78  | 1.51        | 1.42     |
| 14  | A     | 807  | CLA  | C1D-C2D | 3.78  | 1.51        | 1.42     |
| 14  | Z     | 829  | CLA  | C3D-C2D | 3.78  | 1.46        | 1.39     |
| 14  | B     | 830  | CLA  | C3B-C2B | 3.77  | 1.45        | 1.40     |
| 14  | d     | 201  | CLA  | C1D-C2D | 3.77  | 1.51        | 1.42     |
| 17  | Z     | 841  | BCR  | C11-C12 | -3.77 | 1.24        | 1.34     |
| 14  | G     | 806  | CLA  | C3D-C2D | 3.77  | 1.46        | 1.39     |
| 14  | H     | 822  | CLA  | C3D-C2D | 3.76  | 1.46        | 1.39     |
| 14  | W     | 1701 | CLA  | C3D-C2D | 3.76  | 1.46        | 1.39     |
| 14  | B     | 820  | CLA  | C3D-C2D | 3.76  | 1.46        | 1.39     |
| 14  | Z     | 802  | CLA  | C3D-C2D | 3.76  | 1.46        | 1.39     |
| 14  | L     | 201  | CLA  | C3D-C2D | 3.75  | 1.46        | 1.39     |
| 14  | Y     | 816  | CLA  | C3B-C2B | 3.75  | 1.45        | 1.40     |
| 14  | G     | 836  | CLA  | OBD-CAD | 3.75  | 1.27        | 1.22     |
| 14  | H     | 824  | CLA  | C3D-C2D | 3.74  | 1.46        | 1.39     |
| 14  | A     | 840  | CLA  | C1D-C2D | 3.74  | 1.51        | 1.42     |
| 17  | G     | 849  | BCR  | C11-C12 | -3.74 | 1.24        | 1.34     |
| 14  | Z     | 806  | CLA  | C3D-C2D | 3.74  | 1.46        | 1.39     |
| 14  | A     | 816  | CLA  | C1D-C2D | 3.73  | 1.51        | 1.42     |
| 14  | B     | 841  | CLA  | C3B-C2B | 3.73  | 1.45        | 1.40     |
| 14  | J     | 102  | CLA  | C3B-C2B | 3.73  | 1.45        | 1.40     |
| 14  | A     | 832  | CLA  | C3D-C2D | 3.73  | 1.46        | 1.39     |
| 17  | f     | 104  | BCR  | C11-C12 | -3.72 | 1.25        | 1.34     |
| 14  | G     | 839  | CLA  | C3D-C2D | 3.72  | 1.46        | 1.39     |
| 14  | A     | 825  | CLA  | C3D-C2D | 3.72  | 1.46        | 1.39     |
| 14  | B     | 820  | CLA  | C1D-C2D | 3.72  | 1.51        | 1.42     |
| 14  | G     | 816  | CLA  | C1D-C2D | 3.72  | 1.51        | 1.42     |
| 14  | H     | 832  | CLA  | C1D-C2D | 3.71  | 1.51        | 1.42     |
| 14  | G     | 832  | CLA  | C3D-C2D | 3.71  | 1.46        | 1.39     |
| 14  | L     | 202  | CLA  | C3D-C2D | 3.71  | 1.46        | 1.39     |
| 14  | B     | 829  | CLA  | C1C-NC  | -3.71 | 1.32        | 1.37     |
| 14  | G     | 813  | CLA  | OBD-CAD | 3.71  | 1.27        | 1.22     |
| 14  | B     | 830  | CLA  | C1D-C2D | 3.71  | 1.51        | 1.42     |
| 17  | Q     | 202  | BCR  | C11-C12 | -3.70 | 1.25        | 1.34     |
| 14  | B     | 834  | CLA  | C3D-C2D | 3.70  | 1.46        | 1.39     |
| 14  | Y     | 831  | CLA  | C3D-C2D | 3.70  | 1.46        | 1.39     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 830  | CLA  | C1C-NC  | -3.70 | 1.32        | 1.37     |
| 14  | A     | 838  | CLA  | OBD-CAD | 3.70  | 1.27        | 1.22     |
| 14  | H     | 817  | CLA  | C1D-C2D | 3.70  | 1.50        | 1.42     |
| 18  | G     | 851  | LHG  | O7-C7   | 3.69  | 1.44        | 1.34     |
| 14  | B     | 813  | CLA  | C1C-NC  | -3.69 | 1.32        | 1.37     |
| 14  | G     | 822  | CLA  | C1D-C2D | 3.69  | 1.50        | 1.42     |
| 14  | B     | 838  | CLA  | C3B-C2B | 3.69  | 1.45        | 1.40     |
| 17  | F     | 201  | BCR  | C11-C12 | -3.69 | 1.25        | 1.34     |
| 14  | H     | 802  | CLA  | C3B-C2B | 3.68  | 1.45        | 1.40     |
| 14  | H     | 818  | CLA  | C1D-C2D | 3.68  | 1.50        | 1.42     |
| 14  | A     | 821  | CLA  | C3D-C2D | 3.68  | 1.46        | 1.39     |
| 14  | G     | 809  | CLA  | C3D-C2D | 3.68  | 1.46        | 1.39     |
| 17  | L     | 209  | BCR  | C11-C12 | -3.68 | 1.25        | 1.34     |
| 19  | Z     | 847  | LMG  | O7-C10  | 3.68  | 1.44        | 1.34     |
| 14  | Y     | 809  | CLA  | C3D-C2D | 3.66  | 1.46        | 1.39     |
| 14  | Z     | 825  | CLA  | C3B-C2B | 3.66  | 1.45        | 1.40     |
| 14  | G     | 842  | CLA  | C3B-C2B | 3.66  | 1.45        | 1.40     |
| 14  | A     | 823  | CLA  | C1D-C2D | 3.66  | 1.50        | 1.42     |
| 14  | A     | 838  | CLA  | C3C-C2C | 3.65  | 1.44        | 1.36     |
| 14  | A     | 822  | CLA  | C1D-C2D | 3.65  | 1.50        | 1.42     |
| 14  | B     | 803  | CLA  | C3B-C2B | 3.65  | 1.45        | 1.40     |
| 14  | A     | 831  | CLA  | C3D-C2D | 3.64  | 1.46        | 1.39     |
| 14  | Z     | 839  | CLA  | C3D-C2D | 3.64  | 1.46        | 1.39     |
| 14  | B     | 806  | CLA  | C3B-C2B | 3.64  | 1.45        | 1.40     |
| 14  | Z     | 823  | CLA  | C3D-C2D | 3.64  | 1.45        | 1.39     |
| 14  | L     | 202  | CLA  | C3B-C2B | 3.64  | 1.45        | 1.40     |
| 14  | Z     | 809  | CLA  | C1D-C2D | 3.63  | 1.50        | 1.42     |
| 14  | Y     | 819  | CLA  | C1D-C2D | 3.63  | 1.50        | 1.42     |
| 14  | B     | 810  | CLA  | C3D-C2D | 3.63  | 1.45        | 1.39     |
| 14  | A     | 809  | CLA  | C1D-C2D | 3.63  | 1.50        | 1.42     |
| 14  | f     | 102  | CLA  | C3B-C2B | 3.63  | 1.45        | 1.40     |
| 14  | G     | 818  | CLA  | C1D-C2D | 3.62  | 1.50        | 1.42     |
| 14  | B     | 839  | CLA  | OBD-CAD | 3.62  | 1.27        | 1.22     |
| 14  | B     | 802  | CLA  | C3D-C2D | 3.62  | 1.45        | 1.39     |
| 14  | B     | 807  | CLA  | C3D-C2D | 3.62  | 1.45        | 1.39     |
| 14  | Z     | 804  | CLA  | C1D-C2D | 3.62  | 1.50        | 1.42     |
| 14  | A     | 814  | CLA  | C1D-C2D | 3.61  | 1.50        | 1.42     |
| 14  | W     | 1701 | CLA  | C1D-C2D | 3.61  | 1.50        | 1.42     |
| 14  | B     | 812  | CLA  | C3D-C2D | 3.61  | 1.45        | 1.39     |
| 14  | G     | 835  | CLA  | C1D-C2D | 3.61  | 1.50        | 1.42     |
| 14  | Z     | 827  | CLA  | C1C-NC  | -3.60 | 1.32        | 1.37     |
| 14  | G     | 832  | CLA  | OBD-CAD | 3.60  | 1.27        | 1.22     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 810 | CLA  | C3C-C2C | 3.60  | 1.44        | 1.36     |
| 14  | H     | 837 | CLA  | C3B-C2B | 3.60  | 1.45        | 1.40     |
| 14  | B     | 831 | CLA  | OBD-CAD | 3.60  | 1.27        | 1.22     |
| 14  | H     | 802 | CLA  | C1C-NC  | -3.60 | 1.32        | 1.37     |
| 14  | A     | 826 | CLA  | C3D-C2D | 3.60  | 1.45        | 1.39     |
| 14  | H     | 816 | CLA  | C3C-C2C | 3.59  | 1.44        | 1.36     |
| 13  | G     | 801 | CL0  | C1D-C2D | 3.59  | 1.50        | 1.42     |
| 14  | G     | 805 | CLA  | C3C-C2C | 3.59  | 1.44        | 1.36     |
| 17  | Y     | 850 | BCR  | C11-C12 | -3.59 | 1.25        | 1.34     |
| 14  | B     | 801 | CLA  | C1D-C2D | 3.58  | 1.50        | 1.42     |
| 14  | Z     | 813 | CLA  | C1C-NC  | -3.58 | 1.32        | 1.37     |
| 14  | Z     | 804 | CLA  | C3C-C2C | 3.58  | 1.44        | 1.36     |
| 14  | T     | 103 | CLA  | C1D-C2D | 3.58  | 1.50        | 1.42     |
| 14  | H     | 834 | CLA  | C1D-C2D | 3.57  | 1.50        | 1.42     |
| 14  | Y     | 838 | CLA  | MG-NC   | 3.57  | 2.14        | 2.06     |
| 14  | B     | 841 | CLA  | C1D-C2D | 3.57  | 1.50        | 1.42     |
| 14  | A     | 834 | CLA  | C3B-C2B | 3.57  | 1.45        | 1.40     |
| 14  | Y     | 811 | CLA  | C1D-C2D | 3.57  | 1.50        | 1.42     |
| 14  | T     | 101 | CLA  | C1D-C2D | 3.57  | 1.50        | 1.42     |
| 14  | A     | 842 | CLA  | C3D-C2D | 3.56  | 1.45        | 1.39     |
| 14  | Y     | 805 | CLA  | C1D-C2D | 3.56  | 1.50        | 1.42     |
| 14  | A     | 836 | CLA  | C1D-C2D | 3.56  | 1.50        | 1.42     |
| 14  | A     | 828 | CLA  | OBD-CAD | 3.56  | 1.27        | 1.22     |
| 14  | A     | 826 | CLA  | C1D-C2D | 3.56  | 1.50        | 1.42     |
| 19  | B     | 849 | LMG  | O8-C28  | 3.55  | 1.43        | 1.33     |
| 14  | h     | 201 | CLA  | OBD-CAD | 3.55  | 1.27        | 1.22     |
| 14  | Y     | 839 | CLA  | C1D-C2D | 3.55  | 1.50        | 1.42     |
| 14  | Z     | 814 | CLA  | C1D-C2D | 3.55  | 1.50        | 1.42     |
| 14  | G     | 831 | CLA  | C3D-C2D | 3.55  | 1.45        | 1.39     |
| 14  | G     | 838 | CLA  | C3D-C2D | 3.54  | 1.45        | 1.39     |
| 14  | A     | 827 | CLA  | C3D-C2D | 3.54  | 1.45        | 1.39     |
| 14  | B     | 812 | CLA  | C1D-C2D | 3.54  | 1.50        | 1.42     |
| 14  | B     | 835 | CLA  | C1D-C2D | 3.54  | 1.50        | 1.42     |
| 14  | H     | 806 | CLA  | C3B-C2B | 3.54  | 1.45        | 1.40     |
| 14  | G     | 838 | CLA  | C1D-C2D | 3.54  | 1.50        | 1.42     |
| 14  | G     | 813 | CLA  | C3D-C2D | 3.54  | 1.45        | 1.39     |
| 14  | B     | 826 | CLA  | C1C-NC  | -3.54 | 1.32        | 1.37     |
| 14  | B     | 809 | CLA  | C3D-C2D | 3.54  | 1.45        | 1.39     |
| 14  | Z     | 816 | CLA  | C1D-C2D | 3.54  | 1.50        | 1.42     |
| 14  | B     | 832 | CLA  | C1D-C2D | 3.53  | 1.50        | 1.42     |
| 14  | G     | 807 | CLA  | C1D-C2D | 3.53  | 1.50        | 1.42     |
| 17  | e     | 101 | BCR  | C11-C12 | -3.53 | 1.25        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 833  | CLA  | C1D-C2D | 3.53  | 1.50        | 1.42     |
| 17  | J     | 104  | BCR  | C11-C12 | -3.53 | 1.25        | 1.34     |
| 14  | Y     | 804  | CLA  | C1D-C2D | 3.52  | 1.50        | 1.42     |
| 14  | G     | 803  | CLA  | C3B-C2B | 3.52  | 1.45        | 1.40     |
| 14  | H     | 824  | CLA  | C1D-C2D | 3.52  | 1.50        | 1.42     |
| 14  | Y     | 815  | CLA  | C1D-C2D | 3.52  | 1.50        | 1.42     |
| 14  | A     | 837  | CLA  | C1D-C2D | 3.52  | 1.50        | 1.42     |
| 14  | S     | 1102 | CLA  | C1D-C2D | 3.52  | 1.50        | 1.42     |
| 14  | Z     | 827  | CLA  | C3B-C2B | 3.52  | 1.45        | 1.40     |
| 14  | Y     | 854  | CLA  | C3B-C2B | 3.52  | 1.45        | 1.40     |
| 14  | B     | 818  | CLA  | C1C-NC  | -3.51 | 1.32        | 1.37     |
| 14  | Y     | 828  | CLA  | OBD-CAD | 3.51  | 1.27        | 1.22     |
| 14  | H     | 815  | CLA  | C1D-C2D | 3.51  | 1.50        | 1.42     |
| 14  | Y     | 835  | CLA  | MG-NC   | 3.51  | 2.14        | 2.06     |
| 14  | A     | 821  | CLA  | C1D-C2D | 3.51  | 1.50        | 1.42     |
| 14  | Z     | 837  | CLA  | C1D-C2D | 3.51  | 1.50        | 1.42     |
| 17  | V     | 1202 | BCR  | C11-C12 | -3.50 | 1.25        | 1.34     |
| 14  | Z     | 819  | CLA  | C1D-C2D | 3.50  | 1.50        | 1.42     |
| 14  | A     | 810  | CLA  | C1D-C2D | 3.50  | 1.50        | 1.42     |
| 14  | G     | 836  | CLA  | C1D-C2D | 3.50  | 1.50        | 1.42     |
| 14  | H     | 803  | CLA  | C1C-NC  | -3.49 | 1.32        | 1.37     |
| 14  | Q     | 201  | CLA  | C1D-C2D | 3.49  | 1.50        | 1.42     |
| 14  | Y     | 838  | CLA  | C1D-C2D | 3.49  | 1.50        | 1.42     |
| 14  | Y     | 830  | CLA  | C3D-C2D | 3.49  | 1.45        | 1.39     |
| 14  | B     | 814  | CLA  | C1D-C2D | 3.49  | 1.50        | 1.42     |
| 14  | Z     | 804  | CLA  | C3D-C2D | 3.48  | 1.45        | 1.39     |
| 14  | B     | 827  | CLA  | C3D-C2D | 3.48  | 1.45        | 1.39     |
| 14  | K     | 103  | CLA  | C1D-C2D | 3.48  | 1.50        | 1.42     |
| 14  | G     | 812  | CLA  | MG-NC   | 3.47  | 2.14        | 2.06     |
| 14  | H     | 838  | CLA  | C3D-C2D | 3.47  | 1.45        | 1.39     |
| 14  | A     | 818  | CLA  | C3D-C2D | 3.47  | 1.45        | 1.39     |
| 14  | Y     | 803  | CLA  | C1D-C2D | 3.46  | 1.50        | 1.42     |
| 14  | A     | 819  | CLA  | C1D-C2D | 3.46  | 1.50        | 1.42     |
| 14  | B     | 818  | CLA  | C1D-C2D | 3.46  | 1.50        | 1.42     |
| 14  | G     | 837  | CLA  | C1D-C2D | 3.46  | 1.50        | 1.42     |
| 14  | H     | 833  | CLA  | C1D-C2D | 3.46  | 1.50        | 1.42     |
| 14  | U     | 1002 | CLA  | C1C-NC  | -3.45 | 1.32        | 1.37     |
| 14  | S     | 1101 | CLA  | C1D-C2D | 3.45  | 1.50        | 1.42     |
| 14  | A     | 815  | CLA  | C1D-C2D | 3.45  | 1.50        | 1.42     |
| 17  | M     | 101  | BCR  | C11-C12 | -3.45 | 1.25        | 1.34     |
| 14  | Z     | 836  | CLA  | C1D-C2D | 3.45  | 1.50        | 1.42     |
| 14  | H     | 809  | CLA  | C3C-C2C | 3.45  | 1.44        | 1.36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 804  | CLA  | C1D-C2D | 3.45  | 1.50        | 1.42     |
| 17  | G     | 847  | BCR  | C11-C12 | -3.44 | 1.25        | 1.34     |
| 14  | H     | 829  | CLA  | C3B-C2B | 3.44  | 1.45        | 1.40     |
| 14  | A     | 835  | CLA  | C3B-C2B | 3.43  | 1.45        | 1.40     |
| 14  | U     | 1003 | CLA  | C1D-C2D | 3.43  | 1.50        | 1.42     |
| 14  | A     | 808  | CLA  | C1D-C2D | 3.43  | 1.50        | 1.42     |
| 14  | A     | 839  | CLA  | MG-NC   | 3.43  | 2.14        | 2.06     |
| 14  | B     | 810  | CLA  | C1D-C2D | 3.43  | 1.50        | 1.42     |
| 14  | Y     | 820  | CLA  | C1D-C2D | 3.43  | 1.50        | 1.42     |
| 17  | S     | 1104 | BCR  | C11-C12 | -3.43 | 1.25        | 1.34     |
| 14  | A     | 837  | CLA  | C3D-C2D | 3.43  | 1.45        | 1.39     |
| 17  | H     | 840  | BCR  | C11-C12 | -3.43 | 1.25        | 1.34     |
| 14  | G     | 836  | CLA  | C3D-C2D | 3.43  | 1.45        | 1.39     |
| 14  | f     | 101  | CLA  | C1D-C2D | 3.42  | 1.50        | 1.42     |
| 17  | H     | 848  | BCR  | C11-C12 | -3.42 | 1.25        | 1.34     |
| 14  | B     | 801  | CLA  | C3B-C2B | 3.42  | 1.45        | 1.40     |
| 14  | G     | 809  | CLA  | C1D-C2D | 3.41  | 1.50        | 1.42     |
| 14  | G     | 815  | CLA  | C1D-C2D | 3.41  | 1.50        | 1.42     |
| 13  | A     | 801  | CL0  | C3B-C2B | 3.41  | 1.45        | 1.40     |
| 14  | A     | 825  | CLA  | C1D-C2D | 3.41  | 1.50        | 1.42     |
| 14  | G     | 830  | CLA  | C3B-C2B | 3.41  | 1.45        | 1.40     |
| 14  | G     | 813  | CLA  | C1D-C2D | 3.41  | 1.50        | 1.42     |
| 14  | A     | 827  | CLA  | C1D-C2D | 3.41  | 1.50        | 1.42     |
| 14  | H     | 837  | CLA  | MG-NC   | 3.41  | 2.14        | 2.06     |
| 14  | B     | 828  | CLA  | C1D-C2D | 3.40  | 1.50        | 1.42     |
| 14  | Z     | 823  | CLA  | C1D-C2D | 3.40  | 1.50        | 1.42     |
| 14  | B     | 806  | CLA  | C1B-NB  | -3.40 | 1.32        | 1.35     |
| 14  | Z     | 832  | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 17  | B     | 851  | BCR  | C11-C12 | -3.40 | 1.25        | 1.34     |
| 14  | Y     | 840  | CLA  | C1D-C2D | 3.40  | 1.50        | 1.42     |
| 14  | B     | 816  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 14  | K     | 101  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 14  | A     | 813  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 17  | B     | 844  | BCR  | C11-C12 | -3.39 | 1.25        | 1.34     |
| 17  | L     | 203  | BCR  | C11-C12 | -3.39 | 1.25        | 1.34     |
| 14  | Q     | 203  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 14  | B     | 838  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 14  | H     | 835  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 14  | g     | 102  | CLA  | C1D-C2D | 3.39  | 1.50        | 1.42     |
| 19  | H     | 846  | LMG  | C40-C39 | -3.38 | 1.32        | 1.51     |
| 14  | Y     | 822  | CLA  | C1D-C2D | 3.38  | 1.50        | 1.42     |
| 14  | Y     | 821  | CLA  | MG-NC   | 3.38  | 2.14        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 823  | CLA  | C1D-C2D | 3.38  | 1.50        | 1.42     |
| 14  | Q     | 201  | CLA  | C3B-C2B | 3.38  | 1.45        | 1.40     |
| 14  | H     | 803  | CLA  | C3B-C2B | 3.37  | 1.45        | 1.40     |
| 14  | G     | 814  | CLA  | C1D-C2D | 3.37  | 1.50        | 1.42     |
| 17  | J     | 103  | BCR  | C11-C12 | -3.37 | 1.25        | 1.34     |
| 14  | Y     | 833  | CLA  | C1D-C2D | 3.37  | 1.50        | 1.42     |
| 14  | G     | 840  | CLA  | C1D-C2D | 3.37  | 1.50        | 1.42     |
| 14  | B     | 806  | CLA  | C1D-C2D | 3.37  | 1.50        | 1.42     |
| 14  | Y     | 816  | CLA  | C1D-C2D | 3.37  | 1.50        | 1.42     |
| 13  | Y     | 801  | CL0  | C1C-NC  | -3.36 | 1.32        | 1.37     |
| 14  | H     | 836  | CLA  | C1D-C2D | 3.36  | 1.50        | 1.42     |
| 14  | Z     | 829  | CLA  | C1D-C2D | 3.36  | 1.50        | 1.42     |
| 14  | B     | 819  | CLA  | C1D-C2D | 3.36  | 1.50        | 1.42     |
| 14  | A     | 806  | CLA  | C1D-C2D | 3.36  | 1.50        | 1.42     |
| 14  | B     | 837  | CLA  | C1C-NC  | -3.36 | 1.32        | 1.37     |
| 14  | B     | 804  | CLA  | C1C-NC  | -3.36 | 1.32        | 1.37     |
| 14  | A     | 811  | CLA  | C1D-C2D | 3.36  | 1.50        | 1.42     |
| 14  | U     | 1002 | CLA  | C3B-C2B | 3.36  | 1.45        | 1.40     |
| 14  | Y     | 824  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 14  | Y     | 817  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 14  | A     | 817  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 17  | Y     | 849  | BCR  | C11-C12 | -3.35 | 1.25        | 1.34     |
| 17  | A     | 847  | BCR  | C11-C12 | -3.35 | 1.25        | 1.34     |
| 14  | Y     | 821  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 14  | H     | 829  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 14  | Z     | 834  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 14  | h     | 205  | CLA  | C1D-C2D | 3.35  | 1.50        | 1.42     |
| 14  | L     | 202  | CLA  | C3C-C2C | 3.34  | 1.43        | 1.36     |
| 14  | B     | 827  | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 17  | f     | 105  | BCR  | C11-C12 | -3.33 | 1.26        | 1.34     |
| 17  | Y     | 847  | BCR  | C11-C12 | -3.33 | 1.26        | 1.34     |
| 14  | H     | 838  | CLA  | C1D-C2D | 3.33  | 1.50        | 1.42     |
| 17  | G     | 850  | BCR  | C11-C12 | -3.33 | 1.26        | 1.34     |
| 14  | Y     | 825  | CLA  | C1D-C2D | 3.33  | 1.50        | 1.42     |
| 14  | Z     | 828  | CLA  | C1D-C2D | 3.33  | 1.50        | 1.42     |
| 17  | U     | 1005 | BCR  | C11-C12 | -3.33 | 1.26        | 1.34     |
| 14  | G     | 829  | CLA  | MG-NC   | 3.33  | 2.14        | 2.06     |
| 14  | Y     | 809  | CLA  | C1D-C2D | 3.33  | 1.50        | 1.42     |
| 14  | B     | 825  | CLA  | C1D-C2D | 3.33  | 1.50        | 1.42     |
| 14  | A     | 815  | CLA  | C3D-C2D | 3.33  | 1.45        | 1.39     |
| 14  | G     | 804  | CLA  | C1D-C2D | 3.32  | 1.50        | 1.42     |
| 14  | Y     | 826  | CLA  | C1D-C2D | 3.32  | 1.50        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 821  | CLA  | C1D-C2D | 3.32  | 1.50        | 1.42     |
| 14  | Y     | 836  | CLA  | C1D-C2D | 3.32  | 1.50        | 1.42     |
| 17  | A     | 849  | BCR  | C11-C12 | -3.32 | 1.26        | 1.34     |
| 14  | H     | 810  | CLA  | C3B-C2B | 3.32  | 1.45        | 1.40     |
| 14  | Y     | 834  | CLA  | C4B-CHC | 3.32  | 1.50        | 1.41     |
| 14  | H     | 814  | CLA  | C1D-C2D | 3.32  | 1.50        | 1.42     |
| 14  | Z     | 835  | CLA  | C1D-C2D | 3.31  | 1.50        | 1.42     |
| 14  | Y     | 829  | CLA  | MG-NC   | 3.31  | 2.14        | 2.06     |
| 14  | B     | 806  | CLA  | C3D-C2D | 3.31  | 1.45        | 1.39     |
| 17  | Y     | 856  | BCR  | C11-C12 | -3.31 | 1.26        | 1.34     |
| 14  | A     | 839  | CLA  | C1D-C2D | 3.31  | 1.50        | 1.42     |
| 14  | H     | 810  | CLA  | C1D-C2D | 3.31  | 1.50        | 1.42     |
| 19  | H     | 846  | LMG  | C37-C36 | -3.30 | 1.33        | 1.51     |
| 14  | A     | 833  | CLA  | C3D-C2D | 3.30  | 1.45        | 1.39     |
| 17  | L     | 208  | BCR  | C21-C22 | -3.30 | 1.31        | 1.35     |
| 14  | Z     | 806  | CLA  | C1C-NC  | -3.30 | 1.32        | 1.37     |
| 14  | Y     | 835  | CLA  | C1D-C2D | 3.30  | 1.50        | 1.42     |
| 14  | Y     | 803  | CLA  | MG-NC   | 3.30  | 2.14        | 2.06     |
| 14  | B     | 813  | CLA  | C1D-C2D | 3.30  | 1.50        | 1.42     |
| 14  | G     | 834  | CLA  | C1D-C2D | 3.30  | 1.50        | 1.42     |
| 14  | G     | 805  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | L     | 201  | CLA  | OBD-CAD | 3.29  | 1.26        | 1.22     |
| 14  | G     | 843  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | A     | 842  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | A     | 835  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | B     | 822  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | H     | 822  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | B     | 821  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | Z     | 812  | CLA  | C4B-CHC | 3.29  | 1.50        | 1.41     |
| 14  | H     | 828  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | G     | 817  | CLA  | C1D-C2D | 3.29  | 1.50        | 1.42     |
| 14  | H     | 827  | CLA  | C1D-C2D | 3.28  | 1.50        | 1.42     |
| 14  | A     | 829  | CLA  | C1D-C2D | 3.28  | 1.50        | 1.42     |
| 14  | G     | 827  | CLA  | C4B-CHC | 3.28  | 1.50        | 1.41     |
| 14  | Z     | 826  | CLA  | C1D-C2D | 3.28  | 1.50        | 1.42     |
| 14  | B     | 802  | CLA  | C1D-C2D | 3.28  | 1.50        | 1.42     |
| 14  | U     | 1003 | CLA  | MG-NC   | 3.28  | 2.14        | 2.06     |
| 14  | Y     | 810  | CLA  | C1D-C2D | 3.27  | 1.50        | 1.42     |
| 14  | A     | 813  | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 17  | A     | 848  | BCR  | C11-C12 | -3.27 | 1.26        | 1.34     |
| 14  | G     | 828  | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 14  | h     | 201  | CLA  | C1D-C2D | 3.27  | 1.50        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 804  | CLA  | C1D-C2D | 3.27  | 1.50        | 1.42     |
| 14  | j     | 102  | CLA  | C1D-C2D | 3.27  | 1.50        | 1.42     |
| 14  | Z     | 818  | CLA  | C1D-C2D | 3.27  | 1.50        | 1.42     |
| 14  | Z     | 833  | CLA  | MG-NC   | 3.27  | 2.14        | 2.06     |
| 14  | Z     | 825  | CLA  | C1D-C2D | 3.26  | 1.49        | 1.42     |
| 14  | A     | 812  | CLA  | C1D-C2D | 3.26  | 1.49        | 1.42     |
| 14  | Y     | 827  | CLA  | C4B-CHC | 3.25  | 1.50        | 1.41     |
| 14  | G     | 806  | CLA  | C1D-C2D | 3.25  | 1.49        | 1.42     |
| 13  | G     | 801  | CL0  | MG-NC   | 3.24  | 2.14        | 2.06     |
| 14  | Y     | 823  | CLA  | C1D-C2D | 3.24  | 1.49        | 1.42     |
| 14  | A     | 820  | CLA  | C1D-C2D | 3.24  | 1.49        | 1.42     |
| 14  | Y     | 812  | CLA  | C1D-C2D | 3.24  | 1.49        | 1.42     |
| 14  | Y     | 842  | CLA  | C1C-NC  | -3.24 | 1.33        | 1.37     |
| 14  | G     | 815  | CLA  | C3D-C2D | 3.24  | 1.45        | 1.39     |
| 14  | A     | 834  | CLA  | C1D-C2D | 3.24  | 1.49        | 1.42     |
| 14  | Y     | 803  | CLA  | C4C-C3C | 3.24  | 1.50        | 1.45     |
| 14  | Z     | 807  | CLA  | C1C-NC  | -3.24 | 1.33        | 1.37     |
| 14  | Z     | 832  | CLA  | C1D-C2D | 3.24  | 1.49        | 1.42     |
| 19  | H     | 846  | LMG  | C19-C18 | -3.24 | 1.33        | 1.51     |
| 14  | V     | 1201 | CLA  | MG-NC   | 3.24  | 2.14        | 2.06     |
| 14  | B     | 840  | CLA  | C3B-C2B | 3.23  | 1.44        | 1.40     |
| 14  | B     | 839  | CLA  | MG-NC   | 3.23  | 2.13        | 2.06     |
| 14  | Y     | 831  | CLA  | C1D-C2D | 3.23  | 1.49        | 1.42     |
| 14  | S     | 1103 | CLA  | C1D-C2D | 3.23  | 1.49        | 1.42     |
| 14  | Y     | 837  | CLA  | C1D-C2D | 3.23  | 1.49        | 1.42     |
| 14  | Z     | 806  | CLA  | C1D-C2D | 3.22  | 1.49        | 1.42     |
| 14  | g     | 101  | CLA  | C1D-C2D | 3.22  | 1.49        | 1.42     |
| 14  | G     | 824  | CLA  | C1D-C2D | 3.22  | 1.49        | 1.42     |
| 14  | B     | 831  | CLA  | C1C-NC  | -3.21 | 1.33        | 1.37     |
| 14  | G     | 803  | CLA  | MG-NC   | 3.21  | 2.13        | 2.06     |
| 14  | B     | 803  | CLA  | C1D-C2D | 3.21  | 1.49        | 1.42     |
| 14  | Y     | 839  | CLA  | MG-NC   | 3.21  | 2.13        | 2.06     |
| 14  | Y     | 827  | CLA  | C1C-NC  | -3.21 | 1.33        | 1.37     |
| 14  | Y     | 827  | CLA  | MG-NC   | 3.21  | 2.13        | 2.06     |
| 14  | Z     | 821  | CLA  | MG-NC   | 3.21  | 2.13        | 2.06     |
| 14  | H     | 811  | CLA  | C1D-C2D | 3.20  | 1.49        | 1.42     |
| 14  | G     | 819  | CLA  | C1C-NC  | -3.20 | 1.33        | 1.37     |
| 14  | A     | 837  | CLA  | C3B-C2B | 3.20  | 1.44        | 1.40     |
| 14  | Y     | 821  | CLA  | C4B-CHC | 3.20  | 1.49        | 1.41     |
| 14  | H     | 812  | CLA  | C1D-C2D | 3.20  | 1.49        | 1.42     |
| 14  | H     | 806  | CLA  | C1C-NC  | -3.20 | 1.33        | 1.37     |
| 14  | H     | 812  | CLA  | MG-NC   | 3.20  | 2.13        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 834  | CLA  | C1D-C2D | 3.19  | 1.49        | 1.42     |
| 14  | A     | 838  | CLA  | C1D-C2D | 3.19  | 1.49        | 1.42     |
| 14  | H     | 835  | CLA  | C3B-C2B | 3.19  | 1.44        | 1.40     |
| 14  | G     | 827  | CLA  | OBD-CAD | 3.19  | 1.26        | 1.22     |
| 14  | Z     | 838  | CLA  | C1C-NC  | -3.18 | 1.33        | 1.37     |
| 14  | H     | 823  | CLA  | MG-NC   | 3.18  | 2.13        | 2.06     |
| 14  | H     | 807  | CLA  | MG-NC   | 3.18  | 2.13        | 2.06     |
| 14  | H     | 803  | CLA  | C1D-C2D | 3.18  | 1.49        | 1.42     |
| 14  | Z     | 834  | CLA  | MG-NC   | 3.18  | 2.13        | 2.06     |
| 14  | A     | 802  | CLA  | CHD-C4C | 3.18  | 1.50        | 1.41     |
| 14  | H     | 807  | CLA  | C1D-C2D | 3.18  | 1.49        | 1.42     |
| 14  | U     | 1003 | CLA  | C4C-C3C | 3.18  | 1.50        | 1.45     |
| 14  | G     | 820  | CLA  | C1D-C2D | 3.17  | 1.49        | 1.42     |
| 19  | Z     | 847  | LMG  | C40-C39 | -3.17 | 1.33        | 1.51     |
| 19  | Z     | 847  | LMG  | C19-C18 | -3.17 | 1.33        | 1.51     |
| 14  | U     | 1006 | CLA  | C1C-NC  | -3.17 | 1.33        | 1.37     |
| 14  | B     | 833  | CLA  | C1D-C2D | 3.17  | 1.49        | 1.42     |
| 14  | A     | 803  | CLA  | C1D-C2D | 3.16  | 1.49        | 1.42     |
| 14  | Z     | 805  | CLA  | C1D-C2D | 3.16  | 1.49        | 1.42     |
| 14  | Y     | 832  | CLA  | C1D-C2D | 3.16  | 1.49        | 1.42     |
| 14  | H     | 837  | CLA  | C1D-C2D | 3.16  | 1.49        | 1.42     |
| 14  | L     | 202  | CLA  | C1D-C2D | 3.16  | 1.49        | 1.42     |
| 14  | Z     | 821  | CLA  | C1D-C2D | 3.16  | 1.49        | 1.42     |
| 14  | B     | 817  | CLA  | MG-NC   | 3.16  | 2.13        | 2.06     |
| 14  | G     | 833  | CLA  | MG-NC   | 3.16  | 2.13        | 2.06     |
| 14  | G     | 835  | CLA  | MG-NC   | 3.15  | 2.13        | 2.06     |
| 17  | Q     | 204  | BCR  | C11-C12 | -3.15 | 1.26        | 1.34     |
| 14  | B     | 836  | CLA  | C1D-C2D | 3.15  | 1.49        | 1.42     |
| 14  | Y     | 829  | CLA  | C1D-C2D | 3.15  | 1.49        | 1.42     |
| 14  | H     | 837  | CLA  | C1B-CHB | 3.15  | 1.49        | 1.41     |
| 14  | A     | 830  | CLA  | C1D-C2D | 3.15  | 1.49        | 1.42     |
| 17  | K     | 102  | BCR  | C11-C12 | -3.15 | 1.26        | 1.34     |
| 14  | B     | 808  | CLA  | C1C-NC  | -3.15 | 1.33        | 1.37     |
| 14  | U     | 1006 | CLA  | C1D-C2D | 3.14  | 1.49        | 1.42     |
| 17  | B     | 845  | BCR  | C11-C12 | -3.14 | 1.26        | 1.34     |
| 14  | Y     | 816  | CLA  | MG-NC   | 3.14  | 2.13        | 2.06     |
| 14  | Y     | 805  | CLA  | C3C-C2C | 3.14  | 1.43        | 1.36     |
| 14  | Z     | 817  | CLA  | C1D-C2D | 3.14  | 1.49        | 1.42     |
| 14  | B     | 807  | CLA  | C1D-C2D | 3.14  | 1.49        | 1.42     |
| 14  | H     | 833  | CLA  | MG-NC   | 3.14  | 2.13        | 2.06     |
| 14  | Y     | 843  | CLA  | C1D-C2D | 3.14  | 1.49        | 1.42     |
| 14  | X     | 1701 | CLA  | C1D-C2D | 3.14  | 1.49        | 1.42     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | B     | 849 | LMG  | C19-C18 | -3.14 | 1.34        | 1.51     |
| 14  | H     | 802 | CLA  | C4B-NB  | -3.13 | 1.32        | 1.35     |
| 14  | Y     | 825 | CLA  | MG-NC   | 3.13  | 2.13        | 2.06     |
| 19  | B     | 849 | LMG  | C40-C39 | -3.13 | 1.34        | 1.51     |
| 14  | Y     | 823 | CLA  | C1B-CHB | 3.13  | 1.49        | 1.41     |
| 14  | A     | 802 | CLA  | C1D-C2D | 3.13  | 1.49        | 1.42     |
| 14  | K     | 103 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 14  | A     | 824 | CLA  | C1D-C2D | 3.13  | 1.49        | 1.42     |
| 14  | A     | 830 | CLA  | C3B-C2B | 3.13  | 1.44        | 1.40     |
| 14  | H     | 808 | CLA  | C1D-C2D | 3.13  | 1.49        | 1.42     |
| 14  | Y     | 838 | CLA  | C4B-CHC | 3.12  | 1.49        | 1.41     |
| 14  | Y     | 812 | CLA  | MG-NC   | 3.12  | 2.13        | 2.06     |
| 14  | G     | 833 | CLA  | C1D-C2D | 3.12  | 1.49        | 1.42     |
| 14  | A     | 852 | CLA  | MG-NC   | 3.12  | 2.13        | 2.06     |
| 14  | h     | 207 | CLA  | MG-NC   | 3.12  | 2.13        | 2.06     |
| 14  | Y     | 814 | CLA  | C1D-C2D | 3.12  | 1.49        | 1.42     |
| 14  | H     | 827 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 14  | G     | 839 | CLA  | C4B-CHC | 3.12  | 1.49        | 1.41     |
| 14  | Z     | 813 | CLA  | C1D-C2D | 3.12  | 1.49        | 1.42     |
| 14  | Z     | 812 | CLA  | C1D-C2D | 3.11  | 1.49        | 1.42     |
| 14  | B     | 839 | CLA  | C1D-C2D | 3.11  | 1.49        | 1.42     |
| 14  | B     | 831 | CLA  | C1D-C2D | 3.11  | 1.49        | 1.42     |
| 14  | Y     | 829 | CLA  | CHD-C4C | 3.11  | 1.50        | 1.41     |
| 14  | B     | 808 | CLA  | C1D-C2D | 3.11  | 1.49        | 1.42     |
| 14  | B     | 825 | CLA  | C4B-CHC | 3.11  | 1.49        | 1.41     |
| 14  | B     | 801 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 14  | G     | 831 | CLA  | C1D-C2D | 3.11  | 1.49        | 1.42     |
| 14  | G     | 836 | CLA  | MG-NC   | 3.11  | 2.13        | 2.06     |
| 14  | A     | 832 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 14  | G     | 830 | CLA  | C1D-C2D | 3.10  | 1.49        | 1.42     |
| 14  | L     | 206 | CLA  | MG-NC   | 3.10  | 2.13        | 2.06     |
| 14  | G     | 815 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 14  | A     | 817 | CLA  | MG-NC   | 3.10  | 2.13        | 2.06     |
| 14  | Y     | 813 | CLA  | C1D-C2D | 3.10  | 1.49        | 1.42     |
| 14  | Y     | 813 | CLA  | OBD-CAD | 3.10  | 1.26        | 1.22     |
| 14  | B     | 821 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 14  | K     | 101 | CLA  | C1B-CHB | 3.09  | 1.49        | 1.41     |
| 14  | A     | 837 | CLA  | C4B-CHC | 3.09  | 1.49        | 1.41     |
| 13  | Y     | 801 | CL0  | C1D-C2D | 3.08  | 1.49        | 1.42     |
| 14  | B     | 838 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | Z     | 815 | CLA  | C1D-C2D | 3.08  | 1.49        | 1.42     |
| 14  | B     | 805 | CLA  | C3D-C2D | 3.08  | 1.45        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 810  | CLA  | C3B-C2B | 3.08  | 1.44        | 1.40     |
| 14  | G     | 816  | CLA  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 14  | H     | 829  | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 14  | G     | 813  | CLA  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 14  | Z     | 816  | CLA  | C3B-C2B | 3.08  | 1.44        | 1.40     |
| 14  | g     | 101  | CLA  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 14  | d     | 202  | CLA  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 14  | U     | 1004 | CLA  | C1D-C2D | 3.07  | 1.49        | 1.42     |
| 14  | H     | 826  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | A     | 819  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | B     | 837  | CLA  | C1D-C2D | 3.07  | 1.49        | 1.42     |
| 14  | Z     | 824  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | G     | 821  | CLA  | C4B-CHC | 3.07  | 1.49        | 1.41     |
| 14  | Z     | 838  | CLA  | C1D-C2D | 3.07  | 1.49        | 1.42     |
| 14  | G     | 829  | CLA  | C1D-C2D | 3.07  | 1.49        | 1.42     |
| 14  | A     | 831  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 14  | B     | 824  | CLA  | MG-NC   | 3.07  | 2.13        | 2.06     |
| 14  | Y     | 836  | CLA  | C4B-CHC | 3.06  | 1.49        | 1.41     |
| 14  | Z     | 802  | CLA  | C4B-CHC | 3.06  | 1.49        | 1.41     |
| 14  | G     | 839  | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 17  | F     | 203  | BCR  | C11-C12 | -3.06 | 1.26        | 1.34     |
| 14  | B     | 811  | CLA  | C1D-C2D | 3.06  | 1.49        | 1.42     |
| 14  | H     | 816  | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | Z     | 812  | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | H     | 806  | CLA  | C1D-C2D | 3.06  | 1.49        | 1.42     |
| 13  | Y     | 801  | CL0  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 14  | B     | 837  | CLA  | C1B-CHB | 3.05  | 1.49        | 1.41     |
| 14  | H     | 822  | CLA  | MG-NC   | 3.05  | 2.13        | 2.06     |
| 14  | G     | 824  | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 14  | Z     | 839  | CLA  | C1D-C2D | 3.05  | 1.49        | 1.42     |
| 14  | G     | 802  | CLA  | C1D-C2D | 3.05  | 1.49        | 1.42     |
| 14  | Y     | 814  | CLA  | MG-NC   | 3.05  | 2.13        | 2.06     |
| 14  | A     | 805  | CLA  | C1D-C2D | 3.05  | 1.49        | 1.42     |
| 14  | A     | 828  | CLA  | C1D-C2D | 3.05  | 1.49        | 1.42     |
| 14  | H     | 834  | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 19  | Z     | 847  | LMG  | C37-C36 | -3.05 | 1.34        | 1.51     |
| 14  | Y     | 828  | CLA  | C1D-C2D | 3.04  | 1.49        | 1.42     |
| 14  | G     | 830  | CLA  | OBD-CAD | 3.04  | 1.26        | 1.22     |
| 14  | G     | 842  | CLA  | C1D-C2D | 3.04  | 1.49        | 1.42     |
| 14  | Y     | 816  | CLA  | C4B-CHC | 3.04  | 1.49        | 1.41     |
| 14  | Z     | 818  | CLA  | C4B-CHC | 3.04  | 1.49        | 1.41     |
| 14  | Y     | 823  | CLA  | MG-NC   | 3.04  | 2.13        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 808  | CLA  | MG-NC   | 3.04  | 2.13        | 2.06     |
| 14  | B     | 815  | CLA  | C1D-C2D | 3.03  | 1.49        | 1.42     |
| 14  | Z     | 825  | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 19  | B     | 849  | LMG  | C43-C42 | -3.03 | 1.34        | 1.51     |
| 14  | B     | 827  | CLA  | C1D-C2D | 3.03  | 1.49        | 1.42     |
| 17  | Z     | 845  | BCR  | C11-C12 | -3.03 | 1.26        | 1.34     |
| 14  | Y     | 802  | CLA  | C3B-C2B | 3.03  | 1.44        | 1.40     |
| 14  | B     | 840  | CLA  | MG-NC   | 3.03  | 2.13        | 2.06     |
| 14  | Y     | 811  | CLA  | MG-NC   | 3.02  | 2.13        | 2.06     |
| 14  | f     | 102  | CLA  | MG-NC   | 3.02  | 2.13        | 2.06     |
| 14  | Z     | 827  | CLA  | C1D-C2D | 3.02  | 1.49        | 1.42     |
| 14  | J     | 102  | CLA  | MG-NC   | 3.02  | 2.13        | 2.06     |
| 14  | A     | 815  | CLA  | C4B-CHC | 3.02  | 1.49        | 1.41     |
| 14  | Y     | 841  | CLA  | C1D-C2D | 3.02  | 1.49        | 1.42     |
| 14  | A     | 802  | CLA  | MG-NC   | 3.02  | 2.13        | 2.06     |
| 17  | Z     | 842  | BCR  | C11-C12 | -3.02 | 1.26        | 1.34     |
| 14  | J     | 101  | CLA  | C1D-C2D | 3.02  | 1.49        | 1.42     |
| 14  | Z     | 812  | CLA  | CHD-C4C | 3.02  | 1.49        | 1.41     |
| 14  | G     | 839  | CLA  | C1D-C2D | 3.01  | 1.49        | 1.42     |
| 14  | Y     | 840  | CLA  | MG-NC   | 3.01  | 2.13        | 2.06     |
| 14  | B     | 817  | CLA  | C1D-C2D | 3.01  | 1.49        | 1.42     |
| 14  | H     | 804  | CLA  | C4B-CHC | 3.01  | 1.49        | 1.41     |
| 14  | V     | 1201 | CLA  | C4B-CHC | 3.00  | 1.49        | 1.41     |
| 14  | G     | 821  | CLA  | MG-NC   | 3.00  | 2.13        | 2.06     |
| 14  | G     | 831  | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | G     | 810  | CLA  | C1D-C2D | 3.00  | 1.49        | 1.42     |
| 14  | G     | 812  | CLA  | C1D-C2D | 3.00  | 1.49        | 1.42     |
| 14  | B     | 840  | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 14  | A     | 831  | CLA  | C1D-C2D | 3.00  | 1.49        | 1.42     |
| 14  | Y     | 805  | CLA  | C4B-CHC | 3.00  | 1.49        | 1.41     |
| 14  | A     | 838  | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | G     | 807  | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | H     | 816  | CLA  | C1D-C2D | 2.99  | 1.49        | 1.42     |
| 14  | Z     | 808  | CLA  | C3B-C2B | 2.99  | 1.44        | 1.40     |
| 14  | G     | 807  | CLA  | C1B-CHB | 2.99  | 1.49        | 1.41     |
| 14  | G     | 817  | CLA  | C4B-CHC | 2.99  | 1.49        | 1.41     |
| 14  | G     | 823  | CLA  | C1B-CHB | 2.99  | 1.49        | 1.41     |
| 17  | G     | 846  | BCR  | C11-C12 | -2.99 | 1.26        | 1.34     |
| 14  | Y     | 829  | CLA  | C4C-C3C | 2.99  | 1.50        | 1.45     |
| 14  | G     | 814  | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 14  | G     | 837  | CLA  | C4B-CHC | 2.99  | 1.49        | 1.41     |
| 14  | B     | 836  | CLA  | C3B-C2B | 2.98  | 1.44        | 1.40     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 820  | CLA  | MG-NC   | 2.98  | 2.13        | 2.06     |
| 14  | Z     | 810  | CLA  | MG-NC   | 2.98  | 2.13        | 2.06     |
| 14  | H     | 822  | CLA  | C1B-CHB | 2.98  | 1.49        | 1.41     |
| 17  | G     | 848  | BCR  | C11-C12 | -2.98 | 1.26        | 1.34     |
| 14  | Y     | 827  | CLA  | C1D-C2D | 2.97  | 1.49        | 1.42     |
| 14  | G     | 806  | CLA  | C4B-CHC | 2.97  | 1.49        | 1.41     |
| 14  | A     | 802  | CLA  | C3B-C2B | 2.97  | 1.44        | 1.40     |
| 14  | G     | 834  | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 14  | H     | 826  | CLA  | C1D-C2D | 2.97  | 1.49        | 1.42     |
| 14  | T     | 101  | CLA  | C4C-C3C | 2.97  | 1.50        | 1.45     |
| 14  | G     | 840  | CLA  | C4B-CHC | 2.97  | 1.49        | 1.41     |
| 14  | A     | 818  | CLA  | C1D-C2D | 2.97  | 1.49        | 1.42     |
| 19  | B     | 849  | LMG  | C37-C36 | -2.97 | 1.34        | 1.51     |
| 14  | Y     | 814  | CLA  | C4B-CHC | 2.97  | 1.49        | 1.41     |
| 14  | Z     | 808  | CLA  | C1D-C2D | 2.97  | 1.49        | 1.42     |
| 14  | Y     | 815  | CLA  | C4B-CHC | 2.97  | 1.49        | 1.41     |
| 14  | H     | 814  | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 14  | H     | 801  | CLA  | C4B-CHC | 2.97  | 1.49        | 1.41     |
| 14  | G     | 811  | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 14  | H     | 807  | CLA  | C4C-C3C | 2.96  | 1.50        | 1.45     |
| 14  | B     | 812  | CLA  | CHD-C4C | 2.96  | 1.49        | 1.41     |
| 14  | A     | 824  | CLA  | C4B-CHC | 2.96  | 1.49        | 1.41     |
| 14  | H     | 832  | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 14  | Y     | 808  | CLA  | C1C-NC  | -2.96 | 1.33        | 1.37     |
| 17  | Z     | 846  | BCR  | C11-C12 | -2.95 | 1.27        | 1.34     |
| 14  | A     | 834  | CLA  | C4B-CHC | 2.95  | 1.49        | 1.41     |
| 13  | A     | 801  | CL0  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 14  | U     | 1006 | CLA  | C1B-CHB | 2.95  | 1.49        | 1.41     |
| 14  | Y     | 824  | CLA  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 14  | G     | 832  | CLA  | C1D-C2D | 2.94  | 1.49        | 1.42     |
| 14  | B     | 835  | CLA  | C4B-CHC | 2.94  | 1.49        | 1.41     |
| 14  | G     | 828  | CLA  | C1D-C2D | 2.94  | 1.49        | 1.42     |
| 14  | A     | 842  | CLA  | C1B-CHB | 2.94  | 1.49        | 1.41     |
| 14  | Z     | 822  | CLA  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 14  | Z     | 824  | CLA  | C1D-C2D | 2.94  | 1.49        | 1.42     |
| 14  | K     | 101  | CLA  | C1C-NC  | -2.94 | 1.33        | 1.37     |
| 17  | B     | 848  | BCR  | C11-C12 | -2.94 | 1.27        | 1.34     |
| 14  | Y     | 835  | CLA  | C1C-C2C | 2.94  | 1.50        | 1.44     |
| 14  | Z     | 829  | CLA  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 14  | A     | 820  | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 14  | A     | 832  | CLA  | C1D-C2D | 2.93  | 1.49        | 1.42     |
| 14  | G     | 822  | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | H     | 842  | BCR  | C11-C12 | -2.93 | 1.27        | 1.34     |
| 14  | Z     | 832  | CLA  | C4B-CHC | 2.93  | 1.49        | 1.41     |
| 14  | H     | 806  | CLA  | C4B-CHC | 2.93  | 1.49        | 1.41     |
| 14  | G     | 819  | CLA  | CHD-C4C | 2.93  | 1.49        | 1.41     |
| 14  | h     | 206  | CLA  | C4B-CHC | 2.93  | 1.49        | 1.41     |
| 14  | A     | 821  | CLA  | C4B-CHC | 2.93  | 1.49        | 1.41     |
| 14  | Y     | 839  | CLA  | C1B-CHB | 2.93  | 1.49        | 1.41     |
| 14  | G     | 817  | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 14  | Z     | 802  | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 14  | Y     | 802  | CLA  | CHD-C4C | 2.92  | 1.49        | 1.41     |
| 14  | Y     | 807  | CLA  | C4B-CHC | 2.92  | 1.49        | 1.41     |
| 14  | A     | 835  | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 14  | A     | 828  | CLA  | C4B-CHC | 2.92  | 1.49        | 1.41     |
| 14  | H     | 805  | CLA  | C1D-C2D | 2.92  | 1.49        | 1.42     |
| 14  | G     | 828  | CLA  | C4B-CHC | 2.92  | 1.49        | 1.41     |
| 14  | A     | 832  | CLA  | C1B-CHB | 2.92  | 1.49        | 1.41     |
| 14  | X     | 1701 | CLA  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 14  | G     | 825  | CLA  | C1B-CHB | 2.91  | 1.49        | 1.41     |
| 14  | Y     | 835  | CLA  | CHD-C4C | 2.91  | 1.49        | 1.41     |
| 14  | Z     | 831  | CLA  | C1C-NC  | -2.91 | 1.33        | 1.37     |
| 19  | B     | 849  | LMG  | C22-C21 | -2.91 | 1.35        | 1.51     |
| 14  | B     | 829  | CLA  | C1D-C2D | 2.91  | 1.49        | 1.42     |
| 14  | G     | 812  | CLA  | CHD-C4C | 2.91  | 1.49        | 1.41     |
| 14  | Z     | 811  | CLA  | C4B-CHC | 2.91  | 1.49        | 1.41     |
| 14  | G     | 843  | CLA  | CHD-C4C | 2.91  | 1.49        | 1.41     |
| 14  | U     | 1006 | CLA  | MG-NC   | 2.90  | 2.13        | 2.06     |
| 14  | U     | 1004 | CLA  | C1C-NC  | -2.90 | 1.33        | 1.37     |
| 17  | Z     | 842  | BCR  | C30-C25 | -2.90 | 1.49        | 1.53     |
| 14  | G     | 829  | CLA  | C1C-NC  | -2.90 | 1.33        | 1.37     |
| 14  | d     | 201  | CLA  | C1B-CHB | 2.90  | 1.49        | 1.41     |
| 14  | B     | 823  | CLA  | MG-NC   | 2.90  | 2.13        | 2.06     |
| 14  | G     | 819  | CLA  | MG-NC   | 2.90  | 2.13        | 2.06     |
| 14  | B     | 840  | CLA  | C4B-CHC | 2.90  | 1.49        | 1.41     |
| 14  | J     | 102  | CLA  | C4B-CHC | 2.90  | 1.49        | 1.41     |
| 14  | Z     | 831  | CLA  | C1D-C2D | 2.90  | 1.49        | 1.42     |
| 17  | G     | 846  | BCR  | C21-C22 | -2.90 | 1.31        | 1.35     |
| 14  | B     | 832  | CLA  | C1C-NC  | -2.90 | 1.33        | 1.37     |
| 14  | Z     | 805  | CLA  | C1C-NC  | -2.90 | 1.33        | 1.37     |
| 14  | Y     | 811  | CLA  | C4B-CHC | 2.90  | 1.49        | 1.41     |
| 14  | G     | 811  | CLA  | C1D-C2D | 2.90  | 1.49        | 1.42     |
| 14  | B     | 828  | CLA  | C3B-C2B | 2.89  | 1.44        | 1.40     |
| 14  | B     | 809  | CLA  | C1D-C2D | 2.89  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | H     | 802 | CLA  | C1B-NB  | -2.89 | 1.32        | 1.35     |
| 14  | A     | 841 | CLA  | C3B-C2B | 2.89  | 1.44        | 1.40     |
| 17  | f     | 103 | BCR  | C11-C12 | -2.89 | 1.27        | 1.34     |
| 14  | Z     | 825 | CLA  | C4B-CHC | 2.89  | 1.49        | 1.41     |
| 14  | G     | 812 | CLA  | C4B-CHC | 2.89  | 1.49        | 1.41     |
| 14  | Y     | 841 | CLA  | C4B-CHC | 2.89  | 1.49        | 1.41     |
| 14  | G     | 810 | CLA  | C4B-CHC | 2.89  | 1.49        | 1.41     |
| 14  | G     | 808 | CLA  | C1D-C2D | 2.89  | 1.49        | 1.42     |
| 14  | Z     | 827 | CLA  | C4B-NB  | -2.89 | 1.32        | 1.35     |
| 14  | A     | 807 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 14  | B     | 836 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 14  | B     | 804 | CLA  | C1D-C2D | 2.88  | 1.49        | 1.42     |
| 14  | H     | 801 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 14  | H     | 806 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 14  | H     | 803 | CLA  | C4C-C3C | 2.88  | 1.50        | 1.45     |
| 14  | Y     | 817 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 14  | B     | 839 | CLA  | C4B-CHC | 2.88  | 1.49        | 1.41     |
| 14  | H     | 838 | CLA  | C1C-NC  | -2.88 | 1.33        | 1.37     |
| 14  | A     | 812 | CLA  | C4C-C3C | 2.88  | 1.50        | 1.45     |
| 14  | B     | 814 | CLA  | C4B-CHC | 2.88  | 1.49        | 1.41     |
| 14  | G     | 814 | CLA  | C4B-CHC | 2.88  | 1.49        | 1.41     |
| 14  | Y     | 830 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 14  | G     | 832 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 14  | G     | 841 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 13  | A     | 801 | CL0  | MG-NC   | 2.87  | 2.13        | 2.06     |
| 14  | g     | 101 | CLA  | CHD-C4C | 2.87  | 1.49        | 1.41     |
| 14  | G     | 833 | CLA  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 14  | h     | 206 | CLA  | C1D-C2D | 2.87  | 1.49        | 1.42     |
| 14  | Y     | 832 | CLA  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 14  | G     | 841 | CLA  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 14  | Z     | 815 | CLA  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 14  | B     | 807 | CLA  | CHD-C4C | 2.87  | 1.49        | 1.41     |
| 14  | G     | 813 | CLA  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 14  | Y     | 841 | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 14  | B     | 841 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 14  | Y     | 803 | CLA  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 13  | Y     | 801 | CL0  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 14  | G     | 836 | CLA  | CHD-C4C | 2.87  | 1.49        | 1.41     |
| 14  | H     | 816 | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 14  | A     | 824 | CLA  | C1C-C2C | 2.86  | 1.50        | 1.44     |
| 14  | G     | 830 | CLA  | C1B-CHB | 2.86  | 1.49        | 1.41     |
| 14  | H     | 802 | CLA  | C1D-C2D | 2.86  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | f     | 102  | CLA  | C4B-CHC | 2.86  | 1.48        | 1.41     |
| 14  | B     | 802  | CLA  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 14  | S     | 1103 | CLA  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 14  | B     | 823  | CLA  | C4B-CHC | 2.86  | 1.48        | 1.41     |
| 14  | G     | 820  | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 14  | G     | 818  | CLA  | OBD-CAD | 2.86  | 1.26        | 1.22     |
| 14  | h     | 207  | CLA  | C4B-CHC | 2.86  | 1.48        | 1.41     |
| 14  | F     | 202  | CLA  | C1C-NC  | -2.86 | 1.33        | 1.37     |
| 17  | A     | 846  | BCR  | C11-C12 | -2.86 | 1.27        | 1.34     |
| 14  | A     | 842  | CLA  | C1C-C2C | 2.86  | 1.50        | 1.44     |
| 14  | Z     | 811  | CLA  | C1D-C2D | 2.85  | 1.49        | 1.42     |
| 14  | h     | 206  | CLA  | C3D-C2D | 2.85  | 1.44        | 1.39     |
| 14  | h     | 207  | CLA  | C1D-C2D | 2.85  | 1.49        | 1.42     |
| 14  | g     | 102  | CLA  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 14  | A     | 839  | CLA  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 14  | Y     | 819  | CLA  | C1C-NC  | -2.85 | 1.33        | 1.37     |
| 14  | Y     | 836  | CLA  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 14  | U     | 1002 | CLA  | C1D-C2D | 2.85  | 1.49        | 1.42     |
| 14  | Z     | 837  | CLA  | C1C-NC  | -2.85 | 1.33        | 1.37     |
| 14  | G     | 839  | CLA  | CHD-C4C | 2.85  | 1.49        | 1.41     |
| 14  | A     | 834  | CLA  | MG-NC   | 2.85  | 2.13        | 2.06     |
| 14  | Z     | 809  | CLA  | C4B-CHC | 2.85  | 1.48        | 1.41     |
| 14  | Z     | 820  | CLA  | C1D-C2D | 2.84  | 1.49        | 1.42     |
| 14  | L     | 207  | CLA  | C1D-C2D | 2.84  | 1.49        | 1.42     |
| 14  | B     | 813  | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 14  | d     | 202  | CLA  | C1D-C2D | 2.84  | 1.49        | 1.42     |
| 14  | Z     | 814  | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 14  | A     | 825  | CLA  | C4C-C3C | 2.84  | 1.49        | 1.45     |
| 14  | h     | 207  | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 14  | B     | 827  | CLA  | CHD-C4C | 2.84  | 1.49        | 1.41     |
| 14  | Z     | 801  | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 14  | F     | 202  | CLA  | C1D-C2D | 2.84  | 1.49        | 1.42     |
| 14  | A     | 838  | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 14  | B     | 817  | CLA  | CHD-C4C | 2.84  | 1.49        | 1.41     |
| 14  | A     | 827  | CLA  | C4B-CHC | 2.84  | 1.48        | 1.41     |
| 14  | Z     | 838  | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 14  | Y     | 802  | CLA  | C1D-C2D | 2.83  | 1.49        | 1.42     |
| 14  | G     | 805  | CLA  | C1C-NC  | -2.83 | 1.33        | 1.37     |
| 17  | R     | 101  | BCR  | C11-C12 | -2.83 | 1.27        | 1.34     |
| 14  | S     | 1102 | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | A     | 833  | CLA  | C1C-NC  | -2.83 | 1.33        | 1.37     |
| 14  | Y     | 826  | CLA  | C4B-CHC | 2.83  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 805  | CLA  | C1D-C2D | 2.83  | 1.49        | 1.42     |
| 14  | Z     | 805  | CLA  | CHD-C4C | 2.83  | 1.49        | 1.41     |
| 14  | H     | 826  | CLA  | C1B-CHB | 2.83  | 1.48        | 1.41     |
| 14  | L     | 205  | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | A     | 816  | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | H     | 823  | CLA  | C1D-C2D | 2.83  | 1.49        | 1.42     |
| 14  | T     | 101  | CLA  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 14  | G     | 838  | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 14  | Y     | 830  | CLA  | C1D-C2D | 2.82  | 1.49        | 1.42     |
| 14  | B     | 812  | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 14  | G     | 826  | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 14  | H     | 811  | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 14  | G     | 824  | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 14  | A     | 823  | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 14  | G     | 812  | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 14  | S     | 1103 | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 14  | Y     | 818  | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 14  | B     | 811  | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 14  | H     | 826  | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 17  | T     | 102  | BCR  | C11-C12 | -2.82 | 1.27        | 1.34     |
| 14  | H     | 825  | CLA  | C1D-C2D | 2.82  | 1.48        | 1.42     |
| 17  | H     | 845  | BCR  | C11-C12 | -2.82 | 1.27        | 1.34     |
| 14  | j     | 102  | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 14  | L     | 205  | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 14  | Z     | 822  | CLA  | C1D-C2D | 2.82  | 1.48        | 1.42     |
| 14  | H     | 824  | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 14  | Y     | 809  | CLA  | CHD-C4C | 2.81  | 1.49        | 1.41     |
| 14  | Z     | 804  | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 14  | B     | 820  | CLA  | MG-NC   | 2.81  | 2.13        | 2.06     |
| 14  | H     | 830  | CLA  | MG-NC   | 2.81  | 2.12        | 2.06     |
| 14  | A     | 836  | CLA  | CHD-C4C | 2.81  | 1.49        | 1.41     |
| 14  | L     | 207  | CLA  | C1C-NC  | -2.81 | 1.33        | 1.37     |
| 14  | Y     | 817  | CLA  | C4B-CHC | 2.81  | 1.48        | 1.41     |
| 14  | A     | 824  | CLA  | MG-NC   | 2.81  | 2.12        | 2.06     |
| 14  | H     | 809  | CLA  | MG-NC   | 2.80  | 2.12        | 2.06     |
| 14  | B     | 833  | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 14  | H     | 836  | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 14  | H     | 826  | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 14  | H     | 828  | CLA  | C1C-NC  | -2.80 | 1.33        | 1.37     |
| 14  | Z     | 834  | CLA  | C4C-C3C | 2.80  | 1.49        | 1.45     |
| 14  | L     | 205  | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 14  | H     | 808  | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 808  | CLA  | C1C-NC  | -2.80 | 1.33        | 1.37     |
| 14  | G     | 803  | CLA  | C1D-C2D | 2.80  | 1.48        | 1.42     |
| 14  | G     | 805  | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 14  | Y     | 833  | CLA  | C1C-NC  | -2.80 | 1.33        | 1.37     |
| 14  | Z     | 823  | CLA  | C1C-NC  | -2.79 | 1.33        | 1.37     |
| 14  | A     | 840  | CLA  | C1C-NC  | -2.79 | 1.33        | 1.37     |
| 14  | H     | 812  | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 14  | A     | 828  | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | Z     | 831  | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | Y     | 808  | CLA  | C1D-C2D | 2.79  | 1.48        | 1.42     |
| 14  | H     | 811  | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | U     | 1004 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 14  | H     | 812  | CLA  | C4C-C3C | 2.79  | 1.49        | 1.45     |
| 14  | Z     | 820  | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 14  | f     | 101  | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | L     | 206  | CLA  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 14  | Y     | 803  | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 14  | H     | 820  | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 14  | Z     | 810  | CLA  | C1D-C2D | 2.79  | 1.48        | 1.42     |
| 14  | A     | 829  | CLA  | C1C-NC  | -2.78 | 1.33        | 1.37     |
| 14  | B     | 823  | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 14  | B     | 836  | CLA  | CHD-C4C | 2.78  | 1.49        | 1.41     |
| 14  | Z     | 821  | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 14  | U     | 1003 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 14  | Z     | 804  | CLA  | C1B-NB  | -2.78 | 1.32        | 1.35     |
| 14  | A     | 833  | CLA  | C1D-C2D | 2.78  | 1.48        | 1.42     |
| 14  | G     | 806  | CLA  | C1C-NC  | -2.78 | 1.33        | 1.37     |
| 14  | H     | 820  | CLA  | CHD-C4C | 2.78  | 1.49        | 1.41     |
| 14  | A     | 825  | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | H     | 809  | CLA  | C1D-C2D | 2.78  | 1.48        | 1.42     |
| 14  | A     | 830  | CLA  | CHD-C4C | 2.78  | 1.49        | 1.41     |
| 14  | G     | 837  | CLA  | C1C-NC  | -2.78 | 1.33        | 1.37     |
| 14  | B     | 816  | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | B     | 836  | CLA  | C4C-C3C | 2.78  | 1.49        | 1.45     |
| 14  | G     | 834  | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 17  | U     | 1008 | BCR  | C11-C12 | -2.78 | 1.27        | 1.34     |
| 14  | Y     | 819  | CLA  | CHD-C4C | 2.78  | 1.49        | 1.41     |
| 14  | h     | 207  | CLA  | CHD-C4C | 2.78  | 1.49        | 1.41     |
| 17  | d     | 203  | BCR  | C11-C12 | -2.78 | 1.27        | 1.34     |
| 14  | B     | 810  | CLA  | MG-NC   | 2.78  | 2.12        | 2.06     |
| 14  | Z     | 809  | CLA  | C1C-NC  | -2.78 | 1.33        | 1.37     |
| 14  | j     | 102  | CLA  | CHD-C4C | 2.77  | 1.49        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 835  | CLA  | MG-NC   | 2.77  | 2.12        | 2.06     |
| 14  | Z     | 817  | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 14  | B     | 819  | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 14  | G     | 818  | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 14  | A     | 812  | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 14  | A     | 852  | CLA  | C1D-C2D | 2.77  | 1.48        | 1.42     |
| 14  | A     | 822  | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 14  | U     | 1006 | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 14  | G     | 853  | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 14  | A     | 811  | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 14  | A     | 806  | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 14  | Y     | 826  | CLA  | C1C-C2C | 2.77  | 1.49        | 1.44     |
| 14  | Y     | 810  | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 14  | Y     | 806  | CLA  | CHD-C4C | 2.77  | 1.49        | 1.41     |
| 14  | H     | 818  | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | H     | 807  | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | B     | 826  | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 14  | Y     | 815  | CLA  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | A     | 816  | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 14  | G     | 822  | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 14  | G     | 818  | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 17  | Y     | 848  | BCR  | C11-C12 | -2.76 | 1.27        | 1.34     |
| 14  | G     | 838  | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | Y     | 824  | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 17  | Z     | 843  | BCR  | C11-C12 | -2.76 | 1.27        | 1.34     |
| 14  | Y     | 828  | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 14  | A     | 822  | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 14  | H     | 819  | CLA  | C1D-C2D | 2.76  | 1.48        | 1.42     |
| 14  | Y     | 820  | CLA  | MG-NC   | 2.76  | 2.12        | 2.06     |
| 14  | A     | 840  | CLA  | CHD-C4C | 2.76  | 1.49        | 1.41     |
| 14  | L     | 206  | CLA  | C1D-C2D | 2.76  | 1.48        | 1.42     |
| 14  | A     | 805  | CLA  | CHD-C4C | 2.76  | 1.49        | 1.41     |
| 14  | A     | 810  | CLA  | C4B-CHC | 2.75  | 1.48        | 1.41     |
| 14  | F     | 202  | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 14  | A     | 852  | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 14  | Z     | 814  | CLA  | C4B-CHC | 2.75  | 1.48        | 1.41     |
| 14  | G     | 811  | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 14  | Y     | 806  | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | H     | 830  | CLA  | C4B-CHC | 2.75  | 1.48        | 1.41     |
| 14  | B     | 821  | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 14  | Q     | 201  | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | S     | 1101 | CLA  | C1C-NC  | -2.75 | 1.33        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 830  | CLA  | C1C-NC  | -2.75 | 1.33        | 1.37     |
| 14  | A     | 815  | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 14  | Z     | 823  | CLA  | CHD-C4C | 2.75  | 1.49        | 1.41     |
| 14  | H     | 809  | CLA  | C4B-CHC | 2.75  | 1.48        | 1.41     |
| 14  | H     | 831  | CLA  | CHD-C4C | 2.74  | 1.49        | 1.41     |
| 14  | A     | 830  | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | A     | 806  | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | Y     | 804  | CLA  | CHD-C4C | 2.74  | 1.49        | 1.41     |
| 14  | H     | 838  | CLA  | C4B-CHC | 2.74  | 1.48        | 1.41     |
| 14  | A     | 814  | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | H     | 836  | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | Y     | 835  | CLA  | C4C-C3C | 2.74  | 1.49        | 1.45     |
| 14  | B     | 821  | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | X     | 1701 | CLA  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 14  | Q     | 201  | CLA  | C1C-NC  | -2.74 | 1.33        | 1.37     |
| 14  | G     | 827  | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 14  | A     | 812  | CLA  | CHD-C4C | 2.74  | 1.49        | 1.41     |
| 14  | Y     | 838  | CLA  | CHD-C4C | 2.74  | 1.49        | 1.41     |
| 14  | A     | 803  | CLA  | C4B-CHC | 2.74  | 1.48        | 1.41     |
| 14  | A     | 820  | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 14  | Z     | 830  | CLA  | C1C-NC  | -2.73 | 1.33        | 1.37     |
| 14  | B     | 804  | CLA  | CHD-C4C | 2.73  | 1.49        | 1.41     |
| 14  | Y     | 835  | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 14  | A     | 834  | CLA  | CHD-C4C | 2.73  | 1.48        | 1.41     |
| 14  | Z     | 827  | CLA  | C1B-NB  | -2.73 | 1.32        | 1.35     |
| 14  | B     | 838  | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 14  | A     | 823  | CLA  | CHD-C4C | 2.73  | 1.48        | 1.41     |
| 14  | A     | 818  | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 14  | A     | 835  | CLA  | CHD-C4C | 2.73  | 1.48        | 1.41     |
| 14  | G     | 837  | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 14  | G     | 825  | CLA  | C1D-C2D | 2.73  | 1.48        | 1.42     |
| 14  | G     | 853  | CLA  | CHD-C4C | 2.73  | 1.48        | 1.41     |
| 14  | G     | 824  | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 14  | Z     | 839  | CLA  | CHD-C4C | 2.73  | 1.48        | 1.41     |
| 14  | Z     | 836  | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 14  | T     | 103  | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 14  | A     | 826  | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 14  | H     | 831  | CLA  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 14  | Y     | 842  | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 14  | Z     | 833  | CLA  | CHD-C4C | 2.73  | 1.48        | 1.41     |
| 14  | H     | 816  | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 14  | G     | 853  | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 810  | CLA  | CHD-C4C | 2.72  | 1.48        | 1.41     |
| 14  | Q     | 203  | CLA  | MG-NC   | 2.72  | 2.12        | 2.06     |
| 14  | H     | 835  | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 14  | H     | 822  | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 14  | Z     | 835  | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 14  | G     | 836  | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 14  | B     | 839  | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 14  | A     | 803  | CLA  | C1C-C2C | 2.72  | 1.49        | 1.44     |
| 14  | Z     | 827  | CLA  | CHD-C4C | 2.72  | 1.48        | 1.41     |
| 14  | Z     | 807  | CLA  | C1D-C2D | 2.72  | 1.48        | 1.42     |
| 14  | Y     | 830  | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 14  | G     | 803  | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 14  | f     | 101  | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 14  | B     | 805  | CLA  | C4C-C3C | 2.72  | 1.49        | 1.45     |
| 14  | F     | 202  | CLA  | MG-NC   | 2.72  | 2.12        | 2.06     |
| 14  | Y     | 823  | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 14  | Z     | 809  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | f     | 102  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | Z     | 820  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | Z     | 822  | CLA  | C1C-NC  | -2.71 | 1.33        | 1.37     |
| 14  | H     | 804  | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | Y     | 824  | CLA  | C1C-NC  | -2.71 | 1.33        | 1.37     |
| 14  | H     | 814  | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | G     | 840  | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | H     | 805  | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | J     | 101  | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | Y     | 834  | CLA  | C1C-NC  | -2.71 | 1.33        | 1.37     |
| 14  | L     | 201  | CLA  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 14  | Y     | 822  | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 14  | L     | 205  | CLA  | C1D-C2D | 2.71  | 1.48        | 1.42     |
| 14  | G     | 808  | CLA  | C1C-NC  | -2.71 | 1.33        | 1.37     |
| 14  | Y     | 818  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | d     | 202  | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 14  | Y     | 812  | CLA  | C1C-NC  | -2.71 | 1.33        | 1.37     |
| 14  | A     | 821  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | U     | 1003 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 14  | A     | 816  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | B     | 823  | CLA  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 13  | G     | 801  | CL0  | CHD-C4C | 2.71  | 1.48        | 1.41     |
| 14  | H     | 832  | CLA  | C1C-NC  | -2.70 | 1.33        | 1.37     |
| 14  | Y     | 811  | CLA  | CHD-C4C | 2.70  | 1.48        | 1.41     |
| 14  | A     | 830  | CLA  | C4C-C3C | 2.70  | 1.49        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 822 | CLA  | C1C-NC  | -2.70 | 1.33        | 1.37     |
| 14  | Y     | 809 | CLA  | MG-NC   | 2.70  | 2.12        | 2.06     |
| 14  | Z     | 829 | CLA  | C4C-C3C | 2.70  | 1.49        | 1.45     |
| 14  | A     | 805 | CLA  | C1C-NC  | -2.70 | 1.33        | 1.37     |
| 14  | L     | 207 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 14  | Z     | 817 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 14  | Z     | 829 | CLA  | CHD-C4C | 2.70  | 1.48        | 1.41     |
| 14  | H     | 837 | CLA  | C4C-C3C | 2.70  | 1.49        | 1.45     |
| 14  | B     | 818 | CLA  | CHD-C4C | 2.70  | 1.48        | 1.41     |
| 14  | Y     | 812 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 14  | B     | 816 | CLA  | C1C-NC  | -2.70 | 1.33        | 1.37     |
| 14  | L     | 205 | CLA  | CHD-C4C | 2.69  | 1.48        | 1.41     |
| 14  | Z     | 803 | CLA  | CHD-C4C | 2.69  | 1.48        | 1.41     |
| 14  | H     | 823 | CLA  | C4C-C3C | 2.69  | 1.49        | 1.45     |
| 14  | Y     | 825 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 14  | Y     | 812 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 14  | Z     | 809 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 14  | B     | 801 | CLA  | CHD-C4C | 2.69  | 1.48        | 1.41     |
| 14  | Z     | 815 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 14  | B     | 810 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 14  | H     | 818 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 14  | A     | 816 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 14  | Z     | 830 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 14  | f     | 101 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 14  | H     | 833 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 14  | Z     | 806 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 14  | G     | 808 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 14  | Y     | 828 | CLA  | C1C-C2C | 2.69  | 1.49        | 1.44     |
| 14  | Y     | 829 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 14  | H     | 817 | CLA  | CHD-C4C | 2.68  | 1.48        | 1.41     |
| 14  | A     | 805 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | Z     | 825 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | K     | 101 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | H     | 810 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 14  | H     | 838 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | G     | 815 | CLA  | CHD-C4C | 2.68  | 1.48        | 1.41     |
| 14  | Z     | 830 | CLA  | C1D-C2D | 2.68  | 1.48        | 1.42     |
| 14  | B     | 833 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 14  | A     | 815 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 14  | B     | 813 | CLA  | CHD-C4C | 2.68  | 1.48        | 1.41     |
| 14  | Z     | 825 | CLA  | CHD-C4C | 2.68  | 1.48        | 1.41     |
| 14  | H     | 812 | CLA  | CHD-C4C | 2.68  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 808 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | A     | 837 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | Y     | 840 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 14  | J     | 101 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 14  | H     | 815 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 14  | Z     | 838 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | A     | 811 | CLA  | CHD-C4C | 2.68  | 1.48        | 1.41     |
| 14  | B     | 834 | CLA  | MG-NC   | 2.68  | 2.12        | 2.06     |
| 14  | g     | 102 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 14  | G     | 842 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | g     | 101 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 14  | A     | 825 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 14  | H     | 825 | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 14  | g     | 101 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 14  | B     | 820 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | Z     | 813 | CLA  | C4B-NB  | -2.67 | 1.32        | 1.35     |
| 14  | H     | 820 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 14  | Y     | 854 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 14  | g     | 101 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 14  | Q     | 203 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | L     | 201 | CLA  | C1D-C2D | 2.67  | 1.48        | 1.42     |
| 14  | A     | 833 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 14  | Z     | 808 | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 14  | B     | 830 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | Y     | 813 | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 14  | A     | 803 | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 14  | J     | 102 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | B     | 815 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 14  | T     | 103 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 14  | A     | 817 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 14  | Y     | 802 | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 14  | Y     | 820 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | H     | 805 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | Y     | 812 | CLA  | CHD-C4C | 2.67  | 1.48        | 1.41     |
| 14  | B     | 806 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 14  | G     | 835 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | Y     | 831 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 14  | Z     | 837 | CLA  | CHD-C4C | 2.66  | 1.48        | 1.41     |
| 14  | B     | 828 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 14  | h     | 201 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 14  | A     | 841 | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |
| 14  | G     | 825 | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 813  | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | Y     | 833  | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | Z     | 837  | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 14  | J     | 101  | CLA  | CHD-C4C | 2.66  | 1.48        | 1.41     |
| 14  | Y     | 855  | CLA  | C1D-C2D | 2.66  | 1.48        | 1.42     |
| 14  | G     | 827  | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 14  | B     | 802  | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | G     | 804  | CLA  | CHD-C4C | 2.66  | 1.48        | 1.41     |
| 14  | Y     | 810  | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |
| 14  | B     | 816  | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | Z     | 806  | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |
| 14  | J     | 101  | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | Y     | 832  | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |
| 14  | A     | 830  | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 14  | Z     | 801  | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 14  | Y     | 813  | CLA  | CHD-C4C | 2.65  | 1.48        | 1.41     |
| 14  | Z     | 802  | CLA  | CHD-C4C | 2.65  | 1.48        | 1.41     |
| 14  | S     | 1101 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | H     | 823  | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 14  | Y     | 837  | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 14  | g     | 102  | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 14  | K     | 103  | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 14  | B     | 834  | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 14  | H     | 825  | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 14  | H     | 821  | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 14  | B     | 807  | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 14  | A     | 809  | CLA  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 14  | Y     | 825  | CLA  | CHD-C4C | 2.65  | 1.48        | 1.41     |
| 14  | A     | 808  | CLA  | CHD-C4C | 2.65  | 1.48        | 1.41     |
| 14  | Z     | 818  | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 13  | A     | 801  | CL0  | C1D-C2D | 2.65  | 1.48        | 1.42     |
| 14  | A     | 812  | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 14  | Y     | 833  | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 14  | j     | 102  | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 14  | j     | 102  | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 14  | G     | 809  | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 14  | A     | 839  | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | Y     | 806  | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 17  | R     | 102  | BCR  | C21-C22 | -2.64 | 1.32        | 1.35     |
| 14  | A     | 826  | CLA  | CHD-C4C | 2.64  | 1.48        | 1.41     |
| 14  | H     | 831  | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | A     | 825  | CLA  | CHD-C4C | 2.64  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | Y     | 855 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | H     | 807 | CLA  | CHD-C4C | 2.64  | 1.48        | 1.41     |
| 14  | G     | 836 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | Z     | 829 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | B     | 813 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 14  | Z     | 839 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | Y     | 808 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 14  | Z     | 801 | CLA  | C1D-C2D | 2.64  | 1.48        | 1.42     |
| 14  | A     | 809 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 14  | Y     | 822 | CLA  | C1C-NC  | -2.63 | 1.33        | 1.37     |
| 14  | Y     | 813 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 17  | I     | 101 | BCR  | C11-C12 | -2.63 | 1.27        | 1.34     |
| 14  | Y     | 822 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 14  | Z     | 821 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 14  | B     | 809 | CLA  | C1C-NC  | -2.63 | 1.33        | 1.37     |
| 14  | A     | 803 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | G     | 823 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | Y     | 843 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 14  | A     | 813 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | d     | 201 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | Y     | 808 | CLA  | MG-NC   | 2.63  | 2.12        | 2.06     |
| 14  | A     | 823 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | Z     | 810 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | G     | 830 | CLA  | CHD-C4C | 2.62  | 1.48        | 1.41     |
| 14  | B     | 838 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | Y     | 839 | CLA  | C1C-C2C | 2.62  | 1.49        | 1.44     |
| 14  | A     | 810 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | G     | 842 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 13  | A     | 801 | CL0  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 14  | A     | 828 | CLA  | CHD-C4C | 2.62  | 1.48        | 1.41     |
| 14  | H     | 805 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 14  | B     | 811 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 14  | A     | 817 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 14  | L     | 201 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | h     | 205 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | Z     | 816 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | L     | 207 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | G     | 813 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 14  | G     | 810 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 14  | Z     | 824 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | Q     | 201 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | Z     | 815 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 819 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | G     | 816 | CLA  | CHD-C4C | 2.62  | 1.48        | 1.41     |
| 14  | Y     | 810 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | H     | 828 | CLA  | C1B-NB  | -2.62 | 1.32        | 1.35     |
| 14  | A     | 810 | CLA  | CHD-C4C | 2.62  | 1.48        | 1.41     |
| 14  | Z     | 833 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 17  | h     | 202 | BCR  | C11-C12 | -2.62 | 1.27        | 1.34     |
| 14  | G     | 821 | CLA  | CHD-C4C | 2.62  | 1.48        | 1.41     |
| 14  | Z     | 828 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 14  | H     | 819 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 14  | G     | 822 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 14  | H     | 813 | CLA  | C1D-C2D | 2.62  | 1.48        | 1.42     |
| 14  | Z     | 824 | CLA  | CHD-C4C | 2.61  | 1.48        | 1.41     |
| 14  | A     | 832 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | A     | 818 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | H     | 832 | CLA  | CHD-C4C | 2.61  | 1.48        | 1.41     |
| 14  | Y     | 843 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | A     | 837 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 14  | H     | 804 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 14  | B     | 832 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | B     | 822 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 14  | A     | 836 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | B     | 820 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | B     | 810 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | Y     | 807 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | G     | 829 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | Z     | 810 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 14  | Z     | 833 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 14  | Y     | 809 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | Z     | 803 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | H     | 829 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | Z     | 822 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 14  | G     | 825 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 14  | A     | 807 | CLA  | CHD-C4C | 2.61  | 1.48        | 1.41     |
| 14  | A     | 821 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | Z     | 832 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 14  | H     | 815 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 14  | B     | 814 | CLA  | CHD-C4C | 2.61  | 1.48        | 1.41     |
| 14  | B     | 828 | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 14  | G     | 828 | CLA  | MG-NC   | 2.60  | 2.12        | 2.06     |
| 14  | B     | 839 | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | H     | 813 | CLA  | MG-NC   | 2.60  | 2.12        | 2.06     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 821  | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 14  | G     | 805  | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | Y     | 855  | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 14  | G     | 842  | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 14  | B     | 802  | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | K     | 101  | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | T     | 101  | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 14  | G     | 823  | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 14  | B     | 810  | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | H     | 824  | CLA  | C1C-C2C | 2.60  | 1.49        | 1.44     |
| 14  | A     | 806  | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | Y     | 835  | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 14  | H     | 832  | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 14  | G     | 806  | CLA  | MG-NC   | 2.60  | 2.12        | 2.06     |
| 14  | S     | 1101 | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | Z     | 808  | CLA  | CHD-C4C | 2.60  | 1.48        | 1.41     |
| 14  | B     | 811  | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 14  | A     | 833  | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 14  | G     | 822  | CLA  | CHD-C4C | 2.59  | 1.48        | 1.41     |
| 14  | H     | 835  | CLA  | CHD-C4C | 2.59  | 1.48        | 1.41     |
| 14  | Y     | 824  | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 14  | Z     | 837  | CLA  | MG-NC   | 2.59  | 2.12        | 2.06     |
| 14  | A     | 814  | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | B     | 829  | CLA  | CHD-C4C | 2.59  | 1.48        | 1.41     |
| 14  | B     | 824  | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 14  | Z     | 816  | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 14  | Y     | 820  | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | B     | 815  | CLA  | MG-NC   | 2.59  | 2.12        | 2.06     |
| 14  | U     | 1002 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 14  | Z     | 838  | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | G     | 840  | CLA  | CHD-C4C | 2.59  | 1.48        | 1.41     |
| 14  | Z     | 821  | CLA  | CHD-C4C | 2.59  | 1.48        | 1.41     |
| 14  | A     | 809  | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | A     | 838  | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | B     | 817  | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 14  | S     | 1102 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 14  | B     | 824  | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 14  | B     | 812  | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |
| 14  | B     | 836  | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 14  | Y     | 803  | CLA  | CHD-C4C | 2.58  | 1.48        | 1.41     |
| 14  | Z     | 834  | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 14  | G     | 815  | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | J     | 102  | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 14  | Y     | 826  | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 14  | T     | 101  | CLA  | CHD-C4C | 2.58  | 1.48        | 1.41     |
| 14  | Z     | 814  | CLA  | CHD-C4C | 2.58  | 1.48        | 1.41     |
| 14  | H     | 833  | CLA  | CHD-C4C | 2.58  | 1.48        | 1.41     |
| 14  | W     | 1701 | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 14  | A     | 812  | CLA  | MG-NC   | 2.58  | 2.12        | 2.06     |
| 14  | A     | 815  | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 14  | A     | 841  | CLA  | CHD-C4C | 2.58  | 1.48        | 1.41     |
| 14  | d     | 201  | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 14  | Z     | 834  | CLA  | CHD-C4C | 2.58  | 1.48        | 1.41     |
| 14  | h     | 205  | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 14  | B     | 820  | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 14  | B     | 823  | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 14  | B     | 830  | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 14  | Z     | 814  | CLA  | MG-NC   | 2.58  | 2.12        | 2.06     |
| 14  | A     | 829  | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 14  | G     | 816  | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 14  | Y     | 809  | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 14  | H     | 819  | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 14  | h     | 206  | CLA  | MG-NC   | 2.57  | 2.12        | 2.06     |
| 14  | G     | 839  | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | H     | 815  | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 14  | Z     | 815  | CLA  | CHD-C4C | 2.57  | 1.48        | 1.41     |
| 14  | B     | 822  | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 14  | Y     | 822  | CLA  | CHD-C4C | 2.57  | 1.48        | 1.41     |
| 14  | d     | 201  | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 14  | G     | 802  | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 14  | B     | 830  | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | H     | 818  | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 14  | H     | 837  | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 14  | H     | 801  | CLA  | C1D-C2D | 2.57  | 1.48        | 1.42     |
| 14  | L     | 201  | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 14  | H     | 836  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | B     | 833  | CLA  | CHD-C4C | 2.56  | 1.48        | 1.41     |
| 14  | H     | 809  | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 14  | Z     | 820  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | B     | 803  | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 14  | A     | 835  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | A     | 831  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | B     | 836  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | G     | 827  | CLA  | C1D-C2D | 2.56  | 1.48        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 821  | CLA  | CHD-C4C | 2.56  | 1.48        | 1.41     |
| 14  | U     | 1004 | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | Y     | 820  | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 14  | A     | 831  | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | B     | 803  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | A     | 825  | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 14  | Y     | 841  | CLA  | MG-NC   | 2.56  | 2.12        | 2.06     |
| 14  | Z     | 805  | CLA  | C1B-NB  | -2.56 | 1.32        | 1.35     |
| 14  | H     | 803  | CLA  | CHD-C4C | 2.56  | 1.48        | 1.41     |
| 14  | Y     | 832  | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 14  | Z     | 819  | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 14  | H     | 822  | CLA  | CHD-C4C | 2.56  | 1.48        | 1.41     |
| 14  | Y     | 818  | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | B     | 825  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | A     | 839  | CLA  | CHD-C4C | 2.55  | 1.48        | 1.41     |
| 14  | B     | 816  | CLA  | CHD-C4C | 2.55  | 1.48        | 1.41     |
| 14  | B     | 824  | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 14  | H     | 828  | CLA  | CHD-C4C | 2.55  | 1.48        | 1.41     |
| 14  | G     | 817  | CLA  | CHD-C4C | 2.55  | 1.48        | 1.41     |
| 14  | W     | 1701 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 14  | A     | 809  | CLA  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 14  | A     | 802  | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | Z     | 835  | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | Y     | 819  | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 14  | Q     | 203  | CLA  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 14  | A     | 812  | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | H     | 811  | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 14  | Q     | 201  | CLA  | CHD-C4C | 2.55  | 1.48        | 1.41     |
| 14  | Y     | 828  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | f     | 101  | CLA  | C1C-C2C | 2.55  | 1.49        | 1.44     |
| 14  | Y     | 804  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | B     | 805  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | H     | 817  | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 17  | A     | 845  | BCR  | C11-C12 | -2.55 | 1.28        | 1.34     |
| 14  | Y     | 834  | CLA  | C1D-C2D | 2.55  | 1.48        | 1.42     |
| 14  | B     | 807  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | A     | 835  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | Z     | 808  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 14  | Z     | 803  | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 14  | A     | 841  | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | B     | 805  | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | B     | 805  | CLA  | CHD-C4C | 2.54  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 814  | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | Y     | 817  | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 14  | Z     | 828  | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 14  | B     | 831  | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 14  | Z     | 807  | CLA  | C4B-NB  | -2.54 | 1.32        | 1.35     |
| 14  | H     | 837  | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 14  | B     | 824  | CLA  | C1D-C2D | 2.54  | 1.48        | 1.42     |
| 14  | H     | 808  | CLA  | CHD-C4C | 2.54  | 1.48        | 1.41     |
| 14  | A     | 842  | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | A     | 820  | CLA  | C1B-CHB | 2.54  | 1.48        | 1.41     |
| 14  | H     | 833  | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | S     | 1103 | CLA  | CHD-C4C | 2.54  | 1.48        | 1.41     |
| 14  | H     | 814  | CLA  | CHD-C4C | 2.54  | 1.48        | 1.41     |
| 14  | A     | 811  | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 14  | S     | 1103 | CLA  | C1B-CHB | 2.54  | 1.48        | 1.41     |
| 14  | Q     | 203  | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 14  | Y     | 829  | CLA  | C1B-CHB | 2.54  | 1.48        | 1.41     |
| 14  | K     | 103  | CLA  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 13  | A     | 801  | CL0  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 14  | G     | 841  | CLA  | C1D-C2D | 2.53  | 1.48        | 1.42     |
| 14  | G     | 809  | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | H     | 812  | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | B     | 810  | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 14  | Y     | 811  | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 14  | Z     | 819  | CLA  | CHD-C4C | 2.53  | 1.48        | 1.41     |
| 14  | H     | 815  | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 14  | A     | 807  | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 14  | G     | 842  | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | Y     | 804  | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | H     | 825  | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 14  | A     | 823  | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 14  | Y     | 830  | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 14  | A     | 819  | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | Z     | 803  | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 14  | Y     | 817  | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 14  | B     | 806  | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 14  | S     | 1102 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 14  | Y     | 837  | CLA  | CHD-C4C | 2.52  | 1.48        | 1.41     |
| 14  | Z     | 812  | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 14  | H     | 821  | CLA  | CHD-C4C | 2.52  | 1.48        | 1.41     |
| 14  | G     | 819  | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | G     | 837  | CLA  | CHD-C4C | 2.52  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 823  | CLA  | C1C-C2C | 2.52  | 1.49        | 1.44     |
| 14  | G     | 813  | CLA  | CHD-C4C | 2.52  | 1.48        | 1.41     |
| 14  | Y     | 807  | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 14  | G     | 817  | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 14  | H     | 832  | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 14  | H     | 810  | CLA  | MG-NC   | 2.52  | 2.12        | 2.06     |
| 14  | A     | 822  | CLA  | CHD-C4C | 2.52  | 1.48        | 1.41     |
| 14  | G     | 841  | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 14  | G     | 808  | CLA  | CHD-C4C | 2.52  | 1.48        | 1.41     |
| 14  | Y     | 839  | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | A     | 852  | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 14  | h     | 207  | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 14  | S     | 1101 | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 14  | A     | 827  | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | h     | 206  | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 14  | Z     | 829  | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 14  | G     | 843  | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | H     | 821  | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 14  | B     | 841  | CLA  | CHD-C4C | 2.51  | 1.48        | 1.41     |
| 14  | B     | 819  | CLA  | C4B-CHC | 2.51  | 1.48        | 1.41     |
| 14  | B     | 836  | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 14  | W     | 1701 | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | V     | 1201 | CLA  | C1D-C2D | 2.51  | 1.48        | 1.42     |
| 14  | Y     | 825  | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 14  | B     | 808  | CLA  | CHD-C4C | 2.51  | 1.48        | 1.41     |
| 14  | B     | 835  | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 14  | B     | 805  | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 14  | B     | 828  | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | B     | 807  | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 14  | A     | 838  | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 17  | H     | 841  | BCR  | C21-C22 | -2.51 | 1.32        | 1.35     |
| 14  | G     | 832  | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 14  | W     | 1701 | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | A     | 804  | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | G     | 832  | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 14  | B     | 834  | CLA  | C1B-CHB | 2.50  | 1.47        | 1.41     |
| 14  | V     | 1201 | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | Y     | 836  | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | Z     | 819  | CLA  | C1B-CHB | 2.50  | 1.47        | 1.41     |
| 14  | A     | 840  | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 14  | Y     | 816  | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | G     | 803  | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | Z     | 839 | CLA  | MG-NC   | 2.50  | 2.12        | 2.06     |
| 14  | B     | 828 | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | B     | 835 | CLA  | CHD-C4C | 2.50  | 1.48        | 1.41     |
| 14  | A     | 807 | CLA  | C1B-CHB | 2.50  | 1.47        | 1.41     |
| 19  | H     | 846 | LMG  | C22-C21 | -2.50 | 1.33        | 1.51     |
| 14  | Y     | 819 | CLA  | MG-NC   | 2.50  | 2.12        | 2.06     |
| 14  | Z     | 819 | CLA  | C1C-NC  | -2.50 | 1.34        | 1.37     |
| 14  | G     | 816 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 14  | H     | 817 | CLA  | C1C-NC  | -2.50 | 1.34        | 1.37     |
| 14  | Y     | 838 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 14  | Y     | 830 | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 14  | A     | 807 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | A     | 814 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 14  | H     | 835 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | A     | 808 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | A     | 822 | CLA  | MG-NC   | 2.49  | 2.12        | 2.06     |
| 14  | A     | 836 | CLA  | MG-NC   | 2.49  | 2.12        | 2.06     |
| 14  | B     | 815 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 14  | A     | 813 | CLA  | CHD-C4C | 2.49  | 1.48        | 1.41     |
| 14  | Y     | 821 | CLA  | CHD-C4C | 2.49  | 1.48        | 1.41     |
| 14  | H     | 802 | CLA  | CHD-C4C | 2.49  | 1.48        | 1.41     |
| 14  | Y     | 843 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 14  | A     | 841 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 14  | Y     | 839 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 14  | Z     | 811 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 14  | H     | 819 | CLA  | MG-NC   | 2.49  | 2.12        | 2.06     |
| 14  | Q     | 201 | CLA  | C1B-NB  | -2.49 | 1.33        | 1.35     |
| 17  | I     | 101 | BCR  | C1-C6   | -2.49 | 1.50        | 1.53     |
| 14  | Z     | 809 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 14  | G     | 820 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 17  | H     | 845 | BCR  | C30-C25 | -2.49 | 1.50        | 1.53     |
| 14  | A     | 810 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 14  | Z     | 839 | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 14  | H     | 811 | CLA  | CHD-C4C | 2.48  | 1.48        | 1.41     |
| 14  | Z     | 828 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | H     | 811 | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 14  | Z     | 839 | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |
| 14  | Y     | 802 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | G     | 826 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | A     | 842 | CLA  | MG-NC   | 2.48  | 2.12        | 2.06     |
| 14  | h     | 206 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 14  | G     | 816 | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 837  | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | Z     | 835  | CLA  | MG-NC   | 2.48  | 2.12        | 2.06     |
| 14  | B     | 811  | CLA  | CHD-C4C | 2.48  | 1.48        | 1.41     |
| 14  | G     | 830  | CLA  | MG-NC   | 2.48  | 2.12        | 2.06     |
| 14  | Y     | 821  | CLA  | C1C-C2C | 2.48  | 1.49        | 1.44     |
| 14  | G     | 820  | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |
| 14  | Y     | 814  | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 14  | Y     | 827  | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 14  | G     | 809  | CLA  | MG-NC   | 2.48  | 2.12        | 2.06     |
| 14  | U     | 1004 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | H     | 816  | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 14  | H     | 834  | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | U     | 1002 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 14  | B     | 833  | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 14  | A     | 840  | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 14  | Y     | 818  | CLA  | MG-NC   | 2.47  | 2.12        | 2.06     |
| 14  | B     | 810  | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 14  | H     | 823  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | A     | 819  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | A     | 835  | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | A     | 829  | CLA  | MG-NC   | 2.47  | 2.12        | 2.06     |
| 14  | Y     | 813  | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | A     | 852  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | B     | 816  | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | L     | 206  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | Z     | 810  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | A     | 824  | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | G     | 843  | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 14  | Z     | 807  | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | G     | 826  | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 14  | B     | 823  | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 14  | H     | 837  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | B     | 828  | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 14  | H     | 822  | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 14  | Z     | 802  | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 14  | Z     | 804  | CLA  | CHD-C4C | 2.47  | 1.48        | 1.41     |
| 14  | X     | 1701 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 14  | Z     | 828  | CLA  | CHD-C4C | 2.46  | 1.48        | 1.41     |
| 14  | A     | 809  | CLA  | C1B-NB  | -2.46 | 1.33        | 1.35     |
| 14  | B     | 821  | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 14  | B     | 812  | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 14  | h     | 205  | CLA  | CHD-C4C | 2.46  | 1.48        | 1.41     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Y     | 808  | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 14  | B     | 831  | CLA  | CHD-C4C | 2.46  | 1.48        | 1.41     |
| 14  | H     | 802  | CLA  | MG-NC   | 2.46  | 2.12        | 2.06     |
| 14  | L     | 206  | CLA  | C1B-NB  | -2.46 | 1.33        | 1.35     |
| 14  | W     | 1701 | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 14  | Y     | 854  | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 14  | Z     | 835  | CLA  | CHD-C4C | 2.46  | 1.48        | 1.41     |
| 14  | V     | 1201 | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 14  | G     | 826  | CLA  | CHD-C4C | 2.46  | 1.48        | 1.41     |
| 14  | Y     | 834  | CLA  | MG-NC   | 2.46  | 2.12        | 2.06     |
| 14  | L     | 206  | CLA  | C1C-C2C | 2.46  | 1.49        | 1.44     |
| 14  | A     | 821  | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 14  | H     | 836  | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 14  | Y     | 825  | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 14  | H     | 825  | CLA  | CHD-C4C | 2.46  | 1.48        | 1.41     |
| 14  | j     | 102  | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 14  | G     | 802  | CLA  | C1B-NB  | -2.46 | 1.33        | 1.35     |
| 14  | B     | 840  | CLA  | C1D-C2D | 2.46  | 1.48        | 1.42     |
| 14  | Z     | 814  | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 14  | Z     | 820  | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 14  | B     | 814  | CLA  | MG-NC   | 2.45  | 2.12        | 2.06     |
| 14  | h     | 201  | CLA  | C1B-NB  | -2.45 | 1.33        | 1.35     |
| 14  | T     | 103  | CLA  | CHD-C4C | 2.45  | 1.48        | 1.41     |
| 14  | d     | 202  | CLA  | CHD-C4C | 2.45  | 1.48        | 1.41     |
| 14  | Y     | 839  | CLA  | CHD-C4C | 2.45  | 1.48        | 1.41     |
| 14  | Z     | 808  | CLA  | C1B-NB  | -2.45 | 1.33        | 1.35     |
| 14  | Y     | 834  | CLA  | C1C-C2C | 2.45  | 1.49        | 1.44     |
| 14  | G     | 834  | CLA  | C1C-C2C | 2.45  | 1.49        | 1.44     |
| 14  | Z     | 806  | CLA  | CHD-C4C | 2.45  | 1.48        | 1.41     |
| 14  | h     | 205  | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 14  | Z     | 807  | CLA  | MG-NC   | 2.45  | 2.12        | 2.06     |
| 14  | B     | 814  | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 14  | G     | 818  | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 14  | A     | 805  | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 14  | G     | 814  | CLA  | CHD-C4C | 2.45  | 1.48        | 1.41     |
| 14  | Z     | 834  | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | H     | 820  | CLA  | C1B-CHB | 2.44  | 1.47        | 1.41     |
| 14  | B     | 809  | CLA  | MG-NC   | 2.44  | 2.12        | 2.06     |
| 14  | B     | 840  | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 14  | f     | 102  | CLA  | C1B-CHB | 2.44  | 1.47        | 1.41     |
| 14  | Z     | 836  | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 17  | h     | 203  | BCR  | C21-C22 | -2.44 | 1.32        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 831  | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | A     | 811  | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 19  | Z     | 847  | LMG  | C22-C21 | -2.44 | 1.34        | 1.51     |
| 14  | H     | 835  | CLA  | MG-NC   | 2.44  | 2.12        | 2.06     |
| 14  | g     | 102  | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | G     | 822  | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 14  | B     | 834  | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 14  | B     | 826  | CLA  | C1D-C2D | 2.43  | 1.48        | 1.42     |
| 14  | A     | 804  | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 14  | Z     | 832  | CLA  | CHD-C4C | 2.43  | 1.48        | 1.41     |
| 14  | V     | 1201 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | G     | 804  | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 14  | H     | 805  | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 13  | Y     | 801  | CL0  | CHD-C4C | 2.43  | 1.48        | 1.41     |
| 14  | H     | 824  | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | G     | 835  | CLA  | C1B-CHB | 2.43  | 1.47        | 1.41     |
| 14  | T     | 103  | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 14  | G     | 810  | CLA  | MG-NC   | 2.43  | 2.12        | 2.06     |
| 14  | Z     | 820  | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | L     | 202  | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 14  | Z     | 824  | CLA  | MG-NC   | 2.43  | 2.12        | 2.06     |
| 14  | Q     | 203  | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | Z     | 826  | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | H     | 831  | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 14  | Y     | 843  | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 14  | h     | 205  | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 14  | B     | 815  | CLA  | CHD-C4C | 2.42  | 1.48        | 1.41     |
| 14  | B     | 839  | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 14  | G     | 824  | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 14  | H     | 828  | CLA  | MG-NC   | 2.42  | 2.12        | 2.06     |
| 14  | Y     | 828  | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 14  | H     | 825  | CLA  | MG-NC   | 2.42  | 2.12        | 2.06     |
| 14  | H     | 833  | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 14  | H     | 807  | CLA  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 14  | G     | 807  | CLA  | CHD-C4C | 2.42  | 1.48        | 1.41     |
| 14  | Y     | 815  | CLA  | CHD-C4C | 2.42  | 1.48        | 1.41     |
| 14  | H     | 838  | CLA  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 14  | B     | 808  | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 14  | A     | 820  | CLA  | CHD-C4C | 2.42  | 1.48        | 1.41     |
| 14  | L     | 202  | CLA  | MG-NC   | 2.42  | 2.12        | 2.06     |
| 14  | A     | 815  | CLA  | CHD-C4C | 2.42  | 1.48        | 1.41     |
| 14  | B     | 828  | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Y     | 831  | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 14  | B     | 819  | CLA  | CHD-C4C | 2.42  | 1.48        | 1.41     |
| 14  | B     | 803  | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 14  | A     | 804  | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 14  | G     | 842  | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 14  | B     | 830  | CLA  | MG-NC   | 2.41  | 2.12        | 2.06     |
| 14  | A     | 803  | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 14  | B     | 831  | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 14  | H     | 826  | CLA  | CHD-C4C | 2.41  | 1.48        | 1.41     |
| 14  | A     | 814  | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 14  | Y     | 805  | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 14  | Z     | 822  | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 14  | H     | 801  | CLA  | CHD-C4C | 2.41  | 1.48        | 1.41     |
| 14  | B     | 817  | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 14  | T     | 103  | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 14  | G     | 831  | CLA  | C4B-CHC | 2.41  | 1.47        | 1.41     |
| 14  | g     | 102  | CLA  | CHD-C4C | 2.41  | 1.48        | 1.41     |
| 14  | G     | 820  | CLA  | CHD-C4C | 2.41  | 1.48        | 1.41     |
| 14  | K     | 101  | CLA  | C4B-CHC | 2.41  | 1.47        | 1.41     |
| 14  | L     | 206  | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 14  | G     | 807  | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 14  | G     | 831  | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 14  | Y     | 813  | CLA  | MG-NC   | 2.41  | 2.12        | 2.06     |
| 14  | Z     | 839  | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 13  | G     | 801  | CL0  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 17  | S     | 1104 | BCR  | C21-C22 | -2.40 | 1.32        | 1.35     |
| 14  | B     | 840  | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 14  | Y     | 806  | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 14  | B     | 834  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | B     | 832  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | G     | 818  | CLA  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 14  | H     | 827  | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 14  | A     | 814  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | Y     | 840  | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 14  | G     | 811  | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 14  | H     | 836  | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 14  | G     | 802  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | G     | 809  | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 14  | G     | 834  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | d     | 201  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | H     | 820  | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 14  | G     | 802  | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 834  | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 14  | G     | 853  | CLA  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 14  | Y     | 815  | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 14  | Z     | 826  | CLA  | CHD-C4C | 2.40  | 1.48        | 1.41     |
| 14  | K     | 101  | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 14  | H     | 818  | CLA  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 14  | G     | 808  | CLA  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 14  | B     | 802  | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 14  | Z     | 802  | CLA  | C1B-NB  | -2.40 | 1.33        | 1.35     |
| 14  | Z     | 830  | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 14  | A     | 841  | CLA  | C1B-NB  | -2.39 | 1.33        | 1.35     |
| 14  | Z     | 813  | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | H     | 817  | CLA  | MG-NC   | 2.39  | 2.12        | 2.06     |
| 14  | Y     | 823  | CLA  | C1C-NC  | -2.39 | 1.34        | 1.37     |
| 14  | A     | 826  | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 14  | Y     | 837  | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | H     | 821  | CLA  | MG-NC   | 2.39  | 2.11        | 2.06     |
| 14  | A     | 813  | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 14  | Y     | 822  | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | H     | 825  | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 14  | A     | 831  | CLA  | C1B-CHB | 2.39  | 1.47        | 1.41     |
| 14  | X     | 1701 | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 14  | Y     | 837  | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 14  | H     | 821  | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 14  | H     | 830  | CLA  | CHD-C4C | 2.39  | 1.47        | 1.41     |
| 14  | Z     | 833  | CLA  | C1B-CHB | 2.39  | 1.47        | 1.41     |
| 14  | B     | 841  | CLA  | MG-NC   | 2.39  | 2.11        | 2.06     |
| 14  | G     | 836  | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 14  | Z     | 816  | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 14  | G     | 838  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | A     | 831  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | H     | 804  | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 14  | A     | 802  | CLA  | C1B-NB  | -2.38 | 1.33        | 1.35     |
| 14  | Y     | 832  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | Z     | 823  | CLA  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 14  | H     | 809  | CLA  | C1B-CHB | 2.38  | 1.47        | 1.41     |
| 13  | A     | 801  | CL0  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | A     | 805  | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 14  | Y     | 843  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | G     | 837  | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 14  | Y     | 816  | CLA  | C1B-CHB | 2.38  | 1.47        | 1.41     |
| 14  | G     | 829  | CLA  | C1B-CHB | 2.38  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 836  | CLA  | C1B-NB  | -2.38 | 1.33        | 1.35     |
| 14  | S     | 1103 | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 13  | G     | 801  | CL0  | C1B-NB  | -2.38 | 1.33        | 1.35     |
| 14  | H     | 818  | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 14  | G     | 810  | CLA  | C1B-CHB | 2.38  | 1.47        | 1.41     |
| 14  | U     | 1002 | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 14  | G     | 832  | CLA  | C1B-CHB | 2.38  | 1.47        | 1.41     |
| 14  | G     | 835  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | Y     | 810  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | G     | 811  | CLA  | CHD-C4C | 2.38  | 1.47        | 1.41     |
| 14  | Z     | 803  | CLA  | C1D-C2D | 2.37  | 1.47        | 1.42     |
| 14  | A     | 828  | CLA  | C1B-NB  | -2.37 | 1.33        | 1.35     |
| 14  | A     | 802  | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 13  | G     | 801  | CL0  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | H     | 808  | CLA  | MG-NC   | 2.37  | 2.11        | 2.06     |
| 14  | H     | 816  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | B     | 812  | CLA  | MG-NC   | 2.37  | 2.11        | 2.06     |
| 14  | Z     | 808  | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | Y     | 814  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | Z     | 828  | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 14  | X     | 1701 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 14  | X     | 1701 | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | H     | 821  | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | B     | 832  | CLA  | MG-NC   | 2.37  | 2.11        | 2.06     |
| 14  | A     | 830  | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 14  | Z     | 838  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | G     | 825  | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | B     | 827  | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 14  | B     | 809  | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 17  | Z     | 846  | BCR  | C30-C25 | -2.37 | 1.50        | 1.53     |
| 14  | Y     | 833  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | G     | 832  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | G     | 824  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | h     | 206  | CLA  | CHD-C4C | 2.37  | 1.47        | 1.41     |
| 14  | B     | 832  | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | h     | 201  | CLA  | CHD-C4C | 2.36  | 1.47        | 1.41     |
| 14  | Z     | 829  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 14  | B     | 826  | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | H     | 801  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 14  | B     | 840  | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | Y     | 808  | CLA  | CHD-C4C | 2.36  | 1.47        | 1.41     |
| 14  | Z     | 839  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 841  | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 14  | A     | 816  | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 14  | A     | 814  | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 14  | A     | 824  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 14  | B     | 808  | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | A     | 826  | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | H     | 831  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 14  | J     | 101  | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 14  | f     | 101  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 14  | H     | 823  | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | G     | 833  | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 14  | Y     | 831  | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 14  | G     | 822  | CLA  | C1A-CHA | 2.35  | 1.52        | 1.43     |
| 14  | Z     | 823  | CLA  | MG-NC   | 2.35  | 2.11        | 2.06     |
| 14  | B     | 818  | CLA  | MG-NC   | 2.35  | 2.11        | 2.06     |
| 14  | A     | 836  | CLA  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 14  | A     | 822  | CLA  | C1A-CHA | 2.35  | 1.52        | 1.43     |
| 14  | f     | 101  | CLA  | CHD-C4C | 2.35  | 1.47        | 1.41     |
| 14  | Y     | 827  | CLA  | CHD-C4C | 2.35  | 1.47        | 1.41     |
| 14  | A     | 809  | CLA  | CHD-C4C | 2.35  | 1.47        | 1.41     |
| 14  | Z     | 811  | CLA  | C1C-NC  | -2.35 | 1.34        | 1.37     |
| 14  | S     | 1102 | CLA  | CHD-C4C | 2.35  | 1.47        | 1.41     |
| 14  | H     | 834  | CLA  | C1B-NB  | -2.35 | 1.33        | 1.35     |
| 14  | L     | 205  | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | H     | 832  | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | Z     | 808  | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | G     | 820  | CLA  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 14  | B     | 814  | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 14  | G     | 843  | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 13  | G     | 801  | CL0  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | B     | 841  | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | A     | 811  | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | H     | 820  | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 14  | A     | 835  | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 14  | Y     | 802  | CLA  | C1B-NB  | -2.34 | 1.33        | 1.35     |
| 14  | h     | 201  | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | Z     | 816  | CLA  | CHD-C4C | 2.34  | 1.47        | 1.41     |
| 14  | B     | 802  | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 14  | Y     | 813  | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 14  | G     | 838  | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 14  | H     | 813  | CLA  | CHD-C4C | 2.33  | 1.47        | 1.41     |
| 14  | Z     | 818  | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Y     | 805  | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |
| 14  | G     | 809  | CLA  | CHD-C4C | 2.33  | 1.47        | 1.41     |
| 14  | Z     | 818  | CLA  | CHD-C4C | 2.33  | 1.47        | 1.41     |
| 14  | Z     | 831  | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |
| 14  | A     | 834  | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 14  | T     | 101  | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |
| 14  | A     | 841  | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 14  | B     | 833  | CLA  | MG-NC   | 2.33  | 2.11        | 2.06     |
| 17  | i     | 101  | BCR  | C23-C22 | 2.33  | 1.50        | 1.45     |
| 14  | Z     | 814  | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 14  | G     | 826  | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 14  | L     | 206  | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |
| 14  | H     | 830  | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 14  | Y     | 842  | CLA  | C4B-CHC | 2.33  | 1.47        | 1.41     |
| 14  | G     | 812  | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 14  | G     | 840  | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |
| 14  | B     | 818  | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 14  | H     | 812  | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 13  | A     | 801  | CL0  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 14  | G     | 808  | CLA  | C1B-CHB | 2.32  | 1.47        | 1.41     |
| 14  | H     | 824  | CLA  | CHD-C4C | 2.32  | 1.47        | 1.41     |
| 14  | Y     | 839  | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 14  | Y     | 816  | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 14  | Y     | 807  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 14  | L     | 202  | CLA  | CHD-C4C | 2.32  | 1.47        | 1.41     |
| 14  | S     | 1102 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 14  | B     | 835  | CLA  | C1B-CHB | 2.32  | 1.47        | 1.41     |
| 14  | A     | 820  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 14  | H     | 814  | CLA  | C1B-CHB | 2.32  | 1.47        | 1.41     |
| 14  | A     | 838  | CLA  | CHD-C4C | 2.31  | 1.47        | 1.41     |
| 14  | A     | 833  | CLA  | CHD-C4C | 2.31  | 1.47        | 1.41     |
| 14  | Y     | 815  | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 14  | G     | 805  | CLA  | MG-NC   | 2.31  | 2.11        | 2.06     |
| 14  | H     | 835  | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | Z     | 801  | CLA  | CHD-C4C | 2.31  | 1.47        | 1.41     |
| 14  | H     | 813  | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | Z     | 825  | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 13  | A     | 801  | CL0  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 14  | Y     | 818  | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 14  | G     | 837  | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |
| 14  | Y     | 831  | CLA  | CHD-C4C | 2.31  | 1.47        | 1.41     |
| 14  | Y     | 830  | CLA  | C1B-CHB | 2.31  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | A     | 819 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | A     | 813 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | Z     | 826 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | G     | 803 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 14  | A     | 810 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 14  | Y     | 807 | CLA  | CHD-C4C | 2.30  | 1.47        | 1.41     |
| 14  | A     | 819 | CLA  | MG-NC   | 2.30  | 2.11        | 2.06     |
| 14  | H     | 805 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | Y     | 807 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 14  | B     | 831 | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 14  | Y     | 841 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 13  | G     | 801 | CL0  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 14  | B     | 820 | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 14  | Y     | 828 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | H     | 830 | CLA  | C1B-CHB | 2.30  | 1.47        | 1.41     |
| 14  | A     | 818 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 14  | Z     | 804 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 14  | A     | 828 | CLA  | C1C-NC  | -2.29 | 1.34        | 1.37     |
| 14  | H     | 828 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | B     | 804 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 14  | B     | 806 | CLA  | CHD-C4C | 2.29  | 1.47        | 1.41     |
| 14  | A     | 841 | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 14  | Z     | 835 | CLA  | C1B-NB  | -2.29 | 1.33        | 1.35     |
| 17  | H     | 845 | BCR  | C21-C22 | -2.29 | 1.32        | 1.35     |
| 14  | H     | 807 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 14  | Y     | 837 | CLA  | MG-NC   | 2.29  | 2.11        | 2.06     |
| 14  | G     | 811 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 14  | A     | 803 | CLA  | C4C-C3C | 2.28  | 1.49        | 1.45     |
| 14  | G     | 807 | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 14  | H     | 809 | CLA  | CHD-C4C | 2.28  | 1.47        | 1.41     |
| 14  | Z     | 838 | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 14  | Y     | 802 | CLA  | MG-NC   | 2.28  | 2.11        | 2.06     |
| 14  | H     | 804 | CLA  | CHD-C4C | 2.28  | 1.47        | 1.41     |
| 14  | Y     | 840 | CLA  | CHD-C4C | 2.28  | 1.47        | 1.41     |
| 14  | G     | 806 | CLA  | CHD-C4C | 2.28  | 1.47        | 1.41     |
| 14  | G     | 823 | CLA  | CHD-C4C | 2.28  | 1.47        | 1.41     |
| 14  | G     | 813 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 14  | Z     | 801 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 14  | H     | 817 | CLA  | C1B-NB  | -2.28 | 1.33        | 1.35     |
| 14  | Z     | 835 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 14  | Y     | 824 | CLA  | CHD-C4C | 2.28  | 1.47        | 1.41     |
| 14  | A     | 827 | CLA  | C1C-NC  | -2.28 | 1.34        | 1.37     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 803  | CLA  | CHD-C4C | 2.27  | 1.47        | 1.41     |
| 14  | B     | 817  | CLA  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 14  | H     | 813  | CLA  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 14  | U     | 1003 | CLA  | CHD-C4C | 2.27  | 1.47        | 1.41     |
| 14  | H     | 810  | CLA  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 14  | d     | 202  | CLA  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 14  | H     | 806  | CLA  | C1B-NB  | -2.27 | 1.33        | 1.35     |
| 14  | G     | 823  | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | B     | 829  | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 14  | A     | 817  | CLA  | CHD-C4C | 2.27  | 1.47        | 1.41     |
| 14  | Y     | 817  | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 14  | B     | 813  | CLA  | MG-NC   | 2.27  | 2.11        | 2.06     |
| 14  | Z     | 805  | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 14  | Y     | 824  | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 14  | Z     | 837  | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 14  | G     | 825  | CLA  | C1C-C2C | 2.27  | 1.48        | 1.44     |
| 14  | H     | 825  | CLA  | C1C-C2C | 2.27  | 1.48        | 1.44     |
| 14  | Y     | 854  | CLA  | C1D-C2D | 2.27  | 1.47        | 1.42     |
| 14  | H     | 824  | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 14  | B     | 806  | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 14  | A     | 837  | CLA  | C1C-C2C | 2.26  | 1.48        | 1.44     |
| 14  | B     | 838  | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 14  | Z     | 816  | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | Z     | 827  | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | Z     | 830  | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 14  | f     | 102  | CLA  | C1C-C2C | 2.26  | 1.48        | 1.44     |
| 14  | A     | 806  | CLA  | C1C-NC  | -2.26 | 1.34        | 1.37     |
| 14  | A     | 827  | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | Z     | 802  | CLA  | C1D-C2D | 2.26  | 1.47        | 1.42     |
| 14  | G     | 804  | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 14  | Z     | 830  | CLA  | CHD-C4C | 2.26  | 1.47        | 1.41     |
| 14  | Y     | 854  | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |
| 14  | B     | 840  | CLA  | CHD-C4C | 2.26  | 1.47        | 1.41     |
| 14  | T     | 103  | CLA  | C1C-C2C | 2.26  | 1.48        | 1.44     |
| 14  | H     | 827  | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 14  | Y     | 826  | CLA  | C1C-NC  | -2.26 | 1.34        | 1.37     |
| 14  | A     | 818  | CLA  | CHD-C4C | 2.26  | 1.47        | 1.41     |
| 14  | Z     | 807  | CLA  | C4B-CHC | 2.26  | 1.47        | 1.41     |
| 14  | f     | 101  | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 14  | Z     | 822  | CLA  | CHD-C4C | 2.26  | 1.47        | 1.41     |
| 14  | Z     | 817  | CLA  | CHD-C4C | 2.26  | 1.47        | 1.41     |
| 14  | G     | 805  | CLA  | C1B-CHB | 2.26  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 836  | CLA  | CHD-C4C | 2.25  | 1.47        | 1.41     |
| 14  | G     | 815  | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | Z     | 826  | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 14  | A     | 829  | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 14  | A     | 828  | CLA  | C1C-C2C | 2.25  | 1.48        | 1.44     |
| 14  | G     | 833  | CLA  | CHD-C4C | 2.25  | 1.47        | 1.41     |
| 14  | B     | 818  | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 14  | Y     | 836  | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | U     | 1004 | CLA  | CHD-C4C | 2.25  | 1.47        | 1.41     |
| 14  | H     | 838  | CLA  | CHD-C4C | 2.25  | 1.47        | 1.41     |
| 14  | Y     | 831  | CLA  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 14  | G     | 853  | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 14  | B     | 818  | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | Z     | 817  | CLA  | C1B-CHB | 2.25  | 1.47        | 1.41     |
| 14  | Y     | 842  | CLA  | CHD-C4C | 2.25  | 1.47        | 1.41     |
| 14  | K     | 103  | CLA  | CHD-C4C | 2.25  | 1.47        | 1.41     |
| 14  | A     | 816  | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 14  | S     | 1101 | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | A     | 833  | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | G     | 807  | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | K     | 103  | CLA  | C4B-CHC | 2.24  | 1.47        | 1.41     |
| 14  | Y     | 804  | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 14  | L     | 202  | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | G     | 853  | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 14  | H     | 803  | CLA  | MG-NC   | 2.24  | 2.11        | 2.06     |
| 14  | Y     | 827  | CLA  | C1C-C2C | 2.24  | 1.48        | 1.44     |
| 14  | B     | 824  | CLA  | CHD-C4C | 2.24  | 1.47        | 1.41     |
| 14  | H     | 814  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 14  | G     | 838  | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 14  | G     | 839  | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | A     | 840  | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 14  | B     | 821  | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 14  | Z     | 819  | CLA  | MG-NC   | 2.23  | 2.11        | 2.06     |
| 14  | A     | 834  | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | J     | 102  | CLA  | C1B-NB  | -2.23 | 1.33        | 1.35     |
| 14  | G     | 829  | CLA  | CHD-C4C | 2.23  | 1.47        | 1.41     |
| 14  | H     | 836  | CLA  | CHD-C4C | 2.23  | 1.47        | 1.41     |
| 14  | H     | 818  | CLA  | CHD-C4C | 2.23  | 1.47        | 1.41     |
| 14  | B     | 826  | CLA  | MG-NC   | 2.23  | 2.11        | 2.06     |
| 14  | Y     | 823  | CLA  | CHD-C4C | 2.23  | 1.47        | 1.41     |
| 14  | H     | 802  | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 14  | B     | 833  | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | Z     | 835  | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 14  | Y     | 840  | CLA  | C1C-C2C | 2.23  | 1.48        | 1.44     |
| 14  | Y     | 818  | CLA  | C1B-NB  | -2.23 | 1.33        | 1.35     |
| 14  | J     | 102  | CLA  | C1C-C2C | 2.23  | 1.48        | 1.44     |
| 14  | h     | 201  | CLA  | C4B-CHC | 2.22  | 1.47        | 1.41     |
| 14  | B     | 804  | CLA  | C1B-CHB | 2.22  | 1.47        | 1.41     |
| 14  | B     | 827  | CLA  | MG-NC   | 2.22  | 2.11        | 2.06     |
| 14  | Y     | 819  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 14  | B     | 805  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 14  | Y     | 825  | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 14  | G     | 810  | CLA  | CHD-C4C | 2.22  | 1.47        | 1.41     |
| 14  | A     | 820  | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 14  | Y     | 807  | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 14  | Y     | 836  | CLA  | C1C-C2C | 2.22  | 1.48        | 1.44     |
| 17  | G     | 849  | BCR  | C21-C22 | -2.22 | 1.32        | 1.35     |
| 14  | B     | 811  | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 14  | A     | 822  | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 14  | B     | 827  | CLA  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 14  | Z     | 803  | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 14  | B     | 817  | CLA  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 14  | G     | 804  | CLA  | C1B-NB  | -2.21 | 1.33        | 1.35     |
| 14  | A     | 806  | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | Z     | 806  | CLA  | C4B-CHC | 2.21  | 1.47        | 1.41     |
| 14  | U     | 1003 | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | A     | 839  | CLA  | C1C-NC  | -2.21 | 1.34        | 1.37     |
| 14  | Y     | 817  | CLA  | CHD-C4C | 2.21  | 1.47        | 1.41     |
| 13  | Y     | 801  | CL0  | C4B-CHC | 2.21  | 1.47        | 1.41     |
| 14  | H     | 835  | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | G     | 810  | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 14  | H     | 816  | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 14  | F     | 202  | CLA  | CHD-C4C | 2.21  | 1.47        | 1.41     |
| 14  | A     | 811  | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 17  | Z     | 845  | BCR  | C19-C18 | 2.21  | 1.50        | 1.45     |
| 14  | H     | 830  | CLA  | C1D-C2D | 2.21  | 1.47        | 1.42     |
| 14  | Z     | 805  | CLA  | MG-NC   | 2.21  | 2.11        | 2.06     |
| 14  | B     | 838  | CLA  | CHD-C4C | 2.21  | 1.47        | 1.41     |
| 17  | h     | 202  | BCR  | C23-C22 | 2.21  | 1.50        | 1.45     |
| 14  | Z     | 834  | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 14  | H     | 806  | CLA  | CHD-C4C | 2.20  | 1.47        | 1.41     |
| 14  | h     | 207  | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 14  | Y     | 820  | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 14  | H     | 834  | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 809  | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | L     | 207  | CLA  | CHD-C4C | 2.20  | 1.47        | 1.41     |
| 14  | Y     | 835  | CLA  | C1C-NC  | -2.20 | 1.34        | 1.37     |
| 14  | G     | 828  | CLA  | CHD-C4C | 2.20  | 1.47        | 1.41     |
| 14  | H     | 824  | CLA  | C1B-CHB | 2.20  | 1.47        | 1.41     |
| 14  | A     | 802  | CLA  | C4B-CHC | 2.20  | 1.47        | 1.41     |
| 14  | S     | 1101 | CLA  | C4B-NB  | -2.20 | 1.33        | 1.35     |
| 17  | Q     | 204  | BCR  | C30-C25 | -2.20 | 1.50        | 1.53     |
| 14  | G     | 815  | CLA  | MG-NC   | 2.20  | 2.11        | 2.06     |
| 14  | A     | 826  | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 14  | G     | 821  | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 14  | H     | 827  | CLA  | CHD-C4C | 2.19  | 1.47        | 1.41     |
| 14  | Z     | 804  | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 14  | Z     | 812  | CLA  | C1B-NB  | -2.19 | 1.33        | 1.35     |
| 14  | Z     | 804  | CLA  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 14  | G     | 843  | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 14  | Z     | 801  | CLA  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 14  | L     | 201  | CLA  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 14  | Z     | 811  | CLA  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 17  | B     | 848  | BCR  | C30-C25 | -2.19 | 1.50        | 1.53     |
| 14  | B     | 820  | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 14  | G     | 841  | CLA  | MG-NC   | 2.19  | 2.11        | 2.06     |
| 14  | Z     | 813  | CLA  | CHD-C4C | 2.19  | 1.47        | 1.41     |
| 14  | B     | 830  | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 14  | H     | 829  | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 14  | G     | 836  | CLA  | C1C-NC  | -2.18 | 1.34        | 1.37     |
| 14  | G     | 828  | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |
| 14  | H     | 829  | CLA  | CHD-C4C | 2.18  | 1.47        | 1.41     |
| 14  | H     | 829  | CLA  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 14  | B     | 835  | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 14  | Y     | 814  | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 14  | U     | 1002 | CLA  | MG-NC   | 2.18  | 2.11        | 2.06     |
| 14  | B     | 809  | CLA  | CHD-C4C | 2.18  | 1.47        | 1.41     |
| 14  | A     | 804  | CLA  | C1B-CHB | 2.18  | 1.47        | 1.41     |
| 14  | H     | 815  | CLA  | CHD-C4C | 2.18  | 1.47        | 1.41     |
| 14  | F     | 202  | CLA  | C4B-CHC | 2.18  | 1.47        | 1.41     |
| 14  | X     | 1701 | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 14  | B     | 819  | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 14  | H     | 819  | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 14  | Z     | 813  | CLA  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 14  | B     | 812  | CLA  | C1B-CHB | 2.17  | 1.47        | 1.41     |
| 14  | G     | 814  | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 804  | CLA  | C4B-CHC | 2.17  | 1.47        | 1.41     |
| 14  | Z     | 823  | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 14  | B     | 827  | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 14  | B     | 829  | CLA  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 14  | A     | 840  | CLA  | MG-NC   | 2.16  | 2.11        | 2.06     |
| 14  | Y     | 832  | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 14  | f     | 102  | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 14  | H     | 819  | CLA  | CHD-C4C | 2.16  | 1.47        | 1.41     |
| 14  | G     | 827  | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 14  | A     | 823  | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 14  | T     | 101  | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 14  | A     | 832  | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 14  | A     | 818  | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 14  | Y     | 855  | CLA  | CHD-C4C | 2.16  | 1.47        | 1.41     |
| 14  | Z     | 832  | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 14  | Y     | 854  | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 14  | A     | 836  | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 17  | Y     | 846  | BCR  | C11-C12 | -2.16 | 1.29        | 1.34     |
| 14  | H     | 824  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 14  | Y     | 805  | CLA  | MG-NC   | 2.15  | 2.11        | 2.06     |
| 14  | h     | 201  | CLA  | C4B-NB  | -2.15 | 1.33        | 1.35     |
| 17  | F     | 203  | BCR  | C1-C6   | -2.15 | 1.50        | 1.53     |
| 14  | Y     | 804  | CLA  | C1B-CHB | 2.15  | 1.47        | 1.41     |
| 14  | G     | 842  | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 14  | U     | 1002 | CLA  | CHD-C4C | 2.15  | 1.47        | 1.41     |
| 17  | Z     | 845  | BCR  | C23-C22 | 2.15  | 1.50        | 1.45     |
| 14  | G     | 821  | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 14  | Z     | 817  | CLA  | MG-NC   | 2.15  | 2.11        | 2.06     |
| 14  | Y     | 819  | CLA  | C1B-CHB | 2.15  | 1.47        | 1.41     |
| 14  | G     | 831  | CLA  | CHD-C4C | 2.15  | 1.47        | 1.41     |
| 14  | G     | 831  | CLA  | MG-NC   | 2.15  | 2.11        | 2.06     |
| 14  | H     | 823  | CLA  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 14  | G     | 819  | CLA  | C1B-NB  | -2.15 | 1.33        | 1.35     |
| 14  | L     | 205  | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 14  | Z     | 828  | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 14  | B     | 807  | CLA  | C4B-CHC | 2.14  | 1.46        | 1.41     |
| 14  | Z     | 811  | CLA  | CHD-C4C | 2.14  | 1.47        | 1.41     |
| 17  | Z     | 842  | BCR  | C21-C22 | -2.14 | 1.32        | 1.35     |
| 14  | G     | 820  | CLA  | C4B-CHC | 2.14  | 1.46        | 1.41     |
| 14  | A     | 813  | CLA  | C4B-CHC | 2.14  | 1.46        | 1.41     |
| 14  | B     | 819  | CLA  | C1B-CHB | 2.14  | 1.46        | 1.41     |
| 14  | Y     | 840  | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 808  | CLA  | C1B-CHB | 2.14  | 1.46        | 1.41     |
| 14  | B     | 825  | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 14  | A     | 829  | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 14  | Z     | 822  | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 14  | U     | 1006 | CLA  | CHD-C4C | 2.14  | 1.47        | 1.41     |
| 14  | A     | 823  | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | h     | 206  | CLA  | C2A-C1A | -2.13 | 1.47        | 1.52     |
| 14  | H     | 830  | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 15  | B     | 842  | PQN  | C11-C12 | 2.13  | 1.53        | 1.50     |
| 14  | H     | 810  | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | G     | 813  | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 14  | Y     | 814  | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | B     | 835  | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 14  | S     | 1103 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 17  | V     | 1202 | BCR  | C23-C22 | 2.13  | 1.50        | 1.45     |
| 14  | B     | 822  | CLA  | CHD-C4C | 2.13  | 1.47        | 1.41     |
| 14  | B     | 825  | CLA  | CHD-C4C | 2.13  | 1.47        | 1.41     |
| 14  | A     | 826  | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 14  | G     | 829  | CLA  | C4B-NB  | -2.13 | 1.33        | 1.35     |
| 14  | Y     | 812  | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 14  | Z     | 836  | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 14  | Y     | 810  | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 14  | G     | 804  | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 14  | Z     | 835  | CLA  | C4B-NB  | -2.12 | 1.33        | 1.35     |
| 17  | J     | 104  | BCR  | C17-C18 | -2.12 | 1.33        | 1.35     |
| 14  | A     | 808  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 14  | Y     | 829  | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 14  | Y     | 809  | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | L     | 207  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 14  | Z     | 804  | CLA  | C4B-NB  | -2.12 | 1.33        | 1.35     |
| 14  | Z     | 827  | CLA  | MG-NC   | 2.12  | 2.11        | 2.06     |
| 14  | B     | 841  | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | Z     | 815  | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | H     | 801  | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 14  | G     | 817  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 14  | H     | 834  | CLA  | CHD-C4C | 2.11  | 1.47        | 1.41     |
| 14  | H     | 802  | CLA  | C4B-CHC | 2.11  | 1.46        | 1.41     |
| 14  | B     | 805  | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 14  | B     | 825  | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 14  | G     | 835  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 14  | A     | 820  | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 14  | G     | 806  | CLA  | C1B-CHB | 2.11  | 1.46        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | A     | 825 | CLA  | C4B-NB  | -2.11 | 1.33        | 1.35     |
| 14  | A     | 827 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 14  | d     | 202 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 14  | A     | 802 | CLA  | C4B-NB  | -2.11 | 1.33        | 1.35     |
| 14  | Z     | 823 | CLA  | C1B-CHB | 2.11  | 1.46        | 1.41     |
| 14  | Y     | 838 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 14  | Z     | 832 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 14  | A     | 817 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 14  | Z     | 803 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 14  | Y     | 819 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 14  | H     | 827 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 14  | Z     | 807 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 14  | H     | 808 | CLA  | C4B-CHC | 2.10  | 1.46        | 1.41     |
| 14  | A     | 832 | CLA  | MG-NC   | 2.10  | 2.11        | 2.06     |
| 14  | Y     | 855 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 14  | A     | 825 | CLA  | C4B-CHC | 2.10  | 1.46        | 1.41     |
| 14  | Z     | 813 | CLA  | C1B-CHB | 2.10  | 1.46        | 1.41     |
| 14  | Y     | 820 | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 14  | B     | 826 | CLA  | CHD-C4C | 2.10  | 1.47        | 1.41     |
| 14  | Y     | 843 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 14  | Z     | 821 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 17  | Y     | 856 | BCR  | C30-C25 | -2.10 | 1.50        | 1.53     |
| 14  | G     | 830 | CLA  | C4B-CHC | 2.10  | 1.46        | 1.41     |
| 14  | A     | 827 | CLA  | CHD-C4C | 2.10  | 1.47        | 1.41     |
| 14  | Z     | 805 | CLA  | C4B-CHC | 2.09  | 1.46        | 1.41     |
| 14  | G     | 814 | CLA  | C1B-CHB | 2.09  | 1.46        | 1.41     |
| 14  | Y     | 828 | CLA  | CHD-C4C | 2.09  | 1.47        | 1.41     |
| 14  | B     | 830 | CLA  | C4B-CHC | 2.09  | 1.46        | 1.41     |
| 14  | L     | 201 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 14  | A     | 829 | CLA  | C1B-NB  | -2.09 | 1.33        | 1.35     |
| 14  | Z     | 829 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 14  | Z     | 816 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 14  | B     | 837 | CLA  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 14  | G     | 833 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 14  | B     | 822 | CLA  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 14  | B     | 825 | CLA  | C1B-CHB | 2.08  | 1.46        | 1.41     |
| 14  | G     | 843 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 14  | B     | 819 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 14  | A     | 804 | CLA  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 14  | Y     | 822 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 14  | B     | 834 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 14  | B     | 834 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 834  | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 14  | Y     | 836  | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 14  | G     | 838  | CLA  | MG-NC   | 2.07  | 2.11        | 2.06     |
| 14  | Y     | 838  | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 14  | Z     | 805  | CLA  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 14  | Y     | 826  | CLA  | CHD-C4C | 2.07  | 1.47        | 1.41     |
| 14  | A     | 852  | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 14  | B     | 826  | CLA  | C4B-NB  | -2.07 | 1.33        | 1.35     |
| 14  | W     | 1701 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 14  | B     | 804  | CLA  | C4B-NB  | -2.07 | 1.33        | 1.35     |
| 14  | Y     | 841  | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 14  | Y     | 854  | CLA  | CHD-C4C | 2.06  | 1.47        | 1.41     |
| 14  | Y     | 804  | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 14  | Z     | 834  | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 14  | B     | 813  | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 14  | G     | 827  | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 14  | G     | 825  | CLA  | CHD-C4C | 2.06  | 1.47        | 1.41     |
| 14  | A     | 852  | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 14  | A     | 817  | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 14  | G     | 802  | CLA  | MG-NC   | 2.06  | 2.11        | 2.06     |
| 14  | Y     | 831  | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 14  | Y     | 815  | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 14  | A     | 819  | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 14  | A     | 803  | CLA  | C4B-NB  | -2.06 | 1.33        | 1.35     |
| 14  | B     | 808  | CLA  | C4B-NB  | -2.06 | 1.33        | 1.35     |
| 14  | Z     | 836  | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 14  | L     | 207  | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 14  | A     | 806  | CLA  | C1B-CHB | 2.05  | 1.46        | 1.41     |
| 14  | B     | 804  | CLA  | MG-NC   | 2.05  | 2.11        | 2.06     |
| 14  | G     | 820  | CLA  | C4B-NB  | -2.05 | 1.33        | 1.35     |
| 14  | Z     | 802  | CLA  | C1B-CHB | 2.05  | 1.46        | 1.41     |
| 14  | H     | 813  | CLA  | C1B-NB  | -2.05 | 1.33        | 1.35     |
| 14  | Z     | 815  | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 14  | A     | 818  | CLA  | C1B-NB  | -2.05 | 1.33        | 1.35     |
| 14  | H     | 818  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 14  | H     | 827  | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 14  | G     | 839  | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 14  | G     | 843  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 17  | h     | 202  | BCR  | C19-C18 | 2.05  | 1.50        | 1.45     |
| 14  | Z     | 807  | CLA  | CHD-C4C | 2.05  | 1.47        | 1.41     |
| 14  | H     | 805  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 14  | H     | 836  | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | H     | 836 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 14  | Z     | 826 | CLA  | MG-NC   | 2.04  | 2.11        | 2.06     |
| 14  | G     | 816 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 14  | T     | 103 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 14  | Y     | 805 | CLA  | CHD-C4C | 2.04  | 1.46        | 1.41     |
| 14  | Y     | 842 | CLA  | C1B-NB  | -2.04 | 1.33        | 1.35     |
| 14  | A     | 830 | CLA  | C1B-NB  | -2.04 | 1.33        | 1.35     |
| 14  | B     | 836 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 14  | H     | 819 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 14  | A     | 805 | CLA  | C1B-CHB | 2.04  | 1.46        | 1.41     |
| 14  | Y     | 837 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 14  | Z     | 813 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 14  | G     | 803 | CLA  | C1B-CHB | 2.04  | 1.46        | 1.41     |
| 14  | A     | 810 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 14  | G     | 811 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 14  | G     | 813 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 14  | Z     | 809 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 14  | G     | 818 | CLA  | CHD-C4C | 2.03  | 1.46        | 1.41     |
| 14  | d     | 202 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 14  | G     | 811 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | A     | 806 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 14  | Y     | 841 | CLA  | CHD-C4C | 2.03  | 1.46        | 1.41     |
| 17  | B     | 845 | BCR  | C21-C22 | -2.03 | 1.33        | 1.35     |
| 14  | G     | 834 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 14  | G     | 804 | CLA  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 14  | B     | 826 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 14  | G     | 819 | CLA  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 14  | A     | 804 | CLA  | C1B-NB  | -2.03 | 1.33        | 1.35     |
| 14  | Y     | 809 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 14  | B     | 835 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 14  | Z     | 834 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 14  | h     | 201 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 14  | H     | 817 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | d     | 201 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | Y     | 838 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 14  | A     | 842 | CLA  | CHD-C4C | 2.02  | 1.46        | 1.41     |
| 14  | Y     | 821 | CLA  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 14  | Y     | 810 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 14  | A     | 822 | CLA  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 14  | G     | 835 | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 14  | Y     | 826 | CLA  | MG-NC   | 2.02  | 2.11        | 2.06     |
| 14  | H     | 807 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 837  | CLA  | CHD-C4C | 2.02  | 1.46        | 1.41     |
| 14  | H     | 828  | CLA  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 14  | G     | 827  | CLA  | CHD-C4C | 2.01  | 1.46        | 1.41     |
| 14  | U     | 1002 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 14  | B     | 829  | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 14  | G     | 823  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 14  | B     | 831  | CLA  | C4B-CHC | 2.01  | 1.46        | 1.41     |
| 14  | B     | 837  | CLA  | CHD-C4C | 2.01  | 1.46        | 1.41     |
| 14  | H     | 814  | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 14  | A     | 839  | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 14  | B     | 810  | CLA  | CMB-C2B | -2.01 | 1.47        | 1.51     |
| 14  | A     | 821  | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |
| 17  | R     | 102  | BCR  | C14-C13 | -2.00 | 1.33        | 1.35     |
| 14  | G     | 842  | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 14  | Y     | 821  | CLA  | C4C-C3C | 2.00  | 1.48        | 1.45     |
| 14  | G     | 807  | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |

All (6662) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | i     | 101  | BCR  | C16-C17-C18 | 30.09 | 170.25      | 127.31   |
| 17  | A     | 845  | BCR  | C16-C17-C18 | 29.27 | 169.09      | 127.31   |
| 17  | G     | 846  | BCR  | C16-C17-C18 | 28.74 | 168.33      | 127.31   |
| 17  | R     | 101  | BCR  | C16-C17-C18 | 28.38 | 167.81      | 127.31   |
| 17  | A     | 849  | BCR  | C16-C17-C18 | 28.06 | 167.35      | 127.31   |
| 17  | G     | 850  | BCR  | C16-C17-C18 | 28.00 | 167.27      | 127.31   |
| 17  | Y     | 847  | BCR  | C16-C17-C18 | 27.96 | 167.22      | 127.31   |
| 17  | f     | 105  | BCR  | C16-C17-C18 | 27.89 | 167.11      | 127.31   |
| 17  | B     | 843  | BCR  | C16-C17-C18 | 27.71 | 166.86      | 127.31   |
| 17  | S     | 1104 | BCR  | C16-C17-C18 | 27.62 | 166.72      | 127.31   |
| 17  | Y     | 850  | BCR  | C16-C17-C18 | 27.60 | 166.71      | 127.31   |
| 17  | Y     | 851  | BCR  | C16-C17-C18 | 27.50 | 166.55      | 127.31   |
| 17  | Z     | 846  | BCR  | C16-C17-C18 | 27.02 | 165.87      | 127.31   |
| 17  | e     | 101  | BCR  | C20-C21-C22 | 26.86 | 165.64      | 127.31   |
| 17  | J     | 103  | BCR  | C16-C17-C18 | 26.82 | 165.59      | 127.31   |
| 17  | B     | 847  | BCR  | C16-C17-C18 | 26.81 | 165.57      | 127.31   |
| 17  | G     | 849  | BCR  | C16-C17-C18 | 26.62 | 165.31      | 127.31   |
| 17  | Z     | 845  | BCR  | C16-C17-C18 | 26.60 | 165.27      | 127.31   |
| 17  | F     | 203  | BCR  | C16-C17-C18 | 26.44 | 165.05      | 127.31   |
| 17  | Y     | 846  | BCR  | C16-C17-C18 | 26.38 | 164.96      | 127.31   |
| 17  | B     | 844  | BCR  | C16-C17-C18 | 26.37 | 164.95      | 127.31   |
| 17  | I     | 101  | BCR  | C16-C17-C18 | 26.30 | 164.84      | 127.31   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | T     | 102  | BCR  | C16-C17-C18 | 26.23 | 164.75      | 127.31   |
| 17  | e     | 101  | BCR  | C16-C17-C18 | 26.02 | 164.45      | 127.31   |
| 17  | Y     | 848  | BCR  | C16-C17-C18 | 25.90 | 164.28      | 127.31   |
| 17  | H     | 844  | BCR  | C16-C17-C18 | 25.81 | 164.15      | 127.31   |
| 17  | Q     | 204  | BCR  | C16-C17-C18 | 25.78 | 164.11      | 127.31   |
| 17  | U     | 1008 | BCR  | C16-C17-C18 | 25.62 | 163.87      | 127.31   |
| 17  | U     | 1007 | BCR  | C16-C17-C18 | 25.54 | 163.76      | 127.31   |
| 17  | H     | 843  | BCR  | C16-C17-C18 | 25.50 | 163.71      | 127.31   |
| 17  | L     | 208  | BCR  | C16-C17-C18 | 25.39 | 163.55      | 127.31   |
| 17  | L     | 209  | BCR  | C16-C17-C18 | 25.31 | 163.43      | 127.31   |
| 17  | B     | 844  | BCR  | C20-C21-C22 | 25.28 | 163.39      | 127.31   |
| 17  | M     | 101  | BCR  | C16-C17-C18 | 25.24 | 163.33      | 127.31   |
| 17  | h     | 203  | BCR  | C16-C17-C18 | 25.24 | 163.33      | 127.31   |
| 17  | h     | 202  | BCR  | C16-C17-C18 | 25.09 | 163.11      | 127.31   |
| 17  | K     | 102  | BCR  | C16-C17-C18 | 25.08 | 163.11      | 127.31   |
| 17  | Q     | 202  | BCR  | C16-C17-C18 | 25.00 | 162.99      | 127.31   |
| 17  | Y     | 856  | BCR  | C16-C17-C18 | 24.99 | 162.98      | 127.31   |
| 17  | H     | 840  | BCR  | C16-C17-C18 | 24.97 | 162.95      | 127.31   |
| 17  | R     | 101  | BCR  | C20-C21-C22 | 24.96 | 162.93      | 127.31   |
| 17  | V     | 1202 | BCR  | C16-C17-C18 | 24.95 | 162.92      | 127.31   |
| 17  | U     | 1005 | BCR  | C16-C17-C18 | 24.93 | 162.89      | 127.31   |
| 17  | f     | 103  | BCR  | C16-C17-C18 | 24.89 | 162.84      | 127.31   |
| 17  | G     | 847  | BCR  | C16-C17-C18 | 24.85 | 162.78      | 127.31   |
| 17  | Z     | 843  | BCR  | C16-C17-C18 | 24.85 | 162.78      | 127.31   |
| 17  | A     | 848  | BCR  | C16-C17-C18 | 24.84 | 162.76      | 127.31   |
| 17  | B     | 846  | BCR  | C16-C17-C18 | 24.81 | 162.71      | 127.31   |
| 17  | Z     | 842  | BCR  | C16-C17-C18 | 24.78 | 162.68      | 127.31   |
| 17  | I     | 101  | BCR  | C20-C21-C22 | 24.78 | 162.67      | 127.31   |
| 17  | d     | 203  | BCR  | C16-C17-C18 | 24.76 | 162.65      | 127.31   |
| 17  | F     | 201  | BCR  | C16-C17-C18 | 24.65 | 162.49      | 127.31   |
| 17  | Z     | 841  | BCR  | C16-C17-C18 | 24.64 | 162.47      | 127.31   |
| 17  | Y     | 849  | BCR  | C16-C17-C18 | 24.55 | 162.35      | 127.31   |
| 17  | H     | 841  | BCR  | C16-C17-C18 | 24.53 | 162.32      | 127.31   |
| 17  | H     | 848  | BCR  | C16-C17-C18 | 24.45 | 162.20      | 127.31   |
| 17  | R     | 102  | BCR  | C16-C17-C18 | 24.25 | 161.91      | 127.31   |
| 17  | H     | 845  | BCR  | C15-C16-C17 | 24.23 | 173.11      | 123.47   |
| 17  | B     | 851  | BCR  | C16-C17-C18 | 24.21 | 161.87      | 127.31   |
| 17  | B     | 848  | BCR  | C16-C17-C18 | 24.18 | 161.81      | 127.31   |
| 17  | G     | 848  | BCR  | C16-C17-C18 | 23.82 | 161.30      | 127.31   |
| 17  | J     | 104  | BCR  | C16-C17-C18 | 23.60 | 160.99      | 127.31   |
| 17  | B     | 845  | BCR  | C16-C17-C18 | 23.55 | 160.91      | 127.31   |
| 17  | G     | 854  | BCR  | C16-C17-C18 | 23.53 | 160.90      | 127.31   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | T     | 102  | BCR  | C20-C21-C22 | 23.46 | 160.80      | 127.31   |
| 17  | H     | 840  | BCR  | C20-C21-C22 | 23.45 | 160.78      | 127.31   |
| 17  | Y     | 849  | BCR  | C15-C16-C17 | 23.45 | 171.51      | 123.47   |
| 17  | A     | 846  | BCR  | C16-C17-C18 | 23.42 | 160.73      | 127.31   |
| 17  | Y     | 856  | BCR  | C15-C16-C17 | 23.40 | 171.40      | 123.47   |
| 17  | Z     | 841  | BCR  | C15-C16-C17 | 23.35 | 171.30      | 123.47   |
| 17  | H     | 845  | BCR  | C16-C17-C18 | 23.29 | 160.54      | 127.31   |
| 17  | A     | 847  | BCR  | C16-C17-C18 | 23.26 | 160.50      | 127.31   |
| 17  | Y     | 846  | BCR  | C20-C21-C22 | 23.24 | 160.47      | 127.31   |
| 17  | f     | 104  | BCR  | C16-C17-C18 | 23.07 | 160.23      | 127.31   |
| 17  | Z     | 844  | BCR  | C16-C17-C18 | 22.99 | 160.12      | 127.31   |
| 17  | L     | 203  | BCR  | C16-C17-C18 | 22.90 | 159.99      | 127.31   |
| 17  | K     | 102  | BCR  | C20-C21-C22 | 22.87 | 159.95      | 127.31   |
| 17  | H     | 842  | BCR  | C16-C17-C18 | 22.86 | 159.94      | 127.31   |
| 17  | A     | 847  | BCR  | C15-C16-C17 | 22.85 | 170.28      | 123.47   |
| 17  | G     | 848  | BCR  | C20-C21-C22 | 22.72 | 159.74      | 127.31   |
| 17  | Y     | 849  | BCR  | C20-C21-C22 | 22.70 | 159.71      | 127.31   |
| 17  | V     | 1202 | BCR  | C15-C16-C17 | 22.68 | 169.94      | 123.47   |
| 17  | A     | 846  | BCR  | C15-C16-C17 | 22.53 | 169.62      | 123.47   |
| 17  | U     | 1007 | BCR  | C15-C16-C17 | 22.40 | 169.35      | 123.47   |
| 17  | G     | 850  | BCR  | C20-C21-C22 | 22.38 | 159.25      | 127.31   |
| 17  | M     | 101  | BCR  | C15-C16-C17 | 22.37 | 169.29      | 123.47   |
| 17  | B     | 851  | BCR  | C15-C16-C17 | 22.35 | 169.27      | 123.47   |
| 17  | H     | 842  | BCR  | C15-C16-C17 | 22.32 | 169.19      | 123.47   |
| 17  | S     | 1104 | BCR  | C20-C21-C22 | 22.24 | 159.05      | 127.31   |
| 17  | Y     | 848  | BCR  | C15-C16-C17 | 22.16 | 168.86      | 123.47   |
| 17  | d     | 203  | BCR  | C15-C16-C17 | 22.11 | 168.77      | 123.47   |
| 17  | H     | 842  | BCR  | C20-C21-C22 | 22.05 | 158.78      | 127.31   |
| 17  | A     | 849  | BCR  | C20-C21-C22 | 22.02 | 158.74      | 127.31   |
| 17  | L     | 203  | BCR  | C15-C16-C17 | 22.02 | 168.58      | 123.47   |
| 17  | U     | 1008 | BCR  | C15-C16-C17 | 21.98 | 168.51      | 123.47   |
| 17  | G     | 848  | BCR  | C15-C16-C17 | 21.97 | 168.49      | 123.47   |
| 17  | Z     | 844  | BCR  | C15-C16-C17 | 21.95 | 168.44      | 123.47   |
| 17  | f     | 103  | BCR  | C15-C16-C17 | 21.89 | 168.32      | 123.47   |
| 17  | A     | 848  | BCR  | C15-C16-C17 | 21.87 | 168.28      | 123.47   |
| 17  | G     | 847  | BCR  | C15-C16-C17 | 21.84 | 168.22      | 123.47   |
| 17  | A     | 847  | BCR  | C20-C21-C22 | 21.83 | 158.46      | 127.31   |
| 17  | L     | 208  | BCR  | C15-C16-C17 | 21.77 | 168.07      | 123.47   |
| 17  | H     | 848  | BCR  | C15-C16-C17 | 21.71 | 167.95      | 123.47   |
| 17  | Z     | 842  | BCR  | C15-C16-C17 | 21.67 | 167.86      | 123.47   |
| 17  | B     | 845  | BCR  | C15-C16-C17 | 21.64 | 167.80      | 123.47   |
| 17  | h     | 202  | BCR  | C15-C16-C17 | 21.45 | 167.42      | 123.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | H     | 840  | BCR  | C15-C16-C17 | 21.43 | 167.38      | 123.47   |
| 17  | U     | 1005 | BCR  | C15-C16-C17 | 21.33 | 167.17      | 123.47   |
| 17  | f     | 104  | BCR  | C15-C16-C17 | 21.32 | 167.14      | 123.47   |
| 17  | L     | 209  | BCR  | C15-C16-C17 | 21.31 | 167.13      | 123.47   |
| 17  | Z     | 842  | BCR  | C20-C21-C22 | 21.27 | 157.66      | 127.31   |
| 17  | Q     | 204  | BCR  | C15-C16-C17 | 21.22 | 166.94      | 123.47   |
| 17  | B     | 848  | BCR  | C15-C16-C17 | 21.21 | 166.93      | 123.47   |
| 17  | F     | 201  | BCR  | C15-C16-C17 | 21.14 | 166.78      | 123.47   |
| 17  | e     | 101  | BCR  | C15-C16-C17 | 21.14 | 166.77      | 123.47   |
| 17  | Z     | 843  | BCR  | C15-C16-C17 | 21.09 | 166.68      | 123.47   |
| 17  | H     | 843  | BCR  | C15-C16-C17 | 21.06 | 166.61      | 123.47   |
| 17  | K     | 102  | BCR  | C15-C16-C17 | 21.04 | 166.58      | 123.47   |
| 17  | R     | 102  | BCR  | C15-C16-C17 | 21.04 | 166.56      | 123.47   |
| 17  | G     | 854  | BCR  | C15-C16-C17 | 21.02 | 166.53      | 123.47   |
| 17  | I     | 101  | BCR  | C15-C16-C17 | 20.96 | 166.41      | 123.47   |
| 17  | B     | 844  | BCR  | C15-C16-C17 | 20.86 | 166.20      | 123.47   |
| 17  | Z     | 841  | BCR  | C20-C21-C22 | 20.85 | 157.07      | 127.31   |
| 17  | L     | 203  | BCR  | C20-C21-C22 | 20.83 | 157.04      | 127.31   |
| 17  | Z     | 846  | BCR  | C20-C21-C22 | 20.79 | 156.98      | 127.31   |
| 17  | h     | 203  | BCR  | C15-C16-C17 | 20.77 | 166.03      | 123.47   |
| 17  | B     | 843  | BCR  | C20-C21-C22 | 20.72 | 157.01      | 127.30   |
| 17  | i     | 101  | BCR  | C20-C21-C22 | 20.72 | 156.88      | 127.31   |
| 17  | G     | 849  | BCR  | C15-C16-C17 | 20.45 | 165.38      | 123.47   |
| 17  | A     | 848  | BCR  | C20-C21-C22 | 20.45 | 156.50      | 127.31   |
| 17  | G     | 854  | BCR  | C20-C21-C22 | 20.43 | 156.46      | 127.31   |
| 17  | L     | 208  | BCR  | C20-C21-C22 | 20.42 | 156.45      | 127.31   |
| 17  | Y     | 851  | BCR  | C15-C16-C17 | 20.41 | 165.28      | 123.47   |
| 17  | B     | 845  | BCR  | C20-C21-C22 | 20.37 | 156.38      | 127.31   |
| 17  | H     | 841  | BCR  | C15-C16-C17 | 20.34 | 165.14      | 123.47   |
| 17  | J     | 103  | BCR  | C20-C21-C22 | 20.32 | 156.32      | 127.31   |
| 17  | H     | 844  | BCR  | C15-C16-C17 | 20.32 | 165.09      | 123.47   |
| 17  | J     | 104  | BCR  | C15-C16-C17 | 20.31 | 165.09      | 123.47   |
| 17  | H     | 845  | BCR  | C20-C21-C22 | 20.29 | 156.27      | 127.31   |
| 17  | T     | 102  | BCR  | C15-C16-C17 | 20.28 | 165.01      | 123.47   |
| 17  | B     | 847  | BCR  | C15-C16-C17 | 20.27 | 165.00      | 123.47   |
| 17  | Z     | 843  | BCR  | C20-C21-C22 | 20.19 | 156.13      | 127.31   |
| 17  | B     | 846  | BCR  | C15-C16-C17 | 20.18 | 164.82      | 123.47   |
| 17  | U     | 1007 | BCR  | C20-C21-C22 | 20.11 | 156.01      | 127.31   |
| 17  | Y     | 851  | BCR  | C20-C21-C22 | 20.09 | 155.98      | 127.31   |
| 17  | R     | 101  | BCR  | C15-C16-C17 | 20.05 | 164.55      | 123.47   |
| 17  | G     | 850  | BCR  | C15-C16-C17 | 20.05 | 164.54      | 123.47   |
| 17  | A     | 849  | BCR  | C15-C16-C17 | 20.03 | 164.51      | 123.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Z     | 845  | BCR  | C15-C16-C17 | 19.93 | 164.30      | 123.47   |
| 17  | F     | 203  | BCR  | C15-C16-C17 | 19.85 | 164.14      | 123.47   |
| 17  | f     | 103  | BCR  | C20-C21-C22 | 19.80 | 155.56      | 127.31   |
| 17  | Y     | 848  | BCR  | C20-C21-C22 | 19.74 | 155.49      | 127.31   |
| 17  | U     | 1005 | BCR  | C20-C21-C22 | 19.74 | 155.48      | 127.31   |
| 17  | G     | 846  | BCR  | C20-C21-C22 | 19.65 | 155.35      | 127.31   |
| 17  | h     | 203  | BCR  | C20-C21-C22 | 19.61 | 155.29      | 127.31   |
| 17  | Y     | 850  | BCR  | C15-C16-C17 | 19.50 | 163.41      | 123.47   |
| 17  | f     | 105  | BCR  | C20-C21-C22 | 19.50 | 155.13      | 127.31   |
| 17  | G     | 849  | BCR  | C20-C21-C22 | 19.42 | 155.02      | 127.31   |
| 17  | Y     | 846  | BCR  | C15-C16-C17 | 19.39 | 163.19      | 123.47   |
| 17  | R     | 102  | BCR  | C20-C21-C22 | 19.35 | 154.93      | 127.31   |
| 17  | H     | 844  | BCR  | C20-C21-C22 | 19.34 | 154.91      | 127.31   |
| 17  | H     | 841  | BCR  | C20-C21-C22 | 19.24 | 154.76      | 127.31   |
| 17  | B     | 847  | BCR  | C20-C21-C22 | 19.17 | 154.67      | 127.31   |
| 17  | A     | 845  | BCR  | C20-C21-C22 | 19.16 | 154.66      | 127.31   |
| 17  | S     | 1104 | BCR  | C15-C16-C17 | 19.13 | 162.67      | 123.47   |
| 17  | M     | 101  | BCR  | C20-C21-C22 | 19.13 | 154.61      | 127.31   |
| 17  | Y     | 847  | BCR  | C20-C21-C22 | 19.09 | 154.55      | 127.31   |
| 17  | J     | 104  | BCR  | C20-C21-C22 | 18.99 | 154.41      | 127.31   |
| 17  | f     | 104  | BCR  | C20-C21-C22 | 18.91 | 154.30      | 127.31   |
| 17  | A     | 846  | BCR  | C20-C21-C22 | 18.87 | 154.24      | 127.31   |
| 17  | Z     | 844  | BCR  | C20-C21-C22 | 18.87 | 154.23      | 127.31   |
| 17  | B     | 848  | BCR  | C20-C21-C22 | 18.77 | 154.10      | 127.31   |
| 17  | G     | 847  | BCR  | C20-C21-C22 | 18.75 | 154.08      | 127.31   |
| 17  | H     | 843  | BCR  | C20-C21-C22 | 18.64 | 153.91      | 127.31   |
| 17  | i     | 101  | BCR  | C15-C16-C17 | 18.49 | 161.35      | 123.47   |
| 17  | H     | 848  | BCR  | C20-C21-C22 | 18.33 | 153.47      | 127.31   |
| 17  | Z     | 846  | BCR  | C15-C16-C17 | 18.29 | 160.93      | 123.47   |
| 17  | d     | 203  | BCR  | C20-C21-C22 | 18.05 | 153.07      | 127.31   |
| 17  | U     | 1007 | BCR  | C10-C11-C12 | 18.01 | 179.43      | 123.22   |
| 17  | B     | 851  | BCR  | C20-C21-C22 | 17.94 | 152.91      | 127.31   |
| 17  | Q     | 202  | BCR  | C20-C21-C22 | 17.81 | 152.72      | 127.31   |
| 17  | Y     | 856  | BCR  | C20-C21-C22 | 17.77 | 152.66      | 127.31   |
| 17  | G     | 847  | BCR  | C10-C11-C12 | 17.75 | 178.59      | 123.22   |
| 17  | Z     | 845  | BCR  | C10-C11-C12 | 17.60 | 178.14      | 123.22   |
| 17  | V     | 1202 | BCR  | C20-C21-C22 | 17.58 | 152.39      | 127.31   |
| 17  | h     | 202  | BCR  | C20-C21-C22 | 17.50 | 152.29      | 127.31   |
| 17  | B     | 846  | BCR  | C20-C21-C22 | 17.49 | 152.27      | 127.31   |
| 17  | Z     | 845  | BCR  | C20-C21-C22 | 17.49 | 152.27      | 127.31   |
| 17  | Y     | 847  | BCR  | C10-C11-C12 | 17.49 | 177.78      | 123.22   |
| 17  | Q     | 204  | BCR  | C20-C21-C22 | 17.47 | 152.24      | 127.31   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Y     | 850  | BCR  | C20-C21-C22 | 17.47 | 152.24      | 127.31   |
| 17  | G     | 846  | BCR  | C10-C11-C12 | 17.45 | 177.67      | 123.22   |
| 17  | B     | 844  | BCR  | C10-C11-C12 | 17.43 | 177.62      | 123.22   |
| 17  | M     | 101  | BCR  | C10-C11-C12 | 17.29 | 177.19      | 123.22   |
| 17  | L     | 209  | BCR  | C20-C21-C22 | 17.20 | 151.86      | 127.31   |
| 17  | Z     | 843  | BCR  | C11-C10-C9  | 17.19 | 151.84      | 127.31   |
| 17  | f     | 105  | BCR  | C15-C16-C17 | 17.11 | 158.52      | 123.47   |
| 17  | f     | 104  | BCR  | C10-C11-C12 | 17.07 | 176.50      | 123.22   |
| 17  | i     | 101  | BCR  | C10-C11-C12 | 17.06 | 176.46      | 123.22   |
| 17  | J     | 104  | BCR  | C10-C11-C12 | 17.06 | 176.45      | 123.22   |
| 17  | B     | 847  | BCR  | C10-C11-C12 | 16.95 | 176.11      | 123.22   |
| 17  | h     | 202  | BCR  | C10-C11-C12 | 16.93 | 176.05      | 123.22   |
| 17  | T     | 102  | BCR  | C10-C11-C12 | 16.92 | 176.03      | 123.22   |
| 17  | B     | 845  | BCR  | C10-C11-C12 | 16.91 | 175.97      | 123.22   |
| 17  | d     | 203  | BCR  | C10-C11-C12 | 16.87 | 175.86      | 123.22   |
| 17  | H     | 845  | BCR  | C10-C11-C12 | 16.85 | 175.81      | 123.22   |
| 17  | F     | 201  | BCR  | C20-C21-C22 | 16.85 | 151.35      | 127.31   |
| 17  | S     | 1104 | BCR  | C10-C11-C12 | 16.84 | 175.78      | 123.22   |
| 17  | B     | 843  | BCR  | C10-C11-C12 | 16.84 | 175.78      | 123.22   |
| 17  | f     | 103  | BCR  | C10-C11-C12 | 16.81 | 175.69      | 123.22   |
| 17  | Y     | 849  | BCR  | C10-C11-C12 | 16.81 | 175.67      | 123.22   |
| 17  | H     | 841  | BCR  | C10-C11-C12 | 16.80 | 175.64      | 123.22   |
| 17  | H     | 840  | BCR  | C10-C11-C12 | 16.76 | 175.52      | 123.22   |
| 17  | A     | 847  | BCR  | C10-C11-C12 | 16.72 | 175.40      | 123.22   |
| 17  | F     | 203  | BCR  | C20-C21-C22 | 16.71 | 151.16      | 127.31   |
| 17  | I     | 101  | BCR  | C10-C11-C12 | 16.68 | 175.26      | 123.22   |
| 17  | H     | 844  | BCR  | C10-C11-C12 | 16.65 | 175.18      | 123.22   |
| 17  | Y     | 848  | BCR  | C10-C11-C12 | 16.61 | 175.07      | 123.22   |
| 17  | U     | 1005 | BCR  | C10-C11-C12 | 16.59 | 175.00      | 123.22   |
| 17  | A     | 846  | BCR  | C10-C11-C12 | 16.59 | 174.99      | 123.22   |
| 17  | H     | 848  | BCR  | C10-C11-C12 | 16.53 | 174.81      | 123.22   |
| 17  | G     | 848  | BCR  | C10-C11-C12 | 16.51 | 174.74      | 123.22   |
| 17  | A     | 845  | BCR  | C15-C16-C17 | 16.51 | 157.29      | 123.47   |
| 17  | B     | 851  | BCR  | C10-C11-C12 | 16.51 | 174.73      | 123.22   |
| 17  | H     | 842  | BCR  | C10-C11-C12 | 16.50 | 174.71      | 123.22   |
| 17  | A     | 845  | BCR  | C10-C11-C12 | 16.47 | 174.62      | 123.22   |
| 17  | V     | 1202 | BCR  | C10-C11-C12 | 16.39 | 174.37      | 123.22   |
| 17  | L     | 209  | BCR  | C10-C11-C12 | 16.39 | 174.35      | 123.22   |
| 17  | G     | 846  | BCR  | C15-C16-C17 | 16.32 | 156.90      | 123.47   |
| 17  | Y     | 851  | BCR  | C10-C11-C12 | 16.30 | 174.09      | 123.22   |
| 17  | Y     | 847  | BCR  | C15-C16-C17 | 16.22 | 156.70      | 123.47   |
| 17  | Z     | 842  | BCR  | C10-C11-C12 | 16.21 | 173.80      | 123.22   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Q     | 202  | BCR  | C10-C11-C12 | 16.20 | 173.77      | 123.22   |
| 17  | Z     | 843  | BCR  | C10-C11-C12 | 16.16 | 173.65      | 123.22   |
| 17  | A     | 848  | BCR  | C10-C11-C12 | 16.16 | 173.63      | 123.22   |
| 17  | U     | 1008 | BCR  | C20-C21-C22 | 16.09 | 150.28      | 127.31   |
| 17  | K     | 102  | BCR  | C10-C11-C12 | 16.09 | 173.42      | 123.22   |
| 17  | Y     | 850  | BCR  | C10-C11-C12 | 16.06 | 173.34      | 123.22   |
| 17  | G     | 854  | BCR  | C10-C11-C12 | 16.02 | 173.22      | 123.22   |
| 17  | F     | 203  | BCR  | C21-C20-C19 | 15.97 | 173.06      | 123.22   |
| 17  | F     | 203  | BCR  | C10-C11-C12 | 15.93 | 172.93      | 123.22   |
| 17  | h     | 203  | BCR  | C10-C11-C12 | 15.91 | 172.87      | 123.22   |
| 17  | R     | 101  | BCR  | C10-C11-C12 | 15.91 | 172.86      | 123.22   |
| 17  | B     | 843  | BCR  | C15-C16-C17 | 15.82 | 155.88      | 123.47   |
| 17  | G     | 854  | BCR  | C11-C12-C13 | 15.82 | 170.85      | 126.42   |
| 17  | Y     | 856  | BCR  | C21-C20-C19 | 15.77 | 172.44      | 123.22   |
| 17  | J     | 103  | BCR  | C15-C16-C17 | 15.77 | 155.78      | 123.47   |
| 17  | Z     | 841  | BCR  | C10-C11-C12 | 15.77 | 172.42      | 123.22   |
| 17  | f     | 105  | BCR  | C10-C11-C12 | 15.73 | 172.32      | 123.22   |
| 17  | i     | 101  | BCR  | C16-C15-C14 | 15.73 | 155.69      | 123.47   |
| 17  | U     | 1008 | BCR  | C10-C11-C12 | 15.70 | 172.21      | 123.22   |
| 17  | U     | 1008 | BCR  | C21-C20-C19 | 15.66 | 172.08      | 123.22   |
| 17  | F     | 201  | BCR  | C21-C20-C19 | 15.58 | 171.84      | 123.22   |
| 17  | L     | 209  | BCR  | C21-C20-C19 | 15.48 | 171.53      | 123.22   |
| 17  | Q     | 202  | BCR  | C21-C20-C19 | 15.39 | 171.24      | 123.22   |
| 17  | Q     | 204  | BCR  | C10-C11-C12 | 15.39 | 171.24      | 123.22   |
| 17  | Y     | 850  | BCR  | C21-C20-C19 | 15.35 | 171.13      | 123.22   |
| 17  | Z     | 846  | BCR  | C10-C11-C12 | 15.29 | 170.95      | 123.22   |
| 17  | A     | 849  | BCR  | C10-C11-C12 | 15.22 | 170.73      | 123.22   |
| 17  | L     | 208  | BCR  | C10-C11-C12 | 15.22 | 170.71      | 123.22   |
| 17  | R     | 101  | BCR  | C11-C12-C13 | 15.17 | 169.03      | 126.42   |
| 17  | d     | 203  | BCR  | C21-C20-C19 | 15.16 | 170.54      | 123.22   |
| 17  | Z     | 844  | BCR  | C21-C20-C19 | 15.16 | 170.53      | 123.22   |
| 17  | Y     | 846  | BCR  | C10-C11-C12 | 15.10 | 170.34      | 123.22   |
| 17  | H     | 848  | BCR  | C11-C12-C13 | 15.09 | 168.82      | 126.42   |
| 17  | G     | 850  | BCR  | C10-C11-C12 | 15.08 | 170.28      | 123.22   |
| 17  | f     | 104  | BCR  | C21-C20-C19 | 15.08 | 170.26      | 123.22   |
| 17  | B     | 851  | BCR  | C21-C20-C19 | 15.02 | 170.09      | 123.22   |
| 17  | Q     | 204  | BCR  | C21-C20-C19 | 15.01 | 170.07      | 123.22   |
| 17  | L     | 203  | BCR  | C10-C11-C12 | 14.97 | 169.94      | 123.22   |
| 17  | J     | 104  | BCR  | C21-C20-C19 | 14.96 | 169.89      | 123.22   |
| 17  | R     | 102  | BCR  | C10-C11-C12 | 14.95 | 169.88      | 123.22   |
| 17  | Y     | 856  | BCR  | C10-C11-C12 | 14.90 | 169.72      | 123.22   |
| 17  | Z     | 845  | BCR  | C21-C20-C19 | 14.87 | 169.63      | 123.22   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | f     | 105  | BCR  | C16-C15-C14 | 14.87 | 153.94      | 123.47   |
| 17  | J     | 103  | BCR  | C10-C11-C12 | 14.85 | 169.56      | 123.22   |
| 17  | B     | 848  | BCR  | C21-C20-C19 | 14.84 | 169.52      | 123.22   |
| 17  | H     | 844  | BCR  | C21-C20-C19 | 14.82 | 169.46      | 123.22   |
| 17  | F     | 201  | BCR  | C11-C12-C13 | 14.79 | 167.97      | 126.42   |
| 17  | V     | 1202 | BCR  | C21-C20-C19 | 14.77 | 169.30      | 123.22   |
| 17  | f     | 103  | BCR  | C11-C12-C13 | 14.73 | 167.78      | 126.42   |
| 17  | A     | 846  | BCR  | C21-C20-C19 | 14.70 | 169.08      | 123.22   |
| 17  | Y     | 851  | BCR  | C11-C10-C9  | 14.64 | 148.20      | 127.31   |
| 17  | h     | 202  | BCR  | C21-C20-C19 | 14.61 | 168.81      | 123.22   |
| 17  | U     | 1008 | BCR  | C11-C12-C13 | 14.60 | 167.44      | 126.42   |
| 17  | H     | 848  | BCR  | C21-C20-C19 | 14.51 | 168.50      | 123.22   |
| 17  | B     | 848  | BCR  | C10-C11-C12 | 14.50 | 168.46      | 123.22   |
| 17  | L     | 209  | BCR  | C11-C12-C13 | 14.45 | 167.02      | 126.42   |
| 17  | B     | 846  | BCR  | C21-C20-C19 | 14.43 | 168.24      | 123.22   |
| 17  | Q     | 202  | BCR  | C15-C16-C17 | 14.42 | 153.02      | 123.47   |
| 17  | H     | 845  | BCR  | C21-C20-C19 | 14.40 | 168.14      | 123.22   |
| 17  | Y     | 846  | BCR  | C16-C15-C14 | 14.39 | 152.95      | 123.47   |
| 17  | Z     | 841  | BCR  | C21-C20-C19 | 14.38 | 168.08      | 123.22   |
| 17  | e     | 101  | BCR  | C10-C11-C12 | 14.37 | 168.05      | 123.22   |
| 17  | B     | 851  | BCR  | C11-C12-C13 | 14.36 | 166.76      | 126.42   |
| 17  | B     | 845  | BCR  | C21-C20-C19 | 14.34 | 167.97      | 123.22   |
| 17  | Y     | 846  | BCR  | C11-C10-C9  | 14.32 | 147.74      | 127.31   |
| 17  | h     | 203  | BCR  | C21-C20-C19 | 14.30 | 167.85      | 123.22   |
| 17  | G     | 847  | BCR  | C21-C20-C19 | 14.30 | 167.83      | 123.22   |
| 17  | B     | 846  | BCR  | C16-C15-C14 | 14.26 | 152.69      | 123.47   |
| 17  | H     | 843  | BCR  | C21-C20-C19 | 14.23 | 167.63      | 123.22   |
| 17  | h     | 203  | BCR  | C11-C12-C13 | 14.20 | 166.29      | 126.42   |
| 17  | G     | 854  | BCR  | C21-C20-C19 | 14.19 | 167.49      | 123.22   |
| 17  | Z     | 845  | BCR  | C16-C15-C14 | 14.17 | 152.50      | 123.47   |
| 17  | Z     | 846  | BCR  | C11-C12-C13 | 14.17 | 166.22      | 126.42   |
| 17  | R     | 102  | BCR  | C21-C20-C19 | 14.17 | 167.42      | 123.22   |
| 17  | B     | 847  | BCR  | C11-C12-C13 | 14.16 | 166.20      | 126.42   |
| 17  | Y     | 850  | BCR  | C11-C12-C13 | 14.15 | 166.18      | 126.42   |
| 17  | Y     | 848  | BCR  | C11-C12-C13 | 14.14 | 166.13      | 126.42   |
| 17  | U     | 1008 | BCR  | C11-C10-C9  | 14.13 | 147.47      | 127.31   |
| 17  | G     | 849  | BCR  | C10-C11-C12 | 14.12 | 167.29      | 123.22   |
| 17  | f     | 105  | BCR  | C11-C12-C13 | 14.12 | 166.09      | 126.42   |
| 17  | A     | 847  | BCR  | C11-C12-C13 | 14.08 | 165.96      | 126.42   |
| 17  | G     | 854  | BCR  | C16-C15-C14 | 14.05 | 152.25      | 123.47   |
| 17  | G     | 846  | BCR  | C16-C15-C14 | 14.03 | 152.22      | 123.47   |
| 17  | Y     | 849  | BCR  | C11-C12-C13 | 13.98 | 165.69      | 126.42   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Y     | 847  | BCR  | C21-C20-C19 | 13.98 | 166.83      | 123.22   |
| 17  | H     | 841  | BCR  | C21-C20-C19 | 13.95 | 166.76      | 123.22   |
| 17  | Q     | 202  | BCR  | C11-C12-C13 | 13.95 | 165.61      | 126.42   |
| 17  | B     | 847  | BCR  | C21-C20-C19 | 13.95 | 166.75      | 123.22   |
| 17  | A     | 848  | BCR  | C21-C20-C19 | 13.94 | 166.73      | 123.22   |
| 17  | M     | 101  | BCR  | C21-C20-C19 | 13.94 | 166.73      | 123.22   |
| 17  | f     | 103  | BCR  | C21-C20-C19 | 13.93 | 166.68      | 123.22   |
| 17  | Y     | 847  | BCR  | C11-C12-C13 | 13.92 | 165.53      | 126.42   |
| 17  | Y     | 851  | BCR  | C21-C20-C19 | 13.91 | 166.64      | 123.22   |
| 17  | H     | 842  | BCR  | C21-C20-C19 | 13.91 | 166.63      | 123.22   |
| 17  | G     | 846  | BCR  | C21-C20-C19 | 13.86 | 166.48      | 123.22   |
| 17  | S     | 1104 | BCR  | C16-C15-C14 | 13.86 | 151.87      | 123.47   |
| 17  | M     | 101  | BCR  | C11-C12-C13 | 13.86 | 165.35      | 126.42   |
| 17  | J     | 103  | BCR  | C16-C15-C14 | 13.86 | 151.86      | 123.47   |
| 17  | T     | 102  | BCR  | C16-C15-C14 | 13.84 | 151.83      | 123.47   |
| 17  | J     | 104  | BCR  | C11-C12-C13 | 13.81 | 165.22      | 126.42   |
| 17  | Z     | 843  | BCR  | C21-C20-C19 | 13.80 | 166.28      | 123.22   |
| 17  | F     | 203  | BCR  | C16-C15-C14 | 13.79 | 151.73      | 123.47   |
| 17  | A     | 849  | BCR  | C11-C12-C13 | 13.77 | 165.10      | 126.42   |
| 17  | G     | 849  | BCR  | C21-C20-C19 | 13.77 | 166.19      | 123.22   |
| 17  | H     | 844  | BCR  | C16-C15-C14 | 13.77 | 151.67      | 123.47   |
| 17  | S     | 1104 | BCR  | C11-C12-C13 | 13.75 | 165.04      | 126.42   |
| 17  | A     | 845  | BCR  | C21-C20-C19 | 13.72 | 166.04      | 123.22   |
| 17  | H     | 840  | BCR  | C11-C12-C13 | 13.71 | 164.93      | 126.42   |
| 17  | B     | 843  | BCR  | C21-C20-C19 | 13.71 | 166.00      | 123.22   |
| 17  | I     | 101  | BCR  | C11-C12-C13 | 13.71 | 164.93      | 126.42   |
| 17  | Z     | 846  | BCR  | C21-C20-C19 | 13.69 | 165.94      | 123.22   |
| 17  | T     | 102  | BCR  | C11-C12-C13 | 13.68 | 164.86      | 126.42   |
| 17  | J     | 104  | BCR  | C16-C15-C14 | 13.68 | 151.51      | 123.47   |
| 17  | Y     | 847  | BCR  | C16-C15-C14 | 13.68 | 151.50      | 123.47   |
| 17  | L     | 203  | BCR  | C21-C20-C19 | 13.68 | 165.90      | 123.22   |
| 17  | R     | 102  | BCR  | C11-C10-C9  | 13.67 | 146.81      | 127.31   |
| 17  | J     | 103  | BCR  | C21-C20-C19 | 13.64 | 165.80      | 123.22   |
| 17  | f     | 105  | BCR  | C21-C20-C19 | 13.64 | 165.78      | 123.22   |
| 17  | Y     | 850  | BCR  | C16-C15-C14 | 13.62 | 151.38      | 123.47   |
| 17  | Y     | 848  | BCR  | C21-C20-C19 | 13.58 | 165.61      | 123.22   |
| 17  | B     | 845  | BCR  | C11-C12-C13 | 13.57 | 164.54      | 126.42   |
| 17  | A     | 848  | BCR  | C11-C12-C13 | 13.54 | 164.44      | 126.42   |
| 17  | G     | 850  | BCR  | C11-C12-C13 | 13.53 | 164.44      | 126.42   |
| 17  | A     | 847  | BCR  | C21-C20-C19 | 13.52 | 165.41      | 123.22   |
| 17  | Z     | 843  | BCR  | C11-C12-C13 | 13.50 | 164.34      | 126.42   |
| 17  | A     | 845  | BCR  | C11-C12-C13 | 13.49 | 164.32      | 126.42   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | i     | 101  | BCR  | C11-C12-C13 | 13.48 | 164.29      | 126.42   |
| 17  | H     | 841  | BCR  | C11-C12-C13 | 13.47 | 164.24      | 126.42   |
| 17  | B     | 843  | BCR  | C16-C15-C14 | 13.46 | 151.05      | 123.47   |
| 17  | F     | 203  | BCR  | C11-C12-C13 | 13.45 | 164.21      | 126.42   |
| 17  | U     | 1005 | BCR  | C21-C20-C19 | 13.45 | 165.19      | 123.22   |
| 17  | U     | 1007 | BCR  | C21-C20-C19 | 13.44 | 165.15      | 123.22   |
| 17  | K     | 102  | BCR  | C11-C12-C13 | 13.43 | 164.15      | 126.42   |
| 17  | Z     | 846  | BCR  | C11-C10-C9  | 13.40 | 146.44      | 127.31   |
| 17  | H     | 845  | BCR  | C11-C12-C13 | 13.40 | 164.06      | 126.42   |
| 17  | h     | 202  | BCR  | C11-C12-C13 | 13.39 | 164.02      | 126.42   |
| 17  | G     | 846  | BCR  | C11-C12-C13 | 13.37 | 163.97      | 126.42   |
| 17  | G     | 848  | BCR  | C21-C20-C19 | 13.36 | 164.92      | 123.22   |
| 17  | Q     | 204  | BCR  | C11-C12-C13 | 13.36 | 163.94      | 126.42   |
| 17  | i     | 101  | BCR  | C21-C20-C19 | 13.35 | 164.89      | 123.22   |
| 17  | B     | 844  | BCR  | C11-C12-C13 | 13.34 | 163.88      | 126.42   |
| 17  | f     | 104  | BCR  | C16-C15-C14 | 13.32 | 150.75      | 123.47   |
| 17  | Y     | 851  | BCR  | C11-C12-C13 | 13.31 | 163.82      | 126.42   |
| 17  | Z     | 846  | BCR  | C16-C15-C14 | 13.30 | 150.72      | 123.47   |
| 17  | Y     | 850  | BCR  | C11-C10-C9  | 13.29 | 146.28      | 127.31   |
| 17  | U     | 1007 | BCR  | C11-C12-C13 | 13.29 | 163.76      | 126.42   |
| 17  | Q     | 202  | BCR  | C16-C15-C14 | 13.28 | 150.67      | 123.47   |
| 17  | e     | 101  | BCR  | C11-C12-C13 | 13.27 | 163.70      | 126.42   |
| 17  | G     | 850  | BCR  | C16-C15-C14 | 13.21 | 150.54      | 123.47   |
| 17  | Y     | 846  | BCR  | C11-C12-C13 | 13.20 | 163.51      | 126.42   |
| 17  | B     | 843  | BCR  | C11-C12-C13 | 13.16 | 163.38      | 126.42   |
| 17  | G     | 847  | BCR  | C11-C12-C13 | 13.13 | 163.29      | 126.42   |
| 17  | V     | 1202 | BCR  | C11-C12-C13 | 13.12 | 163.27      | 126.42   |
| 17  | A     | 849  | BCR  | C21-C20-C19 | 13.07 | 164.01      | 123.22   |
| 17  | Z     | 842  | BCR  | C21-C20-C19 | 13.04 | 163.92      | 123.22   |
| 17  | h     | 203  | BCR  | C11-C10-C9  | 13.02 | 145.89      | 127.31   |
| 17  | L     | 208  | BCR  | C21-C20-C19 | 13.01 | 163.82      | 123.22   |
| 17  | d     | 203  | BCR  | C16-C15-C14 | 12.94 | 149.99      | 123.47   |
| 17  | Z     | 842  | BCR  | C11-C12-C13 | 12.94 | 162.77      | 126.42   |
| 17  | F     | 201  | BCR  | C10-C11-C12 | 12.93 | 163.58      | 123.22   |
| 17  | G     | 848  | BCR  | C11-C12-C13 | 12.93 | 162.74      | 126.42   |
| 17  | R     | 101  | BCR  | C11-C10-C9  | 12.92 | 145.75      | 127.31   |
| 17  | d     | 203  | BCR  | C11-C12-C13 | 12.91 | 162.68      | 126.42   |
| 17  | G     | 849  | BCR  | C11-C12-C13 | 12.89 | 162.63      | 126.42   |
| 17  | K     | 102  | BCR  | C16-C15-C14 | 12.88 | 149.86      | 123.47   |
| 17  | f     | 104  | BCR  | C11-C12-C13 | 12.88 | 162.60      | 126.42   |
| 17  | H     | 843  | BCR  | C16-C15-C14 | 12.88 | 149.85      | 123.47   |
| 17  | B     | 847  | BCR  | C16-C15-C14 | 12.87 | 149.83      | 123.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 17  | L     | 208  | BCR  | C11-C12-C13 | 12.86  | 162.55      | 126.42   |
| 17  | Z     | 845  | BCR  | C11-C12-C13 | 12.86  | 162.53      | 126.42   |
| 17  | Z     | 844  | BCR  | C16-C15-C14 | 12.82  | 149.74      | 123.47   |
| 17  | A     | 846  | BCR  | C11-C12-C13 | 12.80  | 162.39      | 126.42   |
| 17  | e     | 101  | BCR  | C11-C10-C9  | 12.79  | 145.57      | 127.31   |
| 17  | B     | 848  | BCR  | C16-C15-C14 | 12.77  | 149.64      | 123.47   |
| 17  | K     | 102  | BCR  | C24-C23-C22 | -12.74 | 106.98      | 126.23   |
| 17  | H     | 842  | BCR  | C11-C10-C9  | 12.74  | 145.50      | 127.31   |
| 17  | Z     | 843  | BCR  | C16-C15-C14 | 12.74  | 149.57      | 123.47   |
| 17  | G     | 848  | BCR  | C16-C15-C14 | 12.72  | 149.53      | 123.47   |
| 17  | Q     | 204  | BCR  | C16-C15-C14 | 12.71  | 149.52      | 123.47   |
| 17  | L     | 209  | BCR  | C16-C15-C14 | 12.71  | 149.51      | 123.47   |
| 17  | Z     | 841  | BCR  | C16-C15-C14 | 12.70  | 149.49      | 123.47   |
| 17  | Y     | 856  | BCR  | C16-C15-C14 | 12.69  | 149.48      | 123.47   |
| 17  | H     | 841  | BCR  | C16-C15-C14 | 12.69  | 149.47      | 123.47   |
| 17  | A     | 845  | BCR  | C16-C15-C14 | 12.69  | 149.46      | 123.47   |
| 17  | Y     | 849  | BCR  | C21-C20-C19 | 12.68  | 162.78      | 123.22   |
| 17  | G     | 850  | BCR  | C21-C20-C19 | 12.65  | 162.71      | 123.22   |
| 17  | M     | 101  | BCR  | C11-C10-C9  | 12.63  | 145.34      | 127.31   |
| 17  | B     | 844  | BCR  | C16-C15-C14 | 12.63  | 149.34      | 123.47   |
| 17  | G     | 850  | BCR  | C11-C10-C9  | 12.62  | 145.32      | 127.31   |
| 17  | T     | 102  | BCR  | C11-C10-C9  | 12.61  | 145.31      | 127.31   |
| 17  | H     | 842  | BCR  | C16-C15-C14 | 12.60  | 149.29      | 123.47   |
| 17  | h     | 202  | BCR  | C16-C15-C14 | 12.58  | 149.25      | 123.47   |
| 17  | H     | 840  | BCR  | C21-C20-C19 | 12.58  | 162.47      | 123.22   |
| 17  | L     | 203  | BCR  | C16-C15-C14 | 12.57  | 149.23      | 123.47   |
| 17  | H     | 842  | BCR  | C11-C12-C13 | 12.57  | 161.72      | 126.42   |
| 17  | A     | 849  | BCR  | C11-C10-C9  | 12.55  | 145.22      | 127.31   |
| 17  | R     | 101  | BCR  | C16-C15-C14 | 12.53  | 149.15      | 123.47   |
| 17  | e     | 101  | BCR  | C16-C15-C14 | 12.53  | 149.14      | 123.47   |
| 17  | A     | 846  | BCR  | C16-C15-C14 | 12.52  | 149.11      | 123.47   |
| 17  | e     | 101  | BCR  | C21-C20-C19 | 12.51  | 162.26      | 123.22   |
| 17  | U     | 1005 | BCR  | C11-C12-C13 | 12.50  | 161.52      | 126.42   |
| 17  | Z     | 841  | BCR  | C11-C12-C13 | 12.49  | 161.51      | 126.42   |
| 17  | V     | 1202 | BCR  | C11-C10-C9  | 12.47  | 145.10      | 127.31   |
| 17  | h     | 202  | BCR  | C11-C10-C9  | 12.46  | 145.09      | 127.31   |
| 17  | H     | 844  | BCR  | C11-C12-C13 | 12.45  | 161.39      | 126.42   |
| 17  | B     | 845  | BCR  | C16-C15-C14 | 12.42  | 148.91      | 123.47   |
| 17  | Z     | 842  | BCR  | C16-C15-C14 | 12.39  | 148.86      | 123.47   |
| 17  | B     | 848  | BCR  | C11-C12-C13 | 12.36  | 161.15      | 126.42   |
| 17  | I     | 101  | BCR  | C16-C15-C14 | 12.36  | 148.80      | 123.47   |
| 17  | A     | 849  | BCR  | C16-C15-C14 | 12.33  | 148.73      | 123.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 847  | BCR  | C16-C15-C14 | 12.30 | 148.68      | 123.47   |
| 17  | R     | 102  | BCR  | C16-C15-C14 | 12.28 | 148.62      | 123.47   |
| 17  | G     | 849  | BCR  | C16-C15-C14 | 12.28 | 148.62      | 123.47   |
| 17  | F     | 201  | BCR  | C11-C10-C9  | 12.25 | 144.79      | 127.31   |
| 17  | Z     | 845  | BCR  | C11-C10-C9  | 12.24 | 144.78      | 127.31   |
| 17  | L     | 203  | BCR  | C11-C12-C13 | 12.23 | 160.78      | 126.42   |
| 17  | J     | 103  | BCR  | C11-C12-C13 | 12.23 | 160.76      | 126.42   |
| 17  | Y     | 851  | BCR  | C16-C15-C14 | 12.20 | 148.47      | 123.47   |
| 17  | L     | 203  | BCR  | C11-C10-C9  | 12.19 | 144.71      | 127.31   |
| 17  | Q     | 202  | BCR  | C11-C10-C9  | 12.15 | 144.64      | 127.31   |
| 17  | H     | 840  | BCR  | C16-C15-C14 | 12.10 | 148.26      | 123.47   |
| 17  | B     | 851  | BCR  | C16-C15-C14 | 12.05 | 148.16      | 123.47   |
| 17  | F     | 201  | BCR  | C16-C15-C14 | 11.99 | 148.04      | 123.47   |
| 17  | f     | 103  | BCR  | C11-C10-C9  | 11.98 | 144.41      | 127.31   |
| 17  | A     | 848  | BCR  | C16-C15-C14 | 11.91 | 147.88      | 123.47   |
| 17  | i     | 101  | BCR  | C11-C10-C9  | 11.89 | 144.28      | 127.31   |
| 17  | R     | 102  | BCR  | C11-C12-C13 | 11.84 | 159.67      | 126.42   |
| 17  | Y     | 848  | BCR  | C16-C15-C14 | 11.80 | 147.65      | 123.47   |
| 17  | H     | 848  | BCR  | C16-C15-C14 | 11.80 | 147.64      | 123.47   |
| 17  | f     | 103  | BCR  | C16-C15-C14 | 11.79 | 147.62      | 123.47   |
| 17  | I     | 101  | BCR  | C21-C20-C19 | 11.79 | 160.00      | 123.22   |
| 17  | M     | 101  | BCR  | C16-C15-C14 | 11.77 | 147.57      | 123.47   |
| 17  | U     | 1005 | BCR  | C16-C15-C14 | 11.75 | 147.54      | 123.47   |
| 17  | B     | 844  | BCR  | C11-C10-C9  | 11.61 | 143.88      | 127.31   |
| 17  | e     | 101  | BCR  | C20-C19-C18 | 11.57 | 158.91      | 126.42   |
| 17  | U     | 1007 | BCR  | C16-C15-C14 | 11.56 | 147.16      | 123.47   |
| 17  | h     | 203  | BCR  | C16-C15-C14 | 11.52 | 147.07      | 123.47   |
| 17  | B     | 848  | BCR  | C11-C10-C9  | 11.49 | 143.71      | 127.31   |
| 17  | Y     | 848  | BCR  | C11-C10-C9  | 11.48 | 143.69      | 127.31   |
| 17  | U     | 1008 | BCR  | C16-C15-C14 | 11.45 | 146.92      | 123.47   |
| 17  | R     | 101  | BCR  | C21-C20-C19 | 11.45 | 158.94      | 123.22   |
| 17  | V     | 1202 | BCR  | C16-C15-C14 | 11.44 | 146.91      | 123.47   |
| 17  | G     | 846  | BCR  | C11-C10-C9  | 11.41 | 143.59      | 127.31   |
| 17  | A     | 847  | BCR  | C16-C15-C14 | 11.36 | 146.75      | 123.47   |
| 17  | Y     | 856  | BCR  | C11-C12-C13 | 11.33 | 158.25      | 126.42   |
| 17  | B     | 844  | BCR  | C21-C20-C19 | 11.25 | 158.33      | 123.22   |
| 17  | Y     | 849  | BCR  | C16-C15-C14 | 11.23 | 146.48      | 123.47   |
| 17  | L     | 208  | BCR  | C16-C15-C14 | 11.21 | 146.44      | 123.47   |
| 17  | A     | 849  | BCR  | C20-C19-C18 | 11.14 | 157.71      | 126.42   |
| 17  | H     | 845  | BCR  | C16-C15-C14 | 11.13 | 146.28      | 123.47   |
| 17  | T     | 102  | BCR  | C21-C20-C19 | 11.11 | 157.90      | 123.22   |
| 17  | Y     | 846  | BCR  | C21-C20-C19 | 11.05 | 157.71      | 123.22   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 17  | H     | 841  | BCR  | C11-C10-C9  | 11.05  | 143.08      | 127.31   |
| 17  | T     | 102  | BCR  | C24-C23-C22 | -10.99 | 109.62      | 126.23   |
| 17  | Y     | 856  | BCR  | C11-C10-C9  | 10.96  | 142.96      | 127.31   |
| 17  | i     | 101  | BCR  | C20-C19-C18 | 10.96  | 157.20      | 126.42   |
| 17  | H     | 845  | BCR  | C11-C10-C9  | 10.91  | 142.88      | 127.31   |
| 17  | G     | 848  | BCR  | C11-C10-C9  | 10.90  | 142.87      | 127.31   |
| 17  | G     | 850  | BCR  | C20-C19-C18 | 10.89  | 157.01      | 126.42   |
| 17  | S     | 1104 | BCR  | C21-C20-C19 | 10.85  | 157.07      | 123.22   |
| 17  | G     | 849  | BCR  | C11-C10-C9  | 10.84  | 142.78      | 127.31   |
| 17  | U     | 1007 | BCR  | C11-C10-C9  | 10.83  | 142.76      | 127.31   |
| 17  | H     | 840  | BCR  | C20-C19-C18 | 10.76  | 156.64      | 126.42   |
| 17  | K     | 102  | BCR  | C21-C20-C19 | 10.65  | 156.44      | 123.22   |
| 17  | I     | 101  | BCR  | C20-C19-C18 | 10.64  | 156.32      | 126.42   |
| 17  | Z     | 842  | BCR  | C11-C10-C9  | 10.64  | 142.49      | 127.31   |
| 17  | A     | 845  | BCR  | C20-C19-C18 | 10.63  | 156.27      | 126.42   |
| 17  | J     | 104  | BCR  | C11-C10-C9  | 10.62  | 142.47      | 127.31   |
| 17  | U     | 1007 | BCR  | C20-C19-C18 | 10.56  | 156.08      | 126.42   |
| 17  | A     | 845  | BCR  | C11-C10-C9  | 10.53  | 142.34      | 127.31   |
| 17  | J     | 103  | BCR  | C20-C19-C18 | 10.53  | 156.00      | 126.42   |
| 17  | Y     | 847  | BCR  | C20-C19-C18 | 10.50  | 155.92      | 126.42   |
| 17  | Y     | 849  | BCR  | C20-C19-C18 | 10.49  | 155.87      | 126.42   |
| 17  | I     | 101  | BCR  | C11-C10-C9  | 10.46  | 142.24      | 127.31   |
| 17  | Y     | 846  | BCR  | C20-C19-C18 | 10.46  | 155.80      | 126.42   |
| 17  | R     | 101  | BCR  | C20-C19-C18 | 10.38  | 155.59      | 126.42   |
| 17  | L     | 208  | BCR  | C20-C19-C18 | 10.36  | 155.51      | 126.42   |
| 17  | S     | 1104 | BCR  | C20-C19-C18 | 10.35  | 155.50      | 126.42   |
| 17  | Z     | 846  | BCR  | C20-C19-C18 | 10.27  | 155.25      | 126.42   |
| 17  | Y     | 851  | BCR  | C20-C19-C18 | 10.24  | 155.19      | 126.42   |
| 17  | Y     | 849  | BCR  | C11-C10-C9  | 10.23  | 141.91      | 127.31   |
| 17  | B     | 843  | BCR  | C20-C19-C18 | 10.23  | 155.14      | 126.42   |
| 17  | Y     | 848  | BCR  | C20-C19-C18 | 10.19  | 155.04      | 126.42   |
| 17  | H     | 840  | BCR  | C11-C10-C9  | 10.16  | 141.81      | 127.31   |
| 17  | f     | 105  | BCR  | C20-C19-C18 | 10.13  | 154.88      | 126.42   |
| 17  | G     | 848  | BCR  | C20-C19-C18 | 10.11  | 154.81      | 126.42   |
| 17  | J     | 103  | BCR  | C11-C10-C9  | 10.09  | 141.71      | 127.31   |
| 17  | B     | 844  | BCR  | C20-C19-C18 | 10.07  | 154.72      | 126.42   |
| 17  | Z     | 841  | BCR  | C11-C10-C9  | 10.07  | 141.68      | 127.31   |
| 17  | B     | 847  | BCR  | C20-C19-C18 | 9.95   | 154.37      | 126.42   |
| 17  | K     | 102  | BCR  | C11-C10-C9  | 9.94   | 141.49      | 127.31   |
| 17  | G     | 849  | BCR  | C20-C19-C18 | 9.94   | 154.33      | 126.42   |
| 17  | M     | 101  | BCR  | C20-C19-C18 | 9.93   | 154.31      | 126.42   |
| 17  | Z     | 842  | BCR  | C20-C19-C18 | 9.85   | 154.09      | 126.42   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | H     | 841  | BCR  | C20-C19-C18 | 9.83  | 154.03      | 126.42   |
| 17  | A     | 848  | BCR  | C20-C19-C18 | 9.82  | 154.00      | 126.42   |
| 17  | L     | 209  | BCR  | C11-C10-C9  | 9.82  | 141.32      | 127.31   |
| 13  | Y     | 801  | CL0  | C4A-NA-C1A  | 9.79  | 111.11      | 106.71   |
| 17  | Y     | 847  | BCR  | C11-C10-C9  | 9.76  | 141.24      | 127.31   |
| 17  | A     | 847  | BCR  | C20-C19-C18 | 9.75  | 153.81      | 126.42   |
| 17  | G     | 847  | BCR  | C20-C19-C18 | 9.74  | 153.77      | 126.42   |
| 17  | U     | 1005 | BCR  | C20-C19-C18 | 9.71  | 153.69      | 126.42   |
| 14  | G     | 813  | CLA  | OBD-CAD-C3D | -9.70 | 111.87      | 127.98   |
| 17  | A     | 847  | BCR  | C11-C10-C9  | 9.68  | 141.12      | 127.31   |
| 17  | Z     | 843  | BCR  | C20-C19-C18 | 9.65  | 153.52      | 126.42   |
| 17  | H     | 844  | BCR  | C11-C10-C9  | 9.61  | 141.02      | 127.31   |
| 17  | B     | 845  | BCR  | C11-C10-C9  | 9.61  | 141.02      | 127.31   |
| 17  | K     | 102  | BCR  | C20-C19-C18 | 9.60  | 153.40      | 126.42   |
| 17  | H     | 848  | BCR  | C11-C10-C9  | 9.55  | 140.94      | 127.31   |
| 17  | h     | 202  | BCR  | C20-C19-C18 | 9.55  | 153.25      | 126.42   |
| 17  | H     | 843  | BCR  | C20-C19-C18 | 9.54  | 153.22      | 126.42   |
| 17  | Z     | 845  | BCR  | C20-C19-C18 | 9.52  | 153.15      | 126.42   |
| 17  | B     | 851  | BCR  | C11-C10-C9  | 9.50  | 140.87      | 127.31   |
| 17  | d     | 203  | BCR  | C20-C19-C18 | 9.48  | 153.05      | 126.42   |
| 17  | f     | 105  | BCR  | C11-C10-C9  | 9.46  | 140.81      | 127.31   |
| 17  | A     | 846  | BCR  | C19-C18-C17 | 9.45  | 133.44      | 118.94   |
| 17  | A     | 848  | BCR  | C11-C10-C9  | 9.42  | 140.76      | 127.31   |
| 17  | f     | 103  | BCR  | C20-C19-C18 | 9.41  | 152.84      | 126.42   |
| 17  | T     | 102  | BCR  | C20-C19-C18 | 9.40  | 152.84      | 126.42   |
| 17  | L     | 208  | BCR  | C11-C10-C9  | 9.40  | 140.72      | 127.31   |
| 17  | G     | 846  | BCR  | C20-C19-C18 | 9.40  | 152.82      | 126.42   |
| 17  | Q     | 204  | BCR  | C20-C19-C18 | 9.32  | 152.60      | 126.42   |
| 17  | h     | 203  | BCR  | C20-C19-C18 | 9.30  | 152.56      | 126.42   |
| 17  | G     | 854  | BCR  | C20-C19-C18 | 9.29  | 152.52      | 126.42   |
| 17  | B     | 846  | BCR  | C20-C19-C18 | 9.21  | 152.28      | 126.42   |
| 17  | Y     | 850  | BCR  | C20-C19-C18 | 9.20  | 152.27      | 126.42   |
| 17  | h     | 202  | BCR  | C19-C18-C17 | 9.15  | 132.98      | 118.94   |
| 17  | V     | 1202 | BCR  | C20-C19-C18 | 9.13  | 152.06      | 126.42   |
| 17  | L     | 203  | BCR  | C20-C19-C18 | 9.10  | 151.99      | 126.42   |
| 14  | B     | 810  | CLA  | C2C-C1C-NC  | 8.99  | 118.39      | 109.97   |
| 17  | U     | 1008 | BCR  | C20-C19-C18 | 8.98  | 151.65      | 126.42   |
| 17  | S     | 1104 | BCR  | C11-C10-C9  | 8.98  | 140.12      | 127.31   |
| 17  | f     | 104  | BCR  | C19-C18-C17 | 8.96  | 132.70      | 118.94   |
| 17  | H     | 848  | BCR  | C20-C19-C18 | 8.92  | 151.48      | 126.42   |
| 17  | A     | 846  | BCR  | C11-C10-C9  | 8.89  | 140.00      | 127.31   |
| 17  | B     | 845  | BCR  | C20-C19-C18 | 8.88  | 151.37      | 126.42   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 847  | BCR  | C11-C10-C9  | 8.87  | 139.97      | 127.31   |
| 17  | R     | 102  | BCR  | C20-C19-C18 | 8.87  | 151.32      | 126.42   |
| 17  | A     | 846  | BCR  | C20-C19-C18 | 8.86  | 151.30      | 126.42   |
| 17  | d     | 203  | BCR  | C11-C10-C9  | 8.86  | 139.95      | 127.31   |
| 17  | B     | 851  | BCR  | C20-C19-C18 | 8.85  | 151.27      | 126.42   |
| 17  | F     | 203  | BCR  | C20-C19-C18 | 8.81  | 151.16      | 126.42   |
| 17  | H     | 844  | BCR  | C20-C19-C18 | 8.75  | 150.99      | 126.42   |
| 17  | U     | 1005 | BCR  | C11-C10-C9  | 8.74  | 139.78      | 127.31   |
| 17  | J     | 104  | BCR  | C19-C18-C17 | 8.71  | 132.31      | 118.94   |
| 17  | B     | 843  | BCR  | C11-C10-C9  | 8.71  | 139.74      | 127.31   |
| 17  | B     | 845  | BCR  | C19-C18-C17 | 8.70  | 132.30      | 118.94   |
| 17  | Z     | 841  | BCR  | C20-C19-C18 | 8.69  | 150.84      | 126.42   |
| 17  | Q     | 204  | BCR  | C11-C10-C9  | 8.68  | 139.69      | 127.31   |
| 17  | H     | 842  | BCR  | C19-C18-C17 | 8.67  | 132.25      | 118.94   |
| 17  | H     | 842  | BCR  | C20-C19-C18 | 8.67  | 150.76      | 126.42   |
| 17  | G     | 854  | BCR  | C11-C10-C9  | 8.64  | 139.64      | 127.31   |
| 17  | Z     | 844  | BCR  | C19-C18-C17 | 8.62  | 132.16      | 118.94   |
| 17  | Q     | 202  | BCR  | C20-C19-C18 | 8.58  | 150.52      | 126.42   |
| 17  | Z     | 843  | BCR  | C19-C18-C17 | 8.57  | 132.10      | 118.94   |
| 17  | L     | 209  | BCR  | C20-C19-C18 | 8.52  | 150.36      | 126.42   |
| 14  | G     | 803  | CLA  | OBD-CAD-CBD | -8.49 | 113.76      | 125.89   |
| 14  | Y     | 802  | CLA  | OBD-CAD-CBD | -8.44 | 113.84      | 125.89   |
| 17  | F     | 201  | BCR  | C20-C19-C18 | 8.42  | 150.08      | 126.42   |
| 17  | J     | 104  | BCR  | C20-C19-C18 | 8.42  | 150.07      | 126.42   |
| 17  | B     | 848  | BCR  | C19-C18-C17 | 8.34  | 131.74      | 118.94   |
| 17  | B     | 848  | BCR  | C20-C19-C18 | 8.34  | 149.85      | 126.42   |
| 14  | B     | 834  | CLA  | C4D-C3D-CAD | 8.30  | 113.10      | 108.47   |
| 17  | f     | 104  | BCR  | C11-C10-C9  | 8.19  | 139.00      | 127.31   |
| 17  | H     | 845  | BCR  | C19-C18-C17 | 8.18  | 131.50      | 118.94   |
| 17  | T     | 102  | BCR  | C19-C18-C17 | 8.18  | 131.49      | 118.94   |
| 17  | H     | 845  | BCR  | C20-C19-C18 | 8.09  | 149.14      | 126.42   |
| 17  | F     | 203  | BCR  | C11-C10-C9  | 8.04  | 138.79      | 127.31   |
| 14  | h     | 206  | CLA  | C4D-C3D-CAD | 8.04  | 112.95      | 108.47   |
| 17  | L     | 203  | BCR  | C19-C18-C17 | 8.03  | 131.26      | 118.94   |
| 17  | L     | 209  | BCR  | C19-C18-C17 | 8.02  | 131.25      | 118.94   |
| 14  | B     | 805  | CLA  | O2D-CGD-CBD | 7.96  | 125.41      | 111.27   |
| 17  | A     | 847  | BCR  | C19-C18-C17 | 7.96  | 131.15      | 118.94   |
| 17  | F     | 201  | BCR  | C24-C23-C22 | -7.95 | 114.23      | 126.23   |
| 14  | Y     | 827  | CLA  | OBD-CAD-C3D | -7.92 | 114.84      | 127.98   |
| 13  | A     | 801  | CL0  | C4A-NA-C1A  | 7.91  | 110.26      | 106.71   |
| 14  | A     | 852  | CLA  | OBD-CAD-CBD | -7.89 | 114.62      | 125.89   |
| 14  | Z     | 803  | CLA  | O2D-CGD-CBD | 7.89  | 125.29      | 111.27   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 854  | BCR  | C19-C18-C17 | 7.87  | 131.01      | 118.94   |
| 17  | J     | 104  | BCR  | C36-C18-C17 | -7.86 | 111.91      | 122.92   |
| 13  | G     | 801  | CL0  | O2A-CGA-O1A | -7.85 | 103.79      | 123.59   |
| 17  | f     | 103  | BCR  | C19-C18-C17 | 7.84  | 130.97      | 118.94   |
| 14  | G     | 814  | CLA  | O2D-CGD-CBD | 7.83  | 125.19      | 111.27   |
| 14  | B     | 834  | CLA  | O2D-CGD-CBD | 7.81  | 125.15      | 111.27   |
| 17  | V     | 1202 | BCR  | C37-C22-C21 | -7.77 | 112.04      | 122.92   |
| 17  | A     | 848  | BCR  | C19-C18-C17 | 7.73  | 130.81      | 118.94   |
| 14  | A     | 808  | CLA  | O2D-CGD-CBD | 7.71  | 124.97      | 111.27   |
| 14  | H     | 807  | CLA  | C2C-C1C-NC  | 7.69  | 117.18      | 109.97   |
| 17  | Y     | 856  | BCR  | C20-C19-C18 | 7.68  | 147.98      | 126.42   |
| 14  | h     | 206  | CLA  | C4A-NA-C1A  | 7.66  | 110.15      | 106.71   |
| 17  | Q     | 204  | BCR  | C24-C23-C22 | -7.64 | 114.70      | 126.23   |
| 17  | Y     | 856  | BCR  | C19-C18-C17 | 7.59  | 130.59      | 118.94   |
| 14  | H     | 803  | CLA  | C4A-NA-C1A  | 7.58  | 110.11      | 106.71   |
| 14  | A     | 822  | CLA  | C4A-NA-C1A  | 7.57  | 110.11      | 106.71   |
| 14  | B     | 810  | CLA  | C1C-C2C-C3C | -7.55 | 99.02       | 106.96   |
| 14  | A     | 802  | CLA  | OBD-CAD-CBD | -7.55 | 115.11      | 125.89   |
| 17  | G     | 848  | BCR  | C19-C18-C17 | 7.54  | 130.51      | 118.94   |
| 17  | h     | 202  | BCR  | C37-C22-C21 | -7.52 | 112.39      | 122.92   |
| 14  | G     | 839  | CLA  | C4D-C3D-CAD | 7.48  | 112.64      | 108.47   |
| 14  | H     | 822  | CLA  | C4A-NA-C1A  | 7.46  | 110.06      | 106.71   |
| 14  | B     | 810  | CLA  | OBD-CAD-C3D | -7.46 | 115.60      | 127.98   |
| 14  | Z     | 827  | CLA  | C4A-NA-C1A  | 7.45  | 110.06      | 106.71   |
| 17  | J     | 104  | BCR  | C24-C23-C22 | -7.44 | 114.99      | 126.23   |
| 14  | Z     | 808  | CLA  | C2C-C1C-NC  | 7.44  | 116.94      | 109.97   |
| 14  | G     | 815  | CLA  | C4D-C3D-CAD | 7.43  | 112.61      | 108.47   |
| 14  | G     | 830  | CLA  | C2C-C1C-NC  | 7.42  | 116.93      | 109.97   |
| 17  | L     | 208  | BCR  | C24-C23-C22 | -7.41 | 115.04      | 126.23   |
| 14  | H     | 836  | CLA  | O2D-CGD-CBD | 7.40  | 124.42      | 111.27   |
| 14  | A     | 803  | CLA  | C4D-C3D-CAD | 7.40  | 112.60      | 108.47   |
| 14  | Z     | 807  | CLA  | C4A-NA-C1A  | 7.38  | 110.02      | 106.71   |
| 17  | f     | 103  | BCR  | C36-C18-C17 | -7.37 | 112.60      | 122.92   |
| 14  | Z     | 806  | CLA  | O2D-CGD-CBD | 7.35  | 124.33      | 111.27   |
| 17  | f     | 104  | BCR  | C36-C18-C17 | -7.34 | 112.64      | 122.92   |
| 17  | H     | 843  | BCR  | C19-C18-C17 | 7.34  | 130.21      | 118.94   |
| 14  | H     | 823  | CLA  | C2C-C1C-NC  | 7.34  | 116.85      | 109.97   |
| 14  | G     | 819  | CLA  | O2D-CGD-CBD | 7.34  | 124.31      | 111.27   |
| 14  | Z     | 831  | CLA  | O2D-CGD-CBD | 7.32  | 124.28      | 111.27   |
| 14  | H     | 807  | CLA  | O2D-CGD-CBD | 7.31  | 124.26      | 111.27   |
| 14  | B     | 806  | CLA  | C4D-C3D-CAD | 7.31  | 112.55      | 108.47   |
| 17  | G     | 854  | BCR  | C36-C18-C17 | -7.31 | 112.69      | 122.92   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 803  | CLA  | O2D-CGD-CBD | 7.30  | 124.24      | 111.27   |
| 14  | Z     | 827  | CLA  | C2C-C1C-NC  | 7.29  | 116.81      | 109.97   |
| 17  | B     | 846  | BCR  | C19-C18-C17 | 7.29  | 130.12      | 118.94   |
| 14  | H     | 808  | CLA  | C2C-C1C-NC  | 7.28  | 116.79      | 109.97   |
| 17  | f     | 104  | BCR  | C20-C19-C18 | 7.28  | 146.85      | 126.42   |
| 14  | G     | 808  | CLA  | C4A-NA-C1A  | 7.27  | 109.98      | 106.71   |
| 17  | B     | 851  | BCR  | C19-C18-C17 | 7.27  | 130.09      | 118.94   |
| 14  | A     | 842  | CLA  | C4D-C3D-CAD | 7.25  | 112.51      | 108.47   |
| 17  | R     | 102  | BCR  | C19-C18-C17 | 7.23  | 130.04      | 118.94   |
| 14  | B     | 830  | CLA  | C2C-C1C-NC  | 7.22  | 116.74      | 109.97   |
| 14  | A     | 813  | CLA  | C2C-C1C-NC  | 7.22  | 116.74      | 109.97   |
| 14  | B     | 832  | CLA  | C4A-NA-C1A  | 7.21  | 109.95      | 106.71   |
| 14  | B     | 804  | CLA  | C4A-NA-C1A  | 7.21  | 109.95      | 106.71   |
| 14  | H     | 818  | CLA  | C2C-C1C-NC  | 7.21  | 116.72      | 109.97   |
| 14  | A     | 829  | CLA  | C2C-C1C-NC  | 7.20  | 116.72      | 109.97   |
| 14  | Z     | 813  | CLA  | C2C-C1C-NC  | 7.19  | 116.71      | 109.97   |
| 14  | A     | 822  | CLA  | C2C-C1C-NC  | 7.19  | 116.71      | 109.97   |
| 14  | H     | 832  | CLA  | C2C-C1C-NC  | 7.19  | 116.71      | 109.97   |
| 17  | Z     | 844  | BCR  | C20-C19-C18 | 7.17  | 146.54      | 126.42   |
| 14  | G     | 815  | CLA  | O2D-CGD-CBD | 7.16  | 124.00      | 111.27   |
| 14  | Y     | 825  | CLA  | C2C-C1C-NC  | 7.16  | 116.68      | 109.97   |
| 14  | A     | 804  | CLA  | O2D-CGD-CBD | 7.15  | 123.97      | 111.27   |
| 14  | H     | 824  | CLA  | C4D-C3D-CAD | 7.15  | 112.45      | 108.47   |
| 14  | Y     | 819  | CLA  | O2D-CGD-CBD | 7.13  | 123.93      | 111.27   |
| 17  | B     | 846  | BCR  | C37-C22-C21 | -7.13 | 112.94      | 122.92   |
| 14  | G     | 822  | CLA  | C4A-NA-C1A  | 7.12  | 109.91      | 106.71   |
| 17  | Z     | 845  | BCR  | C19-C18-C17 | 7.12  | 129.86      | 118.94   |
| 14  | A     | 832  | CLA  | C2C-C1C-NC  | 7.11  | 116.63      | 109.97   |
| 14  | A     | 809  | CLA  | C2C-C1C-NC  | 7.09  | 116.62      | 109.97   |
| 17  | U     | 1005 | BCR  | C19-C18-C17 | 7.09  | 129.82      | 118.94   |
| 14  | G     | 822  | CLA  | C2C-C1C-NC  | 7.09  | 116.61      | 109.97   |
| 14  | B     | 841  | CLA  | C4A-NA-C1A  | 7.08  | 109.89      | 106.71   |
| 17  | Y     | 846  | BCR  | C19-C18-C17 | 7.08  | 129.80      | 118.94   |
| 17  | V     | 1202 | BCR  | C27-C26-C25 | -7.07 | 112.46      | 122.73   |
| 14  | Q     | 201  | CLA  | C4A-NA-C1A  | 7.07  | 109.88      | 106.71   |
| 14  | Y     | 804  | CLA  | O2D-CGD-CBD | 7.07  | 123.83      | 111.27   |
| 14  | T     | 103  | CLA  | C2C-C1C-NC  | 7.07  | 116.59      | 109.97   |
| 14  | Z     | 803  | CLA  | C4A-NA-C1A  | 7.05  | 109.88      | 106.71   |
| 14  | A     | 825  | CLA  | C2C-C1C-NC  | 7.04  | 116.57      | 109.97   |
| 14  | A     | 812  | CLA  | C2C-C1C-NC  | 7.03  | 116.56      | 109.97   |
| 14  | Z     | 822  | CLA  | C4D-C3D-CAD | 7.03  | 112.39      | 108.47   |
| 14  | B     | 828  | CLA  | C4D-C3D-CAD | 7.03  | 112.39      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 808  | CLA  | C2C-C1C-NC  | 7.02  | 116.55      | 109.97   |
| 14  | Z     | 814  | CLA  | O2D-CGD-CBD | 7.00  | 123.70      | 111.27   |
| 14  | B     | 809  | CLA  | C4A-NA-C1A  | 6.99  | 109.85      | 106.71   |
| 14  | H     | 819  | CLA  | OBD-CAD-C3D | -6.98 | 116.38      | 127.98   |
| 14  | G     | 816  | CLA  | C2C-C1C-NC  | 6.98  | 116.51      | 109.97   |
| 17  | F     | 203  | BCR  | C33-C5-C6   | -6.98 | 116.69      | 124.53   |
| 17  | Q     | 204  | BCR  | C19-C18-C17 | 6.97  | 129.64      | 118.94   |
| 14  | A     | 809  | CLA  | O2A-C1-C2   | 6.96  | 126.93      | 108.64   |
| 14  | B     | 829  | CLA  | C2C-C1C-NC  | 6.96  | 116.49      | 109.97   |
| 14  | Y     | 811  | CLA  | C2C-C1C-NC  | 6.95  | 116.48      | 109.97   |
| 14  | A     | 830  | CLA  | C2C-C1C-NC  | 6.95  | 116.48      | 109.97   |
| 14  | Z     | 802  | CLA  | C4A-NA-C1A  | 6.94  | 109.83      | 106.71   |
| 14  | Y     | 805  | CLA  | O2D-CGD-CBD | 6.94  | 123.60      | 111.27   |
| 14  | H     | 828  | CLA  | C2C-C1C-NC  | 6.94  | 116.47      | 109.97   |
| 14  | G     | 835  | CLA  | C4D-C3D-CAD | 6.93  | 112.33      | 108.47   |
| 17  | H     | 843  | BCR  | C36-C18-C17 | -6.93 | 113.22      | 122.92   |
| 17  | F     | 203  | BCR  | C19-C18-C17 | 6.93  | 129.57      | 118.94   |
| 14  | B     | 813  | CLA  | C2C-C1C-NC  | 6.93  | 116.46      | 109.97   |
| 14  | U     | 1003 | CLA  | O2D-CGD-CBD | 6.91  | 123.55      | 111.27   |
| 14  | B     | 805  | CLA  | C4D-C3D-CAD | 6.91  | 112.32      | 108.47   |
| 14  | B     | 829  | CLA  | C4A-NA-C1A  | 6.91  | 109.81      | 106.71   |
| 14  | d     | 202  | CLA  | C2C-C1C-NC  | 6.90  | 116.43      | 109.97   |
| 14  | Y     | 831  | CLA  | O2D-CGD-CBD | 6.89  | 123.52      | 111.27   |
| 14  | A     | 831  | CLA  | O2D-CGD-CBD | 6.89  | 123.51      | 111.27   |
| 14  | Y     | 804  | CLA  | C2C-C1C-NC  | 6.89  | 116.43      | 109.97   |
| 14  | Y     | 854  | CLA  | O2D-CGD-CBD | 6.89  | 123.51      | 111.27   |
| 14  | Z     | 805  | CLA  | C2C-C1C-NC  | 6.89  | 116.43      | 109.97   |
| 17  | H     | 848  | BCR  | C19-C18-C17 | 6.89  | 129.51      | 118.94   |
| 14  | B     | 836  | CLA  | C2C-C1C-NC  | 6.87  | 116.41      | 109.97   |
| 14  | H     | 808  | CLA  | C4A-NA-C1A  | 6.87  | 109.80      | 106.71   |
| 14  | Z     | 813  | CLA  | C4A-NA-C1A  | 6.87  | 109.80      | 106.71   |
| 14  | Z     | 823  | CLA  | C2C-C1C-NC  | 6.87  | 116.41      | 109.97   |
| 14  | Q     | 201  | CLA  | C2C-C1C-NC  | 6.87  | 116.41      | 109.97   |
| 17  | Z     | 841  | BCR  | C19-C18-C17 | 6.87  | 129.48      | 118.94   |
| 17  | B     | 848  | BCR  | C36-C18-C17 | -6.86 | 113.31      | 122.92   |
| 14  | G     | 832  | CLA  | C2C-C1C-NC  | 6.86  | 116.40      | 109.97   |
| 17  | Z     | 844  | BCR  | C36-C18-C17 | -6.85 | 113.33      | 122.92   |
| 14  | H     | 821  | CLA  | C2C-C1C-NC  | 6.85  | 116.39      | 109.97   |
| 14  | A     | 830  | CLA  | O2D-CGD-CBD | 6.84  | 123.42      | 111.27   |
| 14  | Y     | 815  | CLA  | O2D-CGD-CBD | 6.84  | 123.42      | 111.27   |
| 13  | G     | 801  | CL0  | C4A-NA-C1A  | 6.83  | 109.78      | 106.71   |
| 14  | A     | 852  | CLA  | O2D-CGD-CBD | 6.83  | 123.40      | 111.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Z     | 845  | BCR  | C37-C22-C21 | -6.82 | 113.36      | 122.92   |
| 14  | Y     | 817  | CLA  | C2C-C1C-NC  | 6.81  | 116.36      | 109.97   |
| 14  | H     | 837  | CLA  | C2C-C1C-NC  | 6.81  | 116.36      | 109.97   |
| 17  | U     | 1008 | BCR  | C37-C22-C21 | -6.81 | 113.38      | 122.92   |
| 14  | G     | 815  | CLA  | C2C-C1C-NC  | 6.81  | 116.35      | 109.97   |
| 14  | B     | 821  | CLA  | C2C-C1C-NC  | 6.80  | 116.34      | 109.97   |
| 14  | G     | 838  | CLA  | C2C-C1C-NC  | 6.80  | 116.34      | 109.97   |
| 14  | B     | 809  | CLA  | O2D-CGD-CBD | 6.79  | 123.33      | 111.27   |
| 14  | G     | 812  | CLA  | C2C-C1C-NC  | 6.79  | 116.33      | 109.97   |
| 14  | Z     | 822  | CLA  | C2C-C1C-NC  | 6.78  | 116.33      | 109.97   |
| 14  | A     | 802  | CLA  | C2C-C1C-NC  | 6.78  | 116.33      | 109.97   |
| 14  | B     | 834  | CLA  | C2C-C1C-NC  | 6.78  | 116.32      | 109.97   |
| 14  | L     | 202  | CLA  | C4A-NA-C1A  | 6.77  | 109.75      | 106.71   |
| 14  | Q     | 201  | CLA  | O2D-CGD-CBD | 6.77  | 123.29      | 111.27   |
| 14  | A     | 833  | CLA  | OBD-CAD-C3D | -6.77 | 116.75      | 127.98   |
| 14  | Y     | 814  | CLA  | O2D-CGD-CBD | 6.76  | 123.29      | 111.27   |
| 17  | G     | 846  | BCR  | C27-C26-C25 | -6.76 | 112.91      | 122.73   |
| 14  | S     | 1102 | CLA  | C2C-C1C-NC  | 6.76  | 116.31      | 109.97   |
| 14  | B     | 820  | CLA  | C2C-C1C-NC  | 6.76  | 116.30      | 109.97   |
| 17  | B     | 845  | BCR  | C36-C18-C17 | -6.76 | 113.45      | 122.92   |
| 14  | B     | 806  | CLA  | C4A-NA-C1A  | 6.76  | 109.74      | 106.71   |
| 14  | Y     | 816  | CLA  | O2D-CGD-CBD | 6.76  | 123.27      | 111.27   |
| 14  | h     | 205  | CLA  | O2A-C1-C2   | 6.75  | 126.39      | 108.64   |
| 14  | A     | 815  | CLA  | C4A-NA-C1A  | 6.75  | 109.74      | 106.71   |
| 14  | Y     | 833  | CLA  | C2C-C1C-NC  | 6.75  | 116.30      | 109.97   |
| 14  | F     | 202  | CLA  | C2C-C1C-NC  | 6.75  | 116.30      | 109.97   |
| 14  | Y     | 808  | CLA  | C4A-NA-C1A  | 6.75  | 109.74      | 106.71   |
| 14  | H     | 828  | CLA  | C4A-NA-C1A  | 6.74  | 109.74      | 106.71   |
| 17  | J     | 103  | BCR  | C36-C18-C17 | -6.74 | 113.48      | 122.92   |
| 14  | Z     | 823  | CLA  | O2D-CGD-CBD | 6.74  | 123.24      | 111.27   |
| 17  | F     | 203  | BCR  | C37-C22-C21 | -6.74 | 113.48      | 122.92   |
| 14  | H     | 801  | CLA  | O2D-CGD-CBD | 6.73  | 123.23      | 111.27   |
| 14  | H     | 832  | CLA  | C4D-C3D-CAD | 6.73  | 112.22      | 108.47   |
| 17  | A     | 847  | BCR  | C36-C18-C17 | -6.73 | 113.50      | 122.92   |
| 14  | Z     | 838  | CLA  | O2D-CGD-CBD | 6.73  | 123.22      | 111.27   |
| 14  | A     | 811  | CLA  | C2C-C1C-NC  | 6.72  | 116.27      | 109.97   |
| 14  | B     | 810  | CLA  | C4D-C3D-CAD | 6.72  | 112.22      | 108.47   |
| 14  | U     | 1004 | CLA  | C2C-C1C-NC  | 6.72  | 116.26      | 109.97   |
| 14  | Y     | 829  | CLA  | C2C-C1C-NC  | 6.72  | 116.26      | 109.97   |
| 14  | K     | 103  | CLA  | C2C-C1C-NC  | 6.72  | 116.26      | 109.97   |
| 14  | G     | 814  | CLA  | CAA-C2A-C3A | -6.71 | 94.40       | 112.78   |
| 14  | B     | 811  | CLA  | O2D-CGD-CBD | 6.71  | 123.19      | 111.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | U     | 1005 | BCR  | C24-C23-C22 | -6.71 | 116.09      | 126.23   |
| 14  | A     | 852  | CLA  | C4D-C3D-CAD | 6.71  | 112.21      | 108.47   |
| 14  | G     | 808  | CLA  | O2D-CGD-CBD | 6.71  | 123.19      | 111.27   |
| 14  | B     | 828  | CLA  | C2C-C1C-NC  | 6.71  | 116.26      | 109.97   |
| 14  | B     | 826  | CLA  | O2D-CGD-CBD | 6.71  | 123.19      | 111.27   |
| 14  | U     | 1004 | CLA  | O2A-C1-C2   | 6.70  | 126.24      | 108.64   |
| 14  | Y     | 839  | CLA  | C2C-C1C-NC  | 6.70  | 116.25      | 109.97   |
| 17  | Z     | 842  | BCR  | C19-C18-C17 | 6.70  | 129.22      | 118.94   |
| 14  | T     | 101  | CLA  | C2C-C1C-NC  | 6.70  | 116.25      | 109.97   |
| 14  | A     | 813  | CLA  | C4D-C3D-CAD | 6.69  | 112.20      | 108.47   |
| 14  | U     | 1002 | CLA  | C4A-NA-C1A  | 6.69  | 109.72      | 106.71   |
| 14  | A     | 816  | CLA  | C2C-C1C-NC  | 6.69  | 116.24      | 109.97   |
| 14  | B     | 807  | CLA  | C2C-C1C-NC  | 6.69  | 116.24      | 109.97   |
| 14  | Y     | 818  | CLA  | O2D-CGD-CBD | 6.68  | 123.14      | 111.27   |
| 14  | A     | 852  | CLA  | C2C-C1C-NC  | 6.68  | 116.23      | 109.97   |
| 14  | g     | 102  | CLA  | C2C-C1C-NC  | 6.68  | 116.23      | 109.97   |
| 14  | B     | 802  | CLA  | C4D-C3D-CAD | 6.68  | 112.19      | 108.47   |
| 17  | B     | 847  | BCR  | C24-C23-C22 | -6.67 | 116.15      | 126.23   |
| 17  | B     | 846  | BCR  | C36-C18-C17 | -6.67 | 113.57      | 122.92   |
| 14  | Z     | 837  | CLA  | C2C-C1C-NC  | 6.67  | 116.22      | 109.97   |
| 14  | B     | 818  | CLA  | C2C-C1C-NC  | 6.67  | 116.22      | 109.97   |
| 17  | Z     | 845  | BCR  | C36-C18-C17 | -6.67 | 113.58      | 122.92   |
| 14  | H     | 831  | CLA  | C2C-C1C-NC  | 6.67  | 116.22      | 109.97   |
| 13  | A     | 801  | CL0  | O2A-CGA-O1A | -6.66 | 106.77      | 123.59   |
| 14  | A     | 804  | CLA  | C4A-NA-C1A  | 6.66  | 109.70      | 106.71   |
| 14  | B     | 809  | CLA  | C4D-C3D-CAD | 6.65  | 112.18      | 108.47   |
| 17  | f     | 105  | BCR  | C37-C22-C21 | -6.65 | 113.61      | 122.92   |
| 14  | A     | 842  | CLA  | C4A-NA-C1A  | 6.65  | 109.69      | 106.71   |
| 14  | V     | 1201 | CLA  | O2D-CGD-CBD | 6.64  | 123.08      | 111.27   |
| 14  | A     | 827  | CLA  | C4D-C3D-CAD | 6.64  | 112.17      | 108.47   |
| 17  | A     | 846  | BCR  | C36-C18-C17 | -6.64 | 113.62      | 122.92   |
| 14  | Z     | 804  | CLA  | C2C-C1C-NC  | 6.63  | 116.18      | 109.97   |
| 14  | Y     | 803  | CLA  | C2C-C1C-NC  | 6.63  | 116.18      | 109.97   |
| 14  | B     | 836  | CLA  | C4D-C3D-CAD | 6.63  | 112.17      | 108.47   |
| 14  | A     | 807  | CLA  | C2C-C1C-NC  | 6.63  | 116.18      | 109.97   |
| 14  | G     | 841  | CLA  | C2C-C1C-NC  | 6.63  | 116.18      | 109.97   |
| 14  | Z     | 833  | CLA  | C2C-C1C-NC  | 6.62  | 116.18      | 109.97   |
| 17  | h     | 202  | BCR  | C36-C18-C17 | -6.62 | 113.65      | 122.92   |
| 14  | B     | 832  | CLA  | C2C-C1C-NC  | 6.62  | 116.18      | 109.97   |
| 14  | B     | 834  | CLA  | C4A-NA-C1A  | 6.61  | 109.68      | 106.71   |
| 14  | Z     | 829  | CLA  | C4A-NA-C1A  | 6.61  | 109.68      | 106.71   |
| 14  | H     | 828  | CLA  | C1C-C2C-C3C | -6.61 | 100.01      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Q     | 203  | CLA  | C2C-C1C-NC  | 6.61  | 116.16      | 109.97   |
| 14  | B     | 823  | CLA  | C2C-C1C-NC  | 6.61  | 116.16      | 109.97   |
| 14  | H     | 838  | CLA  | O2A-C1-C2   | 6.61  | 125.99      | 108.64   |
| 14  | S     | 1101 | CLA  | O2D-CGD-CBD | 6.60  | 123.00      | 111.27   |
| 17  | J     | 103  | BCR  | C19-C18-C17 | 6.60  | 129.06      | 118.94   |
| 14  | Z     | 808  | CLA  | C1C-C2C-C3C | -6.60 | 100.02      | 106.96   |
| 14  | B     | 830  | CLA  | O2D-CGD-CBD | 6.59  | 122.98      | 111.27   |
| 17  | H     | 844  | BCR  | C19-C18-C17 | 6.59  | 129.05      | 118.94   |
| 14  | Z     | 819  | CLA  | C2C-C1C-NC  | 6.59  | 116.14      | 109.97   |
| 14  | H     | 827  | CLA  | C4A-NA-C1A  | 6.59  | 109.67      | 106.71   |
| 14  | Z     | 807  | CLA  | C2C-C1C-NC  | 6.59  | 116.14      | 109.97   |
| 14  | G     | 820  | CLA  | C2C-C1C-NC  | 6.58  | 116.14      | 109.97   |
| 14  | L     | 205  | CLA  | C2C-C1C-NC  | 6.58  | 116.13      | 109.97   |
| 14  | G     | 819  | CLA  | O2A-C1-C2   | 6.58  | 125.92      | 108.64   |
| 14  | Z     | 820  | CLA  | C2C-C1C-NC  | 6.57  | 116.12      | 109.97   |
| 14  | L     | 202  | CLA  | C2C-C1C-NC  | 6.56  | 116.12      | 109.97   |
| 14  | A     | 814  | CLA  | C2C-C1C-NC  | 6.56  | 116.12      | 109.97   |
| 14  | Z     | 830  | CLA  | O2D-CGD-CBD | 6.56  | 122.92      | 111.27   |
| 14  | H     | 815  | CLA  | O2D-CGD-CBD | 6.55  | 122.92      | 111.27   |
| 14  | G     | 836  | CLA  | OBD-CAD-C3D | -6.55 | 117.10      | 127.98   |
| 14  | Y     | 830  | CLA  | C4D-C3D-CAD | 6.55  | 112.12      | 108.47   |
| 14  | Z     | 822  | CLA  | C4A-NA-C1A  | 6.54  | 109.65      | 106.71   |
| 14  | G     | 809  | CLA  | C4D-C3D-CAD | 6.54  | 112.12      | 108.47   |
| 14  | H     | 831  | CLA  | C4D-C3D-CAD | 6.53  | 112.11      | 108.47   |
| 14  | Z     | 806  | CLA  | C4A-NA-C1A  | 6.53  | 109.64      | 106.71   |
| 14  | H     | 825  | CLA  | C2C-C1C-NC  | 6.53  | 116.09      | 109.97   |
| 14  | L     | 201  | CLA  | O2D-CGD-CBD | 6.52  | 122.86      | 111.27   |
| 14  | H     | 835  | CLA  | C4A-NA-C1A  | 6.52  | 109.64      | 106.71   |
| 14  | H     | 812  | CLA  | C2C-C1C-NC  | 6.51  | 116.08      | 109.97   |
| 14  | Z     | 836  | CLA  | C2C-C1C-NC  | 6.51  | 116.07      | 109.97   |
| 14  | H     | 806  | CLA  | O2D-CGD-CBD | 6.50  | 122.83      | 111.27   |
| 14  | B     | 824  | CLA  | C4A-NA-C1A  | 6.50  | 109.63      | 106.71   |
| 14  | B     | 837  | CLA  | O2D-CGD-CBD | 6.50  | 122.82      | 111.27   |
| 14  | G     | 842  | CLA  | C2C-C1C-NC  | 6.50  | 116.06      | 109.97   |
| 14  | H     | 838  | CLA  | C4A-NA-C1A  | 6.50  | 109.63      | 106.71   |
| 14  | B     | 826  | CLA  | C2C-C1C-NC  | 6.50  | 116.06      | 109.97   |
| 17  | Y     | 848  | BCR  | C19-C18-C17 | 6.50  | 128.91      | 118.94   |
| 17  | H     | 848  | BCR  | C34-C9-C10  | -6.49 | 113.83      | 122.92   |
| 14  | Y     | 805  | CLA  | C4D-C3D-CAD | 6.49  | 112.09      | 108.47   |
| 17  | V     | 1202 | BCR  | C31-C1-C6   | -6.49 | 99.77       | 110.30   |
| 14  | Z     | 839  | CLA  | C2C-C1C-NC  | 6.48  | 116.05      | 109.97   |
| 17  | G     | 848  | BCR  | C36-C18-C17 | -6.48 | 113.85      | 122.92   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 819  | CLA  | C1C-C2C-C3C | -6.48 | 100.15      | 106.96   |
| 17  | K     | 102  | BCR  | C19-C18-C17 | 6.47  | 128.88      | 118.94   |
| 14  | G     | 832  | CLA  | C4A-NA-C1A  | 6.47  | 109.62      | 106.71   |
| 14  | U     | 1003 | CLA  | C4D-C3D-CAD | 6.47  | 112.08      | 108.47   |
| 17  | F     | 203  | BCR  | C36-C18-C17 | -6.47 | 113.87      | 122.92   |
| 14  | B     | 812  | CLA  | C2C-C1C-NC  | 6.46  | 116.03      | 109.97   |
| 14  | B     | 841  | CLA  | O2D-CGD-CBD | 6.45  | 122.74      | 111.27   |
| 17  | i     | 101  | BCR  | C36-C18-C17 | -6.45 | 113.89      | 122.92   |
| 14  | Y     | 825  | CLA  | C4A-NA-C1A  | 6.44  | 109.60      | 106.71   |
| 14  | G     | 813  | CLA  | C4D-C3D-CAD | 6.44  | 112.06      | 108.47   |
| 17  | Y     | 847  | BCR  | C19-C18-C17 | 6.44  | 128.82      | 118.94   |
| 14  | Z     | 802  | CLA  | C4D-C3D-CAD | 6.44  | 112.06      | 108.47   |
| 14  | G     | 836  | CLA  | C2C-C1C-NC  | 6.44  | 116.00      | 109.97   |
| 14  | B     | 826  | CLA  | C4D-C3D-CAD | 6.43  | 112.06      | 108.47   |
| 14  | G     | 839  | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 14  | U     | 1003 | CLA  | C2C-C1C-NC  | 6.43  | 115.99      | 109.97   |
| 14  | Y     | 818  | CLA  | C4D-C3D-CAD | 6.42  | 112.05      | 108.47   |
| 14  | Z     | 824  | CLA  | C2C-C1C-NC  | 6.42  | 115.99      | 109.97   |
| 14  | A     | 825  | CLA  | C4A-NA-C1A  | 6.41  | 109.59      | 106.71   |
| 14  | G     | 819  | CLA  | C2C-C1C-NC  | 6.41  | 115.97      | 109.97   |
| 14  | Y     | 843  | CLA  | C2C-C1C-NC  | 6.40  | 115.97      | 109.97   |
| 14  | H     | 801  | CLA  | OBD-CAD-CBD | -6.40 | 116.75      | 125.89   |
| 14  | H     | 824  | CLA  | C1C-C2C-C3C | -6.40 | 100.23      | 106.96   |
| 14  | j     | 102  | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 14  | Z     | 813  | CLA  | O2D-CGD-CBD | 6.39  | 122.63      | 111.27   |
| 14  | G     | 839  | CLA  | C2C-C1C-NC  | 6.39  | 115.96      | 109.97   |
| 17  | Y     | 851  | BCR  | C34-C9-C10  | -6.39 | 113.97      | 122.92   |
| 14  | G     | 825  | CLA  | C4D-C3D-CAD | 6.39  | 112.03      | 108.47   |
| 17  | B     | 851  | BCR  | C37-C22-C21 | -6.39 | 113.97      | 122.92   |
| 14  | B     | 813  | CLA  | O2A-CGA-O1A | -6.38 | 107.48      | 123.59   |
| 14  | Y     | 804  | CLA  | C4A-NA-C1A  | 6.38  | 109.58      | 106.71   |
| 14  | Y     | 830  | CLA  | C2C-C1C-NC  | 6.38  | 115.95      | 109.97   |
| 14  | B     | 821  | CLA  | C4D-C3D-CAD | 6.38  | 112.03      | 108.47   |
| 14  | Y     | 830  | CLA  | C1C-C2C-C3C | -6.37 | 100.25      | 106.96   |
| 14  | Y     | 835  | CLA  | C2C-C1C-NC  | 6.37  | 115.94      | 109.97   |
| 14  | B     | 838  | CLA  | C2C-C1C-NC  | 6.36  | 115.93      | 109.97   |
| 14  | A     | 805  | CLA  | C2C-C1C-NC  | 6.36  | 115.93      | 109.97   |
| 14  | Z     | 807  | CLA  | O2D-CGD-CBD | 6.36  | 122.57      | 111.27   |
| 17  | F     | 203  | BCR  | C23-C22-C21 | 6.35  | 128.69      | 118.94   |
| 14  | K     | 101  | CLA  | C2C-C1C-NC  | 6.35  | 115.92      | 109.97   |
| 14  | A     | 831  | CLA  | C4D-C3D-CAD | 6.35  | 112.01      | 108.47   |
| 14  | G     | 831  | CLA  | C4D-C3D-CAD | 6.35  | 112.01      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Y     | 847  | BCR  | C34-C9-C10  | -6.35 | 114.03      | 122.92   |
| 14  | B     | 831  | CLA  | O2D-CGD-CBD | 6.34  | 122.54      | 111.27   |
| 14  | Y     | 808  | CLA  | O2D-CGD-CBD | 6.34  | 122.53      | 111.27   |
| 14  | A     | 824  | CLA  | C4D-C3D-CAD | 6.34  | 112.00      | 108.47   |
| 17  | A     | 848  | BCR  | C36-C18-C17 | -6.34 | 114.05      | 122.92   |
| 14  | j     | 102  | CLA  | C2C-C1C-NC  | 6.33  | 115.91      | 109.97   |
| 14  | H     | 803  | CLA  | C2C-C1C-NC  | 6.33  | 115.90      | 109.97   |
| 14  | A     | 819  | CLA  | C2C-C1C-NC  | 6.33  | 115.90      | 109.97   |
| 14  | H     | 828  | CLA  | O2D-CGD-CBD | 6.33  | 122.52      | 111.27   |
| 14  | Y     | 824  | CLA  | O2D-CGD-CBD | 6.33  | 122.51      | 111.27   |
| 17  | L     | 209  | BCR  | C33-C5-C6   | -6.32 | 117.43      | 124.53   |
| 14  | H     | 808  | CLA  | C1C-C2C-C3C | -6.32 | 100.31      | 106.96   |
| 14  | Z     | 834  | CLA  | C2C-C1C-NC  | 6.32  | 115.89      | 109.97   |
| 14  | H     | 833  | CLA  | C2C-C1C-NC  | 6.32  | 115.89      | 109.97   |
| 17  | h     | 202  | BCR  | C23-C22-C21 | 6.31  | 128.63      | 118.94   |
| 14  | Z     | 836  | CLA  | C4A-NA-C1A  | 6.31  | 109.54      | 106.71   |
| 14  | X     | 1701 | CLA  | C2C-C1C-NC  | 6.31  | 115.88      | 109.97   |
| 17  | H     | 848  | BCR  | C23-C24-C25 | -6.31 | 109.49      | 127.20   |
| 14  | Y     | 812  | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 14  | Y     | 806  | CLA  | O2D-CGD-CBD | 6.30  | 122.46      | 111.27   |
| 14  | Z     | 832  | CLA  | C4D-C3D-CAD | 6.30  | 111.98      | 108.47   |
| 14  | Z     | 804  | CLA  | C4D-C3D-CAD | 6.30  | 111.98      | 108.47   |
| 14  | L     | 206  | CLA  | C2C-C1C-NC  | 6.30  | 115.87      | 109.97   |
| 17  | d     | 203  | BCR  | C19-C18-C17 | 6.30  | 128.60      | 118.94   |
| 14  | Y     | 811  | CLA  | C1C-C2C-C3C | -6.29 | 100.34      | 106.96   |
| 14  | A     | 821  | CLA  | O2D-CGD-CBD | 6.29  | 122.45      | 111.27   |
| 14  | G     | 804  | CLA  | C4A-NA-C1A  | 6.29  | 109.53      | 106.71   |
| 14  | B     | 801  | CLA  | C2C-C1C-NC  | 6.29  | 115.86      | 109.97   |
| 14  | A     | 809  | CLA  | C4D-C3D-CAD | 6.29  | 111.98      | 108.47   |
| 14  | B     | 835  | CLA  | C4D-C3D-CAD | 6.29  | 111.98      | 108.47   |
| 14  | A     | 805  | CLA  | C4A-NA-C1A  | 6.29  | 109.53      | 106.71   |
| 14  | Y     | 826  | CLA  | O2D-CGD-CBD | 6.28  | 122.43      | 111.27   |
| 14  | Z     | 839  | CLA  | O2A-CGA-O1A | -6.28 | 107.74      | 123.59   |
| 17  | f     | 105  | BCR  | C19-C18-C17 | 6.28  | 128.58      | 118.94   |
| 14  | h     | 206  | CLA  | O2A-CGA-O1A | -6.27 | 107.76      | 123.59   |
| 14  | A     | 817  | CLA  | C2C-C1C-NC  | 6.27  | 115.85      | 109.97   |
| 17  | A     | 849  | BCR  | C34-C9-C10  | -6.27 | 114.14      | 122.92   |
| 14  | G     | 804  | CLA  | C2C-C1C-NC  | 6.27  | 115.85      | 109.97   |
| 14  | U     | 1006 | CLA  | C2C-C1C-NC  | 6.27  | 115.85      | 109.97   |
| 17  | V     | 1202 | BCR  | C19-C18-C17 | 6.27  | 128.56      | 118.94   |
| 14  | Y     | 827  | CLA  | C2C-C1C-NC  | 6.26  | 115.84      | 109.97   |
| 14  | G     | 837  | CLA  | C2C-C1C-NC  | 6.26  | 115.84      | 109.97   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 845  | BCR  | C37-C22-C21 | -6.26 | 114.16      | 122.92   |
| 14  | G     | 803  | CLA  | C2C-C1C-NC  | 6.26  | 115.83      | 109.97   |
| 14  | Z     | 814  | CLA  | C4A-NA-C1A  | 6.25  | 109.52      | 106.71   |
| 14  | G     | 843  | CLA  | C2C-C1C-NC  | 6.25  | 115.83      | 109.97   |
| 14  | Y     | 804  | CLA  | C4D-C3D-CAD | 6.25  | 111.95      | 108.47   |
| 17  | U     | 1008 | BCR  | C27-C26-C25 | -6.24 | 113.67      | 122.73   |
| 14  | Z     | 816  | CLA  | C2C-C1C-NC  | 6.24  | 115.82      | 109.97   |
| 14  | Z     | 823  | CLA  | C4D-C3D-CAD | 6.24  | 111.95      | 108.47   |
| 14  | H     | 809  | CLA  | C2C-C1C-NC  | 6.24  | 115.82      | 109.97   |
| 14  | B     | 838  | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |
| 14  | H     | 814  | CLA  | C2C-C1C-NC  | 6.23  | 115.81      | 109.97   |
| 17  | Q     | 204  | BCR  | C39-C30-C25 | -6.23 | 100.19      | 110.30   |
| 14  | H     | 824  | CLA  | O2D-CGD-CBD | 6.23  | 122.34      | 111.27   |
| 14  | H     | 829  | CLA  | C4A-NA-C1A  | 6.23  | 109.51      | 106.71   |
| 14  | Y     | 840  | CLA  | C4A-NA-C1A  | 6.23  | 109.51      | 106.71   |
| 14  | B     | 817  | CLA  | C2C-C1C-NC  | 6.23  | 115.81      | 109.97   |
| 14  | Y     | 816  | CLA  | C2C-C1C-NC  | 6.23  | 115.81      | 109.97   |
| 17  | B     | 847  | BCR  | C11-C10-C9  | 6.22  | 136.19      | 127.31   |
| 13  | Y     | 801  | CL0  | O2D-CGD-CBD | 6.22  | 122.32      | 111.27   |
| 17  | U     | 1007 | BCR  | C36-C18-C17 | -6.22 | 114.21      | 122.92   |
| 14  | Y     | 810  | CLA  | C2C-C1C-NC  | 6.21  | 115.79      | 109.97   |
| 14  | H     | 810  | CLA  | C2C-C1C-NC  | 6.21  | 115.79      | 109.97   |
| 14  | U     | 1002 | CLA  | C2C-C1C-NC  | 6.21  | 115.79      | 109.97   |
| 17  | L     | 203  | BCR  | C36-C18-C17 | -6.21 | 114.23      | 122.92   |
| 14  | B     | 809  | CLA  | C2C-C1C-NC  | 6.21  | 115.79      | 109.97   |
| 14  | B     | 832  | CLA  | O2D-CGD-CBD | 6.21  | 122.30      | 111.27   |
| 14  | L     | 201  | CLA  | C4A-NA-C1A  | 6.20  | 109.50      | 106.71   |
| 14  | Y     | 838  | CLA  | C4A-NA-C1A  | 6.20  | 109.49      | 106.71   |
| 14  | Y     | 842  | CLA  | O2A-CGA-O1A | -6.20 | 107.94      | 123.59   |
| 14  | G     | 825  | CLA  | C2C-C1C-NC  | 6.20  | 115.78      | 109.97   |
| 14  | Z     | 803  | CLA  | O2A-CGA-O1A | -6.20 | 107.95      | 123.59   |
| 14  | A     | 820  | CLA  | C2C-C1C-NC  | 6.19  | 115.77      | 109.97   |
| 14  | Z     | 809  | CLA  | C2C-C1C-NC  | 6.19  | 115.77      | 109.97   |
| 14  | H     | 809  | CLA  | C4D-C3D-CAD | 6.19  | 111.92      | 108.47   |
| 14  | S     | 1103 | CLA  | C2C-C1C-NC  | 6.19  | 115.77      | 109.97   |
| 14  | h     | 207  | CLA  | O2A-CGA-O1A | -6.18 | 107.99      | 123.59   |
| 14  | B     | 824  | CLA  | C2C-C1C-NC  | 6.18  | 115.76      | 109.97   |
| 14  | A     | 820  | CLA  | C4D-C3D-CAD | 6.18  | 111.92      | 108.47   |
| 14  | Y     | 835  | CLA  | O2D-CGD-CBD | 6.18  | 122.25      | 111.27   |
| 14  | B     | 819  | CLA  | C2C-C1C-NC  | 6.18  | 115.76      | 109.97   |
| 14  | B     | 807  | CLA  | C4A-NA-C1A  | 6.18  | 109.48      | 106.71   |
| 14  | Y     | 831  | CLA  | C2C-C1C-NC  | 6.18  | 115.76      | 109.97   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 849  | BCR  | C32-C1-C6   | 6.18  | 120.31      | 110.30   |
| 14  | Y     | 804  | CLA  | C1C-C2C-C3C | -6.17 | 100.47      | 106.96   |
| 14  | Y     | 808  | CLA  | C2C-C1C-NC  | 6.17  | 115.75      | 109.97   |
| 14  | Z     | 829  | CLA  | C4D-C3D-CAD | 6.17  | 111.91      | 108.47   |
| 14  | G     | 808  | CLA  | C2C-C1C-NC  | 6.16  | 115.75      | 109.97   |
| 14  | Y     | 840  | CLA  | C4D-C3D-CAD | 6.16  | 111.91      | 108.47   |
| 14  | B     | 833  | CLA  | C4A-NA-C1A  | 6.16  | 109.48      | 106.71   |
| 17  | S     | 1104 | BCR  | C33-C5-C6   | -6.16 | 117.61      | 124.53   |
| 17  | U     | 1008 | BCR  | C19-C18-C17 | 6.16  | 128.39      | 118.94   |
| 17  | L     | 209  | BCR  | C34-C9-C10  | -6.16 | 114.30      | 122.92   |
| 14  | Y     | 814  | CLA  | O2A-C1-C2   | 6.16  | 124.81      | 108.64   |
| 14  | Z     | 819  | CLA  | O2D-CGD-CBD | 6.15  | 122.20      | 111.27   |
| 14  | Y     | 840  | CLA  | C2C-C1C-NC  | 6.15  | 115.73      | 109.97   |
| 13  | G     | 801  | CL0  | C2C-C1C-NC  | 6.15  | 115.73      | 109.97   |
| 14  | B     | 831  | CLA  | C2C-C1C-NC  | 6.15  | 115.73      | 109.97   |
| 14  | B     | 809  | CLA  | OBD-CAD-CBD | -6.15 | 117.11      | 125.89   |
| 14  | B     | 809  | CLA  | C1C-C2C-C3C | -6.15 | 100.49      | 106.96   |
| 14  | B     | 831  | CLA  | C4A-NA-C1A  | 6.15  | 109.47      | 106.71   |
| 14  | Y     | 823  | CLA  | O2D-CGD-CBD | 6.15  | 122.19      | 111.27   |
| 14  | B     | 822  | CLA  | O2D-CGD-CBD | 6.15  | 122.19      | 111.27   |
| 14  | G     | 835  | CLA  | C2C-C1C-NC  | 6.15  | 115.73      | 109.97   |
| 14  | g     | 101  | CLA  | C2C-C1C-NC  | 6.15  | 115.73      | 109.97   |
| 14  | A     | 810  | CLA  | C2C-C1C-NC  | 6.14  | 115.72      | 109.97   |
| 17  | B     | 846  | BCR  | C23-C24-C25 | -6.14 | 109.96      | 127.20   |
| 14  | Z     | 817  | CLA  | C2C-C1C-NC  | 6.14  | 115.72      | 109.97   |
| 14  | Y     | 802  | CLA  | C2C-C1C-NC  | 6.14  | 115.72      | 109.97   |
| 14  | X     | 1701 | CLA  | C4D-C3D-CAD | 6.13  | 111.89      | 108.47   |
| 14  | B     | 834  | CLA  | C1C-C2C-C3C | -6.13 | 100.51      | 106.96   |
| 14  | Z     | 826  | CLA  | O2D-CGD-CBD | 6.13  | 122.17      | 111.27   |
| 17  | S     | 1104 | BCR  | C34-C9-C10  | -6.13 | 114.33      | 122.92   |
| 14  | B     | 820  | CLA  | C4D-C3D-CAD | 6.13  | 111.89      | 108.47   |
| 14  | A     | 839  | CLA  | C2C-C1C-NC  | 6.13  | 115.71      | 109.97   |
| 14  | A     | 841  | CLA  | C2C-C1C-NC  | 6.12  | 115.71      | 109.97   |
| 17  | F     | 201  | BCR  | C19-C18-C17 | 6.12  | 128.34      | 118.94   |
| 14  | B     | 819  | CLA  | C4D-C3D-CAD | 6.12  | 111.89      | 108.47   |
| 14  | B     | 830  | CLA  | C4D-C3D-CAD | 6.12  | 111.89      | 108.47   |
| 14  | B     | 803  | CLA  | C4A-NA-C1A  | 6.12  | 109.46      | 106.71   |
| 17  | Y     | 849  | BCR  | C19-C18-C17 | 6.12  | 128.34      | 118.94   |
| 14  | A     | 808  | CLA  | C2C-C1C-NC  | 6.12  | 115.71      | 109.97   |
| 17  | H     | 843  | BCR  | C23-C22-C21 | 6.12  | 128.33      | 118.94   |
| 14  | Z     | 815  | CLA  | O2A-CGA-O1A | -6.12 | 108.15      | 123.59   |
| 17  | B     | 846  | BCR  | C23-C22-C21 | 6.11  | 128.32      | 118.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | S     | 1103 | CLA  | C4D-C3D-CAD | 6.11  | 111.88      | 108.47   |
| 14  | J     | 102  | CLA  | C2C-C1C-NC  | 6.11  | 115.69      | 109.97   |
| 14  | G     | 832  | CLA  | C1C-C2C-C3C | -6.11 | 100.54      | 106.96   |
| 14  | H     | 823  | CLA  | O2D-CGD-CBD | 6.10  | 122.11      | 111.27   |
| 14  | Q     | 201  | CLA  | C4D-C3D-CAD | 6.10  | 111.87      | 108.47   |
| 17  | Z     | 843  | BCR  | C34-C9-C10  | -6.10 | 114.38      | 122.92   |
| 14  | G     | 804  | CLA  | C1C-C2C-C3C | -6.10 | 100.55      | 106.96   |
| 17  | H     | 843  | BCR  | C37-C22-C21 | -6.09 | 114.39      | 122.92   |
| 14  | H     | 819  | CLA  | C4A-NA-C1A  | 6.09  | 109.44      | 106.71   |
| 14  | A     | 818  | CLA  | C4D-C3D-CAD | 6.09  | 111.87      | 108.47   |
| 14  | Y     | 815  | CLA  | C2C-C1C-NC  | 6.09  | 115.68      | 109.97   |
| 17  | R     | 102  | BCR  | C36-C18-C17 | -6.09 | 114.39      | 122.92   |
| 14  | H     | 819  | CLA  | C1C-C2C-C3C | -6.09 | 100.56      | 106.96   |
| 14  | W     | 1701 | CLA  | C2C-C1C-NC  | 6.09  | 115.68      | 109.97   |
| 14  | Y     | 812  | CLA  | C2C-C1C-NC  | 6.09  | 115.68      | 109.97   |
| 14  | A     | 815  | CLA  | C2C-C1C-NC  | 6.09  | 115.68      | 109.97   |
| 14  | H     | 826  | CLA  | C4A-NA-C1A  | 6.08  | 109.44      | 106.71   |
| 14  | H     | 815  | CLA  | C4A-NA-C1A  | 6.08  | 109.44      | 106.71   |
| 14  | A     | 838  | CLA  | C2C-C1C-NC  | 6.08  | 115.67      | 109.97   |
| 14  | G     | 804  | CLA  | C4D-C3D-CAD | 6.08  | 111.86      | 108.47   |
| 14  | S     | 1101 | CLA  | C2C-C1C-NC  | 6.08  | 115.67      | 109.97   |
| 17  | G     | 849  | BCR  | C24-C23-C22 | -6.08 | 117.05      | 126.23   |
| 17  | h     | 202  | BCR  | C27-C26-C25 | -6.08 | 113.91      | 122.73   |
| 14  | H     | 816  | CLA  | O2D-CGD-CBD | 6.07  | 122.06      | 111.27   |
| 14  | A     | 802  | CLA  | O2A-CGA-O1A | -6.07 | 108.27      | 123.59   |
| 14  | Y     | 829  | CLA  | O2A-C1-C2   | 6.07  | 124.59      | 108.64   |
| 14  | Z     | 837  | CLA  | C1C-C2C-C3C | -6.07 | 100.57      | 106.96   |
| 14  | B     | 829  | CLA  | C1C-C2C-C3C | -6.07 | 100.58      | 106.96   |
| 14  | B     | 827  | CLA  | C4D-C3D-CAD | 6.07  | 111.85      | 108.47   |
| 17  | H     | 842  | BCR  | C36-C18-C17 | -6.06 | 114.43      | 122.92   |
| 14  | B     | 815  | CLA  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 14  | H     | 834  | CLA  | O2D-CGD-CBD | 6.06  | 122.04      | 111.27   |
| 14  | Z     | 827  | CLA  | C1C-C2C-C3C | -6.06 | 100.58      | 106.96   |
| 14  | B     | 829  | CLA  | O2A-CGA-O1A | -6.06 | 108.30      | 123.59   |
| 14  | H     | 819  | CLA  | C2C-C1C-NC  | 6.06  | 115.65      | 109.97   |
| 14  | A     | 835  | CLA  | O2D-CGD-CBD | 6.06  | 122.04      | 111.27   |
| 14  | B     | 816  | CLA  | C2C-C1C-NC  | 6.06  | 115.65      | 109.97   |
| 14  | B     | 832  | CLA  | C4D-C3D-CAD | 6.06  | 111.85      | 108.47   |
| 17  | Z     | 843  | BCR  | C36-C18-C17 | -6.05 | 114.45      | 122.92   |
| 14  | A     | 818  | CLA  | O2D-CGD-CBD | 6.05  | 122.02      | 111.27   |
| 17  | Y     | 847  | BCR  | C24-C23-C22 | -6.05 | 117.09      | 126.23   |
| 14  | L     | 206  | CLA  | O2A-CGA-O1A | -6.05 | 108.33      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 807  | CLA  | O2A-CGA-O1A | -6.05 | 108.33      | 123.59   |
| 14  | B     | 827  | CLA  | C2C-C1C-NC  | 6.05  | 115.64      | 109.97   |
| 14  | Y     | 854  | CLA  | OBD-CAD-CBD | -6.04 | 117.26      | 125.89   |
| 14  | Z     | 834  | CLA  | C4D-C3D-CAD | 6.04  | 111.84      | 108.47   |
| 14  | B     | 817  | CLA  | O2A-CGA-O1A | -6.04 | 108.34      | 123.59   |
| 14  | A     | 852  | CLA  | C1C-C2C-C3C | -6.04 | 100.60      | 106.96   |
| 17  | L     | 209  | BCR  | C37-C22-C21 | -6.04 | 114.46      | 122.92   |
| 14  | H     | 802  | CLA  | C2C-C1C-NC  | 6.04  | 115.63      | 109.97   |
| 14  | H     | 824  | CLA  | C2C-C1C-NC  | 6.04  | 115.63      | 109.97   |
| 14  | Y     | 822  | CLA  | C2C-C1C-NC  | 6.04  | 115.63      | 109.97   |
| 14  | G     | 824  | CLA  | C2C-C1C-NC  | 6.04  | 115.63      | 109.97   |
| 18  | Y     | 853  | LHG  | O7-C7-C8    | 6.03  | 122.19      | 111.09   |
| 14  | G     | 822  | CLA  | C4D-C3D-CAD | 6.03  | 111.83      | 108.47   |
| 14  | Y     | 830  | CLA  | C4A-NA-C1A  | 6.03  | 109.42      | 106.71   |
| 14  | A     | 808  | CLA  | O2A-CGA-O1A | -6.03 | 108.38      | 123.59   |
| 14  | B     | 833  | CLA  | O2D-CGD-CBD | 6.02  | 121.97      | 111.27   |
| 14  | A     | 837  | CLA  | C4A-NA-C1A  | 6.02  | 109.41      | 106.71   |
| 17  | G     | 847  | BCR  | C19-C18-C17 | 6.02  | 128.18      | 118.94   |
| 17  | S     | 1104 | BCR  | C36-C18-C17 | -6.02 | 114.49      | 122.92   |
| 14  | Y     | 824  | CLA  | C2C-C1C-NC  | 6.02  | 115.61      | 109.97   |
| 17  | H     | 842  | BCR  | C34-C9-C10  | -6.02 | 114.50      | 122.92   |
| 14  | B     | 839  | CLA  | C2C-C1C-NC  | 6.01  | 115.61      | 109.97   |
| 14  | B     | 828  | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 14  | G     | 815  | CLA  | C1C-C2C-C3C | -6.01 | 100.64      | 106.96   |
| 14  | Z     | 803  | CLA  | C2C-C1C-NC  | 6.01  | 115.60      | 109.97   |
| 14  | Y     | 826  | CLA  | C2C-C1C-NC  | 6.01  | 115.60      | 109.97   |
| 14  | H     | 836  | CLA  | C2C-C1C-NC  | 6.00  | 115.60      | 109.97   |
| 14  | Y     | 805  | CLA  | C4A-NA-C1A  | 6.00  | 109.40      | 106.71   |
| 14  | B     | 837  | CLA  | C2C-C1C-NC  | 6.00  | 115.59      | 109.97   |
| 14  | G     | 822  | CLA  | C1C-C2C-C3C | -6.00 | 100.65      | 106.96   |
| 14  | d     | 201  | CLA  | C2C-C1C-NC  | 6.00  | 115.59      | 109.97   |
| 14  | Z     | 834  | CLA  | O2D-CGD-CBD | 6.00  | 121.92      | 111.27   |
| 14  | A     | 815  | CLA  | C4D-C3D-CAD | 5.99  | 111.81      | 108.47   |
| 14  | H     | 804  | CLA  | C2C-C1C-NC  | 5.99  | 115.59      | 109.97   |
| 14  | B     | 805  | CLA  | C4A-NA-C1A  | 5.99  | 109.40      | 106.71   |
| 14  | H     | 828  | CLA  | O2A-CGA-O1A | -5.99 | 108.47      | 123.59   |
| 14  | H     | 816  | CLA  | C2C-C1C-NC  | 5.99  | 115.58      | 109.97   |
| 17  | H     | 841  | BCR  | C36-C18-C17 | -5.98 | 114.54      | 122.92   |
| 17  | M     | 101  | BCR  | C19-C18-C17 | 5.98  | 128.12      | 118.94   |
| 14  | U     | 1004 | CLA  | O2D-CGD-CBD | 5.98  | 121.89      | 111.27   |
| 14  | Y     | 807  | CLA  | C4D-C3D-CAD | 5.98  | 111.80      | 108.47   |
| 14  | H     | 821  | CLA  | C1C-C2C-C3C | -5.98 | 100.67      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | Y     | 801  | CL0  | C2C-C1C-NC  | 5.98  | 115.57      | 109.97   |
| 14  | Y     | 806  | CLA  | C2C-C1C-NC  | 5.97  | 115.57      | 109.97   |
| 14  | Y     | 832  | CLA  | C4A-NA-C1A  | 5.97  | 109.39      | 106.71   |
| 14  | H     | 801  | CLA  | O2A-CGA-O1A | -5.97 | 108.52      | 123.59   |
| 14  | Y     | 826  | CLA  | C1C-C2C-C3C | -5.97 | 100.68      | 106.96   |
| 14  | Y     | 823  | CLA  | C2C-C1C-NC  | 5.97  | 115.56      | 109.97   |
| 14  | B     | 808  | CLA  | C1C-C2C-C3C | -5.97 | 100.68      | 106.96   |
| 14  | H     | 823  | CLA  | C4D-C3D-CAD | 5.97  | 111.80      | 108.47   |
| 14  | G     | 825  | CLA  | C4A-NA-C1A  | 5.97  | 109.39      | 106.71   |
| 14  | h     | 205  | CLA  | C2C-C1C-NC  | 5.96  | 115.56      | 109.97   |
| 14  | Y     | 842  | CLA  | C2C-C1C-NC  | 5.96  | 115.56      | 109.97   |
| 14  | Z     | 828  | CLA  | C2C-C1C-NC  | 5.96  | 115.56      | 109.97   |
| 17  | F     | 201  | BCR  | C8-C7-C6    | -5.96 | 110.47      | 127.20   |
| 14  | A     | 840  | CLA  | C2C-C1C-NC  | 5.96  | 115.55      | 109.97   |
| 14  | H     | 801  | CLA  | C2C-C1C-NC  | 5.95  | 115.55      | 109.97   |
| 14  | H     | 812  | CLA  | O2A-CGA-O1A | -5.95 | 108.58      | 123.59   |
| 14  | G     | 802  | CLA  | C1-O2A-CGA  | 5.95  | 132.05      | 116.44   |
| 14  | h     | 201  | CLA  | C2C-C1C-NC  | 5.95  | 115.54      | 109.97   |
| 17  | h     | 203  | BCR  | C23-C24-C25 | -5.95 | 110.50      | 127.20   |
| 13  | A     | 801  | CL0  | C2C-C1C-NC  | 5.95  | 115.54      | 109.97   |
| 14  | A     | 833  | CLA  | C2C-C1C-NC  | 5.94  | 115.54      | 109.97   |
| 14  | Y     | 832  | CLA  | O2A-CGA-O1A | -5.94 | 108.59      | 123.59   |
| 17  | H     | 841  | BCR  | C19-C18-C17 | 5.94  | 128.06      | 118.94   |
| 14  | A     | 852  | CLA  | O2A-C1-C2   | 5.94  | 124.25      | 108.64   |
| 17  | U     | 1007 | BCR  | C19-C18-C17 | 5.94  | 128.05      | 118.94   |
| 14  | A     | 842  | CLA  | C2C-C1C-NC  | 5.94  | 115.53      | 109.97   |
| 14  | d     | 201  | CLA  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 14  | G     | 818  | CLA  | O2D-CGD-CBD | 5.93  | 121.81      | 111.27   |
| 14  | A     | 822  | CLA  | C1C-C2C-C3C | -5.93 | 100.72      | 106.96   |
| 14  | H     | 838  | CLA  | O2A-CGA-O1A | -5.93 | 108.62      | 123.59   |
| 13  | G     | 801  | CL0  | O2A-CGA-CBA | 5.93  | 130.53      | 111.91   |
| 14  | Y     | 807  | CLA  | C2C-C1C-NC  | 5.93  | 115.53      | 109.97   |
| 14  | Y     | 820  | CLA  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 14  | U     | 1002 | CLA  | O2A-C1-C2   | 5.93  | 124.21      | 108.64   |
| 14  | A     | 802  | CLA  | O2D-CGD-CBD | 5.92  | 121.79      | 111.27   |
| 14  | Z     | 832  | CLA  | C2C-C1C-NC  | 5.92  | 115.52      | 109.97   |
| 14  | H     | 810  | CLA  | O2D-CGD-CBD | 5.92  | 121.79      | 111.27   |
| 14  | Z     | 804  | CLA  | C4A-NA-C1A  | 5.92  | 109.37      | 106.71   |
| 14  | Y     | 839  | CLA  | O2A-CGA-O1A | -5.92 | 108.66      | 123.59   |
| 14  | B     | 805  | CLA  | C2C-C1C-NC  | 5.91  | 115.51      | 109.97   |
| 17  | Y     | 849  | BCR  | C36-C18-C17 | -5.91 | 114.64      | 122.92   |
| 14  | B     | 811  | CLA  | C2C-C1C-NC  | 5.91  | 115.51      | 109.97   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 811 | CLA  | C2C-C1C-NC  | 5.91  | 115.51      | 109.97   |
| 14  | H     | 814 | CLA  | C4A-NA-C1A  | 5.91  | 109.36      | 106.71   |
| 14  | Q     | 201 | CLA  | C1C-C2C-C3C | -5.91 | 100.75      | 106.96   |
| 17  | Q     | 202 | BCR  | C19-C18-C17 | 5.91  | 128.00      | 118.94   |
| 14  | Y     | 837 | CLA  | C2C-C1C-NC  | 5.91  | 115.50      | 109.97   |
| 14  | B     | 833 | CLA  | C2C-C1C-NC  | 5.90  | 115.50      | 109.97   |
| 14  | Z     | 809 | CLA  | C4A-NA-C1A  | 5.90  | 109.36      | 106.71   |
| 14  | Y     | 839 | CLA  | C4A-NA-C1A  | 5.90  | 109.36      | 106.71   |
| 14  | T     | 103 | CLA  | C1C-C2C-C3C | -5.90 | 100.75      | 106.96   |
| 14  | Y     | 820 | CLA  | O2D-CGD-CBD | 5.90  | 121.76      | 111.27   |
| 14  | Z     | 829 | CLA  | OBD-CAD-C3D | -5.90 | 118.18      | 127.98   |
| 14  | B     | 802 | CLA  | C2C-C1C-NC  | 5.90  | 115.50      | 109.97   |
| 14  | G     | 853 | CLA  | C2C-C1C-NC  | 5.90  | 115.50      | 109.97   |
| 17  | A     | 848 | BCR  | C34-C9-C10  | -5.89 | 114.67      | 122.92   |
| 17  | H     | 840 | BCR  | C19-C18-C17 | 5.89  | 127.98      | 118.94   |
| 14  | H     | 801 | CLA  | C4A-NA-C1A  | 5.89  | 109.35      | 106.71   |
| 14  | Y     | 809 | CLA  | C2C-C1C-NC  | 5.89  | 115.49      | 109.97   |
| 14  | A     | 804 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 14  | A     | 803 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 14  | f     | 102 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 14  | Y     | 833 | CLA  | C1C-C2C-C3C | -5.88 | 100.77      | 106.96   |
| 14  | G     | 823 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 17  | I     | 101 | BCR  | C8-C7-C6    | -5.88 | 110.70      | 127.20   |
| 14  | Z     | 815 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 14  | Z     | 801 | CLA  | C4A-NA-C1A  | 5.87  | 109.35      | 106.71   |
| 14  | H     | 835 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 14  | Y     | 854 | CLA  | C4A-NA-C1A  | 5.87  | 109.35      | 106.71   |
| 14  | H     | 806 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 14  | G     | 833 | CLA  | C4A-NA-C1A  | 5.87  | 109.34      | 106.71   |
| 14  | A     | 814 | CLA  | C4A-NA-C1A  | 5.87  | 109.34      | 106.71   |
| 14  | A     | 838 | CLA  | O2D-CGD-CBD | 5.87  | 121.69      | 111.27   |
| 14  | Y     | 855 | CLA  | C2C-C1C-NC  | 5.86  | 115.47      | 109.97   |
| 14  | G     | 817 | CLA  | C2C-C1C-NC  | 5.86  | 115.46      | 109.97   |
| 14  | G     | 826 | CLA  | C2C-C1C-NC  | 5.86  | 115.46      | 109.97   |
| 14  | G     | 805 | CLA  | C4A-NA-C1A  | 5.86  | 109.34      | 106.71   |
| 14  | B     | 839 | CLA  | O2D-CGD-CBD | 5.86  | 121.68      | 111.27   |
| 14  | G     | 830 | CLA  | C1C-C2C-C3C | -5.86 | 100.80      | 106.96   |
| 14  | J     | 101 | CLA  | C4A-NA-C1A  | 5.86  | 109.34      | 106.71   |
| 14  | H     | 820 | CLA  | C2C-C1C-NC  | 5.85  | 115.46      | 109.97   |
| 14  | A     | 837 | CLA  | C4D-C3D-CAD | 5.85  | 111.73      | 108.47   |
| 14  | G     | 829 | CLA  | C2C-C1C-NC  | 5.85  | 115.45      | 109.97   |
| 14  | A     | 838 | CLA  | O2A-CGA-O1A | -5.85 | 108.83      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | H     | 831 | CLA  | C1C-C2C-C3C | -5.85 | 100.81      | 106.96   |
| 14  | A     | 823 | CLA  | C4A-NA-C1A  | 5.85  | 109.33      | 106.71   |
| 14  | Y     | 808 | CLA  | O2A-CGA-O1A | -5.85 | 108.84      | 123.59   |
| 14  | Z     | 823 | CLA  | C1C-C2C-C3C | -5.84 | 100.81      | 106.96   |
| 14  | B     | 806 | CLA  | C2C-C1C-NC  | 5.84  | 115.44      | 109.97   |
| 17  | H     | 844 | BCR  | C8-C7-C6    | -5.84 | 110.81      | 127.20   |
| 14  | Y     | 825 | CLA  | C1C-C2C-C3C | -5.83 | 100.82      | 106.96   |
| 14  | H     | 829 | CLA  | C2C-C1C-NC  | 5.83  | 115.43      | 109.97   |
| 17  | G     | 849 | BCR  | C37-C22-C21 | -5.83 | 114.76      | 122.92   |
| 14  | B     | 830 | CLA  | C1C-C2C-C3C | -5.83 | 100.83      | 106.96   |
| 14  | H     | 802 | CLA  | C4A-NA-C1A  | 5.82  | 109.32      | 106.71   |
| 14  | B     | 806 | CLA  | C1C-C2C-C3C | -5.82 | 100.84      | 106.96   |
| 17  | B     | 847 | BCR  | C19-C18-C17 | 5.81  | 127.86      | 118.94   |
| 14  | B     | 803 | CLA  | C1C-C2C-C3C | -5.81 | 100.84      | 106.96   |
| 14  | A     | 826 | CLA  | C4D-C3D-CAD | 5.81  | 111.71      | 108.47   |
| 14  | A     | 825 | CLA  | C4D-C3D-CAD | 5.81  | 111.71      | 108.47   |
| 14  | Y     | 839 | CLA  | C4D-C3D-CAD | 5.81  | 111.71      | 108.47   |
| 14  | G     | 807 | CLA  | C4D-C3D-CAD | 5.81  | 111.71      | 108.47   |
| 14  | G     | 807 | CLA  | O2A-C1-C2   | 5.81  | 123.91      | 108.64   |
| 14  | B     | 801 | CLA  | O2A-CGA-O1A | -5.81 | 108.93      | 123.59   |
| 14  | B     | 841 | CLA  | C2C-C1C-NC  | 5.81  | 115.41      | 109.97   |
| 17  | f     | 104 | BCR  | C34-C9-C10  | -5.81 | 114.79      | 122.92   |
| 17  | M     | 101 | BCR  | C37-C22-C21 | -5.81 | 114.79      | 122.92   |
| 14  | A     | 836 | CLA  | C2C-C1C-NC  | 5.81  | 115.41      | 109.97   |
| 14  | Y     | 806 | CLA  | C1C-C2C-C3C | -5.81 | 100.85      | 106.96   |
| 14  | Y     | 822 | CLA  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 14  | J     | 101 | CLA  | C2C-C1C-NC  | 5.80  | 115.41      | 109.97   |
| 14  | Z     | 802 | CLA  | C2C-C1C-NC  | 5.80  | 115.41      | 109.97   |
| 14  | Y     | 819 | CLA  | O2A-CGA-O1A | -5.80 | 108.95      | 123.59   |
| 14  | d     | 202 | CLA  | C1C-C2C-C3C | -5.80 | 100.86      | 106.96   |
| 14  | G     | 843 | CLA  | O2D-CGD-CBD | 5.80  | 121.58      | 111.27   |
| 17  | h     | 203 | BCR  | C34-C9-C8   | 5.80  | 127.21      | 118.08   |
| 14  | H     | 813 | CLA  | C2C-C1C-NC  | 5.79  | 115.40      | 109.97   |
| 14  | B     | 806 | CLA  | O2D-CGD-CBD | 5.79  | 121.55      | 111.27   |
| 14  | B     | 806 | CLA  | O2A-CGA-O1A | -5.79 | 108.99      | 123.59   |
| 14  | G     | 806 | CLA  | C2C-C1C-NC  | 5.78  | 115.39      | 109.97   |
| 14  | A     | 835 | CLA  | C2C-C1C-NC  | 5.78  | 115.39      | 109.97   |
| 14  | Y     | 840 | CLA  | O2D-CGD-CBD | 5.78  | 121.54      | 111.27   |
| 14  | Y     | 832 | CLA  | O2A-C1-C2   | 5.78  | 123.83      | 108.64   |
| 17  | Q     | 204 | BCR  | C27-C26-C25 | -5.78 | 114.34      | 122.73   |
| 14  | Z     | 826 | CLA  | C2C-C1C-NC  | 5.78  | 115.39      | 109.97   |
| 17  | G     | 854 | BCR  | C30-C25-C26 | -5.78 | 114.47      | 122.61   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 809  | CLA  | C1C-C2C-C3C | -5.77 | 100.89      | 106.96   |
| 14  | B     | 810  | CLA  | O2D-CGD-CBD | 5.77  | 121.52      | 111.27   |
| 14  | A     | 803  | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 14  | Z     | 805  | CLA  | O2A-CGA-O1A | -5.76 | 109.05      | 123.59   |
| 14  | L     | 206  | CLA  | C1C-C2C-C3C | -5.76 | 100.90      | 106.96   |
| 14  | U     | 1006 | CLA  | O2A-CGA-O1A | -5.76 | 109.06      | 123.59   |
| 14  | A     | 816  | CLA  | O2D-CGD-CBD | 5.76  | 121.50      | 111.27   |
| 14  | Y     | 810  | CLA  | C1C-C2C-C3C | -5.75 | 100.91      | 106.96   |
| 14  | L     | 202  | CLA  | O2A-CGA-O1A | -5.75 | 109.07      | 123.59   |
| 17  | R     | 102  | BCR  | C24-C23-C22 | -5.75 | 117.54      | 126.23   |
| 17  | H     | 845  | BCR  | C36-C18-C17 | -5.75 | 114.87      | 122.92   |
| 14  | B     | 806  | CLA  | O2A-C1-C2   | 5.75  | 123.75      | 108.64   |
| 14  | Z     | 818  | CLA  | C2C-C1C-NC  | 5.75  | 115.36      | 109.97   |
| 14  | Y     | 825  | CLA  | O2A-C1-C2   | 5.75  | 123.74      | 108.64   |
| 14  | Z     | 804  | CLA  | C1C-C2C-C3C | -5.75 | 100.91      | 106.96   |
| 14  | Z     | 810  | CLA  | C2C-C1C-NC  | 5.75  | 115.36      | 109.97   |
| 17  | U     | 1005 | BCR  | C34-C9-C10  | -5.75 | 114.87      | 122.92   |
| 14  | Y     | 837  | CLA  | C4D-C3D-CAD | 5.75  | 111.67      | 108.47   |
| 14  | B     | 814  | CLA  | O2D-CGD-CBD | 5.74  | 121.48      | 111.27   |
| 14  | G     | 810  | CLA  | C4A-NA-C1A  | 5.74  | 109.29      | 106.71   |
| 14  | H     | 826  | CLA  | C2C-C1C-NC  | 5.74  | 115.35      | 109.97   |
| 14  | G     | 823  | CLA  | C4A-NA-C1A  | 5.74  | 109.29      | 106.71   |
| 13  | G     | 801  | CL0  | C1C-C2C-C3C | -5.74 | 100.92      | 106.96   |
| 14  | W     | 1701 | CLA  | C4A-NA-C1A  | 5.74  | 109.28      | 106.71   |
| 14  | H     | 807  | CLA  | C1C-C2C-C3C | -5.74 | 100.93      | 106.96   |
| 14  | Y     | 837  | CLA  | C1C-C2C-C3C | -5.74 | 100.93      | 106.96   |
| 14  | A     | 808  | CLA  | C1C-C2C-C3C | -5.74 | 100.93      | 106.96   |
| 14  | H     | 805  | CLA  | C2C-C1C-NC  | 5.73  | 115.34      | 109.97   |
| 14  | J     | 102  | CLA  | O2D-CGD-CBD | 5.73  | 121.46      | 111.27   |
| 14  | Z     | 837  | CLA  | O2D-CGD-CBD | 5.73  | 121.46      | 111.27   |
| 14  | G     | 841  | CLA  | C1C-C2C-C3C | -5.73 | 100.93      | 106.96   |
| 17  | Q     | 204  | BCR  | C37-C22-C21 | -5.73 | 114.89      | 122.92   |
| 14  | H     | 819  | CLA  | O2D-CGD-CBD | 5.73  | 121.45      | 111.27   |
| 14  | B     | 815  | CLA  | C1C-C2C-C3C | -5.73 | 100.93      | 106.96   |
| 14  | G     | 807  | CLA  | O2A-CGA-O1A | -5.73 | 109.14      | 123.59   |
| 14  | B     | 801  | CLA  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 14  | U     | 1004 | CLA  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 14  | Z     | 828  | CLA  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 14  | G     | 810  | CLA  | O2D-CGD-CBD | 5.72  | 121.44      | 111.27   |
| 14  | Z     | 831  | CLA  | C2C-C1C-NC  | 5.72  | 115.33      | 109.97   |
| 14  | G     | 824  | CLA  | C4D-C3D-CAD | 5.72  | 111.66      | 108.47   |
| 14  | H     | 816  | CLA  | C4D-C3D-CAD | 5.72  | 111.66      | 108.47   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 827  | CLA  | C4D-C3D-CAD | 5.72  | 111.66      | 108.47   |
| 14  | Z     | 808  | CLA  | C4A-NA-C1A  | 5.72  | 109.28      | 106.71   |
| 14  | H     | 827  | CLA  | C2C-C1C-NC  | 5.71  | 115.33      | 109.97   |
| 14  | A     | 807  | CLA  | C1C-C2C-C3C | -5.71 | 100.95      | 106.96   |
| 14  | A     | 833  | CLA  | O2A-CGA-O1A | -5.71 | 109.18      | 123.59   |
| 14  | Y     | 820  | CLA  | C2C-C1C-NC  | 5.71  | 115.32      | 109.97   |
| 14  | A     | 817  | CLA  | C4A-NA-C1A  | 5.71  | 109.27      | 106.71   |
| 14  | B     | 822  | CLA  | C4D-C3D-CAD | 5.71  | 111.65      | 108.47   |
| 14  | S     | 1102 | CLA  | C1C-C2C-C3C | -5.70 | 100.96      | 106.96   |
| 17  | A     | 849  | BCR  | C33-C5-C6   | -5.70 | 118.12      | 124.53   |
| 14  | A     | 839  | CLA  | C4D-C3D-CAD | 5.70  | 111.65      | 108.47   |
| 14  | A     | 826  | CLA  | C2C-C1C-NC  | 5.70  | 115.31      | 109.97   |
| 14  | H     | 811  | CLA  | C2C-C1C-NC  | 5.70  | 115.31      | 109.97   |
| 13  | G     | 801  | CL0  | O2D-CGD-CBD | 5.70  | 121.39      | 111.27   |
| 14  | G     | 831  | CLA  | O2A-CGA-O1A | -5.70 | 109.22      | 123.59   |
| 14  | H     | 816  | CLA  | O2A-CGA-O1A | -5.69 | 109.22      | 123.59   |
| 17  | H     | 844  | BCR  | C24-C23-C22 | -5.69 | 117.63      | 126.23   |
| 14  | G     | 806  | CLA  | O2D-CGD-CBD | 5.69  | 121.38      | 111.27   |
| 14  | Y     | 854  | CLA  | C2C-C1C-NC  | 5.69  | 115.30      | 109.97   |
| 14  | Z     | 801  | CLA  | O2A-CGA-O1A | -5.68 | 109.25      | 123.59   |
| 14  | Z     | 811  | CLA  | C2C-C1C-NC  | 5.68  | 115.30      | 109.97   |
| 14  | L     | 207  | CLA  | O2D-CGD-CBD | 5.68  | 121.37      | 111.27   |
| 14  | Y     | 843  | CLA  | C1C-C2C-C3C | -5.68 | 100.98      | 106.96   |
| 14  | A     | 816  | CLA  | C1C-C2C-C3C | -5.68 | 100.99      | 106.96   |
| 17  | B     | 851  | BCR  | C36-C18-C17 | -5.68 | 114.97      | 122.92   |
| 14  | G     | 806  | CLA  | C4A-NA-C1A  | 5.68  | 109.26      | 106.71   |
| 14  | Z     | 823  | CLA  | C4A-NA-C1A  | 5.68  | 109.26      | 106.71   |
| 14  | Z     | 821  | CLA  | C2C-C1C-NC  | 5.68  | 115.29      | 109.97   |
| 14  | A     | 852  | CLA  | C4A-NA-C1A  | 5.67  | 109.25      | 106.71   |
| 17  | G     | 848  | BCR  | C30-C25-C26 | -5.67 | 114.63      | 122.61   |
| 14  | B     | 825  | CLA  | C4D-C3D-CAD | 5.67  | 111.63      | 108.47   |
| 14  | A     | 818  | CLA  | O2A-C1-C2   | 5.67  | 123.53      | 108.64   |
| 14  | H     | 817  | CLA  | C4A-NA-C1A  | 5.67  | 109.25      | 106.71   |
| 14  | G     | 837  | CLA  | C4A-NA-C1A  | 5.67  | 109.25      | 106.71   |
| 14  | Y     | 836  | CLA  | O2D-CGD-CBD | 5.66  | 121.33      | 111.27   |
| 14  | B     | 815  | CLA  | C2C-C1C-NC  | 5.66  | 115.28      | 109.97   |
| 14  | Z     | 834  | CLA  | OBD-CAD-C3D | -5.66 | 118.58      | 127.98   |
| 17  | T     | 102  | BCR  | C36-C18-C17 | -5.66 | 115.00      | 122.92   |
| 14  | A     | 811  | CLA  | C1C-C2C-C3C | -5.66 | 101.01      | 106.96   |
| 14  | G     | 831  | CLA  | C2C-C1C-NC  | 5.65  | 115.27      | 109.97   |
| 14  | G     | 820  | CLA  | O2D-CGD-CBD | 5.65  | 121.31      | 111.27   |
| 14  | Z     | 825  | CLA  | O2A-CGA-O1A | -5.65 | 109.33      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 830  | CLA  | C2C-C1C-NC  | 5.65  | 115.27      | 109.97   |
| 17  | Y     | 850  | BCR  | C19-C18-C17 | 5.65  | 127.61      | 118.94   |
| 14  | B     | 814  | CLA  | C2C-C1C-NC  | 5.65  | 115.26      | 109.97   |
| 14  | B     | 821  | CLA  | O2D-CGD-CBD | 5.64  | 121.30      | 111.27   |
| 14  | B     | 837  | CLA  | C4A-NA-C1A  | 5.64  | 109.24      | 106.71   |
| 14  | B     | 838  | CLA  | C4D-C3D-CAD | 5.64  | 111.62      | 108.47   |
| 14  | H     | 808  | CLA  | C4D-C3D-CAD | 5.64  | 111.62      | 108.47   |
| 14  | Z     | 808  | CLA  | C4D-C3D-CAD | 5.64  | 111.61      | 108.47   |
| 14  | G     | 828  | CLA  | C4D-C3D-CAD | 5.64  | 111.61      | 108.47   |
| 14  | B     | 836  | CLA  | C1C-C2C-C3C | -5.64 | 101.03      | 106.96   |
| 14  | G     | 812  | CLA  | C1C-C2C-C3C | -5.64 | 101.03      | 106.96   |
| 14  | Z     | 816  | CLA  | C4A-NA-C1A  | 5.63  | 109.24      | 106.71   |
| 14  | B     | 813  | CLA  | O2A-C1-C2   | 5.63  | 123.44      | 108.64   |
| 14  | H     | 820  | CLA  | C4D-C3D-CAD | 5.63  | 111.61      | 108.47   |
| 14  | f     | 101  | CLA  | O2D-CGD-CBD | 5.63  | 121.27      | 111.27   |
| 14  | H     | 810  | CLA  | C1C-C2C-C3C | -5.62 | 101.04      | 106.96   |
| 14  | U     | 1002 | CLA  | C4D-C3D-CAD | 5.62  | 111.61      | 108.47   |
| 13  | A     | 801  | CL0  | C4D-C3D-CAD | 5.62  | 111.60      | 108.47   |
| 17  | Z     | 843  | BCR  | C8-C7-C6    | -5.62 | 111.42      | 127.20   |
| 14  | G     | 805  | CLA  | C1C-C2C-C3C | -5.62 | 101.05      | 106.96   |
| 14  | H     | 815  | CLA  | C2C-C1C-NC  | 5.62  | 115.23      | 109.97   |
| 14  | A     | 810  | CLA  | C1C-C2C-C3C | -5.62 | 101.05      | 106.96   |
| 17  | Z     | 841  | BCR  | C36-C18-C17 | -5.61 | 115.06      | 122.92   |
| 14  | B     | 815  | CLA  | O2D-CGD-CBD | 5.61  | 121.24      | 111.27   |
| 14  | B     | 820  | CLA  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 14  | F     | 202  | CLA  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 14  | Y     | 822  | CLA  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 14  | Y     | 838  | CLA  | C2C-C1C-NC  | 5.61  | 115.23      | 109.97   |
| 14  | B     | 802  | CLA  | C4A-NA-C1A  | 5.61  | 109.23      | 106.71   |
| 14  | S     | 1103 | CLA  | C4A-NA-C1A  | 5.61  | 109.23      | 106.71   |
| 14  | U     | 1004 | CLA  | C1C-C2C-C3C | -5.61 | 101.06      | 106.96   |
| 14  | G     | 824  | CLA  | C4A-NA-C1A  | 5.61  | 109.23      | 106.71   |
| 17  | J     | 103  | BCR  | C8-C7-C6    | -5.60 | 111.46      | 127.20   |
| 17  | B     | 844  | BCR  | C34-C9-C10  | -5.60 | 115.07      | 122.92   |
| 14  | L     | 206  | CLA  | O2D-CGD-CBD | 5.60  | 121.22      | 111.27   |
| 14  | Y     | 809  | CLA  | C4D-C3D-CAD | 5.60  | 111.59      | 108.47   |
| 14  | B     | 829  | CLA  | O2D-CGD-CBD | 5.60  | 121.22      | 111.27   |
| 14  | H     | 818  | CLA  | C1C-C2C-C3C | -5.60 | 101.07      | 106.96   |
| 14  | B     | 824  | CLA  | C4D-C3D-CAD | 5.60  | 111.59      | 108.47   |
| 14  | G     | 828  | CLA  | C2C-C1C-NC  | 5.60  | 115.22      | 109.97   |
| 14  | Z     | 827  | CLA  | O2D-CGD-CBD | 5.60  | 121.21      | 111.27   |
| 14  | A     | 834  | CLA  | O2A-C1-C2   | 5.60  | 123.34      | 108.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 812  | CLA  | O2A-CGA-O1A | -5.60 | 109.47      | 123.59   |
| 14  | L     | 206  | CLA  | C4D-C3D-CAD | 5.60  | 111.59      | 108.47   |
| 17  | H     | 841  | BCR  | C24-C23-C22 | -5.59 | 117.78      | 126.23   |
| 17  | i     | 101  | BCR  | C37-C22-C21 | -5.59 | 115.09      | 122.92   |
| 14  | h     | 205  | CLA  | C4A-NA-C1A  | 5.59  | 109.22      | 106.71   |
| 14  | A     | 826  | CLA  | C1C-C2C-C3C | -5.59 | 101.08      | 106.96   |
| 14  | A     | 823  | CLA  | C2C-C1C-NC  | 5.59  | 115.21      | 109.97   |
| 14  | G     | 838  | CLA  | C1C-C2C-C3C | -5.59 | 101.08      | 106.96   |
| 17  | B     | 851  | BCR  | C24-C23-C22 | -5.59 | 117.79      | 126.23   |
| 14  | A     | 820  | CLA  | O2A-CGA-O1A | -5.58 | 109.50      | 123.59   |
| 14  | H     | 838  | CLA  | O2D-CGD-CBD | 5.58  | 121.19      | 111.27   |
| 14  | Y     | 814  | CLA  | O2A-CGA-O1A | -5.58 | 109.50      | 123.59   |
| 17  | f     | 105  | BCR  | C23-C24-C25 | -5.58 | 111.53      | 127.20   |
| 17  | Z     | 846  | BCR  | C24-C23-C22 | -5.58 | 117.81      | 126.23   |
| 14  | H     | 801  | CLA  | C4D-C3D-CAD | 5.58  | 111.58      | 108.47   |
| 14  | V     | 1201 | CLA  | C4A-NA-C1A  | 5.58  | 109.21      | 106.71   |
| 14  | Y     | 822  | CLA  | O2D-CGD-CBD | 5.57  | 121.17      | 111.27   |
| 14  | Y     | 843  | CLA  | O2D-CGD-CBD | 5.57  | 121.17      | 111.27   |
| 14  | A     | 804  | CLA  | C1C-C2C-C3C | -5.57 | 101.10      | 106.96   |
| 14  | Y     | 802  | CLA  | C4A-NA-C1A  | 5.57  | 109.21      | 106.71   |
| 14  | J     | 102  | CLA  | O2A-CGA-O1A | -5.57 | 109.53      | 123.59   |
| 14  | H     | 805  | CLA  | C4A-NA-C1A  | 5.57  | 109.21      | 106.71   |
| 14  | B     | 835  | CLA  | C2C-C1C-NC  | 5.57  | 115.19      | 109.97   |
| 14  | Z     | 817  | CLA  | C1C-C2C-C3C | -5.57 | 101.10      | 106.96   |
| 14  | G     | 816  | CLA  | O2A-CGA-O1A | -5.57 | 109.54      | 123.59   |
| 14  | G     | 813  | CLA  | O2D-CGD-CBD | 5.57  | 121.16      | 111.27   |
| 14  | H     | 829  | CLA  | O2D-CGD-CBD | 5.57  | 121.16      | 111.27   |
| 14  | Q     | 203  | CLA  | OBD-CAD-C3D | -5.56 | 118.74      | 127.98   |
| 14  | A     | 828  | CLA  | OBD-CAD-C3D | -5.56 | 118.75      | 127.98   |
| 14  | Q     | 203  | CLA  | C1C-C2C-C3C | -5.56 | 101.11      | 106.96   |
| 17  | H     | 842  | BCR  | C8-C7-C6    | -5.56 | 111.59      | 127.20   |
| 14  | H     | 820  | CLA  | O2D-CGD-CBD | 5.56  | 121.15      | 111.27   |
| 14  | G     | 816  | CLA  | C1C-C2C-C3C | -5.56 | 101.11      | 106.96   |
| 17  | F     | 201  | BCR  | C36-C18-C17 | -5.55 | 115.14      | 122.92   |
| 14  | Y     | 810  | CLA  | O2D-CGD-CBD | 5.55  | 121.13      | 111.27   |
| 14  | Z     | 807  | CLA  | C4D-C3D-CAD | 5.55  | 111.56      | 108.47   |
| 14  | A     | 810  | CLA  | O2D-CGD-CBD | 5.55  | 121.13      | 111.27   |
| 14  | Z     | 805  | CLA  | C4A-NA-C1A  | 5.55  | 109.20      | 106.71   |
| 14  | H     | 813  | CLA  | C4A-NA-C1A  | 5.55  | 109.20      | 106.71   |
| 14  | K     | 103  | CLA  | O2D-CGD-CBD | 5.55  | 121.12      | 111.27   |
| 14  | G     | 826  | CLA  | O2A-CGA-O1A | -5.54 | 109.60      | 123.59   |
| 14  | G     | 836  | CLA  | C4D-C3D-CAD | 5.54  | 111.56      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | Y     | 815 | CLA  | C4A-NA-C1A  | 5.54  | 109.20      | 106.71   |
| 14  | G     | 809 | CLA  | C2C-C1C-NC  | 5.54  | 115.16      | 109.97   |
| 14  | G     | 817 | CLA  | O2A-C1-C2   | 5.54  | 123.18      | 108.64   |
| 14  | Z     | 829 | CLA  | O2D-CGD-CBD | 5.53  | 121.10      | 111.27   |
| 14  | H     | 838 | CLA  | C4D-C3D-CAD | 5.53  | 111.55      | 108.47   |
| 14  | G     | 811 | CLA  | C1C-C2C-C3C | -5.53 | 101.15      | 106.96   |
| 14  | Y     | 830 | CLA  | O2D-CGD-CBD | 5.53  | 121.09      | 111.27   |
| 14  | A     | 804 | CLA  | C4D-C3D-CAD | 5.53  | 111.55      | 108.47   |
| 14  | G     | 839 | CLA  | C1C-C2C-C3C | -5.52 | 101.15      | 106.96   |
| 14  | A     | 819 | CLA  | O2D-CGD-CBD | 5.52  | 121.08      | 111.27   |
| 14  | A     | 821 | CLA  | C2C-C1C-NC  | 5.52  | 115.14      | 109.97   |
| 14  | G     | 843 | CLA  | C4A-NA-C1A  | 5.52  | 109.19      | 106.71   |
| 14  | H     | 823 | CLA  | C1C-C2C-C3C | -5.52 | 101.15      | 106.96   |
| 14  | Y     | 815 | CLA  | C1C-C2C-C3C | -5.52 | 101.15      | 106.96   |
| 14  | Z     | 830 | CLA  | C4A-NA-C1A  | 5.52  | 109.19      | 106.71   |
| 14  | G     | 818 | CLA  | O2A-C1-C2   | 5.52  | 123.14      | 108.64   |
| 14  | G     | 833 | CLA  | C2C-C1C-NC  | 5.52  | 115.14      | 109.97   |
| 14  | A     | 831 | CLA  | C2C-C1C-NC  | 5.52  | 115.14      | 109.97   |
| 14  | G     | 805 | CLA  | C2C-C1C-NC  | 5.52  | 115.14      | 109.97   |
| 14  | G     | 807 | CLA  | C4A-NA-C1A  | 5.52  | 109.19      | 106.71   |
| 14  | Y     | 855 | CLA  | C1C-C2C-C3C | -5.51 | 101.16      | 106.96   |
| 14  | h     | 201 | CLA  | C4D-C3D-CAD | 5.51  | 111.54      | 108.47   |
| 17  | Y     | 848 | BCR  | C34-C9-C10  | -5.51 | 115.20      | 122.92   |
| 17  | Q     | 202 | BCR  | C34-C9-C8   | 5.51  | 126.76      | 118.08   |
| 14  | G     | 839 | CLA  | O2D-CGD-CBD | 5.51  | 121.06      | 111.27   |
| 14  | H     | 830 | CLA  | O2D-CGD-CBD | 5.51  | 121.06      | 111.27   |
| 14  | A     | 842 | CLA  | C1C-C2C-C3C | -5.51 | 101.16      | 106.96   |
| 14  | A     | 832 | CLA  | O2D-CGD-CBD | 5.51  | 121.06      | 111.27   |
| 14  | A     | 817 | CLA  | C1C-C2C-C3C | -5.51 | 101.17      | 106.96   |
| 14  | G     | 833 | CLA  | O2D-CGD-CBD | 5.51  | 121.05      | 111.27   |
| 14  | A     | 842 | CLA  | O2A-CGA-O1A | -5.50 | 109.70      | 123.59   |
| 17  | G     | 847 | BCR  | C37-C22-C21 | -5.50 | 115.21      | 122.92   |
| 14  | A     | 815 | CLA  | O2D-CGD-CBD | 5.50  | 121.05      | 111.27   |
| 17  | Z     | 845 | BCR  | C23-C24-C25 | -5.50 | 111.75      | 127.20   |
| 14  | G     | 803 | CLA  | OBD-CAD-C3D | -5.50 | 118.84      | 127.98   |
| 14  | Z     | 829 | CLA  | C2C-C1C-NC  | 5.50  | 115.13      | 109.97   |
| 14  | H     | 805 | CLA  | C1C-C2C-C3C | -5.50 | 101.17      | 106.96   |
| 17  | A     | 845 | BCR  | C19-C18-C17 | 5.50  | 127.38      | 118.94   |
| 14  | Y     | 803 | CLA  | O2A-CGA-O1A | -5.50 | 109.71      | 123.59   |
| 14  | G     | 833 | CLA  | O2A-C1-C2   | 5.50  | 123.08      | 108.64   |
| 14  | B     | 825 | CLA  | O2A-CGA-O1A | -5.49 | 109.72      | 123.59   |
| 14  | H     | 803 | CLA  | C4D-C3D-CAD | 5.49  | 111.53      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 836  | CLA  | C1C-C2C-C3C | -5.49 | 101.18      | 106.96   |
| 14  | W     | 1701 | CLA  | C4D-C3D-CAD | 5.49  | 111.53      | 108.47   |
| 17  | B     | 843  | BCR  | C34-C9-C8   | 5.49  | 126.72      | 118.08   |
| 14  | Z     | 835  | CLA  | C2C-C1C-NC  | 5.49  | 115.11      | 109.97   |
| 14  | H     | 820  | CLA  | C4A-NA-C1A  | 5.49  | 109.17      | 106.71   |
| 14  | Z     | 805  | CLA  | C1C-C2C-C3C | -5.49 | 101.19      | 106.96   |
| 14  | G     | 810  | CLA  | C2C-C1C-NC  | 5.48  | 115.11      | 109.97   |
| 14  | A     | 829  | CLA  | C1C-C2C-C3C | -5.48 | 101.19      | 106.96   |
| 14  | H     | 815  | CLA  | C1C-C2C-C3C | -5.48 | 101.19      | 106.96   |
| 14  | B     | 822  | CLA  | C2C-C1C-NC  | 5.48  | 115.10      | 109.97   |
| 17  | H     | 844  | BCR  | C36-C18-C17 | -5.48 | 115.25      | 122.92   |
| 14  | A     | 806  | CLA  | C2C-C1C-NC  | 5.47  | 115.10      | 109.97   |
| 17  | G     | 849  | BCR  | C8-C7-C6    | -5.47 | 111.83      | 127.20   |
| 14  | Z     | 806  | CLA  | C2C-C1C-NC  | 5.47  | 115.10      | 109.97   |
| 14  | Y     | 815  | CLA  | C4D-C3D-CAD | 5.47  | 111.52      | 108.47   |
| 14  | H     | 816  | CLA  | O2A-C1-C2   | 5.47  | 123.01      | 108.64   |
| 14  | h     | 205  | CLA  | O2A-CGA-O1A | -5.47 | 109.79      | 123.59   |
| 14  | G     | 813  | CLA  | C2C-C1C-NC  | 5.47  | 115.09      | 109.97   |
| 14  | d     | 201  | CLA  | C4D-C3D-CAD | 5.47  | 111.52      | 108.47   |
| 14  | Y     | 836  | CLA  | C4A-NA-C1A  | 5.47  | 109.16      | 106.71   |
| 14  | G     | 815  | CLA  | C4A-NA-C1A  | 5.46  | 109.16      | 106.71   |
| 14  | A     | 803  | CLA  | O2D-CGD-CBD | 5.46  | 120.97      | 111.27   |
| 14  | H     | 817  | CLA  | C2C-C1C-NC  | 5.46  | 115.09      | 109.97   |
| 14  | G     | 827  | CLA  | O2D-CGD-CBD | 5.46  | 120.97      | 111.27   |
| 14  | Y     | 843  | CLA  | O2A-CGA-O1A | -5.46 | 109.82      | 123.59   |
| 17  | K     | 102  | BCR  | C36-C18-C17 | -5.46 | 115.28      | 122.92   |
| 14  | G     | 807  | CLA  | O2D-CGD-CBD | 5.46  | 120.96      | 111.27   |
| 14  | B     | 801  | CLA  | C1C-C2C-C3C | -5.46 | 101.22      | 106.96   |
| 14  | S     | 1103 | CLA  | C1C-C2C-C3C | -5.46 | 101.22      | 106.96   |
| 14  | H     | 821  | CLA  | C4D-C3D-CAD | 5.46  | 111.51      | 108.47   |
| 17  | Y     | 848  | BCR  | C37-C22-C21 | -5.45 | 115.28      | 122.92   |
| 17  | A     | 845  | BCR  | C34-C9-C10  | -5.45 | 115.29      | 122.92   |
| 14  | B     | 825  | CLA  | C4A-NA-C1A  | 5.45  | 109.16      | 106.71   |
| 14  | H     | 809  | CLA  | C1C-C2C-C3C | -5.45 | 101.22      | 106.96   |
| 14  | Z     | 839  | CLA  | C1C-C2C-C3C | -5.45 | 101.23      | 106.96   |
| 14  | L     | 202  | CLA  | C4D-C3D-CAD | 5.45  | 111.51      | 108.47   |
| 14  | h     | 207  | CLA  | C4A-NA-C1A  | 5.45  | 109.16      | 106.71   |
| 14  | Z     | 807  | CLA  | C1C-C2C-C3C | -5.45 | 101.23      | 106.96   |
| 14  | A     | 820  | CLA  | C1C-C2C-C3C | -5.45 | 101.23      | 106.96   |
| 14  | G     | 807  | CLA  | C2C-C1C-NC  | 5.44  | 115.07      | 109.97   |
| 14  | H     | 824  | CLA  | C4A-NA-C1A  | 5.44  | 109.15      | 106.71   |
| 17  | Z     | 845  | BCR  | C23-C22-C21 | 5.44  | 127.29      | 118.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | f     | 103  | BCR  | C34-C9-C10  | -5.44 | 115.30      | 122.92   |
| 14  | Z     | 814  | CLA  | C2C-C1C-NC  | 5.43  | 115.06      | 109.97   |
| 17  | G     | 850  | BCR  | C34-C9-C10  | -5.43 | 115.31      | 122.92   |
| 14  | Y     | 832  | CLA  | C2C-C1C-NC  | 5.43  | 115.06      | 109.97   |
| 14  | S     | 1101 | CLA  | O2A-CGA-O1A | -5.43 | 109.89      | 123.59   |
| 14  | G     | 802  | CLA  | C2C-C1C-NC  | 5.43  | 115.06      | 109.97   |
| 14  | A     | 809  | CLA  | C4A-NA-C1A  | 5.43  | 109.15      | 106.71   |
| 17  | L     | 208  | BCR  | C19-C18-C17 | 5.43  | 127.27      | 118.94   |
| 14  | A     | 813  | CLA  | C4A-NA-C1A  | 5.43  | 109.14      | 106.71   |
| 14  | H     | 827  | CLA  | C4D-C3D-CAD | 5.42  | 111.50      | 108.47   |
| 17  | Z     | 841  | BCR  | C34-C9-C8   | 5.42  | 126.62      | 118.08   |
| 14  | H     | 836  | CLA  | C4A-NA-C1A  | 5.42  | 109.14      | 106.71   |
| 17  | B     | 848  | BCR  | C37-C22-C21 | -5.42 | 115.33      | 122.92   |
| 14  | S     | 1101 | CLA  | C4D-C3D-CAD | 5.42  | 111.49      | 108.47   |
| 14  | B     | 804  | CLA  | O2A-CGA-O1A | -5.42 | 109.91      | 123.59   |
| 14  | B     | 803  | CLA  | C4D-C3D-CAD | 5.42  | 111.49      | 108.47   |
| 14  | J     | 101  | CLA  | O2D-CGD-CBD | 5.42  | 120.89      | 111.27   |
| 14  | Y     | 814  | CLA  | C2C-C1C-NC  | 5.42  | 115.05      | 109.97   |
| 14  | f     | 101  | CLA  | C2C-C1C-NC  | 5.42  | 115.05      | 109.97   |
| 14  | G     | 823  | CLA  | O2D-CGD-CBD | 5.42  | 120.89      | 111.27   |
| 17  | f     | 105  | BCR  | C36-C18-C17 | -5.41 | 115.34      | 122.92   |
| 14  | B     | 830  | CLA  | C4A-NA-C1A  | 5.41  | 109.14      | 106.71   |
| 14  | H     | 823  | CLA  | O2A-CGA-O1A | -5.41 | 109.94      | 123.59   |
| 14  | B     | 817  | CLA  | O2D-CGD-CBD | 5.41  | 120.88      | 111.27   |
| 14  | G     | 831  | CLA  | C1C-C2C-C3C | -5.41 | 101.27      | 106.96   |
| 14  | Z     | 839  | CLA  | O2A-C1-C2   | 5.41  | 122.85      | 108.64   |
| 14  | G     | 826  | CLA  | C4A-NA-C1A  | 5.41  | 109.14      | 106.71   |
| 14  | B     | 812  | CLA  | C1C-C2C-C3C | -5.41 | 101.27      | 106.96   |
| 14  | L     | 207  | CLA  | C1C-C2C-C3C | -5.41 | 101.27      | 106.96   |
| 14  | H     | 822  | CLA  | C2C-C1C-NC  | 5.40  | 115.03      | 109.97   |
| 17  | U     | 1008 | BCR  | C38-C26-C25 | 5.40  | 130.60      | 124.53   |
| 14  | H     | 838  | CLA  | C2C-C1C-NC  | 5.40  | 115.03      | 109.97   |
| 14  | Y     | 834  | CLA  | C4A-NA-C1A  | 5.40  | 109.14      | 106.71   |
| 14  | g     | 102  | CLA  | C1C-C2C-C3C | -5.40 | 101.28      | 106.96   |
| 14  | G     | 814  | CLA  | C2C-C1C-NC  | 5.40  | 115.03      | 109.97   |
| 14  | G     | 803  | CLA  | C1C-C2C-C3C | -5.40 | 101.28      | 106.96   |
| 14  | G     | 816  | CLA  | C4A-NA-C1A  | 5.39  | 109.13      | 106.71   |
| 14  | B     | 802  | CLA  | C1C-C2C-C3C | -5.39 | 101.29      | 106.96   |
| 14  | h     | 206  | CLA  | C1C-C2C-C3C | -5.39 | 101.29      | 106.96   |
| 14  | A     | 828  | CLA  | C2C-C1C-NC  | 5.39  | 115.02      | 109.97   |
| 14  | Y     | 854  | CLA  | O2A-C1-C2   | 5.39  | 122.80      | 108.64   |
| 14  | Y     | 822  | CLA  | O2A-CGA-O1A | -5.39 | 109.99      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 834  | CLA  | C2C-C1C-NC  | 5.39  | 115.02      | 109.97   |
| 14  | G     | 816  | CLA  | O2D-CGD-CBD | 5.38  | 120.84      | 111.27   |
| 14  | Z     | 839  | CLA  | C4D-C3D-CAD | 5.38  | 111.47      | 108.47   |
| 14  | B     | 825  | CLA  | C1C-C2C-C3C | -5.38 | 101.30      | 106.96   |
| 14  | A     | 832  | CLA  | C1C-C2C-C3C | -5.38 | 101.30      | 106.96   |
| 14  | Y     | 840  | CLA  | C1C-C2C-C3C | -5.38 | 101.30      | 106.96   |
| 14  | A     | 827  | CLA  | C2C-C1C-NC  | 5.38  | 115.01      | 109.97   |
| 14  | B     | 803  | CLA  | C2C-C1C-NC  | 5.38  | 115.01      | 109.97   |
| 14  | A     | 806  | CLA  | O2A-CGA-O1A | -5.38 | 110.02      | 123.59   |
| 14  | G     | 828  | CLA  | O2A-CGA-O1A | -5.37 | 110.03      | 123.59   |
| 14  | Y     | 818  | CLA  | O2A-C1-C2   | 5.37  | 122.76      | 108.64   |
| 14  | G     | 806  | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | Y     | 817  | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 17  | I     | 101  | BCR  | C34-C9-C10  | -5.37 | 115.40      | 122.92   |
| 14  | B     | 839  | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | H     | 813  | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | Y     | 807  | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 14  | Y     | 833  | CLA  | C4A-NA-C1A  | 5.37  | 109.12      | 106.71   |
| 14  | B     | 837  | CLA  | O2A-CGA-O1A | -5.37 | 110.04      | 123.59   |
| 14  | A     | 836  | CLA  | C1C-C2C-C3C | -5.37 | 101.31      | 106.96   |
| 17  | A     | 846  | BCR  | C37-C22-C21 | -5.37 | 115.40      | 122.92   |
| 14  | B     | 832  | CLA  | O2A-CGA-O1A | -5.37 | 110.05      | 123.59   |
| 14  | S     | 1103 | CLA  | O2D-CGD-CBD | 5.37  | 120.80      | 111.27   |
| 14  | G     | 802  | CLA  | O2A-C1-C2   | 5.37  | 122.74      | 108.64   |
| 14  | Y     | 813  | CLA  | C2C-C1C-NC  | 5.36  | 115.00      | 109.97   |
| 17  | B     | 851  | BCR  | C23-C24-C25 | -5.36 | 112.14      | 127.20   |
| 14  | H     | 828  | CLA  | C4D-C3D-CAD | 5.36  | 111.46      | 108.47   |
| 14  | A     | 815  | CLA  | C1C-C2C-C3C | -5.36 | 101.32      | 106.96   |
| 14  | Y     | 808  | CLA  | C4D-C3D-CAD | 5.36  | 111.46      | 108.47   |
| 14  | G     | 837  | CLA  | O2D-CGD-CBD | 5.36  | 120.78      | 111.27   |
| 14  | H     | 833  | CLA  | C1C-C2C-C3C | -5.35 | 101.33      | 106.96   |
| 14  | G     | 832  | CLA  | O2A-CGA-O1A | -5.35 | 110.08      | 123.59   |
| 14  | B     | 811  | CLA  | C4D-C3D-CAD | 5.35  | 111.45      | 108.47   |
| 14  | Y     | 819  | CLA  | C2C-C1C-NC  | 5.35  | 114.99      | 109.97   |
| 14  | H     | 821  | CLA  | O2D-CGD-CBD | 5.35  | 120.78      | 111.27   |
| 14  | Z     | 833  | CLA  | C1C-C2C-C3C | -5.35 | 101.33      | 106.96   |
| 14  | Z     | 838  | CLA  | C4A-NA-C1A  | 5.35  | 109.11      | 106.71   |
| 14  | Z     | 825  | CLA  | O2D-CGD-CBD | 5.35  | 120.77      | 111.27   |
| 17  | V     | 1202 | BCR  | C32-C1-C6   | 5.34  | 118.97      | 110.30   |
| 14  | G     | 843  | CLA  | C1C-C2C-C3C | -5.34 | 101.34      | 106.96   |
| 17  | A     | 845  | BCR  | C8-C7-C6    | -5.34 | 112.20      | 127.20   |
| 14  | G     | 823  | CLA  | C4D-C3D-CAD | 5.34  | 111.45      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | Y     | 833 | CLA  | C4D-C3D-CAD | 5.34  | 111.45      | 108.47   |
| 14  | Y     | 836 | CLA  | C2C-C1C-NC  | 5.34  | 114.97      | 109.97   |
| 17  | h     | 203 | BCR  | C19-C18-C17 | 5.34  | 127.13      | 118.94   |
| 17  | Y     | 849 | BCR  | C33-C5-C6   | -5.34 | 118.54      | 124.53   |
| 14  | H     | 819 | CLA  | C4D-C3D-CAD | 5.34  | 111.44      | 108.47   |
| 14  | B     | 818 | CLA  | O2A-CGA-O1A | -5.33 | 110.13      | 123.59   |
| 14  | Z     | 817 | CLA  | C4D-C3D-CAD | 5.33  | 111.44      | 108.47   |
| 14  | A     | 802 | CLA  | C1C-C2C-C3C | -5.33 | 101.35      | 106.96   |
| 14  | A     | 810 | CLA  | C4D-C3D-CAD | 5.33  | 111.44      | 108.47   |
| 14  | B     | 816 | CLA  | C4A-NA-C1A  | 5.33  | 109.10      | 106.71   |
| 17  | Z     | 845 | BCR  | C8-C7-C6    | -5.33 | 112.25      | 127.20   |
| 14  | Y     | 803 | CLA  | C4D-C3D-CAD | 5.32  | 111.44      | 108.47   |
| 14  | h     | 206 | CLA  | C2C-C1C-NC  | 5.32  | 114.96      | 109.97   |
| 14  | j     | 102 | CLA  | C1C-C2C-C3C | -5.32 | 101.36      | 106.96   |
| 14  | B     | 807 | CLA  | C1C-C2C-C3C | -5.32 | 101.37      | 106.96   |
| 17  | f     | 103 | BCR  | C8-C7-C6    | -5.32 | 112.27      | 127.20   |
| 14  | G     | 808 | CLA  | C1C-C2C-C3C | -5.31 | 101.37      | 106.96   |
| 17  | T     | 102 | BCR  | C23-C24-C25 | -5.31 | 112.28      | 127.20   |
| 14  | B     | 840 | CLA  | C2C-C1C-NC  | 5.31  | 114.95      | 109.97   |
| 14  | Y     | 818 | CLA  | O2A-CGA-O1A | -5.31 | 110.19      | 123.59   |
| 17  | J     | 104 | BCR  | C34-C9-C10  | -5.31 | 115.49      | 122.92   |
| 14  | G     | 803 | CLA  | O2A-CGA-O1A | -5.31 | 110.20      | 123.59   |
| 14  | A     | 825 | CLA  | C1C-C2C-C3C | -5.31 | 101.38      | 106.96   |
| 14  | B     | 822 | CLA  | C4A-NA-C1A  | 5.30  | 109.09      | 106.71   |
| 17  | R     | 101 | BCR  | C7-C8-C9    | -5.30 | 118.23      | 126.23   |
| 14  | H     | 835 | CLA  | C1C-C2C-C3C | -5.30 | 101.39      | 106.96   |
| 14  | Y     | 806 | CLA  | C4A-NA-C1A  | 5.30  | 109.09      | 106.71   |
| 14  | B     | 832 | CLA  | C1C-C2C-C3C | -5.30 | 101.39      | 106.96   |
| 14  | Y     | 832 | CLA  | C4D-C3D-CAD | 5.30  | 111.42      | 108.47   |
| 14  | H     | 825 | CLA  | C4A-NA-C1A  | 5.30  | 109.09      | 106.71   |
| 14  | Z     | 805 | CLA  | O2D-CGD-CBD | 5.30  | 120.68      | 111.27   |
| 14  | H     | 829 | CLA  | C1C-C2C-C3C | -5.29 | 101.39      | 106.96   |
| 14  | Y     | 827 | CLA  | C4D-C3D-CAD | 5.29  | 111.42      | 108.47   |
| 14  | H     | 826 | CLA  | O2A-CGA-O1A | -5.29 | 110.24      | 123.59   |
| 14  | G     | 824 | CLA  | O2A-C1-C2   | 5.29  | 122.53      | 108.64   |
| 14  | G     | 806 | CLA  | O2A-CGA-O1A | -5.29 | 110.25      | 123.59   |
| 14  | G     | 842 | CLA  | C1C-C2C-C3C | -5.29 | 101.40      | 106.96   |
| 17  | H     | 843 | BCR  | C23-C24-C25 | -5.29 | 112.35      | 127.20   |
| 17  | F     | 203 | BCR  | C24-C23-C22 | -5.29 | 118.25      | 126.23   |
| 17  | K     | 102 | BCR  | C34-C9-C8   | 5.29  | 126.41      | 118.08   |
| 14  | G     | 808 | CLA  | O2A-CGA-O1A | -5.29 | 110.25      | 123.59   |
| 14  | G     | 841 | CLA  | C4A-NA-C1A  | 5.28  | 109.08      | 106.71   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 823  | CLA  | O2A-CGA-O1A | -5.28 | 110.25      | 123.59   |
| 17  | Z     | 841  | BCR  | C24-C23-C22 | -5.28 | 118.25      | 126.23   |
| 14  | B     | 811  | CLA  | C1C-C2C-C3C | -5.28 | 101.41      | 106.96   |
| 14  | H     | 804  | CLA  | C1C-C2C-C3C | -5.28 | 101.41      | 106.96   |
| 14  | A     | 814  | CLA  | C1C-C2C-C3C | -5.28 | 101.41      | 106.96   |
| 14  | Y     | 810  | CLA  | C4A-NA-C1A  | 5.28  | 109.08      | 106.71   |
| 14  | L     | 205  | CLA  | C1C-C2C-C3C | -5.27 | 101.41      | 106.96   |
| 14  | Z     | 832  | CLA  | O2D-CGD-CBD | 5.27  | 120.64      | 111.27   |
| 14  | g     | 101  | CLA  | C1C-C2C-C3C | -5.27 | 101.41      | 106.96   |
| 14  | G     | 826  | CLA  | C1C-C2C-C3C | -5.27 | 101.41      | 106.96   |
| 14  | A     | 817  | CLA  | O2D-CGD-CBD | 5.27  | 120.63      | 111.27   |
| 14  | S     | 1103 | CLA  | O2A-CGA-O1A | -5.27 | 110.30      | 123.59   |
| 14  | G     | 820  | CLA  | O2A-CGA-O1A | -5.27 | 110.30      | 123.59   |
| 14  | H     | 832  | CLA  | C1C-C2C-C3C | -5.27 | 101.42      | 106.96   |
| 14  | f     | 102  | CLA  | C4D-C3D-CAD | 5.27  | 111.41      | 108.47   |
| 14  | A     | 840  | CLA  | O2A-C1-C2   | 5.27  | 122.47      | 108.64   |
| 14  | B     | 827  | CLA  | O2A-CGA-O1A | -5.27 | 110.30      | 123.59   |
| 14  | Y     | 818  | CLA  | C2C-C1C-NC  | 5.26  | 114.90      | 109.97   |
| 14  | G     | 822  | CLA  | O2D-CGD-CBD | 5.26  | 120.62      | 111.27   |
| 14  | L     | 207  | CLA  | C2C-C1C-NC  | 5.26  | 114.90      | 109.97   |
| 14  | X     | 1701 | CLA  | C1C-C2C-C3C | -5.26 | 101.42      | 106.96   |
| 14  | Y     | 843  | CLA  | C4D-C3D-CAD | 5.26  | 111.40      | 108.47   |
| 14  | A     | 819  | CLA  | O2A-CGA-O1A | -5.26 | 110.32      | 123.59   |
| 14  | U     | 1003 | CLA  | C1C-C2C-C3C | -5.26 | 101.43      | 106.96   |
| 14  | h     | 201  | CLA  | C1C-C2C-C3C | -5.26 | 101.43      | 106.96   |
| 17  | Q     | 202  | BCR  | C37-C22-C21 | -5.26 | 115.56      | 122.92   |
| 14  | Z     | 830  | CLA  | C2C-C1C-NC  | 5.26  | 114.90      | 109.97   |
| 17  | G     | 848  | BCR  | C33-C5-C6   | -5.26 | 118.63      | 124.53   |
| 14  | G     | 837  | CLA  | O2A-CGA-O1A | -5.25 | 110.33      | 123.59   |
| 17  | G     | 850  | BCR  | C32-C1-C6   | 5.25  | 118.82      | 110.30   |
| 14  | Y     | 803  | CLA  | O2A-C1-C2   | 5.25  | 122.44      | 108.64   |
| 14  | A     | 807  | CLA  | O2A-C1-C2   | 5.25  | 122.44      | 108.64   |
| 14  | H     | 809  | CLA  | C4A-NA-C1A  | 5.25  | 109.07      | 106.71   |
| 14  | Y     | 831  | CLA  | C1C-C2C-C3C | -5.25 | 101.44      | 106.96   |
| 14  | Z     | 836  | CLA  | C4D-C3D-CAD | 5.25  | 111.39      | 108.47   |
| 14  | A     | 838  | CLA  | C4A-NA-C1A  | 5.24  | 109.06      | 106.71   |
| 17  | Y     | 850  | BCR  | C36-C18-C17 | -5.24 | 115.58      | 122.92   |
| 14  | A     | 841  | CLA  | O2A-C1-C2   | 5.24  | 122.40      | 108.64   |
| 14  | J     | 101  | CLA  | C4D-C3D-CAD | 5.24  | 111.39      | 108.47   |
| 14  | B     | 824  | CLA  | O2D-CGD-CBD | 5.24  | 120.57      | 111.27   |
| 14  | U     | 1002 | CLA  | C1C-C2C-C3C | -5.24 | 101.45      | 106.96   |
| 14  | G     | 835  | CLA  | C1C-C2C-C3C | -5.23 | 101.46      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | J     | 101  | CLA  | C1C-C2C-C3C | -5.23 | 101.46      | 106.96   |
| 14  | h     | 205  | CLA  | C1C-C2C-C3C | -5.23 | 101.46      | 106.96   |
| 17  | f     | 104  | BCR  | C24-C23-C22 | -5.23 | 118.33      | 126.23   |
| 17  | G     | 846  | BCR  | C38-C26-C27 | 5.23  | 123.66      | 113.62   |
| 14  | B     | 837  | CLA  | OBD-CAD-C3D | -5.23 | 119.30      | 127.98   |
| 14  | Y     | 807  | CLA  | C4A-NA-C1A  | 5.23  | 109.06      | 106.71   |
| 17  | B     | 851  | BCR  | C34-C9-C10  | -5.22 | 115.60      | 122.92   |
| 14  | Z     | 824  | CLA  | OBD-CAD-C3D | -5.22 | 119.31      | 127.98   |
| 14  | Z     | 833  | CLA  | C4D-C3D-CAD | 5.22  | 111.38      | 108.47   |
| 14  | Y     | 835  | CLA  | C1C-C2C-C3C | -5.22 | 101.47      | 106.96   |
| 14  | Y     | 841  | CLA  | C2C-C1C-NC  | 5.22  | 114.86      | 109.97   |
| 14  | Z     | 801  | CLA  | C2C-C1C-NC  | 5.22  | 114.86      | 109.97   |
| 17  | h     | 202  | BCR  | C8-C7-C6    | -5.22 | 112.54      | 127.20   |
| 14  | G     | 804  | CLA  | O2D-CGD-CBD | 5.22  | 120.54      | 111.27   |
| 14  | Z     | 818  | CLA  | C1C-C2C-C3C | -5.22 | 101.47      | 106.96   |
| 14  | A     | 830  | CLA  | C4A-NA-C1A  | 5.22  | 109.05      | 106.71   |
| 14  | W     | 1701 | CLA  | C1C-C2C-C3C | -5.21 | 101.47      | 106.96   |
| 14  | Y     | 834  | CLA  | C1C-C2C-C3C | -5.21 | 101.47      | 106.96   |
| 14  | Z     | 833  | CLA  | C4A-NA-C1A  | 5.21  | 109.05      | 106.71   |
| 14  | Y     | 827  | CLA  | O2D-CGD-CBD | 5.21  | 120.53      | 111.27   |
| 14  | g     | 101  | CLA  | C4A-NA-C1A  | 5.21  | 109.05      | 106.71   |
| 13  | G     | 801  | CL0  | C4D-C3D-CAD | 5.21  | 111.37      | 108.47   |
| 14  | B     | 812  | CLA  | C4A-NA-C1A  | 5.21  | 109.05      | 106.71   |
| 14  | G     | 836  | CLA  | O2A-C1-C2   | 5.20  | 122.31      | 108.64   |
| 14  | Z     | 822  | CLA  | C1C-C2C-C3C | -5.19 | 101.50      | 106.96   |
| 14  | H     | 813  | CLA  | O2A-C1-C2   | 5.19  | 122.28      | 108.64   |
| 14  | A     | 817  | CLA  | C4D-C3D-CAD | 5.19  | 111.36      | 108.47   |
| 14  | S     | 1101 | CLA  | C4A-NA-C1A  | 5.19  | 109.04      | 106.71   |
| 17  | h     | 202  | BCR  | C34-C9-C10  | -5.19 | 115.66      | 122.92   |
| 14  | G     | 817  | CLA  | C1C-C2C-C3C | -5.19 | 101.50      | 106.96   |
| 14  | B     | 823  | CLA  | C1C-C2C-C3C | -5.19 | 101.50      | 106.96   |
| 14  | G     | 814  | CLA  | C4D-C3D-CAD | 5.18  | 111.36      | 108.47   |
| 14  | A     | 826  | CLA  | O2A-CGA-O1A | -5.18 | 110.51      | 123.59   |
| 14  | A     | 820  | CLA  | O2D-CGD-CBD | 5.18  | 120.47      | 111.27   |
| 14  | Z     | 819  | CLA  | C4D-C3D-CAD | 5.18  | 111.36      | 108.47   |
| 14  | Z     | 839  | CLA  | C4A-NA-C1A  | 5.18  | 109.03      | 106.71   |
| 14  | Q     | 203  | CLA  | O2D-CGD-CBD | 5.18  | 120.47      | 111.27   |
| 17  | U     | 1008 | BCR  | C24-C23-C22 | -5.18 | 118.41      | 126.23   |
| 14  | B     | 828  | CLA  | O2A-C1-C2   | 5.18  | 122.25      | 108.64   |
| 17  | d     | 203  | BCR  | C36-C18-C17 | -5.18 | 115.67      | 122.92   |
| 14  | H     | 835  | CLA  | O2D-CGD-CBD | 5.18  | 120.47      | 111.27   |
| 14  | H     | 816  | CLA  | C4A-NA-C1A  | 5.18  | 109.03      | 106.71   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | Z     | 812 | CLA  | O2A-C1-C2   | 5.18  | 122.24      | 108.64   |
| 14  | H     | 826 | CLA  | O2D-CGD-CBD | 5.18  | 120.46      | 111.27   |
| 14  | B     | 804 | CLA  | C4D-C3D-CAD | 5.17  | 111.36      | 108.47   |
| 14  | Y     | 832 | CLA  | O2D-CGD-CBD | 5.17  | 120.46      | 111.27   |
| 17  | H     | 841 | BCR  | C34-C9-C8   | 5.17  | 126.22      | 118.08   |
| 14  | L     | 207 | CLA  | C4A-NA-C1A  | 5.17  | 109.03      | 106.71   |
| 17  | L     | 209 | BCR  | C8-C7-C6    | -5.17 | 112.69      | 127.20   |
| 14  | L     | 205 | CLA  | O2A-C1-C2   | 5.17  | 122.21      | 108.64   |
| 14  | G     | 820 | CLA  | C1C-C2C-C3C | -5.16 | 101.53      | 106.96   |
| 14  | Y     | 816 | CLA  | O2A-CGA-O1A | -5.16 | 110.56      | 123.59   |
| 14  | G     | 802 | CLA  | O2A-CGA-O1A | -5.16 | 110.57      | 123.59   |
| 14  | H     | 815 | CLA  | O2A-CGA-O1A | -5.16 | 110.57      | 123.59   |
| 14  | Y     | 821 | CLA  | O2D-CGD-CBD | 5.16  | 120.43      | 111.27   |
| 14  | A     | 818 | CLA  | C4A-NA-C1A  | 5.16  | 109.03      | 106.71   |
| 14  | T     | 101 | CLA  | C1C-C2C-C3C | -5.16 | 101.53      | 106.96   |
| 14  | Z     | 824 | CLA  | C1C-C2C-C3C | -5.16 | 101.53      | 106.96   |
| 17  | Z     | 844 | BCR  | C28-C27-C26 | -5.15 | 104.87      | 114.08   |
| 14  | B     | 801 | CLA  | O2A-CGA-CBA | 5.15  | 128.08      | 111.91   |
| 14  | A     | 842 | CLA  | O2A-CGA-CBA | 5.15  | 128.08      | 111.91   |
| 17  | Y     | 846 | BCR  | C36-C18-C17 | -5.15 | 115.71      | 122.92   |
| 14  | Y     | 812 | CLA  | C4D-C3D-CAD | 5.15  | 111.34      | 108.47   |
| 14  | Y     | 840 | CLA  | O2A-CGA-O1A | -5.15 | 110.59      | 123.59   |
| 14  | Z     | 814 | CLA  | O2A-CGA-O1A | -5.15 | 110.60      | 123.59   |
| 14  | Z     | 827 | CLA  | O2A-CGA-O1A | -5.15 | 110.60      | 123.59   |
| 17  | F     | 203 | BCR  | C34-C9-C10  | -5.15 | 115.71      | 122.92   |
| 14  | J     | 102 | CLA  | C1C-C2C-C3C | -5.15 | 101.55      | 106.96   |
| 14  | B     | 813 | CLA  | C4A-NA-C1A  | 5.15  | 109.02      | 106.71   |
| 14  | G     | 839 | CLA  | O2A-CGA-O1A | -5.15 | 110.61      | 123.59   |
| 14  | A     | 814 | CLA  | O2A-CGA-O1A | -5.14 | 110.61      | 123.59   |
| 14  | B     | 833 | CLA  | O2A-CGA-O1A | -5.14 | 110.61      | 123.59   |
| 17  | i     | 101 | BCR  | C34-C9-C8   | 5.14  | 126.18      | 118.08   |
| 17  | A     | 846 | BCR  | C38-C26-C25 | -5.14 | 118.75      | 124.53   |
| 14  | A     | 806 | CLA  | O2A-CGA-CBA | 5.14  | 128.04      | 111.91   |
| 14  | B     | 811 | CLA  | O2A-CGA-O1A | -5.14 | 110.62      | 123.59   |
| 14  | f     | 102 | CLA  | O2D-CGD-CBD | 5.14  | 120.40      | 111.27   |
| 17  | R     | 101 | BCR  | C24-C23-C22 | -5.14 | 118.47      | 126.23   |
| 14  | G     | 802 | CLA  | C1C-C2C-C3C | -5.14 | 101.56      | 106.96   |
| 14  | Y     | 832 | CLA  | O2A-CGA-CBA | 5.14  | 128.02      | 111.91   |
| 14  | Y     | 842 | CLA  | C1C-C2C-C3C | -5.13 | 101.56      | 106.96   |
| 14  | F     | 202 | CLA  | C4A-NA-C1A  | 5.13  | 109.01      | 106.71   |
| 14  | H     | 821 | CLA  | C4A-NA-C1A  | 5.13  | 109.01      | 106.71   |
| 14  | Y     | 839 | CLA  | C1C-C2C-C3C | -5.13 | 101.56      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | V     | 1202 | BCR  | C36-C18-C17 | -5.13 | 115.73      | 122.92   |
| 17  | B     | 843  | BCR  | C36-C18-C17 | -5.13 | 115.73      | 122.92   |
| 17  | Q     | 204  | BCR  | C12-C13-C14 | 5.13  | 126.82      | 118.94   |
| 14  | G     | 802  | CLA  | C4A-NA-C1A  | 5.13  | 109.01      | 106.71   |
| 14  | Y     | 825  | CLA  | C4D-C3D-CAD | 5.13  | 111.33      | 108.47   |
| 17  | A     | 846  | BCR  | C28-C27-C26 | -5.13 | 104.92      | 114.08   |
| 14  | Z     | 831  | CLA  | O2A-CGA-O1A | -5.13 | 110.65      | 123.59   |
| 14  | H     | 822  | CLA  | O2A-CGA-O1A | -5.12 | 110.66      | 123.59   |
| 14  | G     | 826  | CLA  | C4D-C3D-CAD | 5.12  | 111.33      | 108.47   |
| 14  | G     | 835  | CLA  | O2D-CGD-CBD | 5.12  | 120.37      | 111.27   |
| 14  | G     | 841  | CLA  | C4D-C3D-CAD | 5.12  | 111.33      | 108.47   |
| 17  | F     | 203  | BCR  | C38-C26-C25 | -5.12 | 118.78      | 124.53   |
| 17  | Y     | 851  | BCR  | C7-C8-C9    | -5.12 | 118.50      | 126.23   |
| 14  | Z     | 802  | CLA  | C1C-C2C-C3C | -5.12 | 101.58      | 106.96   |
| 14  | A     | 812  | CLA  | C1C-C2C-C3C | -5.12 | 101.58      | 106.96   |
| 14  | Y     | 829  | CLA  | O2D-CGD-CBD | 5.12  | 120.36      | 111.27   |
| 17  | Z     | 843  | BCR  | C33-C5-C6   | -5.11 | 118.78      | 124.53   |
| 14  | A     | 841  | CLA  | C1C-C2C-C3C | -5.11 | 101.58      | 106.96   |
| 14  | G     | 823  | CLA  | C1C-C2C-C3C | -5.11 | 101.58      | 106.96   |
| 17  | H     | 845  | BCR  | C37-C22-C21 | -5.11 | 115.76      | 122.92   |
| 14  | G     | 833  | CLA  | O2A-CGA-O1A | -5.11 | 110.69      | 123.59   |
| 14  | H     | 830  | CLA  | C1C-C2C-C3C | -5.11 | 101.58      | 106.96   |
| 14  | H     | 806  | CLA  | C4A-NA-C1A  | 5.11  | 109.00      | 106.71   |
| 14  | G     | 821  | CLA  | C2C-C1C-NC  | 5.11  | 114.76      | 109.97   |
| 17  | K     | 102  | BCR  | C34-C9-C10  | -5.10 | 115.77      | 122.92   |
| 14  | H     | 830  | CLA  | C4A-NA-C1A  | 5.10  | 109.00      | 106.71   |
| 14  | F     | 202  | CLA  | O2D-CGD-CBD | 5.10  | 120.34      | 111.27   |
| 17  | A     | 848  | BCR  | C8-C7-C6    | -5.10 | 112.87      | 127.20   |
| 17  | V     | 1202 | BCR  | C24-C23-C22 | -5.10 | 118.52      | 126.23   |
| 14  | H     | 809  | CLA  | OBD-CAD-C3D | -5.10 | 119.51      | 127.98   |
| 14  | Y     | 855  | CLA  | O2A-C1-C2   | 5.10  | 122.05      | 108.64   |
| 17  | A     | 849  | BCR  | C24-C23-C22 | -5.10 | 118.53      | 126.23   |
| 17  | V     | 1202 | BCR  | C23-C22-C21 | 5.10  | 126.77      | 118.94   |
| 14  | H     | 804  | CLA  | C4A-NA-C1A  | 5.10  | 109.00      | 106.71   |
| 14  | A     | 808  | CLA  | C4A-NA-C1A  | 5.10  | 109.00      | 106.71   |
| 14  | Y     | 816  | CLA  | C1C-C2C-C3C | -5.10 | 101.60      | 106.96   |
| 14  | G     | 833  | CLA  | C1C-C2C-C3C | -5.10 | 101.60      | 106.96   |
| 14  | Y     | 831  | CLA  | OBD-CAD-C3D | -5.10 | 119.52      | 127.98   |
| 14  | B     | 807  | CLA  | O2A-CGA-O1A | -5.10 | 110.73      | 123.59   |
| 14  | Z     | 809  | CLA  | C1C-C2C-C3C | -5.10 | 101.60      | 106.96   |
| 14  | H     | 817  | CLA  | C1C-C2C-C3C | -5.09 | 101.60      | 106.96   |
| 14  | G     | 818  | CLA  | C2C-C1C-NC  | 5.09  | 114.75      | 109.97   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 828  | CLA  | C1C-C2C-C3C | -5.09 | 101.60      | 106.96   |
| 14  | G     | 836  | CLA  | C1C-C2C-C3C | -5.09 | 101.60      | 106.96   |
| 14  | B     | 820  | CLA  | O2D-CGD-CBD | 5.09  | 120.32      | 111.27   |
| 14  | Y     | 828  | CLA  | C4D-C3D-CAD | 5.09  | 111.31      | 108.47   |
| 17  | U     | 1005 | BCR  | C34-C9-C8   | 5.09  | 126.10      | 118.08   |
| 17  | B     | 843  | BCR  | C19-C18-C17 | 5.09  | 126.75      | 118.94   |
| 14  | L     | 201  | CLA  | O2A-C1-C2   | 5.09  | 122.02      | 108.64   |
| 17  | d     | 203  | BCR  | C24-C23-C22 | -5.09 | 118.54      | 126.23   |
| 14  | A     | 821  | CLA  | C1C-C2C-C3C | -5.09 | 101.61      | 106.96   |
| 17  | e     | 101  | BCR  | C24-C23-C22 | -5.09 | 118.54      | 126.23   |
| 17  | M     | 101  | BCR  | C23-C24-C25 | -5.09 | 112.91      | 127.20   |
| 14  | Y     | 836  | CLA  | C1C-C2C-C3C | -5.09 | 101.61      | 106.96   |
| 14  | Y     | 805  | CLA  | C2C-C1C-NC  | 5.09  | 114.74      | 109.97   |
| 14  | Y     | 813  | CLA  | O2A-CGA-O1A | -5.08 | 110.76      | 123.59   |
| 14  | Z     | 811  | CLA  | C4A-NA-C1A  | 5.08  | 108.99      | 106.71   |
| 14  | Y     | 822  | CLA  | O2A-CGA-CBA | 5.08  | 127.86      | 111.91   |
| 14  | Y     | 821  | CLA  | C2C-C1C-NC  | 5.08  | 114.73      | 109.97   |
| 14  | H     | 824  | CLA  | O2A-CGA-O1A | -5.08 | 110.77      | 123.59   |
| 17  | B     | 845  | BCR  | C33-C5-C6   | -5.08 | 118.82      | 124.53   |
| 14  | Y     | 854  | CLA  | C4D-C3D-CAD | 5.08  | 111.30      | 108.47   |
| 17  | Q     | 204  | BCR  | C8-C7-C6    | -5.08 | 112.94      | 127.20   |
| 14  | B     | 810  | CLA  | C4A-NA-C1A  | 5.08  | 108.99      | 106.71   |
| 14  | f     | 102  | CLA  | C1C-C2C-C3C | -5.08 | 101.62      | 106.96   |
| 14  | H     | 801  | CLA  | C1C-C2C-C3C | -5.07 | 101.62      | 106.96   |
| 14  | H     | 825  | CLA  | C4D-C3D-CAD | 5.07  | 111.30      | 108.47   |
| 14  | G     | 818  | CLA  | O2A-CGA-O1A | -5.07 | 110.79      | 123.59   |
| 14  | Z     | 813  | CLA  | C1C-C2C-C3C | -5.07 | 101.63      | 106.96   |
| 14  | X     | 1701 | CLA  | O2D-CGD-CBD | 5.07  | 120.28      | 111.27   |
| 14  | L     | 202  | CLA  | O2A-CGA-CBA | 5.07  | 127.81      | 111.91   |
| 14  | B     | 835  | CLA  | OBD-CAD-C3D | -5.07 | 119.57      | 127.98   |
| 14  | B     | 809  | CLA  | O2A-CGA-O1A | -5.07 | 110.80      | 123.59   |
| 14  | A     | 823  | CLA  | O2A-CGA-O1A | -5.07 | 110.81      | 123.59   |
| 14  | A     | 840  | CLA  | C4D-C3D-CAD | 5.06  | 111.29      | 108.47   |
| 14  | Y     | 842  | CLA  | C4A-NA-C1A  | 5.06  | 108.98      | 106.71   |
| 14  | H     | 812  | CLA  | O2A-C1-C2   | 5.06  | 121.94      | 108.64   |
| 14  | A     | 806  | CLA  | C4D-C3D-CAD | 5.06  | 111.29      | 108.47   |
| 14  | B     | 803  | CLA  | O2A-CGA-O1A | -5.06 | 110.82      | 123.59   |
| 17  | F     | 203  | BCR  | C12-C13-C14 | 5.06  | 126.70      | 118.94   |
| 17  | Y     | 848  | BCR  | C1-C6-C5    | -5.06 | 115.49      | 122.61   |
| 14  | Z     | 820  | CLA  | C1C-C2C-C3C | -5.06 | 101.64      | 106.96   |
| 17  | Q     | 204  | BCR  | C36-C18-C17 | -5.06 | 115.84      | 122.92   |
| 14  | Y     | 824  | CLA  | O2A-CGA-O1A | -5.06 | 110.83      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 813  | CLA  | C1C-C2C-C3C | -5.06 | 101.64      | 106.96   |
| 14  | A     | 824  | CLA  | C2C-C1C-NC  | 5.05  | 114.71      | 109.97   |
| 14  | Z     | 816  | CLA  | C1C-C2C-C3C | -5.05 | 101.64      | 106.96   |
| 14  | h     | 206  | CLA  | O2D-CGD-CBD | 5.05  | 120.25      | 111.27   |
| 14  | Y     | 842  | CLA  | O2A-CGA-CBA | 5.05  | 127.76      | 111.91   |
| 14  | K     | 101  | CLA  | C1C-C2C-C3C | -5.05 | 101.65      | 106.96   |
| 14  | A     | 816  | CLA  | O2A-CGA-O1A | -5.05 | 110.85      | 123.59   |
| 17  | G     | 850  | BCR  | C31-C1-C6   | -5.05 | 102.11      | 110.30   |
| 14  | H     | 834  | CLA  | O2A-CGA-O1A | -5.05 | 110.86      | 123.59   |
| 14  | Z     | 831  | CLA  | C4D-C3D-CAD | 5.04  | 111.28      | 108.47   |
| 14  | B     | 812  | CLA  | C4D-C3D-CAD | 5.04  | 111.28      | 108.47   |
| 14  | G     | 814  | CLA  | O2A-CGA-O1A | -5.04 | 110.86      | 123.59   |
| 14  | H     | 803  | CLA  | O2A-CGA-O1A | -5.04 | 110.86      | 123.59   |
| 17  | Q     | 204  | BCR  | C34-C9-C10  | -5.04 | 115.86      | 122.92   |
| 14  | U     | 1004 | CLA  | O2A-CGA-O1A | -5.04 | 110.87      | 123.59   |
| 14  | A     | 841  | CLA  | O2A-CGA-O1A | -5.04 | 110.87      | 123.59   |
| 14  | G     | 836  | CLA  | C4A-NA-C1A  | 5.04  | 108.97      | 106.71   |
| 14  | V     | 1201 | CLA  | C4D-C3D-CAD | 5.04  | 111.28      | 108.47   |
| 14  | B     | 808  | CLA  | C4D-C3D-CAD | 5.04  | 111.28      | 108.47   |
| 17  | d     | 203  | BCR  | C34-C9-C10  | -5.03 | 115.87      | 122.92   |
| 14  | B     | 816  | CLA  | O2A-CGA-O1A | -5.03 | 110.89      | 123.59   |
| 14  | K     | 103  | CLA  | C1C-C2C-C3C | -5.03 | 101.67      | 106.96   |
| 14  | B     | 825  | CLA  | C2C-C1C-NC  | 5.03  | 114.69      | 109.97   |
| 14  | B     | 805  | CLA  | O2A-CGA-O1A | -5.03 | 110.89      | 123.59   |
| 14  | A     | 838  | CLA  | C1C-C2C-C3C | -5.03 | 101.67      | 106.96   |
| 14  | B     | 804  | CLA  | C2C-C1C-NC  | 5.03  | 114.68      | 109.97   |
| 14  | A     | 822  | CLA  | O2A-CGA-O1A | -5.03 | 110.90      | 123.59   |
| 17  | H     | 840  | BCR  | C36-C18-C17 | -5.02 | 115.88      | 122.92   |
| 14  | f     | 102  | CLA  | O2A-CGA-O1A | -5.02 | 110.91      | 123.59   |
| 14  | H     | 832  | CLA  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 14  | Y     | 841  | CLA  | O2A-C1-C2   | 5.02  | 121.83      | 108.64   |
| 14  | G     | 820  | CLA  | C4A-NA-C1A  | 5.02  | 108.96      | 106.71   |
| 14  | H     | 813  | CLA  | C4D-C3D-CAD | 5.02  | 111.27      | 108.47   |
| 17  | d     | 203  | BCR  | C37-C22-C21 | -5.02 | 115.89      | 122.92   |
| 14  | Y     | 837  | CLA  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 14  | Y     | 835  | CLA  | C4D-C3D-CAD | 5.02  | 111.27      | 108.47   |
| 14  | S     | 1101 | CLA  | C1C-C2C-C3C | -5.01 | 101.69      | 106.96   |
| 14  | Z     | 810  | CLA  | C4A-NA-C1A  | 5.01  | 108.96      | 106.71   |
| 14  | H     | 821  | CLA  | O2A-CGA-O1A | -5.01 | 110.94      | 123.59   |
| 17  | U     | 1008 | BCR  | C23-C22-C21 | 5.01  | 126.63      | 118.94   |
| 14  | Y     | 855  | CLA  | C4A-NA-C1A  | 5.01  | 108.96      | 106.71   |
| 14  | H     | 809  | CLA  | O2A-CGA-O1A | -5.01 | 110.95      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 820  | CLA  | C4D-C3D-CAD | 5.01  | 111.26      | 108.47   |
| 17  | L     | 208  | BCR  | C34-C9-C8   | 5.01  | 125.97      | 118.08   |
| 14  | H     | 810  | CLA  | O2A-C1-C2   | 5.01  | 121.79      | 108.64   |
| 14  | G     | 806  | CLA  | O2A-CGA-CBA | 5.01  | 127.61      | 111.91   |
| 14  | Y     | 808  | CLA  | C1C-C2C-C3C | -5.00 | 101.70      | 106.96   |
| 14  | Y     | 833  | CLA  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 14  | G     | 840  | CLA  | C2C-C1C-NC  | 5.00  | 114.66      | 109.97   |
| 14  | A     | 833  | CLA  | C4A-NA-C1A  | 5.00  | 108.95      | 106.71   |
| 14  | A     | 839  | CLA  | C1C-C2C-C3C | -5.00 | 101.70      | 106.96   |
| 17  | d     | 203  | BCR  | C12-C13-C14 | 5.00  | 126.61      | 118.94   |
| 17  | Q     | 204  | BCR  | C23-C22-C21 | 5.00  | 126.61      | 118.94   |
| 14  | G     | 830  | CLA  | C4A-NA-C1A  | 5.00  | 108.95      | 106.71   |
| 17  | R     | 101  | BCR  | C34-C9-C10  | -4.99 | 115.93      | 122.92   |
| 14  | H     | 825  | CLA  | C1C-C2C-C3C | -4.99 | 101.71      | 106.96   |
| 17  | Q     | 202  | BCR  | C36-C18-C17 | -4.99 | 115.93      | 122.92   |
| 14  | H     | 833  | CLA  | C4D-C3D-CAD | 4.99  | 111.25      | 108.47   |
| 14  | H     | 824  | CLA  | O2A-CGA-CBA | 4.99  | 127.57      | 111.91   |
| 14  | Z     | 826  | CLA  | C1C-C2C-C3C | -4.99 | 101.71      | 106.96   |
| 14  | B     | 821  | CLA  | C1C-C2C-C3C | -4.99 | 101.71      | 106.96   |
| 14  | G     | 829  | CLA  | O2A-C1-C2   | 4.99  | 121.74      | 108.64   |
| 14  | Y     | 832  | CLA  | C1C-C2C-C3C | -4.98 | 101.72      | 106.96   |
| 14  | B     | 826  | CLA  | C4A-NA-C1A  | 4.98  | 108.95      | 106.71   |
| 17  | Y     | 856  | BCR  | C36-C18-C17 | -4.98 | 115.95      | 122.92   |
| 14  | V     | 1201 | CLA  | C2C-C1C-NC  | 4.98  | 114.64      | 109.97   |
| 14  | Z     | 837  | CLA  | C4A-NA-C1A  | 4.98  | 108.94      | 106.71   |
| 14  | A     | 816  | CLA  | C4A-NA-C1A  | 4.98  | 108.94      | 106.71   |
| 14  | Y     | 834  | CLA  | C2C-C1C-NC  | 4.98  | 114.63      | 109.97   |
| 14  | H     | 802  | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 17  | I     | 101  | BCR  | C19-C18-C17 | 4.97  | 126.57      | 118.94   |
| 14  | B     | 838  | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 14  | H     | 818  | CLA  | C4D-C3D-CAD | 4.97  | 111.24      | 108.47   |
| 14  | Y     | 802  | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 14  | A     | 837  | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 14  | Z     | 838  | CLA  | O2A-CGA-O1A | -4.97 | 111.05      | 123.59   |
| 14  | G     | 830  | CLA  | O2A-CGA-O1A | -4.97 | 111.06      | 123.59   |
| 14  | Z     | 812  | CLA  | C2C-C1C-NC  | 4.97  | 114.62      | 109.97   |
| 17  | S     | 1104 | BCR  | C19-C18-C17 | 4.97  | 126.56      | 118.94   |
| 14  | Z     | 810  | CLA  | C1C-C2C-C3C | -4.96 | 101.74      | 106.96   |
| 14  | Y     | 843  | CLA  | C4A-NA-C1A  | 4.96  | 108.94      | 106.71   |
| 14  | G     | 830  | CLA  | O2D-CGD-CBD | 4.96  | 120.09      | 111.27   |
| 14  | G     | 809  | CLA  | O2A-CGA-O1A | -4.96 | 111.07      | 123.59   |
| 14  | Y     | 822  | CLA  | C4D-C3D-CAD | 4.96  | 111.24      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | Q     | 202 | BCR  | C24-C23-C22 | -4.96 | 118.74      | 126.23   |
| 14  | j     | 102 | CLA  | C4D-C3D-CAD | 4.96  | 111.24      | 108.47   |
| 17  | Z     | 841 | BCR  | C27-C26-C25 | -4.96 | 115.53      | 122.73   |
| 14  | Z     | 811 | CLA  | C1C-C2C-C3C | -4.96 | 101.74      | 106.96   |
| 14  | K     | 101 | CLA  | OBD-CAD-C3D | -4.96 | 122.13      | 127.19   |
| 17  | B     | 845 | BCR  | C24-C23-C22 | -4.96 | 118.74      | 126.23   |
| 13  | A     | 801 | CL0  | C1C-C2C-C3C | -4.96 | 101.74      | 106.96   |
| 14  | Z     | 834 | CLA  | C4A-NA-C1A  | 4.96  | 108.93      | 106.71   |
| 14  | Z     | 832 | CLA  | C1C-C2C-C3C | -4.95 | 101.75      | 106.96   |
| 14  | T     | 101 | CLA  | C4A-NA-C1A  | 4.95  | 108.93      | 106.71   |
| 14  | A     | 814 | CLA  | O2D-CGD-CBD | 4.95  | 120.07      | 111.27   |
| 17  | L     | 209 | BCR  | C7-C8-C9    | -4.95 | 118.75      | 126.23   |
| 14  | Z     | 807 | CLA  | O2A-CGA-O1A | -4.95 | 111.09      | 123.59   |
| 17  | G     | 846 | BCR  | C24-C23-C22 | -4.95 | 118.75      | 126.23   |
| 14  | G     | 811 | CLA  | O2A-CGA-O1A | -4.95 | 111.10      | 123.59   |
| 14  | B     | 825 | CLA  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |
| 14  | A     | 823 | CLA  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |
| 14  | A     | 803 | CLA  | C1C-C2C-C3C | -4.95 | 101.75      | 106.96   |
| 17  | Y     | 856 | BCR  | C37-C22-C21 | -4.95 | 115.99      | 122.92   |
| 14  | H     | 801 | CLA  | O2A-C1-C2   | 4.95  | 121.63      | 108.64   |
| 14  | B     | 841 | CLA  | O2A-CGA-O1A | -4.94 | 111.11      | 123.59   |
| 14  | A     | 832 | CLA  | C4A-NA-C1A  | 4.94  | 108.93      | 106.71   |
| 14  | A     | 803 | CLA  | OBD-CAD-C3D | -4.94 | 119.78      | 127.98   |
| 14  | A     | 830 | CLA  | C1C-C2C-C3C | -4.94 | 101.77      | 106.96   |
| 14  | B     | 813 | CLA  | O2A-CGA-CBA | 4.94  | 127.40      | 111.91   |
| 17  | G     | 849 | BCR  | C19-C18-C17 | 4.94  | 126.52      | 118.94   |
| 17  | Y     | 856 | BCR  | C39-C30-C25 | -4.94 | 102.29      | 110.30   |
| 14  | G     | 819 | CLA  | C4A-NA-C1A  | 4.93  | 108.92      | 106.71   |
| 14  | G     | 825 | CLA  | C1C-C2C-C3C | -4.93 | 101.77      | 106.96   |
| 14  | A     | 819 | CLA  | C1C-C2C-C3C | -4.93 | 101.77      | 106.96   |
| 14  | Y     | 829 | CLA  | C1C-C2C-C3C | -4.93 | 101.77      | 106.96   |
| 14  | Z     | 825 | CLA  | C2C-C1C-NC  | 4.93  | 114.59      | 109.97   |
| 14  | L     | 205 | CLA  | O2A-CGA-O1A | -4.92 | 111.17      | 123.59   |
| 14  | A     | 837 | CLA  | C2C-C1C-NC  | 4.92  | 114.58      | 109.97   |
| 14  | Y     | 826 | CLA  | C4D-C3D-CAD | 4.92  | 111.22      | 108.47   |
| 14  | B     | 807 | CLA  | C4D-C3D-CAD | 4.92  | 111.22      | 108.47   |
| 14  | Y     | 854 | CLA  | O2A-CGA-O1A | -4.92 | 111.17      | 123.59   |
| 14  | G     | 811 | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 14  | Y     | 818 | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 14  | B     | 818 | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 17  | J     | 104 | BCR  | C34-C9-C8   | 4.92  | 125.83      | 118.08   |
| 14  | B     | 822 | CLA  | C1C-C2C-C3C | -4.92 | 101.78      | 106.96   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Q     | 203  | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 14  | H     | 836  | CLA  | C1C-C2C-C3C | -4.92 | 101.79      | 106.96   |
| 14  | G     | 813  | CLA  | OBD-CAD-CBD | -4.92 | 118.87      | 125.89   |
| 14  | X     | 1701 | CLA  | OBD-CAD-C3D | -4.92 | 119.82      | 127.98   |
| 14  | A     | 839  | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 14  | Z     | 818  | CLA  | C4A-NA-C1A  | 4.92  | 108.92      | 106.71   |
| 14  | B     | 828  | CLA  | O2A-CGA-O1A | -4.92 | 111.19      | 123.59   |
| 14  | Z     | 816  | CLA  | O2A-C1-C2   | 4.91  | 121.55      | 108.64   |
| 14  | A     | 824  | CLA  | O2A-CGA-O1A | -4.91 | 111.19      | 123.59   |
| 17  | A     | 845  | BCR  | C27-C26-C25 | -4.91 | 115.60      | 122.73   |
| 13  | A     | 801  | CL0  | O2A-CGA-CBA | 4.91  | 127.32      | 111.91   |
| 14  | B     | 823  | CLA  | C4A-NA-C1A  | 4.91  | 108.91      | 106.71   |
| 17  | G     | 854  | BCR  | C34-C9-C8   | 4.91  | 125.81      | 118.08   |
| 14  | G     | 805  | CLA  | O2A-C1-C2   | 4.91  | 121.54      | 108.64   |
| 14  | G     | 843  | CLA  | O2A-C1-C2   | 4.91  | 121.54      | 108.64   |
| 14  | B     | 819  | CLA  | OBD-CAD-C3D | -4.91 | 119.83      | 127.98   |
| 14  | G     | 826  | CLA  | O2D-CGD-CBD | 4.91  | 119.99      | 111.27   |
| 17  | Z     | 842  | BCR  | C24-C23-C22 | -4.91 | 118.81      | 126.23   |
| 14  | Z     | 803  | CLA  | C1C-C2C-C3C | -4.91 | 101.80      | 106.96   |
| 14  | A     | 822  | CLA  | O2D-CGD-CBD | 4.91  | 119.99      | 111.27   |
| 14  | Z     | 806  | CLA  | C4D-C3D-CAD | 4.91  | 111.21      | 108.47   |
| 14  | Z     | 821  | CLA  | C4D-C3D-CAD | 4.91  | 111.21      | 108.47   |
| 14  | H     | 814  | CLA  | C1C-C2C-C3C | -4.91 | 101.80      | 106.96   |
| 14  | B     | 838  | CLA  | O2D-CGD-CBD | 4.90  | 119.98      | 111.27   |
| 14  | f     | 101  | CLA  | C4D-C3D-CAD | 4.90  | 111.20      | 108.47   |
| 14  | Z     | 835  | CLA  | O2A-CGA-O1A | -4.90 | 111.22      | 123.59   |
| 14  | S     | 1102 | CLA  | C4A-NA-C1A  | 4.90  | 108.91      | 106.71   |
| 14  | A     | 833  | CLA  | C1C-C2C-C3C | -4.90 | 101.81      | 106.96   |
| 14  | A     | 833  | CLA  | C4D-C3D-CAD | 4.90  | 111.20      | 108.47   |
| 14  | d     | 201  | CLA  | C1C-C2C-C3C | -4.90 | 101.81      | 106.96   |
| 14  | G     | 804  | CLA  | O2A-CGA-O1A | -4.89 | 111.25      | 123.59   |
| 14  | G     | 836  | CLA  | O2A-CGA-O1A | -4.89 | 111.25      | 123.59   |
| 14  | G     | 838  | CLA  | C4D-C3D-CAD | 4.89  | 111.20      | 108.47   |
| 14  | G     | 812  | CLA  | C4D-C3D-CAD | 4.89  | 111.20      | 108.47   |
| 14  | G     | 817  | CLA  | O2D-CGD-CBD | 4.89  | 119.95      | 111.27   |
| 14  | G     | 818  | CLA  | O2A-CGA-CBA | 4.89  | 127.24      | 111.91   |
| 14  | A     | 830  | CLA  | O2A-C1-C2   | 4.89  | 121.47      | 108.64   |
| 17  | V     | 1202 | BCR  | C23-C24-C25 | -4.88 | 113.49      | 127.20   |
| 14  | S     | 1101 | CLA  | OBD-CAD-C3D | -4.88 | 119.88      | 127.98   |
| 14  | H     | 817  | CLA  | O2D-CGD-CBD | 4.88  | 119.94      | 111.27   |
| 14  | Z     | 820  | CLA  | O2A-CGA-O1A | -4.88 | 111.28      | 123.59   |
| 14  | A     | 804  | CLA  | O2A-C1-C2   | 4.88  | 121.46      | 108.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Y     | 849  | BCR  | C34-C9-C10  | -4.88 | 116.09      | 122.92   |
| 17  | H     | 848  | BCR  | C24-C23-C22 | -4.88 | 118.87      | 126.23   |
| 14  | H     | 814  | CLA  | C4D-C3D-CAD | 4.88  | 111.19      | 108.47   |
| 14  | A     | 807  | CLA  | C4A-NA-C1A  | 4.88  | 108.90      | 106.71   |
| 14  | A     | 815  | CLA  | O2A-CGA-O1A | -4.87 | 111.30      | 123.59   |
| 14  | Z     | 838  | CLA  | C2C-C1C-NC  | 4.87  | 114.53      | 109.97   |
| 17  | G     | 846  | BCR  | C15-C14-C13 | -4.87 | 120.36      | 127.31   |
| 14  | H     | 816  | CLA  | C1C-C2C-C3C | -4.87 | 101.84      | 106.96   |
| 14  | Z     | 815  | CLA  | C1C-C2C-C3C | -4.86 | 101.84      | 106.96   |
| 14  | G     | 814  | CLA  | C4A-NA-C1A  | 4.86  | 108.89      | 106.71   |
| 14  | G     | 838  | CLA  | O2D-CGD-CBD | 4.86  | 119.91      | 111.27   |
| 14  | Y     | 805  | CLA  | C1C-C2C-C3C | -4.86 | 101.84      | 106.96   |
| 14  | Y     | 807  | CLA  | O2A-C1-C2   | 4.86  | 121.42      | 108.64   |
| 17  | e     | 101  | BCR  | C8-C7-C6    | -4.86 | 113.55      | 127.20   |
| 14  | A     | 803  | CLA  | O2A-CGA-O1A | -4.86 | 111.32      | 123.59   |
| 14  | B     | 835  | CLA  | OBD-CAD-CBD | -4.86 | 118.95      | 125.89   |
| 14  | B     | 828  | CLA  | C1C-C2C-C3C | -4.86 | 101.85      | 106.96   |
| 14  | Y     | 820  | CLA  | C1C-C2C-C3C | -4.86 | 101.85      | 106.96   |
| 17  | Q     | 204  | BCR  | C23-C24-C25 | -4.85 | 113.57      | 127.20   |
| 17  | R     | 102  | BCR  | C37-C22-C21 | -4.85 | 116.12      | 122.92   |
| 14  | Z     | 818  | CLA  | O2D-CGD-CBD | 4.85  | 119.89      | 111.27   |
| 14  | G     | 815  | CLA  | O2A-C1-C2   | 4.85  | 121.39      | 108.64   |
| 14  | Z     | 804  | CLA  | O2A-CGA-O1A | -4.85 | 111.34      | 123.59   |
| 14  | h     | 205  | CLA  | O2A-CGA-CBA | 4.85  | 127.13      | 111.91   |
| 14  | B     | 838  | CLA  | O2A-CGA-O1A | -4.85 | 111.35      | 123.59   |
| 14  | A     | 830  | CLA  | O2A-CGA-O1A | -4.85 | 111.35      | 123.59   |
| 14  | G     | 834  | CLA  | O2A-C1-C2   | 4.85  | 121.38      | 108.64   |
| 14  | Y     | 838  | CLA  | O2A-CGA-O1A | -4.85 | 111.36      | 123.59   |
| 14  | G     | 821  | CLA  | O2A-CGA-O1A | -4.85 | 111.36      | 123.59   |
| 14  | G     | 819  | CLA  | C1C-C2C-C3C | -4.85 | 101.86      | 106.96   |
| 14  | L     | 202  | CLA  | C1C-C2C-C3C | -4.84 | 101.86      | 106.96   |
| 14  | Y     | 806  | CLA  | O2A-CGA-O1A | -4.84 | 111.36      | 123.59   |
| 14  | H     | 831  | CLA  | C4A-NA-C1A  | 4.84  | 108.88      | 106.71   |
| 14  | A     | 835  | CLA  | C4D-C3D-CAD | 4.84  | 111.17      | 108.47   |
| 14  | G     | 821  | CLA  | C4D-C3D-CAD | 4.84  | 111.17      | 108.47   |
| 14  | h     | 207  | CLA  | C2C-C1C-NC  | 4.84  | 114.51      | 109.97   |
| 14  | X     | 1701 | CLA  | C4A-NA-C1A  | 4.84  | 108.88      | 106.71   |
| 14  | H     | 804  | CLA  | C4D-C3D-CAD | 4.84  | 111.17      | 108.47   |
| 14  | Y     | 830  | CLA  | O2A-C1-C2   | 4.84  | 121.36      | 108.64   |
| 17  | G     | 854  | BCR  | C15-C14-C13 | -4.84 | 120.40      | 127.31   |
| 14  | G     | 834  | CLA  | C2C-C1C-NC  | 4.84  | 114.50      | 109.97   |
| 14  | B     | 825  | CLA  | O2A-CGA-CBA | 4.84  | 127.09      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | Y     | 850 | BCR  | C24-C23-C22 | -4.84 | 118.92      | 126.23   |
| 14  | B     | 805 | CLA  | O2A-C1-C2   | 4.84  | 121.35      | 108.64   |
| 14  | A     | 805 | CLA  | O2A-CGA-O1A | -4.83 | 111.39      | 123.59   |
| 14  | L     | 205 | CLA  | C4D-C3D-CAD | 4.83  | 111.17      | 108.47   |
| 17  | A     | 849 | BCR  | C8-C7-C6    | -4.83 | 113.62      | 127.20   |
| 14  | A     | 815 | CLA  | O2A-C1-C2   | 4.83  | 121.34      | 108.64   |
| 14  | B     | 838 | CLA  | O2A-CGA-CBA | 4.83  | 127.07      | 111.91   |
| 14  | A     | 836 | CLA  | O2A-CGA-O1A | -4.83 | 111.40      | 123.59   |
| 14  | A     | 823 | CLA  | C4D-C3D-CAD | 4.83  | 111.16      | 108.47   |
| 14  | H     | 812 | CLA  | C4A-NA-C1A  | 4.83  | 108.88      | 106.71   |
| 14  | B     | 808 | CLA  | C4A-NA-C1A  | 4.83  | 108.88      | 106.71   |
| 14  | H     | 817 | CLA  | O2A-CGA-O1A | -4.83 | 111.41      | 123.59   |
| 14  | Y     | 840 | CLA  | O2A-CGA-CBA | 4.83  | 127.06      | 111.91   |
| 14  | Y     | 819 | CLA  | C4D-C3D-CAD | 4.83  | 111.16      | 108.47   |
| 14  | Z     | 801 | CLA  | C1C-C2C-C3C | -4.82 | 101.89      | 106.96   |
| 17  | L     | 209 | BCR  | C36-C18-C17 | -4.82 | 116.17      | 122.92   |
| 13  | A     | 801 | CL0  | O2D-CGD-CBD | 4.82  | 119.84      | 111.27   |
| 14  | h     | 205 | CLA  | C4D-C3D-CAD | 4.82  | 111.16      | 108.47   |
| 17  | G     | 846 | BCR  | C34-C9-C10  | -4.82 | 116.17      | 122.92   |
| 14  | G     | 822 | CLA  | O2A-CGA-O1A | -4.82 | 111.43      | 123.59   |
| 17  | f     | 105 | BCR  | C24-C23-C22 | -4.82 | 118.95      | 126.23   |
| 14  | H     | 825 | CLA  | O2D-CGD-CBD | 4.82  | 119.83      | 111.27   |
| 17  | F     | 201 | BCR  | C3-C4-C5    | -4.82 | 105.47      | 114.08   |
| 14  | Y     | 806 | CLA  | C4D-C3D-CAD | 4.82  | 111.16      | 108.47   |
| 14  | H     | 811 | CLA  | C1C-C2C-C3C | -4.82 | 101.89      | 106.96   |
| 14  | J     | 102 | CLA  | O2A-CGA-CBA | 4.82  | 127.02      | 111.91   |
| 14  | G     | 853 | CLA  | C1C-C2C-C3C | -4.82 | 101.89      | 106.96   |
| 17  | Y     | 850 | BCR  | C34-C9-C8   | 4.81  | 125.66      | 118.08   |
| 14  | Y     | 820 | CLA  | O2A-CGA-O1A | -4.81 | 111.44      | 123.59   |
| 17  | M     | 101 | BCR  | C36-C18-C17 | -4.81 | 116.18      | 122.92   |
| 14  | B     | 814 | CLA  | CMB-C2B-C3B | 4.81  | 133.68      | 124.68   |
| 14  | A     | 828 | CLA  | O2A-CGA-O1A | -4.81 | 111.45      | 123.59   |
| 14  | Y     | 802 | CLA  | O2A-CGA-O1A | -4.81 | 111.45      | 123.59   |
| 14  | G     | 840 | CLA  | C1C-C2C-C3C | -4.81 | 101.90      | 106.96   |
| 17  | B     | 847 | BCR  | C34-C9-C10  | -4.81 | 116.19      | 122.92   |
| 14  | B     | 837 | CLA  | O2D-CGD-O1D | -4.81 | 114.44      | 123.84   |
| 17  | Y     | 848 | BCR  | C33-C5-C6   | -4.80 | 119.13      | 124.53   |
| 17  | B     | 847 | BCR  | C36-C18-C17 | -4.80 | 116.20      | 122.92   |
| 17  | G     | 849 | BCR  | C34-C9-C10  | -4.80 | 116.20      | 122.92   |
| 14  | A     | 827 | CLA  | C1C-C2C-C3C | -4.80 | 101.91      | 106.96   |
| 14  | G     | 805 | CLA  | O2D-CGD-CBD | 4.80  | 119.79      | 111.27   |
| 14  | Y     | 823 | CLA  | C1C-C2C-C3C | -4.80 | 101.91      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 801  | CLA  | O2A-C1-C2   | 4.79  | 121.24      | 108.64   |
| 14  | Z     | 834  | CLA  | C1C-C2C-C3C | -4.79 | 101.92      | 106.96   |
| 14  | B     | 836  | CLA  | O2D-CGD-CBD | 4.79  | 119.78      | 111.27   |
| 14  | J     | 102  | CLA  | C4D-C3D-CAD | 4.79  | 111.14      | 108.47   |
| 14  | B     | 816  | CLA  | C1C-C2C-C3C | -4.79 | 101.92      | 106.96   |
| 17  | B     | 844  | BCR  | C19-C18-C17 | 4.79  | 126.28      | 118.94   |
| 14  | G     | 843  | CLA  | O2A-CGA-O1A | -4.78 | 111.52      | 123.59   |
| 14  | B     | 815  | CLA  | C4D-C3D-CAD | 4.78  | 111.14      | 108.47   |
| 17  | J     | 103  | BCR  | C34-C9-C8   | 4.78  | 125.61      | 118.08   |
| 14  | B     | 812  | CLA  | O2A-CGA-O1A | -4.78 | 111.52      | 123.59   |
| 14  | Y     | 812  | CLA  | C1C-C2C-C3C | -4.78 | 101.93      | 106.96   |
| 14  | A     | 805  | CLA  | C1C-C2C-C3C | -4.78 | 101.93      | 106.96   |
| 14  | B     | 808  | CLA  | O2D-CGD-CBD | 4.78  | 119.77      | 111.27   |
| 14  | B     | 818  | CLA  | O2A-CGA-CBA | 4.78  | 126.91      | 111.91   |
| 14  | H     | 831  | CLA  | O2D-CGD-CBD | 4.78  | 119.76      | 111.27   |
| 14  | H     | 814  | CLA  | O2D-CGD-CBD | 4.78  | 119.76      | 111.27   |
| 14  | G     | 831  | CLA  | C4A-NA-C1A  | 4.78  | 108.85      | 106.71   |
| 17  | Y     | 850  | BCR  | C34-C9-C10  | -4.78 | 116.23      | 122.92   |
| 14  | B     | 820  | CLA  | OBD-CAD-CBD | -4.77 | 119.08      | 125.89   |
| 14  | Z     | 826  | CLA  | C4A-NA-C1A  | 4.77  | 108.85      | 106.71   |
| 14  | G     | 810  | CLA  | C1C-C2C-C3C | -4.77 | 101.94      | 106.96   |
| 14  | B     | 814  | CLA  | C1C-C2C-C3C | -4.77 | 101.94      | 106.96   |
| 14  | A     | 807  | CLA  | C4D-C3D-CAD | 4.77  | 111.13      | 108.47   |
| 17  | G     | 848  | BCR  | C34-C9-C10  | -4.77 | 116.24      | 122.92   |
| 14  | A     | 809  | CLA  | C1-O2A-CGA  | 4.77  | 128.96      | 116.44   |
| 13  | Y     | 801  | CL0  | C1C-C2C-C3C | -4.77 | 101.94      | 106.96   |
| 17  | i     | 101  | BCR  | C19-C18-C17 | 4.77  | 126.26      | 118.94   |
| 14  | H     | 818  | CLA  | O2A-CGA-O1A | -4.77 | 111.56      | 123.59   |
| 14  | L     | 205  | CLA  | OBD-CAD-CBD | -4.77 | 119.08      | 125.89   |
| 14  | G     | 821  | CLA  | O2A-C1-C2   | 4.77  | 121.17      | 108.64   |
| 14  | G     | 805  | CLA  | C1-C2-C3    | -4.77 | 117.80      | 126.04   |
| 14  | G     | 837  | CLA  | C1C-C2C-C3C | -4.77 | 101.94      | 106.96   |
| 14  | Z     | 839  | CLA  | O2D-CGD-CBD | 4.77  | 119.74      | 111.27   |
| 17  | R     | 101  | BCR  | C8-C7-C6    | -4.76 | 113.82      | 127.20   |
| 14  | Y     | 824  | CLA  | C4A-NA-C1A  | 4.76  | 108.85      | 106.71   |
| 17  | G     | 847  | BCR  | C34-C9-C10  | -4.76 | 116.25      | 122.92   |
| 14  | A     | 813  | CLA  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 14  | G     | 802  | CLA  | C4D-C3D-CAD | 4.76  | 111.13      | 108.47   |
| 17  | H     | 848  | BCR  | C34-C9-C8   | 4.76  | 125.58      | 118.08   |
| 14  | Y     | 833  | CLA  | O2A-C1-C2   | 4.76  | 121.14      | 108.64   |
| 17  | G     | 846  | BCR  | C33-C5-C6   | -4.76 | 119.18      | 124.53   |
| 17  | U     | 1007 | BCR  | C34-C9-C8   | 4.76  | 125.57      | 118.08   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 102  | CLA  | O2D-CGD-CBD | 4.76  | 119.72      | 111.27   |
| 17  | U     | 1005 | BCR  | C37-C22-C21 | -4.75 | 116.26      | 122.92   |
| 14  | Y     | 839  | CLA  | O2D-CGD-CBD | 4.75  | 119.72      | 111.27   |
| 14  | B     | 801  | CLA  | C4D-C3D-CAD | 4.75  | 111.12      | 108.47   |
| 14  | Y     | 830  | CLA  | O2A-CGA-O1A | -4.75 | 111.59      | 123.59   |
| 14  | Y     | 835  | CLA  | O2A-CGA-O1A | -4.75 | 111.60      | 123.59   |
| 14  | B     | 823  | CLA  | O2A-CGA-O1A | -4.75 | 111.61      | 123.59   |
| 14  | G     | 802  | CLA  | O2A-CGA-CBA | 4.75  | 126.80      | 111.91   |
| 14  | A     | 839  | CLA  | O2D-CGD-CBD | 4.75  | 119.70      | 111.27   |
| 14  | A     | 832  | CLA  | C4D-C3D-CAD | 4.75  | 111.12      | 108.47   |
| 14  | Z     | 807  | CLA  | O2A-C1-C2   | 4.74  | 121.11      | 108.64   |
| 17  | G     | 847  | BCR  | C24-C23-C22 | -4.74 | 119.07      | 126.23   |
| 14  | B     | 841  | CLA  | O2D-CGD-O1D | -4.74 | 114.56      | 123.84   |
| 14  | A     | 828  | CLA  | C1C-C2C-C3C | -4.74 | 101.97      | 106.96   |
| 14  | Z     | 818  | CLA  | C4D-C3D-CAD | 4.74  | 111.11      | 108.47   |
| 14  | U     | 1006 | CLA  | O2D-CGD-CBD | 4.74  | 119.69      | 111.27   |
| 14  | H     | 826  | CLA  | O2A-CGA-CBA | 4.74  | 126.78      | 111.91   |
| 14  | L     | 201  | CLA  | C2C-C1C-NC  | 4.74  | 114.41      | 109.97   |
| 14  | G     | 840  | CLA  | O2D-CGD-CBD | 4.74  | 119.69      | 111.27   |
| 14  | A     | 806  | CLA  | C1C-C2C-C3C | -4.74 | 101.97      | 106.96   |
| 14  | Y     | 831  | CLA  | C4A-NA-C1A  | 4.74  | 108.83      | 106.71   |
| 18  | j     | 101  | LHG  | O7-C7-C8    | 4.74  | 121.71      | 111.50   |
| 14  | Z     | 830  | CLA  | C1C-C2C-C3C | -4.73 | 101.98      | 106.96   |
| 17  | H     | 848  | BCR  | C31-C1-C6   | -4.73 | 102.62      | 110.30   |
| 14  | A     | 834  | CLA  | C4A-NA-C1A  | 4.73  | 108.83      | 106.71   |
| 14  | A     | 837  | CLA  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 17  | F     | 203  | BCR  | C35-C13-C14 | -4.73 | 116.30      | 122.92   |
| 14  | K     | 103  | CLA  | C4A-NA-C1A  | 4.73  | 108.83      | 106.71   |
| 14  | G     | 809  | CLA  | C1C-C2C-C3C | -4.73 | 101.98      | 106.96   |
| 14  | Y     | 807  | CLA  | O2A-CGA-O1A | -4.73 | 111.66      | 123.59   |
| 18  | B     | 850  | LHG  | O7-C7-C8    | 4.73  | 121.69      | 111.50   |
| 14  | A     | 825  | CLA  | O2A-C1-C2   | 4.73  | 121.06      | 108.64   |
| 14  | h     | 207  | CLA  | O2A-C1-C2   | 4.73  | 121.06      | 108.64   |
| 14  | Y     | 854  | CLA  | C1C-C2C-C3C | -4.72 | 101.99      | 106.96   |
| 14  | G     | 819  | CLA  | CMB-C2B-C3B | 4.72  | 133.52      | 124.68   |
| 17  | B     | 848  | BCR  | C34-C9-C10  | -4.72 | 116.32      | 122.92   |
| 14  | G     | 824  | CLA  | O2A-CGA-O1A | -4.71 | 111.70      | 123.59   |
| 14  | H     | 804  | CLA  | O2D-CGD-CBD | 4.71  | 119.64      | 111.27   |
| 14  | Y     | 835  | CLA  | O2A-C1-C2   | 4.71  | 121.02      | 108.64   |
| 14  | H     | 812  | CLA  | C1C-C2C-C3C | -4.71 | 102.00      | 106.96   |
| 14  | G     | 841  | CLA  | O2A-C1-C2   | 4.71  | 121.02      | 108.64   |
| 14  | A     | 823  | CLA  | C1C-C2C-C3C | -4.71 | 102.00      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 836  | CLA  | O2D-CGD-CBD | 4.71  | 119.63      | 111.27   |
| 14  | Z     | 811  | CLA  | O2D-CGD-CBD | 4.71  | 119.63      | 111.27   |
| 14  | Y     | 838  | CLA  | C1C-C2C-C3C | -4.71 | 102.01      | 106.96   |
| 14  | B     | 831  | CLA  | C1C-C2C-C3C | -4.71 | 102.01      | 106.96   |
| 14  | Y     | 821  | CLA  | C4D-C3D-CAD | 4.71  | 111.09      | 108.47   |
| 14  | H     | 802  | CLA  | C4D-C3D-CAD | 4.70  | 111.09      | 108.47   |
| 17  | h     | 203  | BCR  | C36-C18-C17 | -4.70 | 116.34      | 122.92   |
| 14  | U     | 1003 | CLA  | O2A-CGA-O1A | -4.70 | 111.74      | 123.59   |
| 14  | Z     | 815  | CLA  | O2D-CGD-CBD | 4.70  | 119.61      | 111.27   |
| 14  | B     | 813  | CLA  | C1C-C2C-C3C | -4.70 | 102.02      | 106.96   |
| 17  | H     | 848  | BCR  | C37-C22-C21 | -4.70 | 116.35      | 122.92   |
| 14  | B     | 809  | CLA  | OBD-CAD-C3D | -4.69 | 120.19      | 127.98   |
| 14  | G     | 825  | CLA  | O2A-CGA-O1A | -4.69 | 111.75      | 123.59   |
| 17  | H     | 844  | BCR  | C37-C22-C21 | -4.69 | 116.35      | 122.92   |
| 14  | Z     | 812  | CLA  | O2D-CGD-CBD | 4.69  | 119.60      | 111.27   |
| 14  | B     | 836  | CLA  | OBD-CAD-C3D | -4.69 | 120.19      | 127.98   |
| 14  | Z     | 803  | CLA  | CMB-C2B-C3B | 4.69  | 133.45      | 124.68   |
| 17  | f     | 104  | BCR  | C7-C8-C9    | -4.69 | 119.15      | 126.23   |
| 14  | B     | 814  | CLA  | O2A-CGA-O1A | -4.68 | 111.77      | 123.59   |
| 14  | L     | 207  | CLA  | CMB-C2B-C3B | 4.68  | 133.44      | 124.68   |
| 17  | f     | 105  | BCR  | C34-C9-C10  | -4.68 | 116.36      | 122.92   |
| 14  | Z     | 803  | CLA  | O2A-CGA-CBA | 4.68  | 126.60      | 111.91   |
| 17  | Q     | 202  | BCR  | C34-C9-C10  | -4.68 | 116.36      | 122.92   |
| 14  | g     | 102  | CLA  | C4D-C3D-CAD | 4.68  | 111.08      | 108.47   |
| 14  | B     | 824  | CLA  | O2A-CGA-O1A | -4.68 | 111.78      | 123.59   |
| 14  | Y     | 811  | CLA  | O2A-C1-C2   | 4.68  | 120.94      | 108.64   |
| 14  | Z     | 837  | CLA  | C4D-C3D-CAD | 4.68  | 111.08      | 108.47   |
| 14  | g     | 102  | CLA  | C4A-NA-C1A  | 4.68  | 108.81      | 106.71   |
| 17  | T     | 102  | BCR  | C34-C9-C10  | -4.68 | 116.37      | 122.92   |
| 17  | i     | 101  | BCR  | C3-C4-C5    | -4.68 | 105.73      | 114.08   |
| 17  | d     | 203  | BCR  | C35-C13-C14 | -4.68 | 116.37      | 122.92   |
| 14  | K     | 103  | CLA  | C4D-C3D-CAD | 4.68  | 111.08      | 108.47   |
| 14  | A     | 805  | CLA  | O2A-C1-C2   | 4.67  | 120.92      | 108.64   |
| 14  | H     | 834  | CLA  | C4A-NA-C1A  | 4.67  | 108.81      | 106.71   |
| 17  | H     | 841  | BCR  | C37-C22-C21 | -4.67 | 116.38      | 122.92   |
| 14  | Y     | 821  | CLA  | O2A-CGA-O1A | -4.67 | 111.81      | 123.59   |
| 14  | H     | 837  | CLA  | O2A-C1-C2   | 4.67  | 120.91      | 108.64   |
| 14  | G     | 825  | CLA  | O2D-CGD-CBD | 4.67  | 119.56      | 111.27   |
| 14  | B     | 827  | CLA  | O2D-CGD-CBD | 4.66  | 119.55      | 111.27   |
| 17  | R     | 101  | BCR  | C36-C18-C17 | -4.66 | 116.39      | 122.92   |
| 14  | T     | 103  | CLA  | C4A-NA-C1A  | 4.66  | 108.80      | 106.71   |
| 14  | H     | 817  | CLA  | O2A-CGA-CBA | 4.66  | 126.53      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 838  | CLA  | O2A-C1-C2   | 4.66  | 120.88      | 108.64   |
| 14  | G     | 824  | CLA  | C1C-C2C-C3C | -4.66 | 102.06      | 106.96   |
| 14  | A     | 806  | CLA  | CAA-C2A-C3A | -4.66 | 100.02      | 112.78   |
| 14  | A     | 822  | CLA  | C4D-C3D-CAD | 4.66  | 111.07      | 108.47   |
| 17  | V     | 1202 | BCR  | C38-C26-C25 | 4.66  | 129.76      | 124.53   |
| 17  | h     | 202  | BCR  | C24-C23-C22 | -4.66 | 119.20      | 126.23   |
| 14  | A     | 831  | CLA  | C4A-NA-C1A  | 4.66  | 108.80      | 106.71   |
| 14  | Y     | 803  | CLA  | C1C-C2C-C3C | -4.66 | 102.06      | 106.96   |
| 17  | R     | 101  | BCR  | C30-C25-C26 | -4.66 | 116.06      | 122.61   |
| 14  | Z     | 819  | CLA  | CMB-C2B-C3B | 4.65  | 133.38      | 124.68   |
| 17  | B     | 844  | BCR  | C37-C22-C23 | 4.65  | 125.41      | 118.08   |
| 14  | A     | 806  | CLA  | O2D-CGD-CBD | 4.65  | 119.54      | 111.27   |
| 14  | Z     | 824  | CLA  | O2D-CGD-CBD | 4.65  | 119.54      | 111.27   |
| 14  | H     | 818  | CLA  | O2A-CGA-CBA | 4.65  | 126.51      | 111.91   |
| 14  | Y     | 838  | CLA  | C4D-C3D-CAD | 4.65  | 111.06      | 108.47   |
| 17  | U     | 1008 | BCR  | C33-C5-C6   | -4.65 | 119.31      | 124.53   |
| 14  | A     | 807  | CLA  | O2A-CGA-O1A | -4.65 | 111.86      | 123.59   |
| 14  | A     | 832  | CLA  | O2A-CGA-O1A | -4.65 | 111.86      | 123.59   |
| 14  | H     | 837  | CLA  | C1C-C2C-C3C | -4.65 | 102.07      | 106.96   |
| 14  | Y     | 809  | CLA  | C1C-C2C-C3C | -4.65 | 102.07      | 106.96   |
| 14  | Y     | 834  | CLA  | O2D-CGD-CBD | 4.65  | 119.52      | 111.27   |
| 14  | Y     | 838  | CLA  | O2D-CGD-CBD | 4.64  | 119.52      | 111.27   |
| 14  | G     | 816  | CLA  | C4D-C3D-CAD | 4.64  | 111.06      | 108.47   |
| 14  | Z     | 831  | CLA  | C4A-NA-C1A  | 4.64  | 108.79      | 106.71   |
| 14  | U     | 1006 | CLA  | C4A-NA-C1A  | 4.64  | 108.79      | 106.71   |
| 19  | Z     | 847  | LMG  | O7-C10-C11  | 4.64  | 121.51      | 111.50   |
| 14  | A     | 840  | CLA  | C1C-C2C-C3C | -4.64 | 102.08      | 106.96   |
| 14  | H     | 822  | CLA  | C4D-C3D-CAD | 4.64  | 111.06      | 108.47   |
| 17  | B     | 847  | BCR  | C37-C22-C21 | -4.64 | 116.42      | 122.92   |
| 14  | G     | 853  | CLA  | OBD-CAD-CBD | -4.64 | 119.27      | 125.89   |
| 14  | Z     | 811  | CLA  | O2A-CGA-O1A | -4.64 | 111.89      | 123.59   |
| 14  | A     | 838  | CLA  | O2A-CGA-CBA | 4.64  | 126.46      | 111.91   |
| 14  | B     | 837  | CLA  | C1C-C2C-C3C | -4.64 | 102.08      | 106.96   |
| 14  | Y     | 822  | CLA  | O2A-C1-C2   | 4.64  | 120.82      | 108.64   |
| 14  | A     | 823  | CLA  | O2A-C1-C2   | 4.63  | 120.81      | 108.64   |
| 14  | G     | 830  | CLA  | OBD-CAD-CBD | -4.63 | 119.27      | 125.89   |
| 14  | G     | 831  | CLA  | OBD-CAD-C3D | -4.63 | 120.29      | 127.98   |
| 14  | G     | 822  | CLA  | O2A-C1-C2   | 4.63  | 120.81      | 108.64   |
| 14  | H     | 805  | CLA  | C4D-C3D-CAD | 4.63  | 111.05      | 108.47   |
| 14  | H     | 822  | CLA  | C1C-C2C-C3C | -4.63 | 102.09      | 106.96   |
| 14  | Z     | 812  | CLA  | C1C-C2C-C3C | -4.63 | 102.09      | 106.96   |
| 14  | A     | 835  | CLA  | C1C-C2C-C3C | -4.63 | 102.09      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 814  | CLA  | O2A-C1-C2   | 4.63  | 120.80      | 108.64   |
| 14  | G     | 838  | CLA  | O2A-CGA-CBA | 4.63  | 126.44      | 111.91   |
| 14  | H     | 820  | CLA  | C1C-C2C-C3C | -4.63 | 102.09      | 106.96   |
| 17  | e     | 101  | BCR  | C19-C18-C17 | 4.63  | 126.04      | 118.94   |
| 14  | B     | 841  | CLA  | C4D-C3D-CAD | 4.63  | 111.05      | 108.47   |
| 14  | A     | 834  | CLA  | O2A-CGA-O1A | -4.63 | 111.92      | 123.59   |
| 14  | G     | 834  | CLA  | O2D-CGD-CBD | 4.62  | 119.49      | 111.27   |
| 17  | V     | 1202 | BCR  | C34-C9-C8   | 4.62  | 125.36      | 118.08   |
| 14  | Z     | 838  | CLA  | O2D-CGD-O1D | -4.62 | 114.80      | 123.84   |
| 14  | Y     | 841  | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 14  | H     | 804  | CLA  | O2A-CGA-O1A | -4.62 | 111.93      | 123.59   |
| 14  | B     | 801  | CLA  | O2D-CGD-CBD | 4.62  | 119.48      | 111.27   |
| 14  | B     | 833  | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 17  | Y     | 851  | BCR  | C32-C1-C6   | 4.62  | 117.79      | 110.30   |
| 14  | H     | 818  | CLA  | O2A-C1-C2   | 4.62  | 120.77      | 108.64   |
| 14  | B     | 819  | CLA  | O2A-CGA-O1A | -4.62 | 111.94      | 123.59   |
| 17  | G     | 849  | BCR  | C36-C18-C17 | -4.61 | 116.46      | 122.92   |
| 14  | G     | 812  | CLA  | O2A-CGA-O1A | -4.61 | 111.95      | 123.59   |
| 14  | Q     | 203  | CLA  | OBD-CAD-CBD | -4.61 | 119.31      | 125.89   |
| 14  | Y     | 818  | CLA  | CMB-C2B-C3B | 4.61  | 133.31      | 124.68   |
| 14  | A     | 812  | CLA  | C4D-C3D-CAD | 4.61  | 111.04      | 108.47   |
| 17  | e     | 101  | BCR  | C36-C18-C17 | -4.61 | 116.47      | 122.92   |
| 14  | B     | 827  | CLA  | OBD-CAD-C3D | -4.61 | 120.33      | 127.98   |
| 14  | Z     | 804  | CLA  | O2A-C1-C2   | 4.61  | 120.75      | 108.64   |
| 17  | M     | 101  | BCR  | C24-C23-C22 | -4.61 | 119.27      | 126.23   |
| 17  | H     | 845  | BCR  | C8-C7-C6    | -4.61 | 114.27      | 127.20   |
| 17  | h     | 202  | BCR  | C33-C5-C6   | -4.61 | 119.36      | 124.53   |
| 14  | Z     | 835  | CLA  | C1C-C2C-C3C | -4.61 | 102.11      | 106.96   |
| 14  | G     | 830  | CLA  | O2A-C1-C2   | 4.60  | 120.74      | 108.64   |
| 14  | A     | 834  | CLA  | C1C-C2C-C3C | -4.60 | 102.12      | 106.96   |
| 17  | Z     | 842  | BCR  | C34-C9-C10  | -4.60 | 116.47      | 122.92   |
| 17  | Z     | 845  | BCR  | C24-C23-C22 | -4.60 | 119.28      | 126.23   |
| 17  | i     | 101  | BCR  | C40-C30-C25 | 4.60  | 117.76      | 110.30   |
| 14  | A     | 834  | CLA  | C4D-C3D-CAD | 4.60  | 111.03      | 108.47   |
| 14  | A     | 819  | CLA  | C4A-NA-C1A  | 4.60  | 108.77      | 106.71   |
| 14  | B     | 821  | CLA  | C4A-NA-C1A  | 4.60  | 108.77      | 106.71   |
| 14  | H     | 827  | CLA  | O2A-C1-C2   | 4.59  | 120.71      | 108.64   |
| 17  | A     | 845  | BCR  | C38-C26-C25 | 4.59  | 129.69      | 124.53   |
| 14  | G     | 838  | CLA  | O2A-CGA-O1A | -4.59 | 112.00      | 123.59   |
| 17  | A     | 847  | BCR  | C24-C23-C22 | -4.59 | 119.29      | 126.23   |
| 14  | G     | 821  | CLA  | O2D-CGD-CBD | 4.59  | 119.43      | 111.27   |
| 14  | Z     | 830  | CLA  | C4D-C3D-CAD | 4.59  | 111.03      | 108.47   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 834  | CLA  | C2C-C1C-NC  | 4.59  | 114.27      | 109.97   |
| 14  | G     | 820  | CLA  | O2A-C1-C2   | 4.59  | 120.70      | 108.64   |
| 14  | H     | 827  | CLA  | O2D-CGD-CBD | 4.59  | 119.42      | 111.27   |
| 17  | Y     | 846  | BCR  | C24-C23-C22 | -4.59 | 119.30      | 126.23   |
| 14  | A     | 818  | CLA  | O2A-CGA-O1A | -4.59 | 112.01      | 123.59   |
| 17  | B     | 851  | BCR  | C23-C22-C21 | 4.59  | 125.98      | 118.94   |
| 14  | H     | 815  | CLA  | C4D-C3D-CAD | 4.59  | 111.03      | 108.47   |
| 14  | G     | 828  | CLA  | OBD-CAD-C3D | -4.59 | 120.36      | 127.98   |
| 14  | A     | 812  | CLA  | O2D-CGD-CBD | 4.59  | 119.42      | 111.27   |
| 14  | H     | 810  | CLA  | O2A-CGA-O1A | -4.58 | 112.02      | 123.59   |
| 17  | G     | 846  | BCR  | C19-C18-C17 | 4.58  | 125.98      | 118.94   |
| 14  | Z     | 812  | CLA  | CMB-C2B-C3B | 4.58  | 133.25      | 124.68   |
| 14  | G     | 804  | CLA  | O2A-C1-C2   | 4.58  | 120.68      | 108.64   |
| 14  | J     | 102  | CLA  | O2A-C1-C2   | 4.58  | 120.67      | 108.64   |
| 14  | Y     | 828  | CLA  | CMB-C2B-C3B | 4.58  | 133.25      | 124.68   |
| 14  | H     | 835  | CLA  | O2A-CGA-O1A | -4.58 | 112.04      | 123.59   |
| 14  | B     | 841  | CLA  | C1C-C2C-C3C | -4.58 | 102.14      | 106.96   |
| 17  | A     | 847  | BCR  | C33-C5-C6   | -4.58 | 119.39      | 124.53   |
| 14  | Y     | 815  | CLA  | O2A-CGA-O1A | -4.57 | 112.05      | 123.59   |
| 14  | L     | 205  | CLA  | O2D-CGD-CBD | 4.57  | 119.39      | 111.27   |
| 14  | Z     | 820  | CLA  | O2D-CGD-CBD | 4.57  | 119.38      | 111.27   |
| 14  | B     | 827  | CLA  | O2A-CGA-CBA | 4.56  | 126.23      | 111.91   |
| 17  | i     | 101  | BCR  | C23-C24-C25 | -4.56 | 114.39      | 127.20   |
| 14  | B     | 824  | CLA  | C1C-C2C-C3C | -4.56 | 102.16      | 106.96   |
| 17  | U     | 1005 | BCR  | C36-C18-C17 | -4.56 | 116.53      | 122.92   |
| 14  | H     | 812  | CLA  | O2D-CGD-CBD | 4.56  | 119.37      | 111.27   |
| 17  | L     | 203  | BCR  | C24-C23-C22 | -4.56 | 119.35      | 126.23   |
| 14  | B     | 812  | CLA  | O2A-C1-C2   | 4.56  | 120.61      | 108.64   |
| 14  | Z     | 814  | CLA  | C4D-C3D-CAD | 4.55  | 111.01      | 108.47   |
| 14  | Z     | 816  | CLA  | O2D-CGD-CBD | 4.55  | 119.36      | 111.27   |
| 14  | B     | 817  | CLA  | C1C-C2C-C3C | -4.55 | 102.17      | 106.96   |
| 17  | B     | 846  | BCR  | C24-C23-C22 | -4.55 | 119.36      | 126.23   |
| 14  | Z     | 812  | CLA  | O2A-CGA-O1A | -4.55 | 112.11      | 123.59   |
| 14  | h     | 201  | CLA  | O2A-CGA-O1A | -4.55 | 112.11      | 123.59   |
| 14  | A     | 803  | CLA  | CMC-C2C-C1C | 4.55  | 131.97      | 125.04   |
| 17  | Z     | 841  | BCR  | C37-C22-C23 | 4.55  | 125.25      | 118.08   |
| 14  | H     | 816  | CLA  | O2A-CGA-CBA | 4.55  | 126.18      | 111.91   |
| 14  | Z     | 835  | CLA  | O2D-CGD-CBD | 4.55  | 119.35      | 111.27   |
| 14  | G     | 840  | CLA  | O2A-CGA-O1A | -4.55 | 112.12      | 123.59   |
| 14  | G     | 816  | CLA  | O2A-CGA-CBA | 4.55  | 126.17      | 111.91   |
| 14  | U     | 1002 | CLA  | O2A-CGA-O1A | -4.54 | 112.13      | 123.59   |
| 14  | L     | 201  | CLA  | O2A-CGA-O1A | -4.54 | 112.14      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | d     | 201  | CLA  | O2D-CGD-CBD | 4.54  | 119.33      | 111.27   |
| 14  | Z     | 835  | CLA  | C4A-NA-C1A  | 4.54  | 108.75      | 106.71   |
| 14  | B     | 827  | CLA  | C1C-C2C-C3C | -4.54 | 102.19      | 106.96   |
| 17  | G     | 850  | BCR  | C33-C5-C6   | -4.53 | 119.44      | 124.53   |
| 14  | B     | 822  | CLA  | O2A-C1-C2   | 4.53  | 120.55      | 108.64   |
| 14  | A     | 830  | CLA  | OBD-CAD-CBD | -4.53 | 119.42      | 125.89   |
| 14  | Z     | 811  | CLA  | C4D-C3D-CAD | 4.53  | 111.00      | 108.47   |
| 14  | Y     | 818  | CLA  | C1C-C2C-C3C | -4.53 | 102.19      | 106.96   |
| 14  | B     | 802  | CLA  | O2D-CGD-CBD | 4.53  | 119.31      | 111.27   |
| 17  | U     | 1008 | BCR  | C36-C18-C17 | -4.53 | 116.58      | 122.92   |
| 14  | U     | 1006 | CLA  | C1C-C2C-C3C | -4.53 | 102.20      | 106.96   |
| 14  | A     | 802  | CLA  | OBD-CAD-C3D | -4.53 | 120.47      | 127.98   |
| 14  | Z     | 819  | CLA  | C4A-NA-C1A  | 4.53  | 108.74      | 106.71   |
| 14  | G     | 818  | CLA  | C4A-NA-C1A  | 4.53  | 108.74      | 106.71   |
| 17  | Q     | 202  | BCR  | C27-C26-C25 | -4.53 | 116.16      | 122.73   |
| 14  | G     | 842  | CLA  | O2A-CGA-O1A | -4.53 | 112.17      | 123.59   |
| 14  | Z     | 824  | CLA  | C4A-NA-C1A  | 4.52  | 108.74      | 106.71   |
| 14  | Y     | 827  | CLA  | C1C-C2C-C3C | -4.52 | 102.20      | 106.96   |
| 14  | G     | 807  | CLA  | C1C-C2C-C3C | -4.52 | 102.20      | 106.96   |
| 14  | h     | 207  | CLA  | O2D-CGD-CBD | 4.52  | 119.30      | 111.27   |
| 14  | B     | 802  | CLA  | O2A-C1-C2   | 4.52  | 120.52      | 108.64   |
| 14  | Y     | 806  | CLA  | O2A-C1-C2   | 4.52  | 120.52      | 108.64   |
| 14  | G     | 821  | CLA  | C1C-C2C-C3C | -4.52 | 102.20      | 106.96   |
| 17  | B     | 843  | BCR  | C34-C9-C10  | -4.52 | 116.59      | 122.92   |
| 17  | B     | 848  | BCR  | C24-C23-C22 | -4.52 | 119.41      | 126.23   |
| 14  | Y     | 823  | CLA  | O2A-CGA-O1A | -4.52 | 112.19      | 123.59   |
| 17  | G     | 848  | BCR  | C23-C24-C25 | -4.52 | 114.52      | 127.20   |
| 17  | i     | 101  | BCR  | C23-C22-C21 | 4.52  | 125.87      | 118.94   |
| 14  | B     | 810  | CLA  | O2A-CGA-O1A | -4.51 | 112.20      | 123.59   |
| 17  | i     | 101  | BCR  | C7-C6-C5    | -4.51 | 110.53      | 121.46   |
| 14  | G     | 814  | CLA  | C1C-C2C-C3C | -4.51 | 102.21      | 106.96   |
| 14  | Z     | 815  | CLA  | O2A-C1-C2   | 4.51  | 120.50      | 108.64   |
| 14  | B     | 839  | CLA  | C4D-C3D-CAD | 4.51  | 110.99      | 108.47   |
| 14  | B     | 840  | CLA  | C4A-NA-C1A  | 4.51  | 108.73      | 106.71   |
| 17  | L     | 208  | BCR  | C37-C22-C21 | -4.51 | 116.61      | 122.92   |
| 14  | A     | 814  | CLA  | C4D-C3D-CAD | 4.51  | 110.98      | 108.47   |
| 14  | A     | 825  | CLA  | O2A-CGA-O1A | -4.51 | 112.21      | 123.59   |
| 14  | A     | 809  | CLA  | O2D-CGD-CBD | 4.51  | 119.28      | 111.27   |
| 14  | G     | 828  | CLA  | C4A-NA-C1A  | 4.50  | 108.73      | 106.71   |
| 14  | G     | 814  | CLA  | O2A-C1-C2   | 4.50  | 120.47      | 108.64   |
| 14  | B     | 841  | CLA  | CAA-C2A-C3A | -4.50 | 100.45      | 112.78   |
| 14  | G     | 834  | CLA  | C1C-C2C-C3C | -4.50 | 102.22      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 831 | CLA  | O2D-CGD-CBD | 4.50  | 119.26      | 111.27   |
| 14  | G     | 831 | CLA  | O2A-CGA-CBA | 4.50  | 126.03      | 111.91   |
| 14  | L     | 202 | CLA  | O2A-C1-C2   | 4.50  | 120.46      | 108.64   |
| 14  | Z     | 808 | CLA  | O2A-CGA-O1A | -4.50 | 112.24      | 123.59   |
| 17  | A     | 846 | BCR  | C34-C9-C10  | -4.50 | 116.62      | 122.92   |
| 14  | B     | 826 | CLA  | OBD-CAD-C3D | -4.50 | 120.51      | 127.98   |
| 17  | L     | 208 | BCR  | C36-C18-C17 | -4.50 | 116.62      | 122.92   |
| 14  | G     | 806 | CLA  | C4D-C3D-CAD | 4.49  | 110.98      | 108.47   |
| 14  | Z     | 822 | CLA  | O2A-CGA-O1A | -4.49 | 112.26      | 123.59   |
| 14  | A     | 825 | CLA  | O2D-CGD-CBD | 4.49  | 119.25      | 111.27   |
| 14  | B     | 831 | CLA  | C4D-C3D-CAD | 4.49  | 110.97      | 108.47   |
| 14  | B     | 813 | CLA  | C4D-C3D-CAD | 4.49  | 110.97      | 108.47   |
| 17  | Y     | 851 | BCR  | C31-C1-C6   | -4.49 | 103.02      | 110.30   |
| 14  | Y     | 839 | CLA  | O2A-CGA-CBA | 4.49  | 125.98      | 111.91   |
| 14  | B     | 819 | CLA  | C1C-C2C-C3C | -4.49 | 102.24      | 106.96   |
| 14  | H     | 805 | CLA  | O2A-CGA-O1A | -4.48 | 112.27      | 123.59   |
| 14  | H     | 825 | CLA  | O2A-CGA-O1A | -4.48 | 112.27      | 123.59   |
| 14  | Y     | 819 | CLA  | C4A-NA-C1A  | 4.48  | 108.72      | 106.71   |
| 17  | B     | 851 | BCR  | C31-C1-C6   | -4.48 | 103.03      | 110.30   |
| 14  | Z     | 821 | CLA  | C4A-NA-C1A  | 4.48  | 108.72      | 106.71   |
| 14  | B     | 836 | CLA  | C4A-NA-C1A  | 4.48  | 108.72      | 106.71   |
| 17  | R     | 102 | BCR  | C7-C8-C9    | -4.48 | 119.47      | 126.23   |
| 14  | Y     | 831 | CLA  | O2A-CGA-O1A | -4.48 | 112.29      | 123.59   |
| 14  | B     | 818 | CLA  | C1C-C2C-C3C | -4.47 | 102.25      | 106.96   |
| 14  | Y     | 806 | CLA  | O2D-CGD-O1D | -4.47 | 115.09      | 123.84   |
| 17  | Z     | 846 | BCR  | C34-C9-C8   | 4.47  | 125.12      | 118.08   |
| 17  | Y     | 846 | BCR  | C34-C9-C10  | -4.47 | 116.66      | 122.92   |
| 14  | G     | 829 | CLA  | O2A-CGA-O1A | -4.47 | 112.31      | 123.59   |
| 14  | Y     | 802 | CLA  | OBD-CAD-C3D | -4.47 | 120.56      | 127.98   |
| 18  | G     | 852 | LHG  | O7-C7-C8    | 4.47  | 121.13      | 111.50   |
| 14  | G     | 828 | CLA  | O2D-CGD-CBD | 4.47  | 119.21      | 111.27   |
| 14  | G     | 811 | CLA  | C4D-C3D-CAD | 4.47  | 110.96      | 108.47   |
| 14  | G     | 819 | CLA  | O2D-CGD-O1D | -4.47 | 115.11      | 123.84   |
| 14  | Y     | 829 | CLA  | CMB-C2B-C3B | 4.47  | 133.03      | 124.68   |
| 14  | A     | 828 | CLA  | C4A-NA-C1A  | 4.46  | 108.71      | 106.71   |
| 17  | K     | 102 | BCR  | C23-C24-C25 | -4.46 | 114.67      | 127.20   |
| 14  | A     | 852 | CLA  | O2A-CGA-O1A | -4.46 | 112.34      | 123.59   |
| 14  | B     | 840 | CLA  | CAC-C3C-C4C | 4.46  | 130.59      | 124.81   |
| 14  | A     | 842 | CLA  | C1-O2A-CGA  | 4.46  | 128.14      | 116.44   |
| 14  | Z     | 835 | CLA  | C4D-C3D-CAD | 4.46  | 110.95      | 108.47   |
| 14  | A     | 832 | CLA  | O2A-C1-C2   | 4.46  | 120.34      | 108.64   |
| 14  | G     | 841 | CLA  | O2D-CGD-CBD | 4.45  | 119.18      | 111.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 812  | CLA  | O2A-CGA-CBA | 4.45  | 125.88      | 111.91   |
| 14  | A     | 836  | CLA  | C4D-C3D-CAD | 4.45  | 110.95      | 108.47   |
| 14  | A     | 816  | CLA  | O2A-C1-C2   | 4.45  | 120.33      | 108.64   |
| 17  | B     | 845  | BCR  | C40-C30-C25 | -4.45 | 103.08      | 110.30   |
| 14  | Z     | 809  | CLA  | O2D-CGD-CBD | 4.45  | 119.17      | 111.27   |
| 14  | Y     | 814  | CLA  | C1C-C2C-C3C | -4.45 | 102.28      | 106.96   |
| 14  | Y     | 818  | CLA  | O2A-CGA-CBA | 4.45  | 125.86      | 111.91   |
| 14  | G     | 829  | CLA  | C1C-C2C-C3C | -4.45 | 102.28      | 106.96   |
| 14  | A     | 819  | CLA  | O2A-C1-C2   | 4.45  | 120.32      | 108.64   |
| 14  | S     | 1103 | CLA  | O2A-CGA-CBA | 4.44  | 125.85      | 111.91   |
| 14  | B     | 805  | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |
| 14  | A     | 818  | CLA  | O2A-CGA-CBA | 4.44  | 125.85      | 111.91   |
| 14  | B     | 822  | CLA  | O2A-CGA-O1A | -4.44 | 112.38      | 123.59   |
| 14  | A     | 812  | CLA  | O2A-C1-C2   | 4.44  | 120.31      | 108.64   |
| 14  | Y     | 813  | CLA  | O2A-C1-C2   | 4.44  | 120.31      | 108.64   |
| 14  | B     | 838  | CLA  | O2A-C1-C2   | 4.44  | 120.31      | 108.64   |
| 14  | B     | 823  | CLA  | C4D-C3D-CAD | 4.44  | 110.95      | 108.47   |
| 14  | B     | 827  | CLA  | C4A-NA-C1A  | 4.44  | 108.70      | 106.71   |
| 14  | f     | 101  | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |
| 14  | H     | 833  | CLA  | O2D-CGD-CBD | 4.44  | 119.15      | 111.27   |
| 14  | G     | 837  | CLA  | CMA-C3A-C4A | 4.44  | 123.69      | 111.77   |
| 14  | G     | 812  | CLA  | O2A-C1-C2   | 4.44  | 120.29      | 108.64   |
| 14  | Y     | 826  | CLA  | C4A-NA-C1A  | 4.43  | 108.70      | 106.71   |
| 17  | G     | 854  | BCR  | C7-C8-C9    | -4.43 | 119.54      | 126.23   |
| 17  | S     | 1104 | BCR  | C34-C9-C8   | 4.43  | 125.06      | 118.08   |
| 14  | H     | 812  | CLA  | CAC-C3C-C4C | 4.43  | 130.55      | 124.81   |
| 14  | Y     | 804  | CLA  | O2A-CGA-O1A | -4.43 | 112.42      | 123.59   |
| 14  | Y     | 828  | CLA  | O2A-CGA-O1A | -4.43 | 112.42      | 123.59   |
| 14  | S     | 1102 | CLA  | O2D-CGD-CBD | 4.42  | 119.13      | 111.27   |
| 14  | L     | 201  | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 14  | Y     | 819  | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 14  | H     | 838  | CLA  | O2A-CGA-CBA | 4.42  | 125.79      | 111.91   |
| 14  | Y     | 854  | CLA  | OBD-CAD-C3D | -4.42 | 120.64      | 127.98   |
| 14  | Z     | 822  | CLA  | O2D-CGD-CBD | 4.42  | 119.12      | 111.27   |
| 14  | A     | 806  | CLA  | C4A-NA-C1A  | 4.42  | 108.69      | 106.71   |
| 14  | B     | 810  | CLA  | CMC-C2C-C1C | 4.42  | 131.77      | 125.04   |
| 14  | h     | 207  | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 14  | G     | 828  | CLA  | C1C-C2C-C3C | -4.41 | 102.31      | 106.96   |
| 17  | A     | 847  | BCR  | C34-C9-C10  | -4.41 | 116.74      | 122.92   |
| 17  | H     | 842  | BCR  | C24-C23-C22 | -4.41 | 119.57      | 126.23   |
| 14  | G     | 817  | CLA  | C4D-C3D-CAD | 4.41  | 110.93      | 108.47   |
| 13  | G     | 801  | CL0  | O2A-C1-C2   | 4.41  | 120.23      | 108.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 826  | CLA  | C4A-NA-C1A  | 4.41  | 108.69      | 106.71   |
| 14  | H     | 805  | CLA  | O2A-CGA-CBA | 4.41  | 125.73      | 111.91   |
| 14  | Z     | 806  | CLA  | C1C-C2C-C3C | -4.41 | 102.33      | 106.96   |
| 14  | H     | 825  | CLA  | O2A-C1-C2   | 4.40  | 120.21      | 108.64   |
| 14  | Z     | 815  | CLA  | C4A-NA-C1A  | 4.40  | 108.69      | 106.71   |
| 17  | G     | 854  | BCR  | C34-C9-C10  | -4.40 | 116.75      | 122.92   |
| 14  | A     | 822  | CLA  | O2A-C1-C2   | 4.40  | 120.21      | 108.64   |
| 14  | A     | 808  | CLA  | O2A-C1-C2   | 4.40  | 120.20      | 108.64   |
| 17  | A     | 849  | BCR  | C34-C9-C8   | 4.40  | 125.01      | 118.08   |
| 14  | f     | 102  | CLA  | O2A-C1-C2   | 4.40  | 120.19      | 108.64   |
| 14  | Y     | 809  | CLA  | O2D-CGD-CBD | 4.40  | 119.08      | 111.27   |
| 14  | H     | 813  | CLA  | O2A-CGA-O1A | -4.40 | 112.49      | 123.59   |
| 14  | H     | 830  | CLA  | O2A-CGA-O1A | -4.40 | 112.50      | 123.59   |
| 14  | H     | 803  | CLA  | CHB-C4A-NA  | 4.39  | 130.59      | 124.51   |
| 14  | A     | 804  | CLA  | O2A-CGA-O1A | -4.39 | 112.51      | 123.59   |
| 14  | f     | 101  | CLA  | C4A-NA-C1A  | 4.39  | 108.68      | 106.71   |
| 14  | A     | 821  | CLA  | O2A-CGA-O1A | -4.39 | 112.52      | 123.59   |
| 14  | B     | 826  | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 14  | L     | 202  | CLA  | O2D-CGD-CBD | 4.39  | 119.06      | 111.27   |
| 17  | J     | 104  | BCR  | C15-C14-C13 | -4.39 | 121.05      | 127.31   |
| 14  | B     | 835  | CLA  | C1C-C2C-C3C | -4.39 | 102.35      | 106.96   |
| 14  | G     | 824  | CLA  | O2A-CGA-CBA | 4.38  | 125.65      | 111.91   |
| 14  | B     | 841  | CLA  | O2A-C1-C2   | 4.38  | 120.14      | 108.64   |
| 17  | F     | 201  | BCR  | C34-C9-C8   | 4.38  | 124.97      | 118.08   |
| 14  | A     | 823  | CLA  | O2A-CGA-CBA | 4.37  | 125.62      | 111.91   |
| 14  | d     | 202  | CLA  | O2D-CGD-CBD | 4.37  | 119.03      | 111.27   |
| 14  | A     | 820  | CLA  | O2A-CGA-CBA | 4.37  | 125.62      | 111.91   |
| 14  | A     | 826  | CLA  | O2D-CGD-CBD | 4.37  | 119.03      | 111.27   |
| 14  | Y     | 809  | CLA  | O2A-CGA-O1A | -4.37 | 112.56      | 123.59   |
| 14  | U     | 1002 | CLA  | OBD-CAD-C3D | -4.37 | 120.73      | 127.98   |
| 14  | K     | 101  | CLA  | C4A-NA-C1A  | 4.37  | 108.67      | 106.71   |
| 14  | U     | 1002 | CLA  | O2D-CGD-CBD | 4.37  | 119.03      | 111.27   |
| 14  | h     | 201  | CLA  | CMB-C2B-C3B | 4.37  | 132.85      | 124.68   |
| 14  | B     | 814  | CLA  | C4D-C3D-CAD | 4.36  | 110.90      | 108.47   |
| 14  | Y     | 823  | CLA  | O2A-C1-C2   | 4.36  | 120.09      | 108.64   |
| 14  | B     | 812  | CLA  | O2D-CGD-CBD | 4.36  | 119.01      | 111.27   |
| 14  | Y     | 811  | CLA  | O2A-CGA-O1A | -4.36 | 112.60      | 123.59   |
| 14  | A     | 812  | CLA  | O2A-CGA-O1A | -4.35 | 112.60      | 123.59   |
| 14  | A     | 831  | CLA  | C1C-C2C-C3C | -4.35 | 102.38      | 106.96   |
| 14  | B     | 825  | CLA  | C1-O2A-CGA  | 4.35  | 127.86      | 116.44   |
| 17  | Y     | 847  | BCR  | C38-C26-C25 | -4.35 | 119.64      | 124.53   |
| 13  | Y     | 801  | CL0  | O2D-CGD-O1D | -4.35 | 115.33      | 123.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 831  | CLA  | C1C-C2C-C3C | -4.35 | 102.38      | 106.96   |
| 17  | Y     | 856  | BCR  | C24-C23-C22 | -4.35 | 119.66      | 126.23   |
| 17  | Z     | 842  | BCR  | C34-C9-C8   | 4.35  | 124.93      | 118.08   |
| 14  | Y     | 816  | CLA  | C4D-C3D-CAD | 4.35  | 110.89      | 108.47   |
| 14  | A     | 817  | CLA  | O2A-CGA-O1A | -4.35 | 112.62      | 123.59   |
| 14  | A     | 807  | CLA  | O2D-CGD-CBD | 4.34  | 118.99      | 111.27   |
| 14  | A     | 813  | CLA  | O2A-CGA-O1A | -4.34 | 112.63      | 123.59   |
| 14  | Y     | 838  | CLA  | O2A-CGA-CBA | 4.34  | 125.53      | 111.91   |
| 14  | A     | 811  | CLA  | C4D-C3D-CAD | 4.34  | 110.89      | 108.47   |
| 14  | L     | 201  | CLA  | O2A-CGA-CBA | 4.34  | 125.53      | 111.91   |
| 14  | Y     | 803  | CLA  | O2A-CGA-CBA | 4.34  | 125.53      | 111.91   |
| 14  | Y     | 817  | CLA  | O2A-C1-C2   | 4.34  | 120.04      | 108.64   |
| 14  | G     | 819  | CLA  | O2A-CGA-O1A | -4.34 | 112.64      | 123.59   |
| 14  | Z     | 804  | CLA  | CAC-C3C-C4C | 4.34  | 130.44      | 124.81   |
| 14  | Y     | 815  | CLA  | O2A-C1-C2   | 4.34  | 120.03      | 108.64   |
| 14  | G     | 817  | CLA  | O2A-CGA-O1A | -4.34 | 112.65      | 123.59   |
| 17  | L     | 203  | BCR  | C34-C9-C8   | 4.33  | 124.91      | 118.08   |
| 14  | Y     | 821  | CLA  | C1C-C2C-C3C | -4.33 | 102.40      | 106.96   |
| 14  | Z     | 832  | CLA  | C4A-NA-C1A  | 4.33  | 108.65      | 106.71   |
| 14  | A     | 829  | CLA  | O2D-CGD-CBD | 4.33  | 118.96      | 111.27   |
| 14  | Z     | 805  | CLA  | O2A-CGA-CBA | 4.33  | 125.49      | 111.91   |
| 14  | A     | 836  | CLA  | CMB-C2B-C3B | 4.33  | 132.77      | 124.68   |
| 14  | G     | 843  | CLA  | C4D-C3D-CAD | 4.33  | 110.88      | 108.47   |
| 14  | H     | 811  | CLA  | C4A-NA-C1A  | 4.32  | 108.65      | 106.71   |
| 14  | A     | 827  | CLA  | CMB-C2B-C3B | 4.32  | 132.75      | 124.68   |
| 14  | A     | 828  | CLA  | CMB-C2B-C3B | 4.32  | 132.75      | 124.68   |
| 14  | Z     | 814  | CLA  | C1C-C2C-C3C | -4.31 | 102.42      | 106.96   |
| 14  | B     | 837  | CLA  | O2A-CGA-CBA | 4.31  | 125.44      | 111.91   |
| 14  | Y     | 813  | CLA  | C1C-C2C-C3C | -4.31 | 102.42      | 106.96   |
| 14  | Y     | 824  | CLA  | O2A-CGA-CBA | 4.31  | 125.44      | 111.91   |
| 14  | G     | 804  | CLA  | O2A-CGA-CBA | 4.31  | 125.43      | 111.91   |
| 14  | Z     | 827  | CLA  | O2A-CGA-CBA | 4.31  | 125.43      | 111.91   |
| 14  | G     | 827  | CLA  | C2C-C1C-NC  | 4.31  | 114.01      | 109.97   |
| 14  | Z     | 805  | CLA  | O2A-C1-C2   | 4.31  | 119.95      | 108.64   |
| 14  | d     | 201  | CLA  | O2A-C1-C2   | 4.30  | 119.94      | 108.64   |
| 17  | H     | 840  | BCR  | C34-C9-C8   | 4.30  | 124.86      | 118.08   |
| 14  | G     | 833  | CLA  | O2A-CGA-CBA | 4.30  | 125.41      | 111.91   |
| 14  | Y     | 816  | CLA  | O2A-CGA-CBA | 4.30  | 125.41      | 111.91   |
| 14  | H     | 808  | CLA  | O2A-CGA-O1A | -4.30 | 112.74      | 123.59   |
| 17  | h     | 203  | BCR  | C34-C9-C10  | -4.30 | 116.90      | 122.92   |
| 14  | A     | 842  | CLA  | O2A-C1-C2   | 4.30  | 119.93      | 108.64   |
| 14  | U     | 1006 | CLA  | C4D-C3D-CAD | 4.30  | 110.87      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 801  | CLA  | OBD-CAD-C3D | -4.30 | 120.85      | 127.98   |
| 14  | H     | 805  | CLA  | O2D-CGD-CBD | 4.29  | 118.90      | 111.27   |
| 17  | G     | 846  | BCR  | C29-C30-C25 | -4.29 | 103.87      | 110.48   |
| 14  | Z     | 805  | CLA  | C4D-C3D-CAD | 4.29  | 110.86      | 108.47   |
| 17  | A     | 848  | BCR  | C24-C23-C22 | -4.29 | 119.75      | 126.23   |
| 14  | U     | 1002 | CLA  | O2D-CGD-O1D | -4.29 | 115.45      | 123.84   |
| 14  | A     | 804  | CLA  | CMB-C2B-C3B | 4.29  | 132.71      | 124.68   |
| 17  | G     | 847  | BCR  | C34-C9-C8   | 4.29  | 124.84      | 118.08   |
| 14  | Z     | 821  | CLA  | O2A-CGA-O1A | -4.29 | 112.77      | 123.59   |
| 14  | Y     | 813  | CLA  | C4A-NA-C1A  | 4.29  | 108.63      | 106.71   |
| 14  | H     | 827  | CLA  | O2A-CGA-O1A | -4.29 | 112.77      | 123.59   |
| 17  | e     | 101  | BCR  | C34-C9-C8   | 4.28  | 124.83      | 118.08   |
| 14  | B     | 816  | CLA  | OBD-CAD-CBD | -4.28 | 119.78      | 125.89   |
| 14  | H     | 828  | CLA  | O2A-C1-C2   | 4.28  | 119.89      | 108.64   |
| 14  | G     | 822  | CLA  | O2A-CGA-CBA | 4.28  | 125.34      | 111.91   |
| 14  | G     | 820  | CLA  | O2A-CGA-CBA | 4.28  | 125.34      | 111.91   |
| 14  | Y     | 843  | CLA  | O2A-CGA-CBA | 4.28  | 125.34      | 111.91   |
| 14  | Y     | 811  | CLA  | C4A-NA-C1A  | 4.28  | 108.63      | 106.71   |
| 14  | H     | 807  | CLA  | O1D-CGD-CBD | -4.28 | 115.73      | 124.48   |
| 14  | U     | 1003 | CLA  | O2A-C1-C2   | 4.28  | 119.88      | 108.64   |
| 14  | H     | 824  | CLA  | CMC-C2C-C1C | 4.27  | 131.55      | 125.04   |
| 17  | G     | 854  | BCR  | C37-C22-C21 | -4.27 | 116.94      | 122.92   |
| 14  | H     | 807  | CLA  | CMA-C3A-C4A | 4.27  | 123.26      | 111.77   |
| 14  | B     | 837  | CLA  | OBD-CAD-CBD | -4.27 | 119.79      | 125.89   |
| 14  | G     | 813  | CLA  | C1C-C2C-C3C | -4.27 | 102.47      | 106.96   |
| 14  | L     | 206  | CLA  | O2A-CGA-CBA | 4.27  | 125.31      | 111.91   |
| 14  | H     | 822  | CLA  | O2D-CGD-CBD | 4.27  | 118.86      | 111.27   |
| 14  | H     | 802  | CLA  | O2A-CGA-O1A | -4.27 | 112.82      | 123.59   |
| 14  | G     | 834  | CLA  | O2A-CGA-O1A | -4.27 | 112.82      | 123.59   |
| 14  | B     | 813  | CLA  | O2D-CGD-CBD | 4.27  | 118.85      | 111.27   |
| 14  | G     | 811  | CLA  | O2A-C1-C2   | 4.27  | 119.85      | 108.64   |
| 17  | A     | 848  | BCR  | C34-C9-C8   | 4.27  | 124.80      | 118.08   |
| 17  | h     | 202  | BCR  | C30-C25-C26 | -4.26 | 116.61      | 122.61   |
| 17  | R     | 102  | BCR  | C15-C14-C13 | -4.26 | 121.23      | 127.31   |
| 14  | f     | 102  | CLA  | O2A-CGA-CBA | 4.26  | 125.28      | 111.91   |
| 14  | Z     | 817  | CLA  | O2A-CGA-O1A | -4.26 | 112.84      | 123.59   |
| 14  | A     | 842  | CLA  | OBD-CAD-C3D | -4.26 | 120.91      | 127.98   |
| 17  | A     | 846  | BCR  | C23-C24-C25 | -4.26 | 115.24      | 127.20   |
| 14  | G     | 823  | CLA  | O2A-CGA-O1A | -4.26 | 112.85      | 123.59   |
| 14  | Z     | 816  | CLA  | O2A-CGA-O1A | -4.26 | 112.85      | 123.59   |
| 14  | G     | 842  | CLA  | O2A-C1-C2   | 4.26  | 119.82      | 108.64   |
| 18  | A     | 851  | LHG  | O7-C7-C8    | 4.25  | 120.67      | 111.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 835  | CLA  | C4D-C3D-CAD | 4.25  | 110.84      | 108.47   |
| 14  | Y     | 855  | CLA  | O2A-CGA-O1A | -4.25 | 112.87      | 123.59   |
| 14  | H     | 807  | CLA  | O2A-CGA-CBA | 4.25  | 125.23      | 111.91   |
| 14  | B     | 840  | CLA  | O2D-CGD-CBD | 4.25  | 118.81      | 111.27   |
| 14  | G     | 803  | CLA  | O2A-C1-C2   | 4.24  | 119.79      | 108.64   |
| 14  | Y     | 804  | CLA  | O2A-C1-C2   | 4.24  | 119.79      | 108.64   |
| 14  | B     | 818  | CLA  | CMB-C2B-C3B | 4.24  | 132.62      | 124.68   |
| 14  | A     | 824  | CLA  | C4A-NA-C1A  | 4.24  | 108.61      | 106.71   |
| 14  | B     | 809  | CLA  | O2A-CGA-CBA | 4.24  | 125.21      | 111.91   |
| 14  | A     | 818  | CLA  | C2C-C1C-NC  | 4.24  | 113.94      | 109.97   |
| 14  | H     | 826  | CLA  | C4D-C3D-CAD | 4.24  | 110.83      | 108.47   |
| 14  | Z     | 837  | CLA  | CMC-C2C-C1C | 4.24  | 131.49      | 125.04   |
| 14  | Z     | 810  | CLA  | OBD-CAD-C3D | -4.24 | 120.94      | 127.98   |
| 14  | Y     | 825  | CLA  | O2A-CGA-O1A | -4.24 | 112.90      | 123.59   |
| 14  | B     | 819  | CLA  | O2A-CGA-CBA | 4.24  | 125.20      | 111.91   |
| 14  | W     | 1701 | CLA  | O2D-CGD-CBD | 4.24  | 118.80      | 111.27   |
| 14  | Y     | 806  | CLA  | O2A-CGA-CBA | 4.24  | 125.20      | 111.91   |
| 14  | A     | 802  | CLA  | C4A-NA-C1A  | 4.24  | 108.61      | 106.71   |
| 17  | B     | 851  | BCR  | C34-C9-C8   | 4.23  | 124.75      | 118.08   |
| 14  | Z     | 816  | CLA  | O2A-CGA-CBA | 4.23  | 125.20      | 111.91   |
| 14  | G     | 839  | CLA  | O2A-C1-C2   | 4.23  | 119.76      | 108.64   |
| 17  | A     | 849  | BCR  | C31-C1-C6   | -4.23 | 103.44      | 110.30   |
| 17  | M     | 101  | BCR  | C34-C9-C8   | 4.23  | 124.74      | 118.08   |
| 14  | H     | 812  | CLA  | C4D-C3D-CAD | 4.23  | 110.83      | 108.47   |
| 14  | Z     | 818  | CLA  | OBD-CAD-C3D | -4.22 | 120.97      | 127.98   |
| 14  | Y     | 827  | CLA  | O2A-CGA-O1A | -4.22 | 112.93      | 123.59   |
| 14  | U     | 1004 | CLA  | O2A-CGA-CBA | 4.22  | 125.16      | 111.91   |
| 14  | Y     | 839  | CLA  | O2A-C1-C2   | 4.22  | 119.73      | 108.64   |
| 14  | A     | 822  | CLA  | O2A-CGA-CBA | 4.22  | 125.15      | 111.91   |
| 14  | A     | 805  | CLA  | O2D-CGD-CBD | 4.22  | 118.77      | 111.27   |
| 14  | Y     | 820  | CLA  | O2A-CGA-CBA | 4.22  | 125.14      | 111.91   |
| 17  | Z     | 846  | BCR  | C27-C26-C25 | -4.22 | 116.61      | 122.73   |
| 14  | Y     | 811  | CLA  | O2D-CGD-CBD | 4.22  | 118.76      | 111.27   |
| 14  | A     | 826  | CLA  | O2A-C1-C2   | 4.22  | 119.71      | 108.64   |
| 14  | Z     | 821  | CLA  | CMA-C3A-C4A | 4.21  | 123.10      | 111.77   |
| 14  | H     | 808  | CLA  | C1-O2A-CGA  | 4.21  | 127.50      | 116.44   |
| 14  | B     | 818  | CLA  | O2D-CGD-CBD | 4.21  | 118.76      | 111.27   |
| 14  | h     | 207  | CLA  | C1-C2-C3    | -4.21 | 118.76      | 126.04   |
| 14  | H     | 837  | CLA  | CMA-C3A-C4A | 4.21  | 123.09      | 111.77   |
| 14  | G     | 810  | CLA  | C4D-C3D-CAD | 4.21  | 110.82      | 108.47   |
| 17  | G     | 850  | BCR  | C8-C7-C6    | -4.21 | 115.37      | 127.20   |
| 14  | H     | 823  | CLA  | O2A-CGA-CBA | 4.21  | 125.13      | 111.91   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | B     | 844  | BCR  | C34-C9-C8   | 4.21  | 124.71      | 118.08   |
| 17  | L     | 203  | BCR  | C33-C5-C6   | -4.21 | 119.80      | 124.53   |
| 17  | R     | 102  | BCR  | C34-C9-C8   | 4.21  | 124.71      | 118.08   |
| 14  | Y     | 841  | CLA  | C4D-C3D-CAD | 4.21  | 110.82      | 108.47   |
| 14  | Z     | 826  | CLA  | O2A-CGA-O1A | -4.21 | 112.97      | 123.59   |
| 14  | G     | 818  | CLA  | C1C-C2C-C3C | -4.21 | 102.53      | 106.96   |
| 14  | A     | 828  | CLA  | C4D-C3D-CAD | 4.21  | 110.82      | 108.47   |
| 14  | G     | 825  | CLA  | O2A-CGA-CBA | 4.20  | 125.10      | 111.91   |
| 14  | Y     | 827  | CLA  | O2A-C1-C2   | 4.20  | 119.69      | 108.64   |
| 14  | Y     | 823  | CLA  | C4A-NA-C1A  | 4.20  | 108.60      | 106.71   |
| 14  | G     | 809  | CLA  | O2A-CGA-CBA | 4.20  | 125.10      | 111.91   |
| 14  | A     | 840  | CLA  | O2D-CGD-CBD | 4.20  | 118.73      | 111.27   |
| 14  | B     | 808  | CLA  | C6-C5-C3    | -4.20 | 102.44      | 113.45   |
| 14  | S     | 1101 | CLA  | O2A-C1-C2   | 4.20  | 119.67      | 108.64   |
| 14  | H     | 821  | CLA  | CMB-C2B-C3B | 4.20  | 132.53      | 124.68   |
| 14  | A     | 826  | CLA  | CMA-C3A-C4A | 4.20  | 123.06      | 111.77   |
| 17  | H     | 845  | BCR  | C37-C22-C23 | 4.20  | 124.69      | 118.08   |
| 14  | Y     | 824  | CLA  | C1C-C2C-C3C | -4.20 | 102.54      | 106.96   |
| 14  | Y     | 816  | CLA  | C4A-NA-C1A  | 4.20  | 108.59      | 106.71   |
| 14  | A     | 811  | CLA  | C4A-NA-C1A  | 4.20  | 108.59      | 106.71   |
| 14  | K     | 101  | CLA  | CAC-C3C-C4C | 4.20  | 130.25      | 124.81   |
| 17  | H     | 840  | BCR  | C24-C23-C22 | -4.19 | 119.90      | 126.23   |
| 14  | H     | 828  | CLA  | O2A-CGA-CBA | 4.19  | 125.07      | 111.91   |
| 17  | R     | 101  | BCR  | C37-C22-C21 | -4.19 | 117.05      | 122.92   |
| 14  | Z     | 809  | CLA  | O2A-CGA-O1A | -4.19 | 113.01      | 123.59   |
| 14  | V     | 1201 | CLA  | O2A-CGA-O1A | -4.19 | 113.01      | 123.59   |
| 14  | G     | 819  | CLA  | C4D-C3D-CAD | 4.19  | 110.81      | 108.47   |
| 14  | d     | 202  | CLA  | CMB-C2B-C3B | 4.19  | 132.51      | 124.68   |
| 17  | Y     | 847  | BCR  | C36-C18-C17 | -4.19 | 117.06      | 122.92   |
| 14  | H     | 804  | CLA  | O2A-CGA-CBA | 4.18  | 125.03      | 111.91   |
| 14  | Z     | 838  | CLA  | O2A-C1-C2   | 4.18  | 119.62      | 108.64   |
| 17  | i     | 101  | BCR  | C1-C6-C7    | 4.18  | 127.60      | 115.78   |
| 14  | B     | 824  | CLA  | CMA-C3A-C4A | 4.18  | 123.00      | 111.77   |
| 14  | A     | 824  | CLA  | O2A-CGA-CBA | 4.18  | 125.02      | 111.91   |
| 17  | H     | 848  | BCR  | C36-C18-C17 | -4.18 | 117.07      | 122.92   |
| 17  | d     | 203  | BCR  | C23-C22-C21 | 4.18  | 125.35      | 118.94   |
| 14  | G     | 832  | CLA  | C4D-C3D-CAD | 4.17  | 110.80      | 108.47   |
| 14  | G     | 841  | CLA  | O2A-CGA-O1A | -4.17 | 113.06      | 123.59   |
| 14  | B     | 804  | CLA  | O2A-CGA-CBA | 4.17  | 125.01      | 111.91   |
| 14  | Y     | 820  | CLA  | C4D-C3D-CAD | 4.17  | 110.80      | 108.47   |
| 14  | H     | 801  | CLA  | O2A-CGA-CBA | 4.17  | 125.00      | 111.91   |
| 14  | Z     | 804  | CLA  | O2D-CGD-CBD | 4.17  | 118.68      | 111.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 830  | CLA  | O2A-C1-C2   | 4.17  | 119.58      | 108.64   |
| 17  | F     | 201  | BCR  | C31-C1-C6   | -4.16 | 103.54      | 110.30   |
| 14  | Z     | 821  | CLA  | C1C-C2C-C3C | -4.16 | 102.58      | 106.96   |
| 17  | Y     | 848  | BCR  | C36-C18-C17 | -4.16 | 117.09      | 122.92   |
| 17  | d     | 203  | BCR  | C28-C27-C26 | -4.16 | 106.65      | 114.08   |
| 14  | H     | 836  | CLA  | C4D-C3D-CAD | 4.16  | 110.79      | 108.47   |
| 14  | A     | 817  | CLA  | O2A-C1-C2   | 4.16  | 119.57      | 108.64   |
| 14  | B     | 836  | CLA  | CMC-C2C-C1C | 4.16  | 131.37      | 125.04   |
| 14  | Y     | 828  | CLA  | C4A-NA-C1A  | 4.16  | 108.58      | 106.71   |
| 14  | B     | 834  | CLA  | CMB-C2B-C3B | 4.16  | 132.45      | 124.68   |
| 17  | H     | 842  | BCR  | C34-C9-C8   | 4.15  | 124.62      | 118.08   |
| 17  | Z     | 842  | BCR  | C8-C7-C6    | -4.15 | 115.54      | 127.20   |
| 17  | G     | 850  | BCR  | C24-C23-C22 | -4.15 | 119.96      | 126.23   |
| 14  | h     | 201  | CLA  | CMC-C2C-C1C | 4.15  | 131.36      | 125.04   |
| 14  | Y     | 840  | CLA  | OBD-CAD-C3D | -4.15 | 121.09      | 127.98   |
| 14  | h     | 206  | CLA  | O2A-CGA-CBA | 4.15  | 124.94      | 111.91   |
| 17  | J     | 103  | BCR  | C3-C4-C5    | -4.15 | 106.66      | 114.08   |
| 17  | F     | 201  | BCR  | C37-C22-C21 | -4.15 | 117.11      | 122.92   |
| 14  | Z     | 835  | CLA  | CMB-C2B-C3B | 4.15  | 132.44      | 124.68   |
| 14  | Y     | 837  | CLA  | O2A-C1-C2   | 4.15  | 119.54      | 108.64   |
| 14  | H     | 809  | CLA  | O2A-CGA-CBA | 4.15  | 124.93      | 111.91   |
| 17  | J     | 103  | BCR  | C37-C22-C21 | -4.15 | 117.11      | 122.92   |
| 14  | A     | 837  | CLA  | O2A-CGA-O1A | -4.15 | 113.13      | 123.59   |
| 14  | H     | 834  | CLA  | C4D-C3D-CAD | 4.14  | 110.78      | 108.47   |
| 14  | L     | 206  | CLA  | CMC-C2C-C1C | 4.14  | 131.35      | 125.04   |
| 17  | U     | 1008 | BCR  | C34-C9-C10  | -4.14 | 117.12      | 122.92   |
| 14  | H     | 833  | CLA  | C4A-NA-C1A  | 4.14  | 108.57      | 106.71   |
| 14  | B     | 817  | CLA  | O2A-CGA-CBA | 4.14  | 124.91      | 111.91   |
| 14  | G     | 827  | CLA  | C4A-NA-C1A  | 4.14  | 108.57      | 106.71   |
| 14  | B     | 825  | CLA  | CMB-C2B-C3B | 4.14  | 132.42      | 124.68   |
| 17  | R     | 102  | BCR  | C37-C22-C23 | 4.14  | 124.60      | 118.08   |
| 17  | G     | 850  | BCR  | C34-C9-C8   | 4.14  | 124.60      | 118.08   |
| 14  | G     | 803  | CLA  | C4A-NA-C1A  | 4.14  | 108.57      | 106.71   |
| 14  | Y     | 819  | CLA  | O2A-C1-C2   | 4.14  | 119.51      | 108.64   |
| 14  | A     | 816  | CLA  | O2A-CGA-CBA | 4.14  | 124.89      | 111.91   |
| 14  | Y     | 830  | CLA  | CMB-C2B-C3B | 4.14  | 132.42      | 124.68   |
| 14  | H     | 803  | CLA  | C1C-C2C-C3C | -4.14 | 102.61      | 106.96   |
| 14  | B     | 833  | CLA  | CAA-C2A-C1A | -4.14 | 98.42       | 111.97   |
| 14  | Z     | 820  | CLA  | O2A-CGA-CBA | 4.14  | 124.89      | 111.91   |
| 14  | Y     | 807  | CLA  | O2D-CGD-CBD | 4.13  | 118.61      | 111.27   |
| 14  | B     | 833  | CLA  | O2A-CGA-CBA | 4.13  | 124.88      | 111.91   |
| 17  | h     | 202  | BCR  | C38-C26-C25 | 4.13  | 129.17      | 124.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Q     | 203  | CLA  | C4D-C3D-CAD | 4.13  | 110.77      | 108.47   |
| 14  | V     | 1201 | CLA  | C1C-C2C-C3C | -4.13 | 102.61      | 106.96   |
| 14  | B     | 840  | CLA  | C1C-C2C-C3C | -4.13 | 102.61      | 106.96   |
| 14  | H     | 802  | CLA  | CMB-C2B-C3B | 4.13  | 132.40      | 124.68   |
| 14  | Y     | 818  | CLA  | OBD-CAD-C3D | -4.13 | 121.13      | 127.98   |
| 14  | Y     | 824  | CLA  | C4D-C3D-CAD | 4.13  | 110.77      | 108.47   |
| 14  | B     | 820  | CLA  | OBD-CAD-C3D | -4.13 | 121.13      | 127.98   |
| 14  | Z     | 828  | CLA  | C4D-C3D-CAD | 4.13  | 110.77      | 108.47   |
| 14  | d     | 201  | CLA  | O2A-CGA-O1A | -4.13 | 113.18      | 123.59   |
| 14  | H     | 801  | CLA  | C1-C2-C3    | -4.12 | 118.91      | 126.04   |
| 17  | B     | 844  | BCR  | C36-C18-C17 | -4.12 | 117.16      | 122.92   |
| 17  | H     | 848  | BCR  | C3-C4-C5    | -4.12 | 106.73      | 114.08   |
| 17  | i     | 101  | BCR  | C34-C9-C10  | -4.12 | 117.16      | 122.92   |
| 14  | Y     | 831  | CLA  | O2A-C1-C2   | 4.11  | 119.45      | 108.64   |
| 14  | A     | 834  | CLA  | O2D-CGD-CBD | 4.11  | 118.58      | 111.27   |
| 14  | Z     | 813  | CLA  | OBD-CAD-C3D | -4.11 | 121.15      | 127.98   |
| 14  | G     | 839  | CLA  | O2A-CGA-CBA | 4.11  | 124.82      | 111.91   |
| 14  | A     | 813  | CLA  | O2A-C1-C2   | 4.11  | 119.44      | 108.64   |
| 14  | H     | 838  | CLA  | C1C-C2C-C3C | -4.11 | 102.63      | 106.96   |
| 14  | H     | 808  | CLA  | OBD-CAD-C3D | -4.11 | 121.16      | 127.98   |
| 14  | Z     | 831  | CLA  | O2A-CGA-CBA | 4.11  | 124.81      | 111.91   |
| 14  | A     | 812  | CLA  | O2A-CGA-CBA | 4.11  | 124.81      | 111.91   |
| 14  | G     | 841  | CLA  | O2A-CGA-CBA | 4.11  | 124.80      | 111.91   |
| 14  | Y     | 834  | CLA  | O2A-C1-C2   | 4.11  | 119.44      | 108.64   |
| 14  | Z     | 833  | CLA  | O2D-CGD-CBD | 4.11  | 118.57      | 111.27   |
| 14  | Z     | 824  | CLA  | O2A-CGA-O1A | -4.10 | 113.24      | 123.59   |
| 14  | Z     | 825  | CLA  | O2A-CGA-CBA | 4.10  | 124.78      | 111.91   |
| 14  | L     | 207  | CLA  | O2A-CGA-O1A | -4.10 | 113.24      | 123.59   |
| 14  | H     | 811  | CLA  | C4D-C3D-CAD | 4.10  | 110.76      | 108.47   |
| 14  | G     | 811  | CLA  | O2A-CGA-CBA | 4.10  | 124.78      | 111.91   |
| 14  | H     | 806  | CLA  | C1C-C2C-C3C | -4.10 | 102.65      | 106.96   |
| 14  | Y     | 810  | CLA  | C4D-C3D-CAD | 4.10  | 110.76      | 108.47   |
| 14  | A     | 813  | CLA  | O2A-CGA-CBA | 4.10  | 124.77      | 111.91   |
| 17  | L     | 209  | BCR  | C23-C22-C21 | 4.10  | 125.23      | 118.94   |
| 14  | G     | 853  | CLA  | CMB-C2B-C3B | 4.10  | 132.34      | 124.68   |
| 14  | A     | 835  | CLA  | C4A-NA-C1A  | 4.09  | 108.55      | 106.71   |
| 14  | A     | 828  | CLA  | O2A-CGA-CBA | 4.09  | 124.76      | 111.91   |
| 17  | R     | 102  | BCR  | C34-C9-C10  | -4.09 | 117.19      | 122.92   |
| 17  | L     | 203  | BCR  | C40-C30-C25 | -4.09 | 103.67      | 110.30   |
| 17  | f     | 103  | BCR  | C38-C26-C25 | 4.09  | 129.12      | 124.53   |
| 14  | H     | 828  | CLA  | CMB-C2B-C3B | 4.09  | 132.33      | 124.68   |
| 17  | Y     | 848  | BCR  | C1-C6-C7    | 4.09  | 127.34      | 115.78   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 850  | LHG  | O7-C7-C8    | 4.09  | 120.31      | 111.50   |
| 14  | Z     | 802  | CLA  | O2A-CGA-O1A | -4.09 | 113.28      | 123.59   |
| 14  | H     | 813  | CLA  | O2D-CGD-CBD | 4.08  | 118.52      | 111.27   |
| 17  | h     | 202  | BCR  | C23-C24-C25 | -4.08 | 115.74      | 127.20   |
| 14  | A     | 827  | CLA  | O2A-CGA-O1A | -4.08 | 113.29      | 123.59   |
| 14  | H     | 820  | CLA  | CMB-C2B-C3B | 4.08  | 132.31      | 124.68   |
| 17  | H     | 848  | BCR  | C38-C26-C25 | -4.08 | 119.94      | 124.53   |
| 14  | Y     | 813  | CLA  | O2D-CGD-CBD | 4.08  | 118.52      | 111.27   |
| 17  | U     | 1007 | BCR  | C23-C24-C25 | -4.08 | 115.75      | 127.20   |
| 14  | Z     | 811  | CLA  | O2A-CGA-CBA | 4.08  | 124.70      | 111.91   |
| 14  | Y     | 833  | CLA  | O1D-CGD-CBD | -4.08 | 116.14      | 124.48   |
| 14  | G     | 811  | CLA  | O2D-CGD-CBD | 4.08  | 118.51      | 111.27   |
| 14  | f     | 102  | CLA  | C4A-NA-C1A  | 4.08  | 108.54      | 106.71   |
| 14  | Y     | 802  | CLA  | O2A-C1-C2   | 4.08  | 119.35      | 108.64   |
| 14  | G     | 803  | CLA  | O2D-CGD-CBD | 4.07  | 118.51      | 111.27   |
| 14  | Z     | 817  | CLA  | O2A-C1-C2   | 4.07  | 119.34      | 108.64   |
| 14  | B     | 819  | CLA  | O2A-C1-C2   | 4.07  | 119.34      | 108.64   |
| 14  | L     | 207  | CLA  | O2A-C1-C2   | 4.07  | 119.34      | 108.64   |
| 14  | A     | 824  | CLA  | C1C-C2C-C3C | -4.07 | 102.67      | 106.96   |
| 14  | G     | 816  | CLA  | O2A-C1-C2   | 4.07  | 119.33      | 108.64   |
| 14  | G     | 830  | CLA  | CED-O2D-CGD | 4.07  | 125.14      | 115.94   |
| 17  | G     | 847  | BCR  | C36-C18-C17 | -4.07 | 117.22      | 122.92   |
| 14  | Y     | 829  | CLA  | C4A-NA-C1A  | 4.07  | 108.54      | 106.71   |
| 14  | U     | 1006 | CLA  | O2A-C1-C2   | 4.07  | 119.33      | 108.64   |
| 17  | G     | 854  | BCR  | C31-C1-C6   | -4.07 | 103.70      | 110.30   |
| 14  | h     | 205  | CLA  | O2D-CGD-CBD | 4.07  | 118.50      | 111.27   |
| 14  | G     | 812  | CLA  | O2D-CGD-CBD | 4.07  | 118.49      | 111.27   |
| 14  | H     | 803  | CLA  | CAC-C3C-C4C | 4.06  | 130.08      | 124.81   |
| 14  | Y     | 840  | CLA  | O2D-CGD-O1D | -4.06 | 115.89      | 123.84   |
| 14  | A     | 814  | CLA  | CAA-C2A-C3A | -4.06 | 101.65      | 112.78   |
| 14  | H     | 824  | CLA  | O2D-CGD-O1D | -4.06 | 115.89      | 123.84   |
| 17  | S     | 1104 | BCR  | C24-C23-C22 | -4.06 | 120.10      | 126.23   |
| 14  | Z     | 814  | CLA  | O2D-CGD-O1D | -4.06 | 115.90      | 123.84   |
| 14  | L     | 202  | CLA  | OBD-CAD-C3D | -4.06 | 121.24      | 127.98   |
| 14  | Z     | 820  | CLA  | O2A-C1-C2   | 4.06  | 119.30      | 108.64   |
| 14  | G     | 840  | CLA  | C4D-C3D-CAD | 4.06  | 110.73      | 108.47   |
| 17  | e     | 101  | BCR  | C39-C30-C25 | -4.06 | 103.72      | 110.30   |
| 14  | G     | 815  | CLA  | CMB-C2B-C3B | 4.06  | 132.27      | 124.68   |
| 14  | A     | 815  | CLA  | O2A-CGA-CBA | 4.05  | 124.63      | 111.91   |
| 14  | B     | 824  | CLA  | O2A-CGA-CBA | 4.05  | 124.63      | 111.91   |
| 17  | Q     | 202  | BCR  | C33-C5-C6   | -4.05 | 119.97      | 124.53   |
| 14  | H     | 826  | CLA  | C1C-C2C-C3C | -4.05 | 102.69      | 106.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | Y     | 801  | CL0  | O2A-CGA-O1A | -4.05 | 113.36      | 123.59   |
| 17  | A     | 849  | BCR  | C37-C22-C23 | 4.05  | 124.46      | 118.08   |
| 14  | A     | 833  | CLA  | O2A-CGA-CBA | 4.05  | 124.62      | 111.91   |
| 14  | G     | 829  | CLA  | C4A-NA-C1A  | 4.05  | 108.53      | 106.71   |
| 14  | A     | 811  | CLA  | O2A-CGA-O1A | -4.05 | 113.38      | 123.59   |
| 17  | A     | 845  | BCR  | C24-C23-C22 | -4.04 | 120.12      | 126.23   |
| 14  | H     | 814  | CLA  | CMA-C3A-C4A | 4.04  | 122.64      | 111.77   |
| 14  | H     | 810  | CLA  | OBD-CAD-CBD | -4.04 | 120.12      | 125.89   |
| 14  | B     | 817  | CLA  | C4A-NA-C1A  | 4.04  | 108.52      | 106.71   |
| 14  | A     | 803  | CLA  | O2A-C1-C2   | 4.04  | 119.25      | 108.64   |
| 14  | A     | 815  | CLA  | CMB-C2B-C3B | 4.04  | 132.24      | 124.68   |
| 14  | Y     | 824  | CLA  | O2A-C1-C2   | 4.04  | 119.25      | 108.64   |
| 17  | Y     | 851  | BCR  | C1-C6-C7    | 4.04  | 127.20      | 115.78   |
| 14  | H     | 807  | CLA  | CAC-C3C-C4C | 4.04  | 130.05      | 124.81   |
| 17  | h     | 202  | BCR  | C31-C1-C6   | -4.03 | 103.75      | 110.30   |
| 14  | H     | 823  | CLA  | C4A-NA-C1A  | 4.03  | 108.52      | 106.71   |
| 14  | B     | 814  | CLA  | C4A-NA-C1A  | 4.03  | 108.52      | 106.71   |
| 14  | B     | 816  | CLA  | CMB-C2B-C3B | 4.03  | 132.22      | 124.68   |
| 14  | A     | 816  | CLA  | C4D-C3D-CAD | 4.03  | 110.72      | 108.47   |
| 14  | G     | 832  | CLA  | O2D-CGD-CBD | 4.03  | 118.43      | 111.27   |
| 17  | f     | 103  | BCR  | C37-C22-C21 | -4.03 | 117.28      | 122.92   |
| 14  | A     | 805  | CLA  | O2A-CGA-CBA | 4.03  | 124.54      | 111.91   |
| 14  | A     | 821  | CLA  | O2A-C1-C2   | 4.03  | 119.22      | 108.64   |
| 14  | Z     | 807  | CLA  | O2A-CGA-CBA | 4.02  | 124.53      | 111.91   |
| 17  | i     | 101  | BCR  | C24-C23-C22 | -4.02 | 120.16      | 126.23   |
| 14  | L     | 205  | CLA  | O2A-CGA-CBA | 4.02  | 124.53      | 111.91   |
| 14  | G     | 805  | CLA  | CMC-C2C-C1C | 4.02  | 131.16      | 125.04   |
| 14  | A     | 805  | CLA  | C4D-C3D-CAD | 4.02  | 110.71      | 108.47   |
| 17  | f     | 105  | BCR  | C34-C9-C8   | 4.02  | 124.41      | 118.08   |
| 17  | G     | 846  | BCR  | C30-C25-C26 | -4.02 | 116.95      | 122.61   |
| 14  | Z     | 812  | CLA  | C4A-NA-C1A  | 4.02  | 108.51      | 106.71   |
| 14  | A     | 808  | CLA  | O2A-CGA-CBA | 4.02  | 124.52      | 111.91   |
| 14  | A     | 809  | CLA  | O2A-CGA-O1A | -4.02 | 113.45      | 123.59   |
| 14  | G     | 832  | CLA  | O2A-CGA-CBA | 4.02  | 124.52      | 111.91   |
| 14  | H     | 806  | CLA  | O2A-CGA-O1A | -4.02 | 113.45      | 123.59   |
| 14  | H     | 829  | CLA  | C4D-C3D-CAD | 4.02  | 110.71      | 108.47   |
| 14  | Y     | 819  | CLA  | O2D-CGD-O1D | -4.02 | 115.98      | 123.84   |
| 14  | Z     | 836  | CLA  | O2D-CGD-CBD | 4.02  | 118.40      | 111.27   |
| 14  | B     | 811  | CLA  | C4A-NA-C1A  | 4.01  | 108.51      | 106.71   |
| 17  | Y     | 851  | BCR  | C34-C9-C8   | 4.01  | 124.40      | 118.08   |
| 17  | U     | 1007 | BCR  | C24-C23-C22 | -4.01 | 120.17      | 126.23   |
| 17  | B     | 847  | BCR  | C3-C4-C5    | -4.01 | 106.92      | 114.08   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 823  | CLA  | CMB-C2B-C3B | 4.01  | 132.18      | 124.68   |
| 14  | G     | 826  | CLA  | O2A-CGA-CBA | 4.01  | 124.48      | 111.91   |
| 17  | A     | 845  | BCR  | C30-C25-C26 | -4.01 | 116.97      | 122.61   |
| 14  | Z     | 813  | CLA  | C4D-C3D-CAD | 4.01  | 110.70      | 108.47   |
| 14  | H     | 813  | CLA  | O2A-CGA-CBA | 4.01  | 124.48      | 111.91   |
| 14  | Y     | 823  | CLA  | O2A-CGA-CBA | 4.01  | 124.48      | 111.91   |
| 14  | U     | 1006 | CLA  | O2A-CGA-CBA | 4.01  | 124.48      | 111.91   |
| 14  | A     | 831  | CLA  | O2A-CGA-O1A | -4.00 | 113.49      | 123.59   |
| 14  | B     | 818  | CLA  | O2A-C1-C2   | 4.00  | 119.16      | 108.64   |
| 17  | A     | 848  | BCR  | C33-C5-C6   | -4.00 | 120.03      | 124.53   |
| 14  | T     | 101  | CLA  | CAC-C3C-C4C | 4.00  | 130.00      | 124.81   |
| 14  | Z     | 829  | CLA  | C1C-C2C-C3C | -4.00 | 102.75      | 106.96   |
| 14  | A     | 824  | CLA  | C3C-C4C-NC  | 4.00  | 115.06      | 110.57   |
| 17  | Y     | 846  | BCR  | C15-C14-C13 | -4.00 | 121.60      | 127.31   |
| 14  | h     | 205  | CLA  | C1-O2A-CGA  | 4.00  | 126.93      | 116.44   |
| 17  | Y     | 850  | BCR  | C8-C7-C6    | -4.00 | 115.98      | 127.20   |
| 17  | Y     | 850  | BCR  | C37-C22-C21 | -3.99 | 117.33      | 122.92   |
| 14  | Z     | 836  | CLA  | O2A-CGA-O1A | -3.99 | 113.52      | 123.59   |
| 14  | B     | 824  | CLA  | CMB-C2B-C3B | 3.99  | 132.15      | 124.68   |
| 14  | B     | 840  | CLA  | O2A-CGA-O1A | -3.99 | 113.52      | 123.59   |
| 14  | G     | 830  | CLA  | C1-O2A-CGA  | 3.99  | 126.91      | 116.44   |
| 14  | H     | 834  | CLA  | C1C-C2C-C3C | -3.99 | 102.76      | 106.96   |
| 14  | B     | 837  | CLA  | CMB-C2B-C3B | 3.99  | 132.14      | 124.68   |
| 14  | Y     | 826  | CLA  | O2A-C1-C2   | 3.99  | 119.11      | 108.64   |
| 14  | B     | 810  | CLA  | C1-O2A-CGA  | 3.99  | 126.91      | 116.44   |
| 14  | B     | 822  | CLA  | O2A-CGA-CBA | 3.99  | 124.42      | 111.91   |
| 19  | H     | 846  | LMG  | O7-C10-C11  | 3.99  | 120.09      | 111.50   |
| 14  | B     | 819  | CLA  | C4A-NA-C1A  | 3.98  | 108.50      | 106.71   |
| 14  | G     | 807  | CLA  | O2A-CGA-CBA | 3.98  | 124.41      | 111.91   |
| 14  | Z     | 825  | CLA  | C4D-C3D-CAD | 3.98  | 110.69      | 108.47   |
| 14  | Z     | 823  | CLA  | O2A-CGA-CBA | 3.98  | 124.41      | 111.91   |
| 17  | e     | 101  | BCR  | C37-C22-C23 | 3.98  | 124.35      | 118.08   |
| 14  | B     | 803  | CLA  | O2A-CGA-CBA | 3.98  | 124.40      | 111.91   |
| 14  | Y     | 831  | CLA  | C4D-C3D-CAD | 3.98  | 110.69      | 108.47   |
| 14  | H     | 815  | CLA  | O2A-C1-C2   | 3.98  | 119.09      | 108.64   |
| 14  | H     | 809  | CLA  | O2D-CGD-CBD | 3.98  | 118.34      | 111.27   |
| 14  | Z     | 826  | CLA  | CMA-C3A-C4A | 3.98  | 122.47      | 111.77   |
| 14  | Z     | 815  | CLA  | O2A-CGA-CBA | 3.98  | 124.39      | 111.91   |
| 14  | G     | 827  | CLA  | C1C-C2C-C3C | -3.98 | 102.78      | 106.96   |
| 14  | H     | 818  | CLA  | CMB-C2B-C3B | 3.98  | 132.12      | 124.68   |
| 14  | Z     | 801  | CLA  | C4D-C3D-CAD | 3.97  | 110.69      | 108.47   |
| 14  | Y     | 802  | CLA  | C4D-C3D-CAD | 3.97  | 110.69      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 821  | CLA  | C4D-C3D-CAD | 3.97  | 110.69      | 108.47   |
| 14  | Z     | 813  | CLA  | CMB-C2B-C3B | 3.97  | 132.11      | 124.68   |
| 14  | B     | 841  | CLA  | CAA-C2A-C1A | -3.97 | 98.95       | 111.97   |
| 14  | Z     | 830  | CLA  | O2A-CGA-O1A | -3.97 | 113.56      | 123.59   |
| 14  | Y     | 841  | CLA  | O2A-CGA-O1A | -3.97 | 113.57      | 123.59   |
| 14  | Z     | 804  | CLA  | CMB-C2B-C3B | 3.97  | 132.11      | 124.68   |
| 14  | H     | 828  | CLA  | CMA-C3A-C4A | 3.97  | 122.44      | 111.77   |
| 14  | A     | 840  | CLA  | C1-O2A-CGA  | 3.97  | 126.85      | 116.44   |
| 14  | U     | 1002 | CLA  | O2A-CGA-CBA | 3.97  | 124.36      | 111.91   |
| 13  | Y     | 801  | CL0  | O2A-C1-C2   | 3.97  | 119.06      | 108.64   |
| 14  | B     | 805  | CLA  | CMB-C2B-C3B | 3.96  | 132.09      | 124.68   |
| 15  | H     | 839  | PQN  | C2M-C2-C3   | -3.96 | 117.93      | 124.40   |
| 14  | Y     | 837  | CLA  | O2A-CGA-O1A | -3.96 | 113.59      | 123.59   |
| 14  | B     | 807  | CLA  | O2A-CGA-CBA | 3.96  | 124.34      | 111.91   |
| 14  | A     | 825  | CLA  | O2A-CGA-CBA | 3.96  | 124.34      | 111.91   |
| 14  | B     | 819  | CLA  | O2D-CGD-CBD | 3.96  | 118.30      | 111.27   |
| 14  | h     | 207  | CLA  | CMB-C2B-C3B | 3.96  | 132.09      | 124.68   |
| 14  | G     | 802  | CLA  | CED-O2D-CGD | 3.96  | 124.89      | 115.94   |
| 17  | H     | 844  | BCR  | C34-C9-C10  | -3.95 | 117.39      | 122.92   |
| 17  | A     | 846  | BCR  | C24-C23-C22 | -3.95 | 120.26      | 126.23   |
| 17  | B     | 845  | BCR  | C8-C7-C6    | -3.95 | 116.11      | 127.20   |
| 14  | Y     | 811  | CLA  | O2A-CGA-CBA | 3.95  | 124.31      | 111.91   |
| 14  | U     | 1003 | CLA  | O2D-CGD-O1D | -3.95 | 116.11      | 123.84   |
| 17  | Z     | 845  | BCR  | C3-C4-C5    | -3.95 | 107.02      | 114.08   |
| 14  | Z     | 814  | CLA  | O2A-C1-C2   | 3.95  | 119.02      | 108.64   |
| 14  | A     | 806  | CLA  | CMB-C2B-C3B | 3.95  | 132.07      | 124.68   |
| 14  | Z     | 821  | CLA  | O2D-CGD-CBD | 3.95  | 118.28      | 111.27   |
| 14  | A     | 842  | CLA  | O2D-CGD-CBD | 3.94  | 118.28      | 111.27   |
| 17  | Z     | 842  | BCR  | C37-C22-C23 | 3.94  | 124.29      | 118.08   |
| 14  | h     | 205  | CLA  | CED-O2D-CGD | 3.94  | 124.86      | 115.94   |
| 17  | J     | 103  | BCR  | C24-C23-C22 | -3.94 | 120.28      | 126.23   |
| 17  | B     | 845  | BCR  | C34-C9-C8   | 3.94  | 124.29      | 118.08   |
| 14  | Y     | 823  | CLA  | C4D-C3D-CAD | 3.94  | 110.67      | 108.47   |
| 14  | Z     | 826  | CLA  | O2A-C1-C2   | 3.94  | 118.98      | 108.64   |
| 14  | A     | 830  | CLA  | O2D-CGD-O1D | -3.94 | 116.14      | 123.84   |
| 17  | Z     | 844  | BCR  | C15-C14-C13 | -3.93 | 121.66      | 127.30   |
| 14  | H     | 817  | CLA  | O2A-C1-C2   | 3.93  | 118.97      | 108.64   |
| 14  | Y     | 835  | CLA  | C4A-NA-C1A  | 3.93  | 108.47      | 106.71   |
| 14  | A     | 833  | CLA  | O2A-C1-C2   | 3.92  | 118.95      | 108.64   |
| 17  | I     | 101  | BCR  | C24-C23-C22 | -3.92 | 120.31      | 126.23   |
| 14  | Y     | 843  | CLA  | CMB-C2B-C3B | 3.92  | 132.02      | 124.68   |
| 14  | B     | 813  | CLA  | CAC-C3C-C4C | 3.92  | 129.90      | 124.81   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 828  | CLA  | C1C-C2C-C3C | -3.92 | 102.83      | 106.96   |
| 14  | H     | 817  | CLA  | C4D-C3D-CAD | 3.92  | 110.66      | 108.47   |
| 14  | G     | 809  | CLA  | O2D-CGD-CBD | 3.92  | 118.23      | 111.27   |
| 14  | B     | 808  | CLA  | O2A-CGA-O1A | -3.92 | 113.70      | 123.59   |
| 14  | U     | 1002 | CLA  | C3C-C4C-NC  | 3.92  | 114.96      | 110.57   |
| 14  | U     | 1006 | CLA  | CMA-C3A-C4A | 3.91  | 122.30      | 111.77   |
| 14  | Y     | 827  | CLA  | O2A-CGA-CBA | 3.91  | 124.19      | 111.91   |
| 14  | Y     | 829  | CLA  | C4D-C3D-CAD | 3.91  | 110.65      | 108.47   |
| 14  | Y     | 836  | CLA  | C4D-C3D-CAD | 3.91  | 110.65      | 108.47   |
| 14  | A     | 825  | CLA  | CAC-C3C-C4C | 3.91  | 129.88      | 124.81   |
| 17  | Z     | 841  | BCR  | C30-C25-C26 | -3.91 | 117.11      | 122.61   |
| 14  | L     | 207  | CLA  | O2A-CGA-CBA | 3.91  | 124.18      | 111.91   |
| 14  | G     | 838  | CLA  | CMB-C2B-C3B | 3.91  | 131.99      | 124.68   |
| 14  | B     | 829  | CLA  | O2A-C1-C2   | 3.91  | 118.91      | 108.64   |
| 14  | B     | 816  | CLA  | C4D-C3D-CAD | 3.91  | 110.65      | 108.47   |
| 17  | Y     | 848  | BCR  | C34-C9-C8   | 3.91  | 124.24      | 118.08   |
| 17  | Y     | 848  | BCR  | C24-C23-C22 | -3.91 | 120.33      | 126.23   |
| 14  | H     | 821  | CLA  | O2A-C1-C2   | 3.91  | 118.91      | 108.64   |
| 14  | G     | 809  | CLA  | C4A-NA-C1A  | 3.91  | 108.46      | 106.71   |
| 14  | H     | 821  | CLA  | O2A-CGA-CBA | 3.91  | 124.17      | 111.91   |
| 14  | Z     | 832  | CLA  | CMB-C2B-C3B | 3.91  | 131.99      | 124.68   |
| 14  | H     | 817  | CLA  | CMB-C2B-C3B | 3.91  | 131.99      | 124.68   |
| 14  | S     | 1101 | CLA  | O2A-CGA-CBA | 3.90  | 124.16      | 111.91   |
| 14  | Z     | 803  | CLA  | O1D-CGD-CBD | -3.90 | 116.50      | 124.48   |
| 14  | Y     | 821  | CLA  | C4A-NA-C1A  | 3.90  | 108.46      | 106.71   |
| 14  | F     | 202  | CLA  | CMB-C2B-C3B | 3.90  | 131.98      | 124.68   |
| 14  | H     | 838  | CLA  | OBD-CAD-C3D | -3.90 | 121.50      | 127.98   |
| 14  | Z     | 815  | CLA  | OBD-CAD-CBD | -3.90 | 120.32      | 125.89   |
| 14  | H     | 803  | CLA  | O2D-CGD-CBD | 3.90  | 118.20      | 111.27   |
| 17  | J     | 104  | BCR  | C8-C7-C6    | -3.90 | 116.25      | 127.20   |
| 18  | G     | 851  | LHG  | O7-C7-C8    | 3.90  | 119.90      | 111.50   |
| 14  | Z     | 818  | CLA  | CMB-C2B-C3B | 3.90  | 131.97      | 124.68   |
| 17  | H     | 840  | BCR  | C34-C9-C10  | -3.90 | 117.46      | 122.92   |
| 17  | Z     | 845  | BCR  | C15-C14-C13 | -3.90 | 121.75      | 127.31   |
| 14  | Y     | 809  | CLA  | C4A-NA-C1A  | 3.90  | 108.46      | 106.71   |
| 14  | B     | 838  | CLA  | OBD-CAD-C3D | -3.90 | 121.51      | 127.98   |
| 14  | Y     | 825  | CLA  | C1-O2A-CGA  | 3.90  | 126.67      | 116.44   |
| 14  | B     | 839  | CLA  | C4A-NA-C1A  | 3.89  | 108.46      | 106.71   |
| 14  | A     | 831  | CLA  | CMB-C2B-C3B | 3.89  | 131.96      | 124.68   |
| 14  | H     | 832  | CLA  | C4A-NA-C1A  | 3.89  | 108.46      | 106.71   |
| 14  | H     | 826  | CLA  | O2A-C1-C2   | 3.89  | 118.86      | 108.64   |
| 14  | G     | 806  | CLA  | O2D-CGD-O1D | -3.89 | 116.23      | 123.84   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | S     | 1104 | BCR  | C15-C14-C13 | -3.89 | 121.76      | 127.31   |
| 17  | Y     | 848  | BCR  | C23-C22-C21 | 3.89  | 124.91      | 118.94   |
| 14  | A     | 803  | CLA  | CMB-C2B-C3B | 3.89  | 131.96      | 124.68   |
| 14  | Y     | 821  | CLA  | CMC-C2C-C1C | 3.89  | 130.96      | 125.04   |
| 14  | G     | 810  | CLA  | CMB-C2B-C3B | 3.89  | 131.96      | 124.68   |
| 17  | f     | 103  | BCR  | C27-C26-C25 | -3.89 | 117.09      | 122.73   |
| 14  | G     | 837  | CLA  | C4D-C3D-CAD | 3.89  | 110.64      | 108.47   |
| 17  | H     | 841  | BCR  | C15-C14-C13 | -3.89 | 121.76      | 127.31   |
| 14  | Z     | 839  | CLA  | O2A-CGA-CBA | 3.89  | 124.11      | 111.91   |
| 14  | Y     | 817  | CLA  | O2D-CGD-CBD | 3.89  | 118.17      | 111.27   |
| 17  | e     | 101  | BCR  | C34-C9-C10  | -3.89 | 117.48      | 122.92   |
| 14  | Z     | 815  | CLA  | OBD-CAD-C3D | -3.89 | 121.53      | 127.98   |
| 14  | G     | 827  | CLA  | O2A-C1-C2   | 3.88  | 118.84      | 108.64   |
| 14  | G     | 814  | CLA  | CBA-CAA-C2A | 3.88  | 125.33      | 113.86   |
| 14  | G     | 816  | CLA  | CMA-C3A-C4A | 3.88  | 122.21      | 111.77   |
| 14  | Y     | 822  | CLA  | CMC-C2C-C1C | 3.88  | 130.95      | 125.04   |
| 14  | G     | 814  | CLA  | O1D-CGD-CBD | -3.88 | 116.54      | 124.48   |
| 14  | Y     | 813  | CLA  | C4D-C3D-CAD | 3.88  | 110.63      | 108.47   |
| 17  | f     | 105  | BCR  | C15-C14-C13 | -3.88 | 121.78      | 127.31   |
| 14  | H     | 822  | CLA  | CAA-C2A-C1A | -3.88 | 99.27       | 111.97   |
| 14  | Y     | 829  | CLA  | O2A-CGA-O1A | -3.88 | 113.81      | 123.59   |
| 14  | G     | 805  | CLA  | C4D-C3D-CAD | 3.87  | 110.63      | 108.47   |
| 14  | U     | 1003 | CLA  | CAC-C3C-C4C | 3.87  | 129.83      | 124.81   |
| 14  | Z     | 822  | CLA  | CMB-C2B-C3B | 3.87  | 131.92      | 124.68   |
| 17  | Z     | 845  | BCR  | C7-C8-C9    | -3.87 | 120.39      | 126.23   |
| 14  | H     | 827  | CLA  | C1C-C2C-C3C | -3.87 | 102.89      | 106.96   |
| 14  | H     | 823  | CLA  | CMA-C3A-C4A | 3.86  | 122.16      | 111.77   |
| 17  | B     | 843  | BCR  | C15-C14-C13 | -3.86 | 121.80      | 127.31   |
| 17  | A     | 848  | BCR  | C37-C22-C21 | -3.86 | 117.51      | 122.92   |
| 14  | Y     | 828  | CLA  | O2D-CGD-CBD | 3.86  | 118.13      | 111.27   |
| 14  | S     | 1103 | CLA  | O2D-CGD-O1D | -3.86 | 116.29      | 123.84   |
| 14  | d     | 202  | CLA  | C4A-NA-C1A  | 3.86  | 108.44      | 106.71   |
| 17  | f     | 103  | BCR  | C23-C24-C25 | -3.86 | 116.37      | 127.20   |
| 17  | R     | 101  | BCR  | C19-C18-C17 | 3.86  | 124.86      | 118.94   |
| 14  | H     | 811  | CLA  | O2D-CGD-CBD | 3.86  | 118.12      | 111.27   |
| 14  | Y     | 833  | CLA  | C1-O2A-CGA  | 3.86  | 126.56      | 116.44   |
| 17  | G     | 846  | BCR  | C28-C27-C26 | -3.85 | 107.19      | 114.08   |
| 17  | H     | 841  | BCR  | C34-C9-C10  | -3.85 | 117.52      | 122.92   |
| 14  | G     | 836  | CLA  | O2D-CGD-CBD | 3.85  | 118.11      | 111.27   |
| 14  | Z     | 802  | CLA  | CHB-C4A-NA  | 3.85  | 129.84      | 124.51   |
| 14  | Y     | 805  | CLA  | O2A-C1-C2   | 3.85  | 118.76      | 108.64   |
| 14  | h     | 201  | CLA  | O2A-C1-C2   | 3.85  | 118.76      | 108.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 809  | CLA  | O1D-CGD-CBD | -3.85 | 116.60      | 124.48   |
| 14  | Z     | 835  | CLA  | O2A-CGA-CBA | 3.85  | 123.99      | 111.91   |
| 14  | Z     | 802  | CLA  | CMB-C2B-C3B | 3.85  | 131.88      | 124.68   |
| 14  | Y     | 841  | CLA  | C4A-NA-C1A  | 3.85  | 108.44      | 106.71   |
| 14  | Y     | 837  | CLA  | C4A-NA-C1A  | 3.85  | 108.44      | 106.71   |
| 14  | A     | 814  | CLA  | O2A-CGA-CBA | 3.85  | 123.98      | 111.91   |
| 14  | H     | 831  | CLA  | CMB-C2B-C3B | 3.85  | 131.87      | 124.68   |
| 14  | G     | 828  | CLA  | O2A-CGA-CBA | 3.84  | 123.97      | 111.91   |
| 17  | e     | 101  | BCR  | C33-C5-C6   | -3.84 | 120.21      | 124.53   |
| 13  | A     | 801  | CL0  | CAC-C3C-C4C | 3.84  | 129.79      | 124.81   |
| 14  | G     | 819  | CLA  | O2A-CGA-CBA | 3.84  | 123.95      | 111.91   |
| 14  | Y     | 817  | CLA  | C4A-NA-C1A  | 3.84  | 108.43      | 106.71   |
| 14  | G     | 829  | CLA  | O2D-CGD-CBD | 3.84  | 118.09      | 111.27   |
| 14  | S     | 1101 | CLA  | O2D-CGD-O1D | -3.84 | 116.34      | 123.84   |
| 17  | J     | 104  | BCR  | C33-C5-C6   | -3.84 | 120.22      | 124.53   |
| 14  | h     | 207  | CLA  | O2A-CGA-CBA | 3.84  | 123.95      | 111.91   |
| 14  | H     | 802  | CLA  | O2A-C1-C2   | 3.83  | 118.71      | 108.64   |
| 17  | I     | 101  | BCR  | C36-C18-C17 | -3.83 | 117.56      | 122.92   |
| 14  | Y     | 808  | CLA  | O2A-CGA-CBA | 3.83  | 123.92      | 111.91   |
| 14  | B     | 816  | CLA  | O2A-CGA-CBA | 3.83  | 123.92      | 111.91   |
| 14  | Y     | 840  | CLA  | O2A-C1-C2   | 3.83  | 118.70      | 108.64   |
| 14  | G     | 838  | CLA  | O2A-C1-C2   | 3.83  | 118.69      | 108.64   |
| 14  | Y     | 828  | CLA  | O2A-CGA-CBA | 3.83  | 123.92      | 111.91   |
| 14  | G     | 810  | CLA  | O2D-CGD-O1D | -3.83 | 116.36      | 123.84   |
| 17  | H     | 845  | BCR  | C39-C30-C25 | -3.83 | 104.09      | 110.30   |
| 14  | G     | 842  | CLA  | C4A-NA-C1A  | 3.83  | 108.43      | 106.71   |
| 14  | B     | 835  | CLA  | O2D-CGD-CBD | 3.83  | 118.07      | 111.27   |
| 14  | Y     | 814  | CLA  | O2A-CGA-CBA | 3.82  | 123.91      | 111.91   |
| 14  | G     | 834  | CLA  | C4A-NA-C1A  | 3.82  | 108.42      | 106.71   |
| 17  | Q     | 204  | BCR  | C35-C13-C14 | -3.82 | 117.57      | 122.92   |
| 14  | G     | 827  | CLA  | O2A-CGA-O1A | -3.82 | 113.95      | 123.59   |
| 14  | B     | 811  | CLA  | O2D-CGD-O1D | -3.82 | 116.37      | 123.84   |
| 14  | G     | 809  | CLA  | O2A-C1-C2   | 3.82  | 118.67      | 108.64   |
| 17  | A     | 845  | BCR  | C23-C22-C21 | 3.82  | 124.80      | 118.94   |
| 14  | U     | 1004 | CLA  | C1-C2-C3    | -3.82 | 119.44      | 126.04   |
| 17  | B     | 844  | BCR  | C33-C5-C6   | -3.82 | 120.24      | 124.53   |
| 14  | Z     | 810  | CLA  | C4D-C3D-CAD | 3.81  | 110.60      | 108.47   |
| 17  | B     | 846  | BCR  | C15-C14-C13 | -3.81 | 121.83      | 127.30   |
| 17  | R     | 101  | BCR  | C34-C9-C8   | 3.81  | 124.09      | 118.08   |
| 14  | H     | 837  | CLA  | O2D-CGD-CBD | 3.81  | 118.05      | 111.27   |
| 17  | B     | 848  | BCR  | C7-C8-C9    | -3.81 | 120.47      | 126.23   |
| 17  | Y     | 856  | BCR  | C7-C8-C9    | -3.81 | 120.47      | 126.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 805  | CLA  | O2D-CGD-O1D | -3.81 | 116.39      | 123.84   |
| 14  | Y     | 830  | CLA  | CMC-C2C-C1C | 3.81  | 130.84      | 125.04   |
| 14  | B     | 835  | CLA  | C4A-NA-C1A  | 3.81  | 108.42      | 106.71   |
| 14  | G     | 808  | CLA  | O2A-CGA-CBA | 3.81  | 123.86      | 111.91   |
| 14  | Z     | 803  | CLA  | O2A-C1-C2   | 3.81  | 118.64      | 108.64   |
| 14  | H     | 833  | CLA  | CAC-C3C-C4C | 3.81  | 129.75      | 124.81   |
| 14  | Y     | 843  | CLA  | O2A-C1-C2   | 3.81  | 118.64      | 108.64   |
| 17  | G     | 848  | BCR  | C28-C27-C26 | -3.81 | 107.28      | 114.08   |
| 14  | A     | 827  | CLA  | O2D-CGD-CBD | 3.81  | 118.03      | 111.27   |
| 17  | i     | 101  | BCR  | C39-C30-C25 | -3.81 | 104.13      | 110.30   |
| 14  | G     | 823  | CLA  | O2A-C1-C2   | 3.81  | 118.64      | 108.64   |
| 17  | H     | 840  | BCR  | C3-C4-C5    | -3.80 | 107.28      | 114.08   |
| 14  | A     | 802  | CLA  | C4D-C3D-CAD | 3.80  | 110.59      | 108.47   |
| 14  | Y     | 817  | CLA  | O2A-CGA-O1A | -3.80 | 113.99      | 123.59   |
| 14  | Y     | 825  | CLA  | O2D-CGD-CBD | 3.80  | 118.02      | 111.27   |
| 14  | Y     | 828  | CLA  | C2C-C1C-NC  | 3.80  | 113.53      | 109.97   |
| 14  | H     | 810  | CLA  | C4A-NA-C1A  | 3.80  | 108.41      | 106.71   |
| 14  | A     | 829  | CLA  | C4A-NA-C1A  | 3.80  | 108.41      | 106.71   |
| 14  | A     | 842  | CLA  | CMC-C2C-C1C | 3.80  | 130.82      | 125.04   |
| 17  | Y     | 856  | BCR  | C3-C4-C5    | -3.80 | 107.30      | 114.08   |
| 14  | A     | 827  | CLA  | OBD-CAD-C3D | -3.80 | 121.68      | 127.98   |
| 14  | Y     | 811  | CLA  | C4D-C3D-CAD | 3.80  | 110.59      | 108.47   |
| 14  | Y     | 842  | CLA  | O2A-C1-C2   | 3.79  | 118.61      | 108.64   |
| 14  | S     | 1101 | CLA  | CMB-C2B-C3B | 3.79  | 131.78      | 124.68   |
| 14  | S     | 1102 | CLA  | C4D-C3D-CAD | 3.79  | 110.58      | 108.47   |
| 14  | G     | 835  | CLA  | OBD-CAD-C3D | -3.79 | 121.69      | 127.98   |
| 14  | H     | 823  | CLA  | O2A-C1-C2   | 3.79  | 118.59      | 108.64   |
| 14  | B     | 805  | CLA  | O2D-CGD-O1D | -3.78 | 116.44      | 123.84   |
| 14  | H     | 835  | CLA  | CMC-C2C-C1C | 3.78  | 130.80      | 125.04   |
| 17  | A     | 848  | BCR  | C30-C25-C26 | -3.78 | 117.29      | 122.61   |
| 14  | H     | 803  | CLA  | CED-O2D-CGD | 3.78  | 124.49      | 115.94   |
| 14  | G     | 835  | CLA  | C4A-NA-C1A  | 3.78  | 108.41      | 106.71   |
| 14  | Z     | 838  | CLA  | C1C-C2C-C3C | -3.78 | 102.98      | 106.96   |
| 14  | Y     | 837  | CLA  | CMB-C2B-C3B | 3.78  | 131.75      | 124.68   |
| 14  | B     | 811  | CLA  | OBD-CAD-C3D | -3.78 | 121.71      | 127.98   |
| 14  | Y     | 830  | CLA  | O1D-CGD-CBD | -3.78 | 116.75      | 124.48   |
| 17  | G     | 850  | BCR  | C7-C6-C5    | -3.78 | 112.31      | 121.46   |
| 14  | A     | 808  | CLA  | C6-C5-C3    | -3.78 | 103.56      | 113.45   |
| 14  | H     | 806  | CLA  | O2A-CGA-CBA | 3.78  | 123.76      | 111.91   |
| 14  | Z     | 817  | CLA  | O2D-CGD-CBD | 3.77  | 117.98      | 111.27   |
| 17  | L     | 209  | BCR  | C24-C23-C22 | -3.77 | 120.53      | 126.23   |
| 14  | A     | 809  | CLA  | O2A-CGA-CBA | 3.77  | 123.75      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 838  | CLA  | CMC-C2C-C1C | 3.77  | 130.79      | 125.04   |
| 14  | Y     | 817  | CLA  | C4D-C3D-CAD | 3.77  | 110.57      | 108.47   |
| 14  | H     | 802  | CLA  | C4-C3-C5    | 3.77  | 121.62      | 115.27   |
| 14  | G     | 834  | CLA  | CMB-C2B-C3B | 3.77  | 131.74      | 124.68   |
| 14  | B     | 823  | CLA  | O2A-C1-C2   | 3.77  | 118.55      | 108.64   |
| 14  | Y     | 831  | CLA  | O2D-CGD-O1D | -3.77 | 116.47      | 123.84   |
| 14  | d     | 201  | CLA  | O2A-CGA-CBA | 3.77  | 123.74      | 111.91   |
| 14  | Z     | 831  | CLA  | O1D-CGD-CBD | -3.77 | 116.77      | 124.48   |
| 14  | H     | 804  | CLA  | O2A-C1-C2   | 3.77  | 118.54      | 108.64   |
| 14  | Y     | 832  | CLA  | CMB-C2B-C3B | 3.77  | 131.72      | 124.68   |
| 17  | Y     | 847  | BCR  | C38-C26-C27 | 3.77  | 120.85      | 113.62   |
| 17  | H     | 842  | BCR  | C23-C24-C25 | -3.76 | 116.63      | 127.20   |
| 17  | H     | 843  | BCR  | C39-C30-C25 | -3.76 | 104.19      | 110.30   |
| 14  | Y     | 812  | CLA  | O2D-CGD-CBD | 3.76  | 117.95      | 111.27   |
| 17  | e     | 101  | BCR  | C37-C22-C21 | -3.76 | 117.65      | 122.92   |
| 17  | L     | 203  | BCR  | C15-C14-C13 | -3.76 | 121.94      | 127.31   |
| 17  | Y     | 851  | BCR  | C33-C5-C4   | 3.76  | 120.84      | 113.62   |
| 14  | Q     | 203  | CLA  | O2D-CGD-O1D | -3.76 | 116.48      | 123.84   |
| 13  | A     | 801  | CL0  | O2A-C1-C2   | 3.76  | 118.52      | 108.64   |
| 17  | T     | 102  | BCR  | C34-C9-C8   | 3.76  | 124.00      | 118.08   |
| 17  | S     | 1104 | BCR  | C3-C4-C5    | -3.76 | 107.36      | 114.08   |
| 14  | Z     | 831  | CLA  | O2A-C1-C2   | 3.76  | 118.52      | 108.64   |
| 14  | Y     | 826  | CLA  | O2A-CGA-O1A | -3.76 | 114.11      | 123.59   |
| 14  | Z     | 806  | CLA  | O1D-CGD-CBD | -3.76 | 116.80      | 124.48   |
| 14  | U     | 1003 | CLA  | CMC-C2C-C1C | 3.76  | 130.76      | 125.04   |
| 17  | Z     | 842  | BCR  | C36-C18-C17 | -3.76 | 117.66      | 122.92   |
| 14  | A     | 829  | CLA  | O2A-CGA-O1A | -3.76 | 114.11      | 123.59   |
| 14  | H     | 830  | CLA  | O1D-CGD-CBD | -3.76 | 116.80      | 124.48   |
| 14  | Z     | 831  | CLA  | CMA-C3A-C4A | 3.75  | 121.86      | 111.77   |
| 14  | Z     | 836  | CLA  | O2A-C1-C2   | 3.75  | 118.50      | 108.64   |
| 17  | G     | 850  | BCR  | C28-C27-C26 | -3.75 | 107.37      | 114.08   |
| 14  | B     | 807  | CLA  | CMB-C2B-C3B | 3.75  | 131.70      | 124.68   |
| 17  | B     | 848  | BCR  | C33-C5-C6   | -3.75 | 120.31      | 124.53   |
| 14  | Z     | 806  | CLA  | O2A-CGA-O1A | -3.75 | 114.13      | 123.59   |
| 14  | Y     | 810  | CLA  | CMB-C2B-C3B | 3.75  | 131.69      | 124.68   |
| 17  | Z     | 842  | BCR  | C37-C22-C21 | -3.75 | 117.67      | 122.92   |
| 14  | Z     | 823  | CLA  | CMB-C2B-C3B | 3.75  | 131.69      | 124.68   |
| 14  | A     | 808  | CLA  | O1D-CGD-CBD | -3.75 | 116.82      | 124.48   |
| 17  | Q     | 204  | BCR  | C34-C9-C8   | 3.75  | 123.98      | 118.08   |
| 17  | f     | 104  | BCR  | C15-C14-C13 | -3.74 | 121.97      | 127.31   |
| 14  | U     | 1003 | CLA  | C4A-NA-C1A  | 3.74  | 108.39      | 106.71   |
| 14  | h     | 206  | CLA  | CMB-C2B-C3B | 3.74  | 131.68      | 124.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 847  | BCR  | C38-C26-C25 | -3.74 | 120.33      | 124.53   |
| 17  | Z     | 846  | BCR  | C38-C26-C25 | 3.74  | 128.73      | 124.53   |
| 14  | K     | 103  | CLA  | CMA-C3A-C4A | 3.74  | 121.83      | 111.77   |
| 14  | G     | 813  | CLA  | C4A-NA-C1A  | 3.74  | 108.39      | 106.71   |
| 14  | G     | 837  | CLA  | O2D-CGD-O1D | -3.74 | 116.53      | 123.84   |
| 17  | Z     | 841  | BCR  | C3-C4-C5    | -3.74 | 107.40      | 114.08   |
| 17  | L     | 208  | BCR  | C34-C9-C10  | -3.74 | 117.69      | 122.92   |
| 14  | H     | 833  | CLA  | OBD-CAD-CBD | -3.74 | 120.56      | 125.89   |
| 14  | G     | 821  | CLA  | O2A-CGA-CBA | 3.74  | 123.64      | 111.91   |
| 14  | B     | 840  | CLA  | CMC-C2C-C1C | 3.74  | 130.73      | 125.04   |
| 14  | A     | 831  | CLA  | O2A-C1-C2   | 3.73  | 118.45      | 108.64   |
| 14  | A     | 818  | CLA  | O1D-CGD-CBD | -3.73 | 116.84      | 124.48   |
| 17  | H     | 842  | BCR  | C15-C14-C13 | -3.73 | 121.98      | 127.31   |
| 14  | Y     | 819  | CLA  | CMB-C2B-C3B | 3.73  | 131.66      | 124.68   |
| 14  | B     | 824  | CLA  | O2A-C1-C2   | 3.73  | 118.45      | 108.64   |
| 14  | A     | 805  | CLA  | CAC-C3C-C4C | 3.73  | 129.65      | 124.81   |
| 14  | G     | 817  | CLA  | C1-O2A-CGA  | 3.73  | 126.24      | 116.44   |
| 17  | Q     | 204  | BCR  | C40-C30-C25 | 3.73  | 116.35      | 110.30   |
| 14  | A     | 819  | CLA  | O2A-CGA-CBA | 3.73  | 123.61      | 111.91   |
| 17  | L     | 203  | BCR  | C3-C4-C5    | -3.73 | 107.42      | 114.08   |
| 14  | Z     | 828  | CLA  | O2D-CGD-CBD | 3.73  | 117.89      | 111.27   |
| 14  | A     | 852  | CLA  | OBD-CAD-C3D | -3.73 | 121.79      | 127.98   |
| 14  | A     | 814  | CLA  | CAA-CBA-CGA | -3.73 | 102.37      | 113.25   |
| 14  | A     | 829  | CLA  | O2A-C1-C2   | 3.73  | 118.42      | 108.64   |
| 14  | G     | 839  | CLA  | OBD-CAD-C3D | -3.72 | 121.80      | 127.98   |
| 14  | Z     | 808  | CLA  | OBD-CAD-CBD | -3.72 | 120.57      | 125.89   |
| 17  | A     | 846  | BCR  | C33-C5-C6   | -3.72 | 120.35      | 124.53   |
| 14  | H     | 815  | CLA  | O2A-CGA-CBA | 3.72  | 123.59      | 111.91   |
| 14  | B     | 817  | CLA  | C4D-C3D-CAD | 3.72  | 110.55      | 108.47   |
| 14  | H     | 837  | CLA  | C4D-C3D-CAD | 3.72  | 110.55      | 108.47   |
| 17  | Y     | 847  | BCR  | C34-C9-C8   | 3.72  | 123.94      | 118.08   |
| 14  | A     | 820  | CLA  | CMA-C3A-C4A | 3.72  | 121.77      | 111.77   |
| 14  | A     | 836  | CLA  | C4A-NA-C1A  | 3.72  | 108.38      | 106.71   |
| 17  | V     | 1202 | BCR  | C33-C5-C6   | -3.72 | 120.35      | 124.53   |
| 14  | Z     | 812  | CLA  | O2A-CGA-CBA | 3.72  | 123.57      | 111.91   |
| 14  | Z     | 822  | CLA  | OBD-CAD-C3D | -3.72 | 121.81      | 127.98   |
| 14  | Y     | 821  | CLA  | O2A-CGA-CBA | 3.71  | 123.57      | 111.91   |
| 17  | Q     | 204  | BCR  | C38-C26-C27 | 3.71  | 120.75      | 113.62   |
| 14  | Z     | 825  | CLA  | C4A-NA-C1A  | 3.71  | 108.38      | 106.71   |
| 14  | Z     | 817  | CLA  | OBD-CAD-CBD | -3.71 | 120.59      | 125.89   |
| 14  | B     | 841  | CLA  | O2A-CGA-CBA | 3.71  | 123.56      | 111.91   |
| 14  | G     | 830  | CLA  | O2A-CGA-CBA | 3.71  | 123.56      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 829  | CLA  | O2A-CGA-CBA | 3.71  | 123.56      | 111.91   |
| 14  | Y     | 814  | CLA  | C4D-C3D-CAD | 3.71  | 110.54      | 108.47   |
| 14  | G     | 840  | CLA  | O2A-C1-C2   | 3.71  | 118.39      | 108.64   |
| 17  | S     | 1104 | BCR  | C8-C7-C6    | -3.71 | 116.78      | 127.20   |
| 14  | Y     | 804  | CLA  | O2D-CGD-O1D | -3.71 | 116.58      | 123.84   |
| 14  | A     | 827  | CLA  | C4A-NA-C1A  | 3.71  | 108.37      | 106.71   |
| 14  | B     | 806  | CLA  | OBD-CAD-C3D | -3.71 | 121.82      | 127.98   |
| 14  | Z     | 829  | CLA  | CMB-C2B-C3B | 3.71  | 131.62      | 124.68   |
| 17  | T     | 102  | BCR  | C8-C7-C6    | -3.71 | 116.79      | 127.20   |
| 14  | B     | 806  | CLA  | CMC-C2C-C1C | 3.71  | 130.69      | 125.04   |
| 14  | B     | 801  | CLA  | C1-O2A-CGA  | 3.71  | 126.17      | 116.44   |
| 14  | T     | 103  | CLA  | O2D-CGD-CBD | 3.70  | 117.85      | 111.27   |
| 14  | A     | 829  | CLA  | C4D-C3D-CAD | 3.70  | 110.53      | 108.47   |
| 17  | Y     | 851  | BCR  | C4-C5-C6    | -3.70 | 117.36      | 122.73   |
| 14  | B     | 829  | CLA  | O1D-CGD-CBD | -3.70 | 116.91      | 124.48   |
| 14  | Q     | 201  | CLA  | O2A-CGA-O1A | -3.70 | 114.25      | 123.59   |
| 14  | Y     | 826  | CLA  | CMC-C2C-C1C | 3.70  | 130.67      | 125.04   |
| 14  | Z     | 807  | CLA  | CMA-C3A-C4A | 3.70  | 121.71      | 111.77   |
| 14  | B     | 817  | CLA  | OBD-CAD-C3D | -3.70 | 121.84      | 127.98   |
| 14  | Y     | 827  | CLA  | C3C-C4C-NC  | 3.70  | 114.72      | 110.57   |
| 17  | G     | 846  | BCR  | C8-C7-C6    | -3.70 | 116.82      | 127.20   |
| 14  | B     | 810  | CLA  | O2A-C1-C2   | 3.69  | 118.34      | 108.64   |
| 17  | i     | 101  | BCR  | C7-C8-C9    | -3.69 | 120.65      | 126.23   |
| 14  | G     | 829  | CLA  | C4D-C3D-CAD | 3.69  | 110.53      | 108.47   |
| 14  | A     | 828  | CLA  | O2A-C1-C2   | 3.69  | 118.34      | 108.64   |
| 17  | B     | 851  | BCR  | C3-C4-C5    | -3.69 | 107.49      | 114.08   |
| 17  | Y     | 846  | BCR  | C12-C13-C14 | 3.69  | 124.61      | 118.94   |
| 14  | H     | 811  | CLA  | CED-O2D-CGD | 3.69  | 124.28      | 115.94   |
| 17  | I     | 101  | BCR  | C23-C24-C25 | -3.69 | 116.84      | 127.20   |
| 14  | Z     | 823  | CLA  | O2A-C1-C2   | 3.69  | 118.33      | 108.64   |
| 14  | B     | 802  | CLA  | O2A-CGA-O1A | -3.69 | 114.29      | 123.59   |
| 14  | G     | 843  | CLA  | O2A-CGA-CBA | 3.69  | 123.48      | 111.91   |
| 17  | H     | 845  | BCR  | C24-C23-C22 | -3.69 | 120.67      | 126.23   |
| 14  | B     | 804  | CLA  | O2A-C1-C2   | 3.68  | 118.31      | 108.64   |
| 17  | Y     | 848  | BCR  | C38-C26-C25 | -3.68 | 120.39      | 124.53   |
| 14  | G     | 823  | CLA  | O2A-CGA-CBA | 3.68  | 123.45      | 111.91   |
| 14  | Y     | 810  | CLA  | CMC-C2C-C1C | 3.68  | 130.64      | 125.04   |
| 14  | A     | 839  | CLA  | O2A-C1-C2   | 3.68  | 118.30      | 108.64   |
| 14  | A     | 841  | CLA  | C4D-C3D-CAD | 3.68  | 110.52      | 108.47   |
| 17  | Y     | 847  | BCR  | C37-C22-C21 | -3.68 | 117.78      | 122.92   |
| 14  | H     | 807  | CLA  | C4A-NA-C1A  | 3.67  | 108.36      | 106.71   |
| 14  | A     | 836  | CLA  | O2A-C1-C2   | 3.67  | 118.29      | 108.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 826  | CLA  | O2A-C1-C2   | 3.67  | 118.29      | 108.64   |
| 14  | G     | 808  | CLA  | O2A-C1-C2   | 3.67  | 118.29      | 108.64   |
| 14  | H     | 809  | CLA  | CMC-C2C-C1C | 3.67  | 130.63      | 125.04   |
| 14  | H     | 822  | CLA  | O2A-CGA-CBA | 3.67  | 123.43      | 111.91   |
| 17  | f     | 105  | BCR  | C23-C22-C21 | 3.67  | 124.57      | 118.94   |
| 14  | A     | 833  | CLA  | O2D-CGD-CBD | 3.67  | 117.79      | 111.27   |
| 14  | B     | 804  | CLA  | CMB-C2B-C3B | 3.67  | 131.54      | 124.68   |
| 14  | Y     | 807  | CLA  | CMC-C2C-C1C | 3.67  | 130.62      | 125.04   |
| 14  | B     | 840  | CLA  | OBD-CAD-C3D | -3.67 | 121.89      | 127.98   |
| 14  | d     | 202  | CLA  | OBD-CAD-CBD | -3.66 | 120.66      | 125.89   |
| 14  | Y     | 815  | CLA  | O2D-CGD-O1D | -3.66 | 116.67      | 123.84   |
| 14  | Z     | 809  | CLA  | C4D-C3D-CAD | 3.66  | 110.51      | 108.47   |
| 14  | B     | 834  | CLA  | O1D-CGD-CBD | -3.66 | 116.99      | 124.48   |
| 14  | Y     | 804  | CLA  | O2A-CGA-CBA | 3.66  | 123.40      | 111.91   |
| 14  | A     | 810  | CLA  | C4A-NA-C1A  | 3.66  | 108.35      | 106.71   |
| 14  | A     | 821  | CLA  | CMB-C2B-C3B | 3.66  | 131.53      | 124.68   |
| 14  | Y     | 855  | CLA  | O2A-CGA-CBA | 3.66  | 123.39      | 111.91   |
| 14  | A     | 821  | CLA  | O2A-CGA-CBA | 3.66  | 123.39      | 111.91   |
| 14  | A     | 826  | CLA  | CMC-C2C-C1C | 3.66  | 130.61      | 125.04   |
| 14  | G     | 825  | CLA  | OBD-CAD-C3D | -3.66 | 121.91      | 127.98   |
| 17  | H     | 841  | BCR  | C7-C8-C9    | -3.66 | 120.71      | 126.23   |
| 14  | Y     | 814  | CLA  | C1-O2A-CGA  | 3.66  | 126.04      | 116.44   |
| 18  | A     | 850  | LHG  | O8-C23-C24  | 3.66  | 123.38      | 111.91   |
| 14  | Y     | 817  | CLA  | O2A-CGA-CBA | 3.65  | 123.38      | 111.91   |
| 14  | G     | 820  | CLA  | O2D-CGD-O1D | -3.65 | 116.69      | 123.84   |
| 14  | Y     | 841  | CLA  | O2D-CGD-CBD | 3.65  | 117.76      | 111.27   |
| 17  | h     | 203  | BCR  | C24-C23-C22 | -3.65 | 120.72      | 126.23   |
| 14  | Z     | 830  | CLA  | O2A-CGA-CBA | 3.65  | 123.37      | 111.91   |
| 17  | f     | 104  | BCR  | C39-C30-C25 | -3.65 | 104.38      | 110.30   |
| 14  | G     | 853  | CLA  | O2D-CGD-CBD | 3.65  | 117.75      | 111.27   |
| 14  | H     | 835  | CLA  | CMA-C3A-C4A | 3.65  | 121.58      | 111.77   |
| 14  | A     | 811  | CLA  | O2D-CGD-CBD | 3.65  | 117.75      | 111.27   |
| 14  | L     | 206  | CLA  | CMB-C2B-C3B | 3.65  | 131.50      | 124.68   |
| 14  | B     | 807  | CLA  | O2D-CGD-CBD | 3.65  | 117.75      | 111.27   |
| 14  | U     | 1004 | CLA  | CMB-C2B-C3B | 3.65  | 131.50      | 124.68   |
| 14  | G     | 821  | CLA  | C4A-NA-C1A  | 3.65  | 108.34      | 106.71   |
| 17  | A     | 846  | BCR  | C30-C25-C24 | 3.65  | 126.09      | 115.78   |
| 14  | L     | 205  | CLA  | C1-O2A-CGA  | 3.64  | 126.00      | 116.44   |
| 14  | Y     | 809  | CLA  | CMB-C2B-C3B | 3.64  | 131.49      | 124.68   |
| 14  | G     | 809  | CLA  | CMB-C2B-C3B | 3.64  | 131.49      | 124.68   |
| 14  | Y     | 829  | CLA  | O2D-CGD-O1D | -3.64 | 116.73      | 123.84   |
| 14  | G     | 815  | CLA  | O2A-CGA-O1A | -3.64 | 114.41      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | A     | 846 | BCR  | C23-C22-C21 | 3.64  | 124.52      | 118.94   |
| 14  | A     | 839 | CLA  | O2A-CGA-O1A | -3.64 | 114.42      | 123.59   |
| 17  | Q     | 202 | BCR  | C38-C26-C25 | 3.64  | 128.61      | 124.53   |
| 14  | H     | 802 | CLA  | O2A-CGA-CBA | 3.63  | 123.31      | 111.91   |
| 14  | B     | 814 | CLA  | O1D-CGD-CBD | -3.63 | 117.05      | 124.48   |
| 15  | G     | 844 | PQN  | C11-C12-C13 | -3.63 | 120.74      | 126.79   |
| 17  | G     | 849 | BCR  | C33-C5-C6   | -3.63 | 120.45      | 124.53   |
| 17  | I     | 101 | BCR  | C35-C13-C14 | -3.63 | 117.84      | 122.92   |
| 14  | G     | 836 | CLA  | C1-C2-C3    | -3.63 | 120.88      | 126.75   |
| 14  | h     | 201 | CLA  | C4A-NA-C1A  | 3.63  | 108.34      | 106.71   |
| 14  | A     | 804 | CLA  | O1D-CGD-CBD | -3.63 | 117.06      | 124.48   |
| 17  | Z     | 844 | BCR  | C37-C22-C21 | -3.62 | 117.85      | 122.92   |
| 14  | H     | 802 | CLA  | CHB-C4A-NA  | 3.62  | 129.52      | 124.51   |
| 14  | Y     | 807 | CLA  | O2A-CGA-CBA | 3.62  | 123.27      | 111.91   |
| 14  | Z     | 809 | CLA  | O2A-C1-C2   | 3.62  | 118.15      | 108.64   |
| 14  | Y     | 809 | CLA  | CAC-C3C-C4C | 3.62  | 129.50      | 124.81   |
| 14  | G     | 814 | CLA  | O2A-CGA-CBA | 3.62  | 123.26      | 111.91   |
| 14  | Z     | 814 | CLA  | O2A-CGA-CBA | 3.62  | 123.25      | 111.91   |
| 17  | h     | 203 | BCR  | C37-C22-C21 | -3.62 | 117.86      | 122.92   |
| 17  | G     | 854 | BCR  | C24-C23-C22 | -3.61 | 120.77      | 126.23   |
| 17  | f     | 103 | BCR  | C34-C9-C8   | 3.61  | 123.77      | 118.08   |
| 14  | B     | 812 | CLA  | O2A-CGA-CBA | 3.61  | 123.25      | 111.91   |
| 17  | G     | 850 | BCR  | C37-C22-C21 | -3.61 | 117.86      | 122.92   |
| 14  | B     | 826 | CLA  | O2A-CGA-O1A | -3.61 | 114.48      | 123.59   |
| 14  | Z     | 816 | CLA  | CMA-C3A-C4A | 3.61  | 121.48      | 111.77   |
| 14  | A     | 816 | CLA  | O2D-CGD-O1D | -3.61 | 116.78      | 123.84   |
| 14  | h     | 207 | CLA  | CMA-C3A-C4A | 3.61  | 121.47      | 111.77   |
| 14  | G     | 829 | CLA  | CMB-C2B-C3B | 3.61  | 131.43      | 124.68   |
| 14  | A     | 812 | CLA  | C4A-NA-C1A  | 3.61  | 108.33      | 106.71   |
| 14  | d     | 202 | CLA  | C4D-C3D-CAD | 3.60  | 110.48      | 108.47   |
| 17  | G     | 849 | BCR  | C34-C9-C8   | 3.60  | 123.76      | 118.08   |
| 17  | A     | 849 | BCR  | C1-C6-C7    | 3.60  | 125.97      | 115.78   |
| 17  | h     | 203 | BCR  | C38-C26-C25 | -3.60 | 120.48      | 124.53   |
| 14  | Y     | 812 | CLA  | O2A-CGA-CBA | 3.60  | 123.21      | 111.91   |
| 14  | H     | 837 | CLA  | C4A-NA-C1A  | 3.60  | 108.33      | 106.71   |
| 14  | Y     | 839 | CLA  | CMC-C2C-C1C | 3.60  | 130.52      | 125.04   |
| 14  | B     | 805 | CLA  | O2A-CGA-CBA | 3.60  | 123.21      | 111.91   |
| 14  | H     | 834 | CLA  | O2A-CGA-CBA | 3.60  | 123.20      | 111.91   |
| 13  | A     | 801 | CL0  | CMC-C2C-C1C | 3.60  | 130.52      | 125.04   |
| 14  | G     | 806 | CLA  | O2A-C1-C2   | 3.59  | 118.08      | 108.64   |
| 14  | H     | 810 | CLA  | CMA-C3A-C4A | 3.59  | 121.43      | 111.77   |
| 17  | h     | 202 | BCR  | C30-C25-C24 | 3.59  | 125.94      | 115.78   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Y     | 847  | BCR  | C39-C30-C25 | -3.59 | 104.48      | 110.30   |
| 14  | Z     | 804  | CLA  | CMC-C2C-C1C | 3.59  | 130.50      | 125.04   |
| 14  | H     | 827  | CLA  | O2A-CGA-CBA | 3.59  | 123.17      | 111.91   |
| 14  | f     | 101  | CLA  | O2D-CGD-O1D | -3.59 | 116.82      | 123.84   |
| 14  | Z     | 802  | CLA  | OBD-CAD-C3D | -3.59 | 122.03      | 127.98   |
| 14  | Y     | 839  | CLA  | C3C-C4C-NC  | 3.59  | 114.59      | 110.57   |
| 17  | Z     | 845  | BCR  | C33-C5-C4   | 3.59  | 120.50      | 113.62   |
| 14  | Y     | 825  | CLA  | O2A-CGA-CBA | 3.58  | 123.16      | 111.91   |
| 14  | Y     | 803  | CLA  | C4A-NA-C1A  | 3.58  | 108.32      | 106.71   |
| 17  | Z     | 841  | BCR  | C8-C7-C6    | -3.58 | 117.14      | 127.20   |
| 14  | J     | 102  | CLA  | CMC-C2C-C1C | 3.58  | 130.49      | 125.04   |
| 14  | Z     | 812  | CLA  | C4D-C3D-CAD | 3.58  | 110.47      | 108.47   |
| 14  | B     | 826  | CLA  | CMB-C2B-C3B | 3.58  | 131.38      | 124.68   |
| 14  | H     | 803  | CLA  | O2A-CGA-CBA | 3.58  | 123.14      | 111.91   |
| 14  | Y     | 809  | CLA  | O2A-CGA-CBA | 3.58  | 123.14      | 111.91   |
| 14  | Z     | 822  | CLA  | CMA-C3A-C4A | 3.58  | 121.39      | 111.77   |
| 14  | G     | 807  | CLA  | CMC-C2C-C1C | 3.58  | 130.49      | 125.04   |
| 14  | B     | 829  | CLA  | CMB-C2B-C3B | 3.58  | 131.37      | 124.68   |
| 14  | H     | 807  | CLA  | OBD-CAD-CBD | -3.58 | 120.78      | 125.89   |
| 14  | G     | 853  | CLA  | C4D-C3D-CAD | 3.58  | 110.47      | 108.47   |
| 17  | G     | 850  | BCR  | C1-C6-C7    | 3.58  | 125.90      | 115.78   |
| 14  | A     | 802  | CLA  | CGD-CBD-CAD | -3.58 | 99.15       | 110.73   |
| 17  | A     | 849  | BCR  | C7-C6-C5    | -3.57 | 112.81      | 121.46   |
| 14  | Y     | 803  | CLA  | O2D-CGD-O1D | -3.57 | 116.85      | 123.84   |
| 14  | Y     | 815  | CLA  | CMB-C2B-C3B | 3.57  | 131.36      | 124.68   |
| 14  | G     | 803  | CLA  | C4D-C3D-CAD | 3.57  | 110.46      | 108.47   |
| 14  | H     | 820  | CLA  | CED-O2D-CGD | 3.57  | 124.02      | 115.94   |
| 17  | A     | 845  | BCR  | C36-C18-C17 | -3.57 | 117.92      | 122.92   |
| 14  | G     | 803  | CLA  | O2A-CGA-CBA | 3.57  | 123.11      | 111.91   |
| 14  | Z     | 803  | CLA  | C4D-C3D-CAD | 3.57  | 110.46      | 108.47   |
| 17  | Y     | 846  | BCR  | C37-C22-C21 | -3.57 | 117.92      | 122.92   |
| 17  | U     | 1007 | BCR  | C34-C9-C10  | -3.57 | 117.92      | 122.92   |
| 14  | G     | 812  | CLA  | O2A-CGA-CBA | 3.57  | 123.11      | 111.91   |
| 14  | B     | 818  | CLA  | CAC-C3C-C4C | 3.57  | 129.44      | 124.81   |
| 14  | A     | 811  | CLA  | O2A-CGA-CBA | 3.57  | 123.10      | 111.91   |
| 14  | G     | 842  | CLA  | O2A-CGA-CBA | 3.57  | 123.10      | 111.91   |
| 17  | L     | 209  | BCR  | C27-C26-C25 | -3.57 | 117.55      | 122.73   |
| 14  | Z     | 816  | CLA  | C4D-C3D-CAD | 3.57  | 110.46      | 108.47   |
| 14  | V     | 1201 | CLA  | CMB-C2B-C3B | 3.56  | 131.35      | 124.68   |
| 14  | B     | 823  | CLA  | CMB-C2B-C3B | 3.56  | 131.35      | 124.68   |
| 17  | Y     | 849  | BCR  | C30-C25-C26 | -3.56 | 117.59      | 122.61   |
| 14  | H     | 813  | CLA  | C1-O2A-CGA  | 3.56  | 125.79      | 116.44   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 840  | CLA  | OBD-CAD-CBD | -3.56 | 120.80      | 125.89   |
| 14  | Z     | 834  | CLA  | O2D-CGD-O1D | -3.56 | 116.87      | 123.84   |
| 14  | A     | 811  | CLA  | O2A-C1-C2   | 3.56  | 117.99      | 108.64   |
| 14  | Y     | 842  | CLA  | C1-O2A-CGA  | 3.56  | 125.79      | 116.44   |
| 14  | A     | 805  | CLA  | O2D-CGD-O1D | -3.56 | 116.88      | 123.84   |
| 14  | A     | 823  | CLA  | CMB-C2B-C3B | 3.56  | 131.34      | 124.68   |
| 14  | Z     | 822  | CLA  | O2A-CGA-CBA | 3.56  | 123.08      | 111.91   |
| 17  | A     | 846  | BCR  | C34-C9-C8   | 3.56  | 123.69      | 118.08   |
| 14  | B     | 811  | CLA  | OBD-CAD-CBD | -3.56 | 120.81      | 125.89   |
| 14  | Y     | 812  | CLA  | C4-C3-C5    | 3.56  | 121.25      | 115.27   |
| 14  | H     | 806  | CLA  | O2A-C1-C2   | 3.56  | 117.98      | 108.64   |
| 14  | G     | 842  | CLA  | C4-C3-C5    | 3.55  | 121.25      | 115.27   |
| 14  | Z     | 809  | CLA  | CMA-C3A-C4A | 3.55  | 121.33      | 111.77   |
| 14  | A     | 839  | CLA  | O2A-CGA-CBA | 3.55  | 123.06      | 111.91   |
| 14  | Y     | 818  | CLA  | O1D-CGD-CBD | -3.55 | 117.21      | 124.48   |
| 14  | Y     | 813  | CLA  | CMB-C2B-C3B | 3.55  | 131.32      | 124.68   |
| 18  | H     | 847  | LHG  | O7-C7-C8    | 3.55  | 119.16      | 111.50   |
| 14  | G     | 818  | CLA  | CMB-C2B-C3B | 3.55  | 131.32      | 124.68   |
| 17  | T     | 102  | BCR  | C37-C22-C21 | -3.55 | 117.95      | 122.92   |
| 14  | Y     | 837  | CLA  | O2A-CGA-CBA | 3.55  | 123.05      | 111.91   |
| 17  | L     | 203  | BCR  | C39-C30-C25 | 3.55  | 116.06      | 110.30   |
| 14  | Y     | 815  | CLA  | O2A-CGA-CBA | 3.55  | 123.04      | 111.91   |
| 17  | L     | 209  | BCR  | C36-C18-C19 | -3.55 | 112.49      | 118.08   |
| 14  | A     | 828  | CLA  | O2D-CGD-CBD | 3.55  | 117.57      | 111.27   |
| 14  | L     | 201  | CLA  | C4D-C3D-CAD | 3.54  | 110.45      | 108.47   |
| 14  | G     | 833  | CLA  | C4D-C3D-CAD | 3.54  | 110.45      | 108.47   |
| 14  | G     | 827  | CLA  | O2A-CGA-CBA | 3.54  | 123.03      | 111.91   |
| 14  | B     | 806  | CLA  | OBD-CAD-CBD | -3.54 | 120.83      | 125.89   |
| 14  | A     | 818  | CLA  | CMB-C2B-C3B | 3.54  | 131.31      | 124.68   |
| 14  | B     | 836  | CLA  | O2D-CGD-O1D | -3.54 | 116.91      | 123.84   |
| 14  | Y     | 814  | CLA  | CMA-C3A-C4A | 3.54  | 121.29      | 111.77   |
| 14  | G     | 815  | CLA  | O2D-CGD-O1D | -3.54 | 116.92      | 123.84   |
| 14  | A     | 841  | CLA  | CMA-C3A-C4A | 3.54  | 121.29      | 111.77   |
| 14  | Y     | 832  | CLA  | CED-O2D-CGD | 3.54  | 123.94      | 115.94   |
| 14  | Y     | 808  | CLA  | CMB-C2B-C3B | 3.54  | 131.30      | 124.68   |
| 17  | G     | 848  | BCR  | C7-C8-C9    | -3.54 | 120.89      | 126.23   |
| 17  | U     | 1008 | BCR  | C3-C4-C5    | -3.54 | 107.76      | 114.08   |
| 14  | A     | 837  | CLA  | CMA-C3A-C4A | 3.54  | 121.28      | 111.77   |
| 17  | A     | 845  | BCR  | C31-C1-C6   | -3.54 | 104.56      | 110.30   |
| 14  | B     | 814  | CLA  | O2A-CGA-CBA | 3.53  | 123.00      | 111.91   |
| 14  | Y     | 835  | CLA  | CMC-C2C-C1C | 3.53  | 130.42      | 125.04   |
| 17  | F     | 203  | BCR  | C34-C9-C8   | 3.53  | 123.64      | 118.08   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | Z     | 801 | CLA  | C1-O2A-CGA  | 3.53  | 125.71      | 116.44   |
| 14  | Z     | 824 | CLA  | O2A-C1-C2   | 3.53  | 117.92      | 108.64   |
| 14  | g     | 102 | CLA  | CMB-C2B-C3B | 3.53  | 131.28      | 124.68   |
| 14  | Y     | 820 | CLA  | O2A-C1-C2   | 3.53  | 117.91      | 108.64   |
| 14  | Z     | 838 | CLA  | C3C-C4C-NC  | 3.53  | 114.53      | 110.57   |
| 18  | Y     | 852 | LHG  | O8-C23-C24  | 3.53  | 122.98      | 111.91   |
| 14  | Y     | 834 | CLA  | O2A-CGA-O1A | -3.53 | 114.69      | 123.59   |
| 14  | A     | 822 | CLA  | CMA-C3A-C4A | 3.52  | 121.25      | 111.77   |
| 14  | H     | 837 | CLA  | CAC-C3C-C4C | 3.52  | 129.38      | 124.81   |
| 14  | Z     | 819 | CLA  | CMC-C2C-C1C | 3.52  | 130.41      | 125.04   |
| 14  | B     | 826 | CLA  | O2A-C1-C2   | 3.52  | 117.89      | 108.64   |
| 14  | d     | 202 | CLA  | CMA-C3A-C4A | 3.52  | 121.24      | 111.77   |
| 14  | Y     | 855 | CLA  | C4D-C3D-CAD | 3.52  | 110.43      | 108.47   |
| 14  | B     | 819 | CLA  | CMB-C2B-C3B | 3.52  | 131.27      | 124.68   |
| 14  | A     | 824 | CLA  | O2A-C1-C2   | 3.52  | 117.89      | 108.64   |
| 14  | Z     | 812 | CLA  | CMC-C2C-C1C | 3.52  | 130.40      | 125.04   |
| 14  | B     | 835 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 17  | A     | 849 | BCR  | C37-C22-C21 | -3.52 | 118.00      | 122.92   |
| 14  | Y     | 822 | CLA  | O2D-CGD-O1D | -3.52 | 116.96      | 123.84   |
| 14  | G     | 813 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 14  | G     | 816 | CLA  | CAC-C3C-C4C | 3.52  | 129.37      | 124.81   |
| 14  | G     | 812 | CLA  | C4A-NA-C1A  | 3.51  | 108.29      | 106.71   |
| 14  | H     | 816 | CLA  | CMA-C3A-C4A | 3.51  | 121.22      | 111.77   |
| 14  | J     | 101 | CLA  | O2D-CGD-O1D | -3.51 | 116.97      | 123.84   |
| 14  | A     | 840 | CLA  | O2A-CGA-O1A | -3.51 | 114.73      | 123.59   |
| 14  | A     | 803 | CLA  | CAC-C3C-C4C | 3.51  | 129.37      | 124.81   |
| 14  | Y     | 827 | CLA  | C1-O2A-CGA  | 3.51  | 125.66      | 116.44   |
| 14  | f     | 101 | CLA  | OBD-CAD-C3D | -3.51 | 122.15      | 127.98   |
| 17  | h     | 203 | BCR  | C33-C5-C6   | -3.51 | 120.59      | 124.53   |
| 14  | Z     | 832 | CLA  | CED-O2D-CGD | 3.51  | 123.87      | 115.94   |
| 17  | i     | 101 | BCR  | C15-C14-C13 | -3.51 | 122.30      | 127.31   |
| 14  | Z     | 811 | CLA  | O2A-C1-C2   | 3.51  | 117.86      | 108.64   |
| 17  | B     | 848 | BCR  | C34-C9-C8   | 3.51  | 123.60      | 118.08   |
| 17  | I     | 101 | BCR  | C4-C5-C6    | -3.51 | 117.64      | 122.73   |
| 17  | H     | 841 | BCR  | C33-C5-C6   | -3.51 | 120.59      | 124.53   |
| 14  | h     | 207 | CLA  | C4D-C3D-CAD | 3.51  | 110.43      | 108.47   |
| 14  | Y     | 827 | CLA  | CMA-C3A-C4A | 3.51  | 121.20      | 111.77   |
| 14  | Y     | 855 | CLA  | C16-C15-C13 | -3.51 | 104.59      | 115.92   |
| 14  | Z     | 838 | CLA  | C4D-C3D-CAD | 3.50  | 110.42      | 108.47   |
| 14  | h     | 201 | CLA  | O2A-CGA-CBA | 3.50  | 122.90      | 111.91   |
| 14  | Z     | 816 | CLA  | C1-O2A-CGA  | 3.50  | 125.63      | 116.44   |
| 14  | G     | 810 | CLA  | CMA-C3A-C4A | 3.50  | 121.19      | 111.77   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 804  | CLA  | CAC-C3C-C4C | 3.50  | 129.35      | 124.81   |
| 14  | Z     | 806  | CLA  | CED-O2D-CGD | 3.50  | 123.86      | 115.94   |
| 14  | B     | 833  | CLA  | O1D-CGD-CBD | -3.50 | 117.32      | 124.48   |
| 14  | G     | 817  | CLA  | O2A-CGA-CBA | 3.50  | 122.89      | 111.91   |
| 14  | B     | 820  | CLA  | CMB-C2B-C3B | 3.50  | 131.22      | 124.68   |
| 17  | U     | 1008 | BCR  | C8-C7-C6    | -3.50 | 117.38      | 127.20   |
| 17  | Z     | 845  | BCR  | C33-C5-C6   | -3.50 | 120.60      | 124.53   |
| 17  | J     | 104  | BCR  | C37-C22-C21 | -3.50 | 118.03      | 122.92   |
| 17  | G     | 854  | BCR  | C28-C27-C26 | -3.49 | 107.84      | 114.08   |
| 17  | Y     | 849  | BCR  | C30-C25-C24 | 3.49  | 125.66      | 115.78   |
| 14  | g     | 101  | CLA  | CAC-C3C-C4C | 3.49  | 129.34      | 124.81   |
| 17  | J     | 104  | BCR  | C40-C30-C25 | 3.49  | 115.96      | 110.30   |
| 14  | Y     | 804  | CLA  | CMC-C2C-C1C | 3.49  | 130.36      | 125.04   |
| 14  | H     | 838  | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 14  | B     | 828  | CLA  | O2D-CGD-CBD | 3.49  | 117.47      | 111.27   |
| 14  | B     | 813  | CLA  | OBD-CAD-C3D | -3.49 | 122.19      | 127.98   |
| 17  | G     | 848  | BCR  | C8-C7-C6    | -3.49 | 117.41      | 127.20   |
| 14  | H     | 818  | CLA  | C3C-C4C-NC  | 3.48  | 114.48      | 110.57   |
| 14  | A     | 818  | CLA  | C1-O2A-CGA  | 3.48  | 125.58      | 116.44   |
| 14  | H     | 813  | CLA  | CMB-C2B-C3B | 3.48  | 131.19      | 124.68   |
| 14  | A     | 817  | CLA  | O2A-CGA-CBA | 3.48  | 122.83      | 111.91   |
| 17  | Y     | 851  | BCR  | C7-C6-C5    | -3.48 | 113.03      | 121.46   |
| 14  | G     | 809  | CLA  | CAC-C3C-C4C | 3.48  | 129.32      | 124.81   |
| 17  | V     | 1202 | BCR  | C7-C8-C9    | -3.48 | 120.98      | 126.23   |
| 17  | e     | 101  | BCR  | C2-C1-C6    | -3.48 | 105.12      | 110.48   |
| 17  | F     | 201  | BCR  | C7-C8-C9    | -3.48 | 120.98      | 126.23   |
| 14  | Y     | 816  | CLA  | O2A-C1-C2   | 3.48  | 117.78      | 108.64   |
| 14  | B     | 830  | CLA  | O1D-CGD-CBD | -3.48 | 117.37      | 124.48   |
| 14  | Y     | 811  | CLA  | CMB-C2B-C3B | 3.48  | 131.18      | 124.68   |
| 14  | B     | 803  | CLA  | CHB-C4A-NA  | 3.48  | 129.32      | 124.51   |
| 14  | Y     | 824  | CLA  | C3C-C4C-NC  | 3.47  | 114.47      | 110.57   |
| 14  | G     | 828  | CLA  | C3C-C4C-NC  | 3.47  | 114.46      | 110.57   |
| 17  | J     | 103  | BCR  | C34-C9-C10  | -3.47 | 118.06      | 122.92   |
| 17  | F     | 203  | BCR  | C23-C24-C25 | -3.47 | 117.45      | 127.20   |
| 14  | A     | 820  | CLA  | C4-C3-C5    | 3.47  | 121.11      | 115.27   |
| 14  | B     | 804  | CLA  | C1C-C2C-C3C | -3.47 | 103.31      | 106.96   |
| 17  | G     | 846  | BCR  | C34-C9-C8   | 3.47  | 123.54      | 118.08   |
| 14  | Y     | 816  | CLA  | CMA-C3A-C4A | 3.47  | 121.09      | 111.77   |
| 14  | B     | 801  | CLA  | CHB-C4A-NA  | 3.47  | 129.30      | 124.51   |
| 17  | H     | 845  | BCR  | C23-C24-C25 | -3.46 | 117.47      | 127.20   |
| 17  | K     | 102  | BCR  | C15-C14-C13 | -3.46 | 122.37      | 127.31   |
| 17  | Y     | 849  | BCR  | C24-C23-C22 | -3.46 | 121.01      | 126.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 802 | CLA  | CGD-CBD-CAD | 3.46  | 121.93      | 110.73   |
| 14  | A     | 830 | CLA  | C4D-C3D-CAD | 3.46  | 110.40      | 108.47   |
| 14  | G     | 831 | CLA  | O2A-C1-C2   | 3.46  | 117.72      | 108.64   |
| 14  | H     | 806 | CLA  | C3C-C4C-NC  | 3.46  | 114.45      | 110.57   |
| 14  | Q     | 201 | CLA  | OBD-CAD-C3D | -3.46 | 122.24      | 127.98   |
| 14  | h     | 207 | CLA  | OBD-CAD-C3D | -3.46 | 122.24      | 127.98   |
| 17  | Y     | 846 | BCR  | C34-C9-C8   | 3.46  | 123.52      | 118.08   |
| 17  | A     | 847 | BCR  | C30-C25-C26 | -3.45 | 117.75      | 122.61   |
| 14  | H     | 829 | CLA  | O2D-CGD-O1D | -3.45 | 117.08      | 123.84   |
| 13  | Y     | 801 | CL0  | CED-O2D-CGD | 3.45  | 123.75      | 115.94   |
| 17  | Z     | 842 | BCR  | C39-C30-C25 | -3.45 | 104.70      | 110.30   |
| 14  | B     | 813 | CLA  | C1-C2-C3    | -3.45 | 120.08      | 126.04   |
| 14  | G     | 814 | CLA  | CAC-C3C-C4C | 3.45  | 129.29      | 124.81   |
| 14  | B     | 816 | CLA  | OBD-CAD-C3D | -3.45 | 122.25      | 127.98   |
| 14  | L     | 206 | CLA  | O2A-C1-C2   | 3.45  | 117.70      | 108.64   |
| 14  | A     | 811 | CLA  | CMA-C3A-C4A | 3.45  | 121.05      | 111.77   |
| 14  | Y     | 808 | CLA  | CMA-C3A-C4A | 3.45  | 121.04      | 111.77   |
| 14  | Y     | 840 | CLA  | CMB-C2B-C3B | 3.45  | 131.12      | 124.68   |
| 14  | A     | 803 | CLA  | O2A-CGA-CBA | 3.45  | 122.72      | 111.91   |
| 14  | Y     | 833 | CLA  | O2A-CGA-O1A | -3.45 | 114.90      | 123.59   |
| 14  | L     | 207 | CLA  | C4D-C3D-CAD | 3.44  | 110.39      | 108.47   |
| 17  | H     | 845 | BCR  | C34-C9-C8   | 3.44  | 123.50      | 118.08   |
| 17  | B     | 848 | BCR  | C15-C14-C13 | -3.44 | 122.40      | 127.31   |
| 14  | A     | 824 | CLA  | OBD-CAD-C3D | -3.44 | 122.27      | 127.98   |
| 14  | A     | 808 | CLA  | CMC-C2C-C1C | 3.44  | 130.28      | 125.04   |
| 17  | B     | 844 | BCR  | C23-C22-C21 | -3.44 | 113.66      | 118.94   |
| 14  | B     | 819 | CLA  | C3C-C4C-NC  | 3.44  | 114.43      | 110.57   |
| 14  | Y     | 834 | CLA  | CMB-C2B-C3B | 3.44  | 131.11      | 124.68   |
| 14  | G     | 813 | CLA  | O2A-CGA-O1A | -3.44 | 114.92      | 123.59   |
| 14  | H     | 827 | CLA  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 14  | G     | 840 | CLA  | C4A-NA-C1A  | 3.43  | 108.25      | 106.71   |
| 14  | A     | 821 | CLA  | C4A-NA-C1A  | 3.43  | 108.25      | 106.71   |
| 14  | G     | 825 | CLA  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 14  | G     | 831 | CLA  | CMB-C2B-C3B | 3.43  | 131.10      | 124.68   |
| 14  | Z     | 811 | CLA  | CMB-C2B-C3B | 3.43  | 131.09      | 124.68   |
| 14  | Y     | 854 | CLA  | O2A-CGA-CBA | 3.43  | 122.67      | 111.91   |
| 14  | A     | 837 | CLA  | O2A-C1-C2   | 3.43  | 117.64      | 108.64   |
| 14  | A     | 835 | CLA  | O2D-CGD-O1D | -3.43 | 117.14      | 123.84   |
| 17  | Y     | 851 | BCR  | C37-C22-C23 | 3.43  | 123.48      | 118.08   |
| 14  | Z     | 810 | CLA  | O2D-CGD-CBD | 3.43  | 117.36      | 111.27   |
| 14  | Z     | 821 | CLA  | O2A-C1-C2   | 3.43  | 117.64      | 108.64   |
| 14  | A     | 841 | CLA  | C4A-NA-C1A  | 3.43  | 108.25      | 106.71   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | H     | 843  | BCR  | C40-C30-C25 | 3.43  | 115.86      | 110.30   |
| 14  | B     | 810  | CLA  | O2A-CGA-CBA | 3.43  | 122.66      | 111.91   |
| 14  | Z     | 822  | CLA  | O2A-C1-C2   | 3.43  | 117.64      | 108.64   |
| 17  | B     | 845  | BCR  | C34-C9-C10  | -3.43 | 118.12      | 122.92   |
| 14  | A     | 833  | CLA  | CMB-C2B-C3B | 3.42  | 131.09      | 124.68   |
| 14  | H     | 811  | CLA  | CMA-C3A-C4A | 3.42  | 120.97      | 111.77   |
| 14  | Y     | 841  | CLA  | O2A-CGA-CBA | 3.42  | 122.65      | 111.91   |
| 14  | H     | 824  | CLA  | OBD-CAD-C3D | -3.42 | 122.30      | 127.98   |
| 14  | Z     | 817  | CLA  | C1-O2A-CGA  | 3.42  | 125.42      | 116.44   |
| 14  | Z     | 826  | CLA  | O2A-CGA-CBA | 3.42  | 122.64      | 111.91   |
| 14  | J     | 102  | CLA  | CMA-C3A-C4A | 3.42  | 120.97      | 111.77   |
| 14  | Z     | 834  | CLA  | CAC-C3C-C4C | 3.42  | 129.25      | 124.81   |
| 14  | Z     | 817  | CLA  | CMB-C2B-C3B | 3.42  | 131.08      | 124.68   |
| 14  | Y     | 803  | CLA  | CAC-C3C-C4C | 3.42  | 129.24      | 124.81   |
| 14  | Z     | 825  | CLA  | C1C-C2C-C3C | -3.42 | 103.36      | 106.96   |
| 14  | G     | 822  | CLA  | CMB-C2B-C3B | 3.42  | 131.07      | 124.68   |
| 17  | Y     | 851  | BCR  | C37-C22-C21 | -3.41 | 118.14      | 122.92   |
| 17  | Z     | 846  | BCR  | C34-C9-C10  | -3.41 | 118.14      | 122.92   |
| 17  | B     | 845  | BCR  | C37-C22-C23 | 3.41  | 123.46      | 118.08   |
| 14  | H     | 836  | CLA  | CMC-C2C-C1C | 3.41  | 130.24      | 125.04   |
| 14  | Y     | 805  | CLA  | O2A-CGA-O1A | -3.41 | 114.98      | 123.59   |
| 17  | G     | 847  | BCR  | C23-C24-C25 | -3.41 | 117.62      | 127.20   |
| 17  | Z     | 845  | BCR  | C1-C6-C7    | 3.41  | 125.43      | 115.78   |
| 14  | L     | 205  | CLA  | CMB-C2B-C3B | 3.41  | 131.06      | 124.68   |
| 14  | Y     | 835  | CLA  | O2D-CGD-O1D | -3.41 | 117.17      | 123.84   |
| 14  | Z     | 817  | CLA  | C4A-NA-C1A  | 3.41  | 108.24      | 106.71   |
| 14  | H     | 837  | CLA  | O2A-CGA-O1A | -3.41 | 114.99      | 123.59   |
| 14  | H     | 832  | CLA  | CMA-C3A-C4A | 3.41  | 120.93      | 111.77   |
| 14  | A     | 819  | CLA  | CMB-C2B-C3B | 3.41  | 131.05      | 124.68   |
| 14  | L     | 201  | CLA  | O1D-CGD-CBD | -3.41 | 117.52      | 124.48   |
| 14  | Z     | 808  | CLA  | O2A-C1-C2   | 3.41  | 117.59      | 108.64   |
| 14  | Z     | 827  | CLA  | O2A-C1-C2   | 3.41  | 117.59      | 108.64   |
| 14  | G     | 823  | CLA  | CMC-C2C-C1C | 3.41  | 130.22      | 125.04   |
| 14  | H     | 830  | CLA  | C1-C2-C3    | -3.40 | 120.16      | 126.04   |
| 14  | H     | 825  | CLA  | O2A-CGA-CBA | 3.40  | 122.59      | 111.91   |
| 14  | H     | 824  | CLA  | O2A-C1-C2   | 3.40  | 117.58      | 108.64   |
| 17  | Z     | 843  | BCR  | C7-C8-C9    | -3.40 | 121.09      | 126.23   |
| 14  | B     | 807  | CLA  | CHB-C4A-NA  | 3.40  | 129.22      | 124.51   |
| 17  | V     | 1202 | BCR  | C34-C9-C10  | -3.40 | 118.16      | 122.92   |
| 14  | A     | 815  | CLA  | CGD-CBD-CAD | -3.40 | 99.72       | 110.73   |
| 14  | U     | 1006 | CLA  | CGD-CBD-CAD | -3.40 | 99.72       | 110.73   |
| 14  | B     | 817  | CLA  | O1D-CGD-CBD | -3.40 | 117.53      | 124.48   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | U     | 1008 | BCR  | C23-C24-C25 | -3.40 | 117.66      | 127.20   |
| 14  | A     | 804  | CLA  | O2A-CGA-CBA | 3.40  | 122.57      | 111.91   |
| 14  | H     | 810  | CLA  | C1-O2A-CGA  | 3.40  | 125.36      | 116.44   |
| 14  | Z     | 833  | CLA  | OBD-CAD-CBD | -3.40 | 121.04      | 125.89   |
| 17  | I     | 101  | BCR  | C1-C6-C5    | -3.40 | 117.83      | 122.61   |
| 14  | H     | 805  | CLA  | O2A-C1-C2   | 3.40  | 117.56      | 108.64   |
| 14  | B     | 835  | CLA  | CMA-C3A-C4A | 3.39  | 120.89      | 111.77   |
| 17  | I     | 101  | BCR  | C7-C8-C9    | -3.39 | 121.11      | 126.23   |
| 14  | Z     | 822  | CLA  | C3C-C4C-NC  | 3.39  | 114.37      | 110.57   |
| 14  | B     | 840  | CLA  | CMA-C3A-C4A | 3.39  | 120.89      | 111.77   |
| 14  | h     | 201  | CLA  | CAC-C3C-C4C | 3.39  | 129.21      | 124.81   |
| 14  | A     | 830  | CLA  | CAC-C3C-C4C | 3.39  | 129.21      | 124.81   |
| 14  | L     | 201  | CLA  | C3C-C4C-NC  | 3.39  | 114.37      | 110.57   |
| 14  | Y     | 819  | CLA  | O2A-CGA-CBA | 3.39  | 122.54      | 111.91   |
| 14  | h     | 201  | CLA  | O2D-CGD-CBD | 3.38  | 117.28      | 111.27   |
| 14  | H     | 830  | CLA  | O2A-CGA-CBA | 3.38  | 122.52      | 111.91   |
| 14  | A     | 814  | CLA  | O2A-C1-C2   | 3.38  | 117.52      | 108.64   |
| 14  | Z     | 830  | CLA  | CMA-C3A-C4A | 3.38  | 120.86      | 111.77   |
| 15  | B     | 842  | PQN  | C2M-C2-C3   | -3.38 | 118.89      | 124.40   |
| 14  | Z     | 807  | CLA  | O1D-CGD-CBD | -3.38 | 117.57      | 124.48   |
| 14  | G     | 840  | CLA  | CMB-C2B-C3B | 3.38  | 131.00      | 124.68   |
| 14  | h     | 207  | CLA  | O2D-CGD-O1D | -3.38 | 117.23      | 123.84   |
| 14  | Y     | 802  | CLA  | O2D-CGD-CBD | 3.38  | 117.27      | 111.27   |
| 14  | G     | 819  | CLA  | C1-O2A-CGA  | 3.38  | 125.30      | 116.44   |
| 14  | A     | 828  | CLA  | CMC-C2C-C1C | 3.38  | 130.18      | 125.04   |
| 14  | Y     | 814  | CLA  | C4A-NA-C1A  | 3.37  | 108.22      | 106.71   |
| 17  | Y     | 851  | BCR  | C39-C30-C25 | -3.37 | 104.83      | 110.30   |
| 14  | G     | 828  | CLA  | C5-C3-C2    | -3.37 | 114.29      | 121.12   |
| 14  | Y     | 809  | CLA  | O2A-C1-C2   | 3.37  | 117.50      | 108.64   |
| 14  | S     | 1103 | CLA  | CMC-C2C-C1C | 3.37  | 130.18      | 125.04   |
| 14  | Y     | 834  | CLA  | O2A-CGA-CBA | 3.37  | 122.49      | 111.91   |
| 14  | Z     | 835  | CLA  | O2A-C1-C2   | 3.37  | 117.49      | 108.64   |
| 14  | Y     | 840  | CLA  | CMC-C2C-C1C | 3.37  | 130.17      | 125.04   |
| 14  | B     | 805  | CLA  | CAC-C3C-C4C | 3.37  | 129.18      | 124.81   |
| 17  | M     | 101  | BCR  | C33-C5-C6   | -3.37 | 120.75      | 124.53   |
| 17  | B     | 843  | BCR  | C3-C4-C5    | -3.37 | 108.07      | 114.08   |
| 14  | Z     | 817  | CLA  | OBD-CAD-C3D | -3.37 | 122.39      | 127.98   |
| 14  | J     | 102  | CLA  | C1-O2A-CGA  | 3.37  | 125.27      | 116.44   |
| 13  | G     | 801  | CL0  | C1-O2A-CGA  | 3.37  | 125.27      | 116.44   |
| 14  | Z     | 831  | CLA  | C3C-C4C-NC  | 3.37  | 114.34      | 110.57   |
| 17  | B     | 847  | BCR  | C8-C7-C6    | -3.37 | 117.75      | 127.20   |
| 14  | G     | 828  | CLA  | O2A-C1-C2   | 3.37  | 117.48      | 108.64   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 817  | CLA  | CAC-C3C-C4C | 3.36  | 129.17      | 124.81   |
| 14  | Z     | 806  | CLA  | O2A-C1-C2   | 3.36  | 117.47      | 108.64   |
| 14  | Y     | 837  | CLA  | CMC-C2C-C1C | 3.36  | 130.16      | 125.04   |
| 14  | A     | 820  | CLA  | O2A-C1-C2   | 3.36  | 117.47      | 108.64   |
| 17  | f     | 103  | BCR  | C30-C25-C26 | -3.36 | 117.88      | 122.61   |
| 14  | B     | 825  | CLA  | C4-C3-C5    | 3.36  | 120.92      | 115.27   |
| 17  | i     | 101  | BCR  | C33-C5-C4   | 3.36  | 120.07      | 113.62   |
| 14  | U     | 1004 | CLA  | O2D-CGD-O1D | -3.36 | 117.27      | 123.84   |
| 14  | A     | 821  | CLA  | O2D-CGD-O1D | -3.36 | 117.27      | 123.84   |
| 14  | H     | 816  | CLA  | CMC-C2C-C1C | 3.36  | 130.15      | 125.04   |
| 17  | S     | 1104 | BCR  | C37-C22-C23 | 3.36  | 123.37      | 118.08   |
| 14  | G     | 837  | CLA  | O2A-CGA-CBA | 3.36  | 122.44      | 111.91   |
| 14  | Y     | 842  | CLA  | CMB-C2B-C3B | 3.36  | 130.96      | 124.68   |
| 17  | Y     | 847  | BCR  | C7-C8-C9    | -3.36 | 121.17      | 126.23   |
| 17  | B     | 845  | BCR  | C7-C6-C5    | -3.35 | 113.34      | 121.46   |
| 14  | H     | 802  | CLA  | CAA-C2A-C1A | 3.35  | 122.96      | 111.97   |
| 14  | B     | 806  | CLA  | CMB-C2B-C3B | 3.35  | 130.95      | 124.68   |
| 17  | Y     | 851  | BCR  | C24-C23-C22 | -3.35 | 121.17      | 126.23   |
| 14  | H     | 833  | CLA  | CMB-C2B-C3B | 3.35  | 130.95      | 124.68   |
| 17  | Z     | 841  | BCR  | C34-C9-C10  | -3.35 | 118.23      | 122.92   |
| 17  | Z     | 843  | BCR  | C8-C9-C10   | 3.35  | 124.08      | 118.94   |
| 14  | G     | 802  | CLA  | CMB-C2B-C3B | 3.35  | 130.94      | 124.68   |
| 14  | Z     | 826  | CLA  | O2D-CGD-O1D | -3.35 | 117.29      | 123.84   |
| 14  | G     | 817  | CLA  | C4A-NA-C1A  | 3.35  | 108.21      | 106.71   |
| 14  | Z     | 814  | CLA  | C4-C3-C5    | 3.35  | 120.90      | 115.27   |
| 17  | d     | 203  | BCR  | C7-C8-C9    | -3.35 | 121.18      | 126.23   |
| 17  | Y     | 856  | BCR  | C34-C9-C10  | -3.35 | 118.24      | 122.92   |
| 14  | B     | 840  | CLA  | C1-O2A-CGA  | 3.34  | 125.22      | 116.44   |
| 14  | J     | 102  | CLA  | CMB-C2B-C3B | 3.34  | 130.94      | 124.68   |
| 17  | h     | 203  | BCR  | C15-C14-C13 | -3.34 | 122.54      | 127.31   |
| 14  | B     | 811  | CLA  | O2A-CGA-CBA | 3.34  | 122.40      | 111.91   |
| 14  | A     | 817  | CLA  | CMC-C2C-C1C | 3.34  | 130.13      | 125.04   |
| 14  | A     | 810  | CLA  | CMC-C2C-C1C | 3.34  | 130.13      | 125.04   |
| 14  | H     | 822  | CLA  | CED-O2D-CGD | 3.34  | 123.50      | 115.94   |
| 14  | B     | 823  | CLA  | O2A-CGA-CBA | 3.34  | 122.40      | 111.91   |
| 18  | G     | 851  | LHG  | O8-C23-C24  | 3.34  | 122.40      | 111.91   |
| 14  | H     | 824  | CLA  | CMB-C2B-C3B | 3.34  | 130.93      | 124.68   |
| 14  | G     | 828  | CLA  | C4-C3-C5    | 3.34  | 120.89      | 115.27   |
| 14  | Q     | 203  | CLA  | CMB-C2B-C3B | 3.34  | 130.93      | 124.68   |
| 14  | H     | 810  | CLA  | O2A-CGA-CBA | 3.34  | 122.39      | 111.91   |
| 14  | H     | 823  | CLA  | C3C-C4C-NC  | 3.34  | 114.32      | 110.57   |
| 14  | Y     | 855  | CLA  | OBD-CAD-CBD | -3.34 | 121.12      | 125.89   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | S     | 1104 | BCR  | C33-C5-C4   | 3.34  | 120.03      | 113.62   |
| 17  | H     | 845  | BCR  | C34-C9-C10  | -3.34 | 118.25      | 122.92   |
| 14  | G     | 830  | CLA  | CMA-C3A-C4A | 3.34  | 120.74      | 111.77   |
| 14  | Z     | 807  | CLA  | OBD-CAD-C3D | -3.34 | 122.44      | 127.98   |
| 14  | Z     | 809  | CLA  | O2A-CGA-CBA | 3.33  | 122.37      | 111.91   |
| 14  | G     | 815  | CLA  | O2A-CGA-CBA | 3.33  | 122.37      | 111.91   |
| 14  | Y     | 805  | CLA  | CBC-CAC-C3C | -3.33 | 103.24      | 112.43   |
| 14  | G     | 817  | CLA  | CMC-C2C-C1C | 3.33  | 130.12      | 125.04   |
| 17  | Z     | 845  | BCR  | C34-C9-C10  | -3.33 | 118.25      | 122.92   |
| 14  | Y     | 841  | CLA  | CMB-C2B-C3B | 3.33  | 130.91      | 124.68   |
| 17  | U     | 1007 | BCR  | C37-C22-C23 | 3.33  | 123.33      | 118.08   |
| 14  | B     | 837  | CLA  | C4D-C3D-CAD | 3.33  | 110.33      | 108.47   |
| 14  | Y     | 825  | CLA  | CMB-C2B-C3B | 3.33  | 130.91      | 124.68   |
| 17  | Y     | 851  | BCR  | C40-C30-C25 | 3.33  | 115.70      | 110.30   |
| 14  | Y     | 821  | CLA  | CMB-C2B-C3B | 3.33  | 130.90      | 124.68   |
| 14  | B     | 832  | CLA  | O2A-CGA-CBA | 3.33  | 122.35      | 111.91   |
| 14  | Y     | 843  | CLA  | O2D-CGD-O1D | -3.33 | 117.33      | 123.84   |
| 14  | Z     | 801  | CLA  | O2A-CGA-CBA | 3.33  | 122.35      | 111.91   |
| 14  | G     | 820  | CLA  | CMB-C2B-C3B | 3.33  | 130.90      | 124.68   |
| 14  | B     | 821  | CLA  | O1D-CGD-CBD | -3.33 | 117.68      | 124.48   |
| 14  | A     | 841  | CLA  | O2A-CGA-CBA | 3.33  | 122.34      | 111.91   |
| 17  | J     | 104  | BCR  | C31-C1-C6   | -3.33 | 104.91      | 110.30   |
| 17  | A     | 845  | BCR  | C34-C9-C8   | 3.32  | 123.31      | 118.08   |
| 17  | Y     | 848  | BCR  | C33-C5-C4   | 3.32  | 120.00      | 113.62   |
| 17  | B     | 845  | BCR  | C33-C5-C4   | 3.32  | 120.00      | 113.62   |
| 14  | H     | 836  | CLA  | O2D-CGD-O1D | -3.32 | 117.34      | 123.84   |
| 14  | B     | 817  | CLA  | O2A-C1-C2   | 3.32  | 117.37      | 108.64   |
| 14  | H     | 833  | CLA  | CMC-C2C-C1C | 3.32  | 130.10      | 125.04   |
| 14  | H     | 834  | CLA  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 14  | G     | 814  | CLA  | C1-O2A-CGA  | 3.32  | 125.16      | 116.44   |
| 14  | G     | 824  | CLA  | C3C-C4C-NC  | 3.32  | 114.29      | 110.57   |
| 17  | H     | 843  | BCR  | C24-C23-C22 | -3.32 | 121.22      | 126.23   |
| 14  | G     | 809  | CLA  | CMA-C3A-C4A | 3.32  | 120.69      | 111.77   |
| 14  | Y     | 812  | CLA  | O2A-C1-C2   | 3.32  | 117.35      | 108.64   |
| 17  | J     | 103  | BCR  | C15-C14-C13 | -3.31 | 122.58      | 127.31   |
| 17  | L     | 209  | BCR  | C8-C9-C10   | 3.31  | 124.03      | 118.94   |
| 14  | B     | 812  | CLA  | O2D-CGD-O1D | -3.31 | 117.36      | 123.84   |
| 14  | H     | 809  | CLA  | C1-O2A-CGA  | 3.31  | 125.14      | 116.44   |
| 17  | K     | 102  | BCR  | C30-C25-C26 | -3.31 | 117.95      | 122.61   |
| 14  | H     | 808  | CLA  | O2D-CGD-CBD | 3.31  | 117.15      | 111.27   |
| 14  | G     | 802  | CLA  | CHB-C4A-NA  | 3.31  | 129.09      | 124.51   |
| 17  | B     | 851  | BCR  | C4-C5-C6    | -3.31 | 117.93      | 122.73   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | H     | 840  | BCR  | C37-C22-C23 | 3.31  | 123.29      | 118.08   |
| 14  | G     | 832  | CLA  | CHB-C4A-NA  | 3.31  | 129.08      | 124.51   |
| 14  | Z     | 829  | CLA  | CAC-C3C-C4C | 3.30  | 129.10      | 124.81   |
| 14  | Z     | 806  | CLA  | CAC-C3C-C4C | 3.30  | 129.10      | 124.81   |
| 14  | Y     | 843  | CLA  | C1-O2A-CGA  | 3.30  | 125.11      | 116.44   |
| 17  | Z     | 845  | BCR  | C1-C6-C5    | -3.30 | 117.96      | 122.61   |
| 14  | j     | 102  | CLA  | CMB-C2B-C3B | 3.30  | 130.86      | 124.68   |
| 14  | Y     | 808  | CLA  | O2D-CGD-O1D | -3.30 | 117.38      | 123.84   |
| 14  | A     | 836  | CLA  | O2A-CGA-CBA | 3.30  | 122.28      | 111.91   |
| 14  | L     | 205  | CLA  | CMC-C2C-C1C | 3.30  | 130.07      | 125.04   |
| 14  | G     | 838  | CLA  | CMC-C2C-C1C | 3.30  | 130.07      | 125.04   |
| 14  | Z     | 826  | CLA  | CMB-C2B-C3B | 3.30  | 130.85      | 124.68   |
| 14  | G     | 841  | CLA  | C4-C3-C5    | 3.30  | 120.82      | 115.27   |
| 17  | H     | 841  | BCR  | C33-C5-C4   | 3.30  | 119.95      | 113.62   |
| 14  | Z     | 819  | CLA  | CED-O2D-CGD | 3.30  | 123.40      | 115.94   |
| 14  | A     | 818  | CLA  | C1C-C2C-C3C | -3.30 | 103.49      | 106.96   |
| 14  | Y     | 821  | CLA  | O2A-C1-C2   | 3.30  | 117.30      | 108.64   |
| 17  | G     | 854  | BCR  | C38-C26-C25 | -3.30 | 120.83      | 124.53   |
| 17  | A     | 846  | BCR  | C36-C18-C19 | -3.30 | 112.88      | 118.08   |
| 14  | U     | 1003 | CLA  | O2A-CGA-CBA | 3.30  | 122.25      | 111.91   |
| 14  | A     | 816  | CLA  | C1-O2A-CGA  | 3.30  | 125.09      | 116.44   |
| 17  | H     | 844  | BCR  | C40-C30-C25 | 3.29  | 115.64      | 110.30   |
| 14  | Z     | 810  | CLA  | CED-O2D-CGD | 3.29  | 123.39      | 115.94   |
| 14  | A     | 810  | CLA  | O2D-CGD-O1D | -3.29 | 117.40      | 123.84   |
| 14  | H     | 838  | CLA  | C3C-C4C-NC  | 3.29  | 114.27      | 110.57   |
| 14  | B     | 838  | CLA  | O2D-CGD-O1D | -3.29 | 117.40      | 123.84   |
| 14  | Y     | 828  | CLA  | CMC-C2C-C1C | 3.29  | 130.05      | 125.04   |
| 14  | H     | 808  | CLA  | O2A-CGA-CBA | 3.29  | 122.24      | 111.91   |
| 14  | L     | 206  | CLA  | C1-O2A-CGA  | 3.29  | 125.08      | 116.44   |
| 14  | Y     | 802  | CLA  | O2A-CGA-CBA | 3.29  | 122.23      | 111.91   |
| 14  | A     | 824  | CLA  | O2D-CGD-CBD | 3.29  | 117.11      | 111.27   |
| 14  | Z     | 823  | CLA  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |
| 17  | Y     | 847  | BCR  | C30-C25-C24 | 3.29  | 125.08      | 115.78   |
| 14  | H     | 823  | CLA  | OBD-CAD-C3D | -3.29 | 122.53      | 127.98   |
| 14  | Z     | 838  | CLA  | CMA-C3A-C4A | 3.28  | 120.60      | 111.77   |
| 14  | Z     | 830  | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 14  | S     | 1103 | CLA  | CMA-C3A-C4A | 3.28  | 120.60      | 111.77   |
| 14  | H     | 809  | CLA  | O2A-C1-C2   | 3.28  | 117.26      | 108.64   |
| 17  | B     | 851  | BCR  | C28-C27-C26 | -3.28 | 108.22      | 114.08   |
| 14  | B     | 830  | CLA  | OBD-CAD-C3D | -3.28 | 122.53      | 127.98   |
| 14  | B     | 837  | CLA  | O2A-C1-C2   | 3.28  | 117.26      | 108.64   |
| 17  | Z     | 841  | BCR  | C28-C27-C26 | -3.28 | 108.22      | 114.08   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 839  | CLA  | CMC-C2C-C1C | 3.28  | 130.04      | 125.04   |
| 14  | Z     | 827  | CLA  | CMB-C2B-C3B | 3.28  | 130.82      | 124.68   |
| 17  | H     | 844  | BCR  | C1-C6-C7    | 3.28  | 125.06      | 115.78   |
| 14  | G     | 829  | CLA  | O2A-CGA-CBA | 3.28  | 122.20      | 111.91   |
| 17  | Z     | 842  | BCR  | C36-C18-C19 | -3.28 | 112.91      | 118.08   |
| 14  | Y     | 822  | CLA  | CMB-C2B-C3B | 3.28  | 130.81      | 124.68   |
| 14  | Y     | 806  | CLA  | CMB-C2B-C3B | 3.28  | 130.81      | 124.68   |
| 14  | G     | 808  | CLA  | C4D-C3D-CAD | 3.28  | 110.30      | 108.47   |
| 14  | Z     | 824  | CLA  | C4D-C3D-CAD | 3.28  | 110.30      | 108.47   |
| 17  | U     | 1005 | BCR  | C36-C18-C19 | -3.27 | 112.92      | 118.08   |
| 14  | H     | 816  | CLA  | CMB-C2B-C3B | 3.27  | 130.80      | 124.68   |
| 14  | Z     | 810  | CLA  | CMB-C2B-C3B | 3.27  | 130.80      | 124.68   |
| 17  | B     | 845  | BCR  | C1-C6-C7    | 3.27  | 125.03      | 115.78   |
| 14  | Y     | 819  | CLA  | C1-C2-C3    | -3.27 | 120.39      | 126.04   |
| 17  | H     | 844  | BCR  | C33-C5-C4   | 3.27  | 119.90      | 113.62   |
| 14  | A     | 802  | CLA  | O1D-CGD-CBD | -3.27 | 117.79      | 124.48   |
| 14  | B     | 817  | CLA  | OBD-CAD-CBD | -3.27 | 121.22      | 125.89   |
| 14  | Z     | 818  | CLA  | CMA-C3A-C4A | 3.27  | 120.56      | 111.77   |
| 14  | Y     | 816  | CLA  | O2D-CGD-O1D | -3.27 | 117.45      | 123.84   |
| 14  | B     | 819  | CLA  | CMC-C2C-C1C | 3.27  | 130.01      | 125.04   |
| 14  | B     | 829  | CLA  | C4D-C3D-CAD | 3.27  | 110.29      | 108.47   |
| 14  | Y     | 823  | CLA  | O2D-CGD-O1D | -3.27 | 117.45      | 123.84   |
| 14  | Z     | 827  | CLA  | CBC-CAC-C3C | -3.27 | 103.43      | 112.43   |
| 14  | Y     | 833  | CLA  | OBD-CAD-C3D | -3.27 | 122.56      | 127.98   |
| 14  | A     | 834  | CLA  | O2A-CGA-CBA | 3.27  | 122.16      | 111.91   |
| 17  | G     | 846  | BCR  | C37-C22-C21 | -3.27 | 118.35      | 122.92   |
| 17  | H     | 842  | BCR  | C37-C22-C21 | -3.26 | 118.35      | 122.92   |
| 14  | A     | 840  | CLA  | C4A-NA-C1A  | 3.26  | 108.17      | 106.71   |
| 17  | V     | 1202 | BCR  | C1-C6-C7    | 3.26  | 125.00      | 115.78   |
| 14  | Y     | 841  | CLA  | C1-O2A-CGA  | 3.26  | 124.99      | 116.44   |
| 14  | A     | 840  | CLA  | O2A-CGA-CBA | 3.26  | 122.13      | 111.91   |
| 14  | B     | 807  | CLA  | CAC-C3C-C4C | 3.26  | 129.04      | 124.81   |
| 14  | B     | 825  | CLA  | C4-C3-C2    | -3.26 | 115.32      | 123.68   |
| 14  | Z     | 825  | CLA  | O1D-CGD-CBD | -3.26 | 117.82      | 124.48   |
| 14  | G     | 841  | CLA  | C3C-C4C-NC  | 3.26  | 114.22      | 110.57   |
| 14  | Y     | 835  | CLA  | O2A-CGA-CBA | 3.26  | 122.12      | 111.91   |
| 14  | A     | 837  | CLA  | O2A-CGA-CBA | 3.26  | 122.12      | 111.91   |
| 14  | U     | 1002 | CLA  | CED-O2D-CGD | 3.25  | 123.30      | 115.94   |
| 17  | A     | 848  | BCR  | C7-C8-C9    | -3.25 | 121.32      | 126.23   |
| 14  | A     | 802  | CLA  | O2A-C1-C2   | 3.25  | 117.18      | 108.64   |
| 14  | H     | 835  | CLA  | OBD-CAD-C3D | -3.25 | 122.58      | 127.98   |
| 14  | G     | 836  | CLA  | O2A-CGA-CBA | 3.25  | 122.11      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | f     | 104  | BCR  | C34-C9-C8   | 3.25  | 123.20      | 118.08   |
| 14  | B     | 824  | CLA  | C3C-C4C-NC  | 3.25  | 114.22      | 110.57   |
| 14  | A     | 835  | CLA  | CMC-C2C-C1C | 3.25  | 129.99      | 125.04   |
| 14  | G     | 834  | CLA  | C4D-C3D-CAD | 3.25  | 110.28      | 108.47   |
| 14  | G     | 822  | CLA  | OBD-CAD-C3D | -3.25 | 122.59      | 127.98   |
| 14  | Z     | 839  | CLA  | CMA-C3A-C4A | 3.24  | 120.49      | 111.77   |
| 14  | Y     | 815  | CLA  | CMA-C3A-C4A | 3.24  | 120.49      | 111.77   |
| 14  | L     | 201  | CLA  | OBD-CAD-C3D | -3.24 | 122.60      | 127.98   |
| 14  | U     | 1006 | CLA  | C3C-C4C-NC  | 3.24  | 114.20      | 110.57   |
| 14  | A     | 831  | CLA  | O2A-CGA-CBA | 3.24  | 122.08      | 111.91   |
| 14  | A     | 818  | CLA  | CAC-C3C-C4C | 3.24  | 129.01      | 124.81   |
| 14  | B     | 834  | CLA  | CHB-C4A-NA  | 3.24  | 128.99      | 124.51   |
| 14  | Y     | 838  | CLA  | C4-C3-C5    | 3.24  | 120.72      | 115.27   |
| 17  | A     | 847  | BCR  | C30-C25-C24 | 3.24  | 124.94      | 115.78   |
| 14  | Y     | 824  | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 14  | G     | 816  | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 14  | J     | 102  | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 17  | Y     | 856  | BCR  | C8-C7-C6    | -3.24 | 118.11      | 127.20   |
| 14  | Z     | 819  | CLA  | CMA-C3A-C4A | 3.24  | 120.47      | 111.77   |
| 14  | G     | 840  | CLA  | O2A-CGA-CBA | 3.23  | 122.06      | 111.91   |
| 14  | Y     | 837  | CLA  | OBD-CAD-C3D | -3.23 | 122.61      | 127.98   |
| 14  | Z     | 825  | CLA  | CMB-C2B-C3B | 3.23  | 130.73      | 124.68   |
| 14  | A     | 830  | CLA  | O2A-CGA-CBA | 3.23  | 122.06      | 111.91   |
| 17  | G     | 847  | BCR  | C7-C8-C9    | -3.23 | 121.35      | 126.23   |
| 14  | Y     | 837  | CLA  | O2D-CGD-O1D | -3.23 | 117.52      | 123.84   |
| 14  | B     | 802  | CLA  | O2A-CGA-CBA | 3.23  | 122.05      | 111.91   |
| 17  | h     | 203  | BCR  | C40-C30-C25 | -3.23 | 105.06      | 110.30   |
| 14  | A     | 832  | CLA  | O2A-CGA-CBA | 3.23  | 122.03      | 111.91   |
| 14  | H     | 804  | CLA  | CMC-C2C-C1C | 3.23  | 129.95      | 125.04   |
| 14  | G     | 814  | CLA  | CMC-C2C-C1C | 3.22  | 129.95      | 125.04   |
| 17  | U     | 1008 | BCR  | C7-C8-C9    | -3.22 | 121.36      | 126.23   |
| 14  | Y     | 855  | CLA  | CMB-C2B-C3B | 3.22  | 130.71      | 124.68   |
| 17  | B     | 846  | BCR  | C39-C30-C25 | -3.22 | 105.07      | 110.30   |
| 14  | A     | 840  | CLA  | CMA-C3A-C4A | 3.22  | 120.43      | 111.77   |
| 14  | Z     | 820  | CLA  | C4D-C3D-CAD | 3.22  | 110.27      | 108.47   |
| 17  | Z     | 844  | BCR  | C39-C30-C25 | -3.22 | 105.08      | 110.30   |
| 14  | Z     | 805  | CLA  | OBD-CAD-C3D | -3.22 | 122.63      | 127.98   |
| 14  | Z     | 821  | CLA  | CED-O2D-CGD | 3.22  | 123.22      | 115.94   |
| 14  | Y     | 820  | CLA  | CMB-C2B-C3B | 3.22  | 130.70      | 124.68   |
| 14  | B     | 807  | CLA  | CAA-C2A-C3A | -3.22 | 103.96      | 112.78   |
| 14  | h     | 206  | CLA  | O2A-C1-C2   | 3.22  | 117.10      | 108.64   |
| 14  | B     | 826  | CLA  | O2A-CGA-CBA | 3.22  | 122.01      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 848  | BCR  | C15-C14-C13 | -3.22 | 122.72      | 127.31   |
| 14  | Y     | 833  | CLA  | OBD-CAD-CBD | -3.22 | 121.30      | 125.89   |
| 14  | A     | 825  | CLA  | CMC-C2C-C1C | 3.22  | 129.94      | 125.04   |
| 17  | G     | 848  | BCR  | C38-C26-C25 | -3.22 | 120.92      | 124.53   |
| 14  | B     | 829  | CLA  | CED-O2D-CGD | 3.22  | 123.21      | 115.94   |
| 14  | G     | 807  | CLA  | CMA-C3A-C4A | 3.22  | 120.42      | 111.77   |
| 14  | B     | 841  | CLA  | CMA-C3A-C4A | 3.22  | 120.42      | 111.77   |
| 14  | Z     | 802  | CLA  | CMC-C2C-C1C | 3.22  | 129.94      | 125.04   |
| 14  | H     | 810  | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 17  | V     | 1202 | BCR  | C30-C25-C26 | -3.21 | 118.08      | 122.61   |
| 14  | B     | 841  | CLA  | CAC-C3C-C2C | 3.21  | 133.02      | 127.53   |
| 14  | Z     | 806  | CLA  | O2A-CGA-CBA | 3.21  | 121.97      | 111.91   |
| 14  | Q     | 203  | CLA  | CMA-C3A-C4A | 3.21  | 120.39      | 111.77   |
| 17  | M     | 101  | BCR  | C23-C22-C21 | 3.21  | 123.86      | 118.94   |
| 14  | S     | 1103 | CLA  | OBD-CAD-C3D | -3.21 | 122.66      | 127.98   |
| 14  | A     | 824  | CLA  | CMC-C2C-C1C | 3.21  | 129.92      | 125.04   |
| 17  | Y     | 856  | BCR  | C33-C5-C6   | -3.20 | 120.93      | 124.53   |
| 14  | Z     | 826  | CLA  | C4D-C3D-CAD | 3.20  | 110.26      | 108.47   |
| 14  | Y     | 826  | CLA  | CMA-C3A-C4A | 3.20  | 120.38      | 111.77   |
| 14  | d     | 201  | CLA  | C1-O2A-CGA  | 3.20  | 124.85      | 116.44   |
| 14  | G     | 806  | CLA  | CMB-C2B-C3B | 3.20  | 130.67      | 124.68   |
| 14  | Y     | 805  | CLA  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 14  | g     | 101  | CLA  | CMC-C2C-C1C | 3.20  | 129.91      | 125.04   |
| 17  | L     | 208  | BCR  | C31-C1-C6   | -3.20 | 105.11      | 110.30   |
| 14  | Z     | 823  | CLA  | C1-O2A-CGA  | 3.20  | 124.84      | 116.44   |
| 14  | Z     | 808  | CLA  | CBC-CAC-C3C | -3.20 | 103.61      | 112.43   |
| 14  | Y     | 827  | CLA  | OBD-CAD-CBD | -3.20 | 121.33      | 125.89   |
| 14  | H     | 823  | CLA  | CMC-C2C-C1C | 3.20  | 129.91      | 125.04   |
| 14  | B     | 806  | CLA  | O2A-CGA-CBA | 3.20  | 121.94      | 111.91   |
| 14  | G     | 813  | CLA  | CAC-C3C-C4C | 3.20  | 128.96      | 124.81   |
| 14  | A     | 806  | CLA  | CMC-C2C-C1C | 3.20  | 129.91      | 125.04   |
| 14  | Y     | 813  | CLA  | O2A-CGA-CBA | 3.19  | 121.93      | 111.91   |
| 17  | A     | 846  | BCR  | C24-C25-C26 | -3.19 | 113.72      | 121.46   |
| 14  | Y     | 835  | CLA  | CMB-C2B-C3B | 3.19  | 130.66      | 124.68   |
| 17  | K     | 102  | BCR  | C37-C22-C23 | 3.19  | 123.11      | 118.08   |
| 14  | Z     | 824  | CLA  | O2A-CGA-CBA | 3.19  | 121.93      | 111.91   |
| 14  | Y     | 841  | CLA  | CMC-C2C-C1C | 3.19  | 129.90      | 125.04   |
| 14  | Y     | 836  | CLA  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 14  | B     | 821  | CLA  | CED-O2D-CGD | 3.19  | 123.15      | 115.94   |
| 14  | T     | 103  | CLA  | CMA-C3A-C4A | 3.19  | 120.35      | 111.77   |
| 14  | G     | 809  | CLA  | OBD-CAD-C3D | -3.19 | 122.69      | 127.98   |
| 14  | Z     | 828  | CLA  | C3C-C4C-NC  | 3.19  | 114.15      | 110.57   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 850  | BCR  | C37-C22-C23 | 3.19  | 123.10      | 118.08   |
| 14  | Y     | 825  | CLA  | CMC-C2C-C1C | 3.19  | 129.89      | 125.04   |
| 17  | f     | 104  | BCR  | C31-C1-C6   | -3.19 | 105.13      | 110.30   |
| 17  | G     | 848  | BCR  | C38-C26-C27 | 3.19  | 119.74      | 113.62   |
| 14  | f     | 102  | CLA  | OBD-CAD-CBD | -3.19 | 121.34      | 125.89   |
| 14  | B     | 824  | CLA  | OBD-CAD-C3D | -3.18 | 122.69      | 127.98   |
| 14  | Y     | 819  | CLA  | CMA-C3A-C4A | 3.18  | 120.33      | 111.77   |
| 13  | Y     | 801  | CL0  | O2A-CGA-CBA | 3.18  | 121.89      | 111.91   |
| 14  | B     | 802  | CLA  | CMC-C2C-C1C | 3.18  | 129.88      | 125.04   |
| 14  | B     | 836  | CLA  | CMA-C3A-C4A | 3.18  | 120.32      | 111.77   |
| 14  | Y     | 807  | CLA  | O2D-CGD-O1D | -3.18 | 117.62      | 123.84   |
| 14  | Z     | 801  | CLA  | CAA-C2A-C3A | -3.18 | 104.07      | 112.78   |
| 14  | G     | 812  | CLA  | CMA-C3A-C4A | 3.18  | 120.32      | 111.77   |
| 14  | Z     | 824  | CLA  | CMA-C3A-C4A | 3.18  | 120.32      | 111.77   |
| 14  | Z     | 809  | CLA  | C4-C3-C5    | 3.18  | 120.62      | 115.27   |
| 14  | g     | 102  | CLA  | CED-O2D-CGD | 3.18  | 123.12      | 115.94   |
| 14  | Y     | 830  | CLA  | C3C-C4C-NC  | 3.18  | 114.13      | 110.57   |
| 14  | Y     | 806  | CLA  | CAA-C2A-C3A | -3.18 | 104.08      | 112.78   |
| 14  | G     | 827  | CLA  | C3C-C4C-NC  | 3.18  | 114.13      | 110.57   |
| 14  | Y     | 814  | CLA  | C3C-C4C-NC  | 3.17  | 114.13      | 110.57   |
| 14  | Z     | 813  | CLA  | O1D-CGD-CBD | -3.17 | 117.99      | 124.48   |
| 17  | f     | 104  | BCR  | C3-C4-C5    | -3.17 | 108.41      | 114.08   |
| 14  | h     | 201  | CLA  | OBD-CAD-C3D | -3.17 | 122.71      | 127.98   |
| 14  | Y     | 855  | CLA  | CHB-C4A-NA  | 3.17  | 128.90      | 124.51   |
| 14  | H     | 828  | CLA  | CBC-CAC-C3C | -3.17 | 103.69      | 112.43   |
| 14  | Y     | 842  | CLA  | C4D-C3D-CAD | 3.17  | 110.24      | 108.47   |
| 14  | A     | 804  | CLA  | CHB-C4A-NA  | 3.17  | 128.90      | 124.51   |
| 14  | Z     | 801  | CLA  | CHB-C4A-NA  | 3.17  | 128.90      | 124.51   |
| 14  | Z     | 835  | CLA  | O2D-CGD-O1D | -3.17 | 117.64      | 123.84   |
| 17  | f     | 104  | BCR  | C1-C6-C7    | 3.17  | 124.74      | 115.78   |
| 17  | A     | 845  | BCR  | C3-C4-C5    | -3.17 | 108.42      | 114.08   |
| 13  | G     | 801  | CL0  | O2D-CGD-O1D | -3.17 | 117.64      | 123.84   |
| 14  | Z     | 804  | CLA  | CHB-C4A-NA  | 3.17  | 128.89      | 124.51   |
| 14  | A     | 811  | CLA  | C1-O2A-CGA  | 3.17  | 124.75      | 116.44   |
| 17  | G     | 848  | BCR  | C37-C22-C23 | 3.16  | 123.06      | 118.08   |
| 14  | Z     | 831  | CLA  | CMB-C2B-C3B | 3.16  | 130.60      | 124.68   |
| 14  | B     | 828  | CLA  | C4-C3-C5    | 3.16  | 120.59      | 115.27   |
| 14  | G     | 813  | CLA  | CMA-C3A-C4A | 3.16  | 120.28      | 111.77   |
| 17  | A     | 847  | BCR  | C7-C8-C9    | -3.16 | 121.45      | 126.23   |
| 17  | F     | 203  | BCR  | C7-C8-C9    | -3.16 | 121.46      | 126.23   |
| 17  | Z     | 842  | BCR  | C33-C5-C6   | -3.16 | 120.98      | 124.53   |
| 17  | U     | 1005 | BCR  | C8-C7-C6    | -3.16 | 118.32      | 127.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 832  | CLA  | CAC-C3C-C4C | 3.16  | 128.91      | 124.81   |
| 14  | A     | 807  | CLA  | O2A-CGA-CBA | 3.16  | 121.81      | 111.91   |
| 14  | G     | 826  | CLA  | O2D-CGD-O1D | -3.16 | 117.67      | 123.84   |
| 14  | B     | 832  | CLA  | CMB-C2B-C3B | 3.16  | 130.58      | 124.68   |
| 14  | A     | 807  | CLA  | CMA-C3A-C4A | 3.16  | 120.25      | 111.77   |
| 14  | A     | 841  | CLA  | CAA-C2A-C3A | -3.16 | 104.14      | 112.78   |
| 14  | Z     | 832  | CLA  | CMC-C2C-C1C | 3.16  | 129.84      | 125.04   |
| 14  | G     | 833  | CLA  | C1-C2-C3    | -3.15 | 120.59      | 126.04   |
| 14  | H     | 814  | CLA  | CED-O2D-CGD | 3.15  | 123.07      | 115.94   |
| 14  | G     | 829  | CLA  | CMA-C3A-C4A | 3.15  | 120.25      | 111.77   |
| 19  | Z     | 847  | LMG  | C8-O7-C10   | -3.15 | 110.03      | 117.79   |
| 14  | X     | 1701 | CLA  | CMC-C2C-C1C | 3.15  | 129.84      | 125.04   |
| 14  | G     | 817  | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 14  | H     | 836  | CLA  | C3C-C4C-NC  | 3.15  | 114.11      | 110.57   |
| 14  | A     | 852  | CLA  | O1D-CGD-CBD | -3.15 | 118.04      | 124.48   |
| 14  | J     | 102  | CLA  | C4-C3-C5    | 3.15  | 120.56      | 115.27   |
| 14  | U     | 1004 | CLA  | C4D-C3D-CAD | 3.15  | 110.22      | 108.47   |
| 14  | B     | 836  | CLA  | CAC-C3C-C4C | 3.15  | 128.89      | 124.81   |
| 14  | Z     | 808  | CLA  | CMC-C2C-C1C | 3.14  | 129.83      | 125.04   |
| 14  | B     | 816  | CLA  | CMA-C3A-C4A | 3.14  | 120.22      | 111.77   |
| 14  | B     | 808  | CLA  | O2A-CGA-CBA | 3.14  | 121.77      | 111.91   |
| 14  | Y     | 830  | CLA  | O2A-CGA-CBA | 3.14  | 121.76      | 111.91   |
| 17  | B     | 843  | BCR  | C37-C22-C23 | 3.14  | 121.53      | 114.60   |
| 14  | Y     | 820  | CLA  | CMA-C3A-C4A | 3.14  | 120.21      | 111.77   |
| 14  | A     | 804  | CLA  | CMC-C2C-C1C | 3.14  | 129.82      | 125.04   |
| 14  | H     | 813  | CLA  | CED-O2D-CGD | 3.14  | 123.03      | 115.94   |
| 14  | Z     | 802  | CLA  | CAA-C2A-C1A | 3.14  | 122.25      | 111.97   |
| 17  | F     | 203  | BCR  | C33-C5-C4   | 3.13  | 119.64      | 113.62   |
| 14  | H     | 808  | CLA  | CHC-C1C-C2C | -3.13 | 118.05      | 126.72   |
| 14  | G     | 818  | CLA  | CED-O2D-CGD | 3.13  | 123.02      | 115.94   |
| 14  | J     | 102  | CLA  | CAC-C3C-C4C | 3.13  | 128.88      | 124.81   |
| 14  | Q     | 201  | CLA  | O2A-CGA-CBA | 3.13  | 121.74      | 111.91   |
| 18  | B     | 850  | LHG  | C5-O7-C7    | -3.13 | 110.08      | 117.79   |
| 14  | G     | 837  | CLA  | OBD-CAD-CBD | -3.13 | 121.42      | 125.89   |
| 14  | B     | 804  | CLA  | CHB-C4A-NA  | 3.13  | 128.84      | 124.51   |
| 14  | G     | 828  | CLA  | CMC-C2C-C1C | 3.13  | 129.80      | 125.04   |
| 14  | A     | 803  | CLA  | C3C-C4C-NC  | 3.13  | 114.08      | 110.57   |
| 14  | Y     | 833  | CLA  | C1-C2-C3    | -3.13 | 120.64      | 126.04   |
| 14  | H     | 817  | CLA  | OBD-CAD-C3D | -3.12 | 122.79      | 127.98   |
| 14  | A     | 841  | CLA  | C1-C2-C3    | -3.12 | 120.64      | 126.04   |
| 14  | A     | 842  | CLA  | C3C-C4C-NC  | 3.12  | 114.08      | 110.57   |
| 14  | B     | 840  | CLA  | CED-O2D-CGD | 3.12  | 123.00      | 115.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 813 | CLA  | O2A-C1-C2   | 3.12  | 116.84      | 108.64   |
| 17  | Z     | 846 | BCR  | C3-C4-C5    | -3.12 | 108.50      | 114.08   |
| 14  | A     | 835 | CLA  | CAC-C3C-C4C | 3.12  | 128.86      | 124.81   |
| 14  | G     | 828 | CLA  | CMB-C2B-C3B | 3.12  | 130.51      | 124.68   |
| 17  | f     | 104 | BCR  | C37-C22-C21 | -3.12 | 118.56      | 122.92   |
| 14  | H     | 828 | CLA  | CHC-C1C-C2C | -3.12 | 118.10      | 126.72   |
| 14  | B     | 822 | CLA  | CMB-C2B-C3B | 3.12  | 130.51      | 124.68   |
| 14  | B     | 805 | CLA  | O1D-CGD-CBD | -3.12 | 118.11      | 124.48   |
| 17  | A     | 847 | BCR  | C8-C7-C6    | -3.12 | 118.45      | 127.20   |
| 14  | L     | 202 | CLA  | CAA-C2A-C1A | 3.12  | 122.19      | 111.97   |
| 17  | I     | 101 | BCR  | C37-C22-C23 | 3.12  | 122.98      | 118.08   |
| 14  | Y     | 805 | CLA  | CMC-C2C-C1C | 3.11  | 129.78      | 125.04   |
| 14  | B     | 808 | CLA  | CMC-C2C-C1C | 3.11  | 129.78      | 125.04   |
| 14  | A     | 827 | CLA  | O2A-CGA-CBA | 3.11  | 121.67      | 111.91   |
| 14  | B     | 803 | CLA  | C4-C3-C5    | 3.11  | 120.51      | 115.27   |
| 17  | G     | 854 | BCR  | C38-C26-C27 | 3.11  | 119.59      | 113.62   |
| 14  | B     | 801 | CLA  | O2A-C1-C2   | 3.11  | 116.81      | 108.64   |
| 14  | G     | 805 | CLA  | O2A-CGA-O1A | -3.11 | 115.74      | 123.59   |
| 14  | H     | 816 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | Z     | 833 | CLA  | OBD-CAD-C3D | -3.11 | 122.82      | 127.98   |
| 14  | H     | 801 | CLA  | O1D-CGD-CBD | -3.11 | 118.12      | 124.48   |
| 14  | G     | 834 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 17  | Y     | 856 | BCR  | C23-C24-C25 | -3.11 | 118.47      | 127.20   |
| 14  | Z     | 813 | CLA  | OBD-CAD-CBD | -3.11 | 121.45      | 125.89   |
| 14  | A     | 820 | CLA  | C4A-NA-C1A  | 3.11  | 108.10      | 106.71   |
| 14  | h     | 206 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 17  | B     | 851 | BCR  | C2-C1-C6    | 3.11  | 115.26      | 110.48   |
| 14  | Y     | 839 | CLA  | C1-C2-C3    | -3.11 | 121.72      | 126.75   |
| 14  | A     | 832 | CLA  | C3C-C4C-NC  | 3.11  | 114.05      | 110.57   |
| 14  | A     | 802 | CLA  | O2A-CGA-CBA | 3.11  | 121.65      | 111.91   |
| 14  | A     | 823 | CLA  | O2D-CGD-O1D | -3.11 | 117.77      | 123.84   |
| 14  | H     | 819 | CLA  | O2D-CGD-O1D | -3.11 | 117.77      | 123.84   |
| 14  | G     | 841 | CLA  | CMC-C2C-C1C | 3.11  | 129.77      | 125.04   |
| 14  | A     | 828 | CLA  | C1-C2-C3    | -3.10 | 120.67      | 126.04   |
| 14  | Y     | 808 | CLA  | C3C-C4C-NC  | 3.10  | 114.05      | 110.57   |
| 14  | A     | 819 | CLA  | C4D-C3D-CAD | 3.10  | 110.20      | 108.47   |
| 14  | h     | 207 | CLA  | CMC-C2C-C1C | 3.10  | 129.76      | 125.04   |
| 14  | G     | 810 | CLA  | C3C-C4C-NC  | 3.10  | 114.05      | 110.57   |
| 14  | H     | 808 | CLA  | CAC-C3C-C4C | 3.10  | 128.84      | 124.81   |
| 14  | H     | 808 | CLA  | CBC-CAC-C3C | -3.10 | 103.88      | 112.43   |
| 14  | Z     | 802 | CLA  | O2A-CGA-CBA | 3.10  | 121.64      | 111.91   |
| 14  | G     | 821 | CLA  | CED-O2D-CGD | 3.10  | 122.95      | 115.94   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 802  | CLA  | O2D-CGD-O1D | -3.10 | 117.77      | 123.84   |
| 14  | B     | 834  | CLA  | O2D-CGD-O1D | -3.10 | 117.78      | 123.84   |
| 14  | Y     | 824  | CLA  | CMA-C3A-C4A | 3.10  | 120.11      | 111.77   |
| 14  | f     | 101  | CLA  | CMB-C2B-C3B | 3.10  | 130.48      | 124.68   |
| 14  | X     | 1701 | CLA  | O2D-CGD-O1D | -3.10 | 117.78      | 123.84   |
| 14  | Y     | 832  | CLA  | CMC-C2C-C1C | 3.10  | 129.76      | 125.04   |
| 14  | H     | 837  | CLA  | C3C-C4C-NC  | 3.10  | 114.05      | 110.57   |
| 14  | Z     | 816  | CLA  | CED-O2D-CGD | 3.10  | 122.94      | 115.94   |
| 17  | Y     | 849  | BCR  | C34-C9-C8   | 3.10  | 122.95      | 118.08   |
| 14  | A     | 834  | CLA  | CED-O2D-CGD | 3.10  | 122.94      | 115.94   |
| 17  | K     | 102  | BCR  | C33-C5-C6   | -3.10 | 121.05      | 124.53   |
| 19  | Z     | 847  | LMG  | O7-C10-O9   | -3.10 | 116.22      | 123.70   |
| 14  | Z     | 808  | CLA  | O2A-CGA-CBA | 3.09  | 121.62      | 111.91   |
| 14  | H     | 815  | CLA  | CMA-C3A-C4A | 3.09  | 120.09      | 111.77   |
| 14  | H     | 808  | CLA  | CMC-C2C-C1C | 3.09  | 129.75      | 125.04   |
| 14  | H     | 825  | CLA  | CMB-C2B-C3B | 3.09  | 130.46      | 124.68   |
| 14  | H     | 822  | CLA  | CMA-C3A-C4A | 3.09  | 120.08      | 111.77   |
| 17  | B     | 848  | BCR  | C23-C24-C25 | -3.09 | 118.53      | 127.20   |
| 14  | A     | 838  | CLA  | O2D-CGD-O1D | -3.09 | 117.80      | 123.84   |
| 14  | H     | 819  | CLA  | CMC-C2C-C1C | 3.09  | 129.74      | 125.04   |
| 14  | B     | 831  | CLA  | OBD-CAD-C3D | -3.09 | 122.85      | 127.98   |
| 14  | H     | 814  | CLA  | CAA-CBA-CGA | 3.09  | 120.22      | 113.59   |
| 14  | Z     | 804  | CLA  | O2A-CGA-CBA | 3.09  | 121.59      | 111.91   |
| 14  | A     | 818  | CLA  | CMC-C2C-C1C | 3.09  | 129.74      | 125.04   |
| 14  | A     | 840  | CLA  | CMB-C2B-C3B | 3.09  | 130.45      | 124.68   |
| 14  | G     | 825  | CLA  | CMC-C2C-C1C | 3.08  | 129.74      | 125.04   |
| 14  | A     | 814  | CLA  | O2D-CGD-O1D | -3.08 | 117.81      | 123.84   |
| 14  | f     | 101  | CLA  | C3C-C4C-NC  | 3.08  | 114.03      | 110.57   |
| 14  | G     | 805  | CLA  | CMA-C3A-C4A | 3.08  | 120.06      | 111.77   |
| 14  | B     | 835  | CLA  | CAC-C3C-C4C | 3.08  | 128.81      | 124.81   |
| 14  | h     | 206  | CLA  | OBD-CAD-CBD | 3.08  | 130.30      | 125.89   |
| 14  | G     | 815  | CLA  | C1-O2A-CGA  | 3.08  | 124.53      | 116.44   |
| 14  | H     | 833  | CLA  | CMA-C3A-C4A | 3.08  | 120.05      | 111.77   |
| 14  | H     | 819  | CLA  | OBD-CAD-CBD | -3.08 | 121.49      | 125.89   |
| 14  | H     | 824  | CLA  | C4-C3-C5    | 3.08  | 120.45      | 115.27   |
| 17  | U     | 1005 | BCR  | C32-C1-C6   | -3.08 | 105.31      | 110.30   |
| 14  | A     | 820  | CLA  | OBD-CAD-C3D | -3.08 | 122.87      | 127.98   |
| 14  | Z     | 807  | CLA  | C3C-C4C-NC  | 3.08  | 114.02      | 110.57   |
| 14  | H     | 831  | CLA  | O2D-CGD-O1D | -3.08 | 117.82      | 123.84   |
| 14  | G     | 829  | CLA  | CED-O2D-CGD | 3.07  | 122.89      | 115.94   |
| 14  | G     | 833  | CLA  | O1D-CGD-CBD | -3.07 | 118.19      | 124.48   |
| 17  | Q     | 202  | BCR  | C23-C24-C25 | -3.07 | 118.57      | 127.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 835  | CLA  | CAC-C3C-C4C | 3.07  | 128.80      | 124.81   |
| 14  | G     | 827  | CLA  | CMC-C2C-C1C | 3.07  | 129.72      | 125.04   |
| 17  | R     | 101  | BCR  | C37-C22-C23 | 3.07  | 122.92      | 118.08   |
| 17  | d     | 203  | BCR  | C8-C7-C6    | -3.07 | 118.58      | 127.20   |
| 17  | Y     | 849  | BCR  | C37-C22-C21 | -3.07 | 118.62      | 122.92   |
| 17  | Z     | 842  | BCR  | C38-C26-C25 | -3.07 | 121.08      | 124.53   |
| 14  | H     | 816  | CLA  | OBD-CAD-C3D | -3.07 | 122.89      | 127.98   |
| 14  | Z     | 837  | CLA  | CED-O2D-CGD | 3.07  | 122.88      | 115.94   |
| 14  | h     | 205  | CLA  | CGD-CBD-CAD | -3.07 | 100.80      | 110.73   |
| 13  | G     | 801  | CL0  | C1-C2-C3    | -3.07 | 120.74      | 126.04   |
| 14  | V     | 1201 | CLA  | O2A-C1-C2   | 3.07  | 116.69      | 108.64   |
| 14  | A     | 820  | CLA  | OBD-CAD-CBD | -3.07 | 121.52      | 125.89   |
| 17  | G     | 854  | BCR  | C30-C25-C24 | 3.06  | 124.45      | 115.78   |
| 14  | U     | 1002 | CLA  | C1-O2A-CGA  | 3.06  | 124.48      | 116.44   |
| 14  | Y     | 827  | CLA  | CMC-C2C-C1C | 3.06  | 129.71      | 125.04   |
| 14  | Y     | 809  | CLA  | C4-C3-C5    | 3.06  | 120.42      | 115.27   |
| 14  | H     | 834  | CLA  | OBD-CAD-C3D | -3.06 | 122.89      | 127.98   |
| 14  | Y     | 831  | CLA  | C1-O2A-CGA  | 3.06  | 124.48      | 116.44   |
| 14  | G     | 815  | CLA  | CMD-C2D-C3D | -3.06 | 118.95      | 124.68   |
| 14  | F     | 202  | CLA  | CMA-C3A-C4A | 3.06  | 120.00      | 111.77   |
| 14  | A     | 831  | CLA  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |
| 14  | H     | 821  | CLA  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |
| 14  | A     | 814  | CLA  | CMA-C3A-C4A | 3.06  | 120.00      | 111.77   |
| 14  | Y     | 837  | CLA  | OBD-CAD-CBD | -3.06 | 121.52      | 125.89   |
| 14  | H     | 831  | CLA  | CHB-C4A-NA  | 3.06  | 128.74      | 124.51   |
| 14  | Y     | 818  | CLA  | C1-C2-C3    | -3.06 | 120.75      | 126.04   |
| 14  | J     | 102  | CLA  | C4A-NA-C1A  | 3.06  | 108.08      | 106.71   |
| 14  | G     | 803  | CLA  | CMC-C2C-C1C | 3.06  | 129.70      | 125.04   |
| 14  | Z     | 836  | CLA  | O2A-CGA-CBA | 3.06  | 121.50      | 111.91   |
| 14  | Z     | 815  | CLA  | C4D-C3D-CAD | 3.06  | 110.17      | 108.47   |
| 14  | B     | 833  | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 14  | G     | 827  | CLA  | OBD-CAD-C3D | -3.06 | 122.91      | 127.98   |
| 14  | Z     | 813  | CLA  | CMC-C2C-C3C | 3.06  | 134.41      | 126.12   |
| 17  | F     | 203  | BCR  | C3-C4-C5    | -3.06 | 108.62      | 114.08   |
| 14  | H     | 838  | CLA  | CAC-C3C-C2C | 3.06  | 132.75      | 127.53   |
| 17  | Y     | 848  | BCR  | C28-C27-C26 | -3.06 | 108.62      | 114.08   |
| 14  | Y     | 817  | CLA  | CMA-C3A-C4A | 3.05  | 119.98      | 111.77   |
| 14  | d     | 201  | CLA  | CMA-C3A-C4A | 3.05  | 119.98      | 111.77   |
| 14  | H     | 836  | CLA  | O1D-CGD-CBD | -3.05 | 118.24      | 124.48   |
| 14  | Y     | 841  | CLA  | C3C-C4C-NC  | 3.05  | 113.99      | 110.57   |
| 14  | H     | 815  | CLA  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 17  | B     | 851  | BCR  | C27-C26-C25 | -3.05 | 118.30      | 122.73   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 838  | CLA  | CMA-C3A-C4A | 3.05  | 119.97      | 111.77   |
| 14  | Y     | 808  | CLA  | CMC-C2C-C1C | 3.05  | 129.68      | 125.04   |
| 17  | H     | 842  | BCR  | C36-C18-C19 | -3.05 | 113.27      | 118.08   |
| 14  | H     | 803  | CLA  | O2A-C1-C2   | 3.05  | 116.65      | 108.64   |
| 14  | G     | 835  | CLA  | CMA-C3A-C4A | 3.05  | 119.97      | 111.77   |
| 14  | B     | 826  | CLA  | CMA-C3A-C4A | 3.05  | 119.97      | 111.77   |
| 14  | V     | 1201 | CLA  | C3C-C4C-NC  | 3.05  | 113.99      | 110.57   |
| 14  | T     | 103  | CLA  | CMC-C2C-C1C | 3.05  | 129.68      | 125.04   |
| 14  | H     | 812  | CLA  | CMB-C2B-C3B | 3.05  | 130.38      | 124.68   |
| 17  | Y     | 856  | BCR  | C36-C18-C19 | -3.04 | 113.28      | 118.08   |
| 17  | Y     | 856  | BCR  | C30-C25-C26 | -3.04 | 118.33      | 122.61   |
| 14  | G     | 811  | CLA  | CMA-C3A-C4A | 3.04  | 119.95      | 111.77   |
| 14  | Z     | 802  | CLA  | O2A-C1-C2   | 3.04  | 116.63      | 108.64   |
| 14  | Y     | 828  | CLA  | O2A-C1-C2   | 3.04  | 116.63      | 108.64   |
| 14  | B     | 807  | CLA  | C4-C3-C5    | 3.04  | 120.39      | 115.27   |
| 14  | f     | 102  | CLA  | OBD-CAD-C3D | -3.04 | 122.93      | 127.98   |
| 14  | Y     | 820  | CLA  | CAC-C3C-C4C | 3.04  | 128.75      | 124.81   |
| 14  | F     | 202  | CLA  | C4D-C3D-CAD | 3.04  | 110.17      | 108.47   |
| 17  | H     | 843  | BCR  | C35-C13-C12 | 3.04  | 121.31      | 114.60   |
| 14  | A     | 827  | CLA  | C3C-C4C-NC  | 3.04  | 113.98      | 110.57   |
| 14  | H     | 803  | CLA  | CHC-C1C-C2C | -3.04 | 118.32      | 126.72   |
| 17  | f     | 103  | BCR  | C3-C4-C5    | -3.04 | 108.66      | 114.08   |
| 14  | A     | 806  | CLA  | CHB-C4A-NA  | 3.04  | 128.71      | 124.51   |
| 14  | G     | 827  | CLA  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 14  | B     | 815  | CLA  | OBD-CAD-C3D | -3.03 | 122.94      | 127.98   |
| 14  | A     | 832  | CLA  | CMA-C3A-C4A | 3.03  | 119.93      | 111.77   |
| 14  | Y     | 811  | CLA  | CMA-C3A-C4A | 3.03  | 119.93      | 111.77   |
| 17  | L     | 203  | BCR  | C23-C24-C25 | -3.03 | 118.68      | 127.20   |
| 14  | A     | 829  | CLA  | O2A-CGA-CBA | 3.03  | 121.43      | 111.91   |
| 14  | B     | 827  | CLA  | CMB-C2B-C3B | 3.03  | 130.35      | 124.68   |
| 14  | B     | 830  | CLA  | CMA-C3A-C4A | 3.03  | 119.92      | 111.77   |
| 14  | A     | 826  | CLA  | CMB-C2B-C3B | 3.03  | 130.35      | 124.68   |
| 17  | h     | 202  | BCR  | C36-C18-C19 | -3.03 | 113.30      | 118.08   |
| 17  | Z     | 843  | BCR  | C24-C23-C22 | -3.03 | 121.66      | 126.23   |
| 17  | Y     | 847  | BCR  | C30-C25-C26 | -3.03 | 118.35      | 122.61   |
| 14  | H     | 832  | CLA  | OBD-CAD-C3D | -3.03 | 122.95      | 127.98   |
| 14  | B     | 834  | CLA  | CMC-C2C-C1C | 3.03  | 129.65      | 125.04   |
| 14  | G     | 816  | CLA  | OBD-CAD-C3D | -3.03 | 122.96      | 127.98   |
| 14  | Y     | 802  | CLA  | CBC-CAC-C3C | -3.02 | 104.09      | 112.43   |
| 14  | A     | 825  | CLA  | CMB-C2B-C3B | 3.02  | 130.33      | 124.68   |
| 14  | V     | 1201 | CLA  | O2A-CGA-CBA | 3.02  | 121.39      | 111.91   |
| 14  | H     | 815  | CLA  | CMB-C2B-C3B | 3.02  | 130.33      | 124.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 819  | CLA  | CAC-C3C-C4C | 3.02  | 128.73      | 124.81   |
| 14  | Y     | 842  | CLA  | O2D-CGD-CBD | 3.02  | 116.64      | 111.27   |
| 17  | h     | 203  | BCR  | C37-C22-C23 | 3.02  | 122.83      | 118.08   |
| 14  | H     | 807  | CLA  | CED-O2D-CGD | 3.02  | 122.77      | 115.94   |
| 14  | G     | 838  | CLA  | C4A-NA-C1A  | 3.02  | 108.06      | 106.71   |
| 14  | B     | 818  | CLA  | C4D-C3D-CAD | 3.02  | 110.15      | 108.47   |
| 14  | H     | 805  | CLA  | CMC-C2C-C1C | 3.02  | 129.63      | 125.04   |
| 17  | Z     | 845  | BCR  | C12-C13-C14 | 3.02  | 123.57      | 118.94   |
| 14  | Y     | 805  | CLA  | O1D-CGD-CBD | -3.02 | 118.31      | 124.48   |
| 14  | U     | 1006 | CLA  | C1-O2A-CGA  | 3.02  | 124.36      | 116.44   |
| 14  | Y     | 836  | CLA  | CMC-C2C-C1C | 3.02  | 129.63      | 125.04   |
| 14  | G     | 808  | CLA  | O2D-CGD-O1D | -3.02 | 117.94      | 123.84   |
| 14  | B     | 829  | CLA  | CHB-C4A-NA  | 3.01  | 128.68      | 124.51   |
| 14  | K     | 101  | CLA  | CMB-C2B-C3B | 3.01  | 130.32      | 124.68   |
| 14  | G     | 821  | CLA  | CMC-C2C-C1C | 3.01  | 129.63      | 125.04   |
| 14  | B     | 820  | CLA  | C4A-NA-C1A  | 3.01  | 108.06      | 106.71   |
| 17  | G     | 849  | BCR  | C40-C30-C25 | 3.01  | 115.18      | 110.30   |
| 15  | Z     | 840  | PQN  | C14-C13-C15 | 3.01  | 120.34      | 115.27   |
| 14  | Y     | 820  | CLA  | OBD-CAD-CBD | -3.01 | 121.59      | 125.89   |
| 15  | A     | 843  | PQN  | C14-C13-C15 | 3.01  | 120.33      | 115.27   |
| 14  | U     | 1006 | CLA  | CAC-C3C-C4C | 3.01  | 128.71      | 124.81   |
| 14  | B     | 805  | CLA  | C1-O2A-CGA  | 3.01  | 124.34      | 116.44   |
| 17  | G     | 849  | BCR  | C32-C1-C6   | -3.01 | 105.42      | 110.30   |
| 14  | A     | 840  | CLA  | C4-C3-C5    | 3.01  | 120.33      | 115.27   |
| 14  | H     | 824  | CLA  | C1-O2A-CGA  | 3.01  | 124.33      | 116.44   |
| 14  | B     | 823  | CLA  | CMA-C3A-C4A | 3.00  | 119.85      | 111.77   |
| 14  | G     | 822  | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 14  | G     | 825  | CLA  | CMA-C3A-C4A | 3.00  | 119.84      | 111.77   |
| 14  | Z     | 805  | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.72   |
| 14  | G     | 835  | CLA  | CMC-C2C-C1C | 3.00  | 129.61      | 125.04   |
| 14  | G     | 827  | CLA  | CMB-C2B-C3B | 3.00  | 130.29      | 124.68   |
| 14  | Y     | 821  | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 14  | Z     | 813  | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 17  | H     | 844  | BCR  | C33-C5-C6   | -3.00 | 121.16      | 124.53   |
| 14  | G     | 829  | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 14  | A     | 818  | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 14  | A     | 818  | CLA  | CMA-C3A-C4A | 3.00  | 119.83      | 111.77   |
| 17  | A     | 845  | BCR  | C7-C8-C9    | -3.00 | 121.71      | 126.23   |
| 14  | H     | 809  | CLA  | CMA-C3A-C4A | 3.00  | 119.83      | 111.77   |
| 14  | A     | 829  | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 14  | Y     | 810  | CLA  | CMA-C3A-C4A | 3.00  | 119.82      | 111.77   |
| 14  | H     | 817  | CLA  | O1D-CGD-CBD | -2.99 | 118.36      | 124.48   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 828  | CLA  | O2A-CGA-CBA | 2.99  | 121.31      | 111.91   |
| 14  | H     | 825  | CLA  | CMC-C2C-C1C | 2.99  | 129.60      | 125.04   |
| 14  | Y     | 828  | CLA  | C3C-C4C-NC  | 2.99  | 113.93      | 110.57   |
| 14  | Z     | 806  | CLA  | C1-O2A-CGA  | 2.99  | 124.30      | 116.44   |
| 14  | Z     | 817  | CLA  | CED-O2D-CGD | 2.99  | 122.71      | 115.94   |
| 17  | H     | 845  | BCR  | C7-C8-C9    | -2.99 | 121.71      | 126.23   |
| 17  | G     | 846  | BCR  | C30-C25-C24 | 2.99  | 124.24      | 115.78   |
| 14  | Y     | 833  | CLA  | CMC-C2C-C1C | 2.99  | 129.59      | 125.04   |
| 14  | G     | 816  | CLA  | CHC-C1C-C2C | -2.99 | 118.45      | 126.72   |
| 14  | A     | 825  | CLA  | CED-O2D-CGD | 2.99  | 122.70      | 115.94   |
| 17  | Z     | 844  | BCR  | C37-C22-C23 | 2.99  | 122.79      | 118.08   |
| 14  | A     | 827  | CLA  | CMC-C2C-C1C | 2.99  | 129.59      | 125.04   |
| 17  | B     | 844  | BCR  | C7-C8-C9    | -2.99 | 121.72      | 126.23   |
| 14  | Z     | 817  | CLA  | O2A-CGA-CBA | 2.99  | 121.28      | 111.91   |
| 14  | Z     | 801  | CLA  | O2D-CGD-CBD | 2.99  | 116.58      | 111.27   |
| 14  | H     | 835  | CLA  | C1-O2A-CGA  | 2.99  | 124.28      | 116.44   |
| 14  | G     | 817  | CLA  | CMA-C3A-C4A | 2.99  | 119.80      | 111.77   |
| 14  | Z     | 809  | CLA  | CMC-C2C-C1C | 2.99  | 129.59      | 125.04   |
| 17  | A     | 847  | BCR  | C38-C26-C27 | 2.99  | 119.35      | 113.62   |
| 17  | H     | 840  | BCR  | C32-C1-C6   | -2.98 | 105.46      | 110.30   |
| 14  | B     | 841  | CLA  | C1-C2-C3    | -2.98 | 120.88      | 126.04   |
| 17  | Z     | 841  | BCR  | C38-C26-C27 | 2.98  | 119.35      | 113.62   |
| 14  | Y     | 854  | CLA  | O2D-CGD-O1D | -2.98 | 118.01      | 123.84   |
| 14  | B     | 840  | CLA  | O2D-CGD-O1D | -2.98 | 118.01      | 123.84   |
| 14  | B     | 824  | CLA  | O2D-CGD-O1D | -2.98 | 118.01      | 123.84   |
| 14  | G     | 805  | CLA  | CMB-C2B-C3B | 2.98  | 130.25      | 124.68   |
| 14  | d     | 202  | CLA  | CMC-C2C-C1C | 2.98  | 129.57      | 125.04   |
| 14  | Y     | 831  | CLA  | CMB-C2B-C3B | 2.98  | 130.25      | 124.68   |
| 19  | Z     | 847  | LMG  | C7-O1-C1    | -2.98 | 107.92      | 113.74   |
| 14  | G     | 817  | CLA  | C4-C3-C5    | 2.98  | 120.28      | 115.27   |
| 14  | Z     | 805  | CLA  | O2D-CGD-O1D | -2.98 | 118.02      | 123.84   |
| 14  | B     | 806  | CLA  | CHB-C4A-NA  | 2.98  | 128.63      | 124.51   |
| 14  | H     | 825  | CLA  | C3C-C4C-NC  | 2.98  | 113.91      | 110.57   |
| 14  | Y     | 805  | CLA  | CAC-C3C-C4C | 2.97  | 128.67      | 124.81   |
| 14  | A     | 820  | CLA  | CMC-C2C-C1C | 2.97  | 129.57      | 125.04   |
| 14  | G     | 833  | CLA  | CMC-C2C-C1C | 2.97  | 129.57      | 125.04   |
| 17  | h     | 202  | BCR  | C34-C9-C8   | 2.97  | 122.76      | 118.08   |
| 14  | G     | 834  | CLA  | C3C-C4C-NC  | 2.97  | 113.90      | 110.57   |
| 14  | H     | 830  | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 17  | i     | 101  | BCR  | C33-C5-C6   | -2.97 | 121.19      | 124.53   |
| 14  | B     | 826  | CLA  | O1D-CGD-CBD | -2.97 | 118.41      | 124.48   |
| 14  | U     | 1006 | CLA  | CED-O2D-CGD | 2.97  | 122.65      | 115.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | V     | 1202 | BCR  | C7-C6-C5    | -2.97 | 114.27      | 121.46   |
| 14  | G     | 831  | CLA  | OBD-CAD-CBD | -2.97 | 121.66      | 125.89   |
| 17  | H     | 840  | BCR  | C8-C7-C6    | -2.97 | 118.87      | 127.20   |
| 14  | Y     | 805  | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 14  | G     | 820  | CLA  | CMA-C3A-C4A | 2.96  | 119.74      | 111.77   |
| 17  | H     | 848  | BCR  | C36-C18-C19 | -2.96 | 113.41      | 118.08   |
| 14  | G     | 826  | CLA  | CMA-C3A-C4A | 2.96  | 119.74      | 111.77   |
| 14  | Z     | 836  | CLA  | CMC-C2C-C1C | 2.96  | 129.55      | 125.04   |
| 17  | Z     | 846  | BCR  | C30-C25-C26 | -2.96 | 118.44      | 122.61   |
| 14  | B     | 802  | CLA  | CMB-C2B-C3B | 2.96  | 130.22      | 124.68   |
| 14  | B     | 831  | CLA  | CMA-C3A-C4A | 2.96  | 119.73      | 111.77   |
| 17  | H     | 844  | BCR  | C1-C6-C5    | -2.96 | 118.44      | 122.61   |
| 17  | B     | 848  | BCR  | C35-C13-C14 | -2.96 | 118.78      | 122.92   |
| 14  | G     | 809  | CLA  | CMC-C2C-C1C | 2.96  | 129.55      | 125.04   |
| 14  | H     | 826  | CLA  | C3C-C4C-NC  | 2.96  | 113.89      | 110.57   |
| 14  | Z     | 821  | CLA  | O2A-CGA-CBA | 2.96  | 121.20      | 111.91   |
| 14  | Z     | 804  | CLA  | CED-O2D-CGD | 2.96  | 122.63      | 115.94   |
| 14  | B     | 838  | CLA  | C3C-C4C-NC  | 2.96  | 113.89      | 110.57   |
| 17  | M     | 101  | BCR  | C1-C6-C7    | 2.96  | 124.15      | 115.78   |
| 14  | Z     | 821  | CLA  | CAC-C3C-C4C | 2.96  | 128.65      | 124.81   |
| 14  | V     | 1201 | CLA  | CMC-C2C-C1C | 2.96  | 129.54      | 125.04   |
| 14  | L     | 205  | CLA  | O2D-CGD-O1D | -2.96 | 118.06      | 123.84   |
| 14  | H     | 803  | CLA  | CMB-C2B-C1B | 2.95  | 133.00      | 128.46   |
| 14  | L     | 207  | CLA  | CMC-C2C-C1C | 2.95  | 129.54      | 125.04   |
| 14  | B     | 826  | CLA  | C1-C2-C3    | -2.95 | 120.93      | 126.04   |
| 14  | G     | 822  | CLA  | CMA-C3A-C4A | 2.95  | 119.71      | 111.77   |
| 14  | Z     | 822  | CLA  | CMC-C2C-C1C | 2.95  | 129.54      | 125.04   |
| 14  | B     | 813  | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 14  | H     | 815  | CLA  | CED-O2D-CGD | 2.95  | 122.61      | 115.94   |
| 17  | Y     | 851  | BCR  | C3-C4-C5    | -2.95 | 108.81      | 114.08   |
| 14  | X     | 1701 | CLA  | C3C-C4C-NC  | 2.95  | 113.88      | 110.57   |
| 14  | Y     | 814  | CLA  | O1D-CGD-CBD | -2.95 | 118.45      | 124.48   |
| 14  | Z     | 805  | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 17  | H     | 845  | BCR  | C3-C4-C5    | -2.95 | 108.81      | 114.08   |
| 14  | H     | 826  | CLA  | CHB-C4A-NA  | 2.95  | 128.59      | 124.51   |
| 14  | Y     | 836  | CLA  | OBD-CAD-C3D | -2.95 | 123.09      | 127.98   |
| 14  | G     | 814  | CLA  | CAA-CBA-CGA | -2.95 | 104.64      | 113.25   |
| 14  | G     | 831  | CLA  | CMC-C2C-C1C | 2.95  | 129.53      | 125.04   |
| 14  | H     | 812  | CLA  | C1-C2-C3    | -2.95 | 120.95      | 126.04   |
| 14  | X     | 1701 | CLA  | CMA-C3A-C4A | 2.95  | 119.69      | 111.77   |
| 14  | K     | 103  | CLA  | O2D-CGD-O1D | -2.95 | 118.08      | 123.84   |
| 14  | Z     | 822  | CLA  | C4-C3-C5    | 2.94  | 120.22      | 115.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 855  | CLA  | CMC-C2C-C1C | 2.94  | 129.52      | 125.04   |
| 14  | Z     | 801  | CLA  | CED-O2D-CGD | 2.94  | 122.60      | 115.94   |
| 14  | Y     | 854  | CLA  | O1D-CGD-CBD | -2.94 | 118.46      | 124.48   |
| 14  | A     | 852  | CLA  | CBC-CAC-C3C | -2.94 | 104.32      | 112.43   |
| 14  | G     | 822  | CLA  | CMC-C2C-C1C | 2.94  | 129.52      | 125.04   |
| 17  | Y     | 847  | BCR  | C28-C27-C26 | -2.94 | 108.82      | 114.08   |
| 14  | B     | 835  | CLA  | CMC-C2C-C1C | 2.94  | 129.52      | 125.04   |
| 14  | G     | 853  | CLA  | OBD-CAD-C3D | -2.94 | 123.10      | 127.98   |
| 14  | Y     | 802  | CLA  | CAC-C3C-C4C | 2.94  | 128.62      | 124.81   |
| 14  | G     | 834  | CLA  | C6-C5-C3    | -2.94 | 105.75      | 113.45   |
| 14  | A     | 826  | CLA  | O2A-CGA-CBA | 2.94  | 121.13      | 111.91   |
| 14  | A     | 829  | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 14  | A     | 814  | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 17  | I     | 101  | BCR  | C40-C30-C25 | 2.94  | 115.06      | 110.30   |
| 17  | Z     | 843  | BCR  | C36-C18-C19 | -2.94 | 113.45      | 118.08   |
| 14  | Y     | 818  | CLA  | CHB-C4A-NA  | 2.94  | 128.57      | 124.51   |
| 14  | G     | 830  | CLA  | OBD-CAD-C3D | -2.94 | 123.11      | 127.98   |
| 14  | A     | 852  | CLA  | CMC-C2C-C1C | 2.94  | 129.51      | 125.04   |
| 14  | G     | 833  | CLA  | C1-O2A-CGA  | 2.93  | 124.14      | 116.44   |
| 14  | G     | 835  | CLA  | C3C-C4C-NC  | 2.93  | 113.86      | 110.57   |
| 14  | B     | 801  | CLA  | CHC-C1C-C2C | -2.93 | 118.61      | 126.72   |
| 14  | H     | 827  | CLA  | C4C-C3C-C2C | -2.93 | 102.62      | 106.90   |
| 14  | A     | 819  | CLA  | C1-C2-C3    | -2.93 | 120.97      | 126.04   |
| 14  | G     | 834  | CLA  | OBD-CAD-C3D | -2.93 | 123.11      | 127.98   |
| 14  | H     | 816  | CLA  | C3C-C4C-NC  | 2.93  | 113.86      | 110.57   |
| 14  | H     | 832  | CLA  | CAC-C3C-C4C | 2.93  | 128.61      | 124.81   |
| 14  | B     | 825  | CLA  | CMC-C2C-C1C | 2.93  | 129.50      | 125.04   |
| 14  | B     | 813  | CLA  | CHC-C1C-C2C | -2.93 | 118.62      | 126.72   |
| 17  | T     | 102  | BCR  | C36-C18-C19 | -2.93 | 113.46      | 118.08   |
| 14  | G     | 805  | CLA  | OBD-CAD-C3D | -2.93 | 123.12      | 127.98   |
| 14  | V     | 1201 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 14  | Z     | 812  | CLA  | O1D-CGD-CBD | -2.93 | 118.50      | 124.48   |
| 14  | U     | 1006 | CLA  | OBD-CAD-CBD | -2.93 | 121.71      | 125.89   |
| 14  | Z     | 831  | CLA  | OBD-CAD-C3D | -2.93 | 123.12      | 127.98   |
| 14  | Y     | 828  | CLA  | OBD-CAD-C3D | -2.93 | 123.12      | 127.98   |
| 14  | B     | 840  | CLA  | O2A-C1-C2   | 2.93  | 116.32      | 108.64   |
| 14  | G     | 804  | CLA  | CHB-C4A-NA  | 2.93  | 128.56      | 124.51   |
| 14  | G     | 802  | CLA  | C1-C2-C3    | -2.93 | 120.98      | 126.04   |
| 17  | J     | 103  | BCR  | C38-C26-C25 | 2.92  | 127.81      | 124.53   |
| 17  | B     | 851  | BCR  | C7-C8-C9    | -2.92 | 121.82      | 126.23   |
| 14  | L     | 202  | CLA  | C3C-C4C-NC  | 2.92  | 113.85      | 110.57   |
| 18  | G     | 852  | LHG  | O8-C23-C24  | 2.92  | 121.08      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Z     | 846  | BCR  | C24-C25-C26 | 2.92  | 128.54      | 121.46   |
| 14  | Z     | 803  | CLA  | O2D-CGD-O1D | -2.92 | 118.12      | 123.84   |
| 13  | A     | 801  | CL0  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 17  | Y     | 856  | BCR  | C34-C9-C8   | 2.92  | 122.68      | 118.08   |
| 14  | G     | 818  | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 14  | Z     | 838  | CLA  | O2A-CGA-CBA | 2.92  | 121.07      | 111.91   |
| 14  | Q     | 201  | CLA  | O1D-CGD-CBD | -2.92 | 118.51      | 124.48   |
| 14  | G     | 826  | CLA  | C4-C3-C5    | 2.92  | 120.18      | 115.27   |
| 14  | Y     | 824  | CLA  | CED-O2D-CGD | 2.92  | 122.54      | 115.94   |
| 17  | H     | 844  | BCR  | C3-C4-C5    | -2.92 | 108.87      | 114.08   |
| 17  | S     | 1104 | BCR  | C1-C6-C7    | 2.92  | 124.03      | 115.78   |
| 14  | B     | 834  | CLA  | OBD-CAD-C3D | -2.92 | 123.14      | 127.98   |
| 14  | Y     | 829  | CLA  | O2A-CGA-CBA | 2.91  | 121.05      | 111.91   |
| 14  | Y     | 826  | CLA  | CMB-C2B-C3B | 2.91  | 130.13      | 124.68   |
| 14  | G     | 818  | CLA  | C3C-C4C-NC  | 2.91  | 113.84      | 110.57   |
| 14  | Y     | 834  | CLA  | CMC-C2C-C1C | 2.91  | 129.47      | 125.04   |
| 14  | Y     | 809  | CLA  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |
| 14  | A     | 829  | CLA  | CHC-C1C-C2C | -2.91 | 118.67      | 126.72   |
| 14  | H     | 833  | CLA  | OBD-CAD-C3D | -2.91 | 123.15      | 127.98   |
| 14  | A     | 834  | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 14  | G     | 839  | CLA  | CMC-C2C-C1C | 2.91  | 129.47      | 125.04   |
| 17  | A     | 848  | BCR  | C27-C26-C25 | -2.91 | 118.51      | 122.73   |
| 14  | Z     | 839  | CLA  | C1-C2-C3    | -2.91 | 121.01      | 126.04   |
| 13  | G     | 801  | CL0  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 14  | A     | 831  | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.81   |
| 14  | Y     | 854  | CLA  | C1-C2-C3    | -2.91 | 121.01      | 126.04   |
| 17  | Q     | 202  | BCR  | C3-C4-C5    | -2.91 | 108.89      | 114.08   |
| 17  | B     | 843  | BCR  | C33-C5-C6   | -2.91 | 121.26      | 124.53   |
| 14  | A     | 839  | CLA  | CMA-C3A-C4A | 2.91  | 119.59      | 111.77   |
| 17  | K     | 102  | BCR  | C37-C22-C21 | -2.91 | 118.85      | 122.92   |
| 14  | d     | 201  | CLA  | C3C-C4C-NC  | 2.91  | 113.83      | 110.57   |
| 14  | G     | 824  | CLA  | CED-O2D-CGD | 2.91  | 122.51      | 115.94   |
| 14  | Y     | 804  | CLA  | CMA-C3A-C4A | 2.91  | 119.58      | 111.77   |
| 14  | L     | 207  | CLA  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 17  | L     | 203  | BCR  | C33-C5-C4   | 2.90  | 119.19      | 113.62   |
| 14  | g     | 101  | CLA  | CMA-C3A-C4A | 2.90  | 119.58      | 111.77   |
| 17  | Y     | 847  | BCR  | C40-C30-C25 | 2.90  | 115.01      | 110.30   |
| 15  | Z     | 840  | PQN  | C15-C13-C12 | -2.90 | 115.24      | 121.12   |
| 14  | A     | 815  | CLA  | C3C-C4C-NC  | 2.90  | 113.83      | 110.57   |
| 14  | A     | 833  | CLA  | OBD-CAD-CBD | -2.90 | 121.75      | 125.89   |
| 14  | B     | 823  | CLA  | CED-O2D-CGD | 2.90  | 122.50      | 115.94   |
| 13  | G     | 801  | CL0  | CMC-C2C-C1C | 2.90  | 129.46      | 125.04   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 822 | CLA  | CED-O2D-CGD | 2.90  | 122.50      | 115.94   |
| 17  | B     | 843 | BCR  | C8-C7-C6    | -2.90 | 119.06      | 127.20   |
| 14  | Z     | 827 | CLA  | CHC-C1C-C2C | -2.90 | 118.70      | 126.72   |
| 14  | H     | 806 | CLA  | O1D-CGD-CBD | -2.90 | 118.55      | 124.48   |
| 17  | A     | 847 | BCR  | C37-C22-C21 | -2.90 | 118.86      | 122.92   |
| 14  | A     | 836 | CLA  | C1-O2A-CGA  | 2.90  | 124.04      | 116.44   |
| 14  | B     | 840 | CLA  | C3C-C4C-NC  | 2.90  | 113.82      | 110.57   |
| 14  | Z     | 805 | CLA  | CED-O2D-CGD | 2.90  | 122.49      | 115.94   |
| 17  | d     | 203 | BCR  | C23-C24-C25 | -2.89 | 119.08      | 127.20   |
| 14  | Z     | 824 | CLA  | CMB-C2B-C3B | 2.89  | 130.09      | 124.68   |
| 14  | Z     | 809 | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 14  | Y     | 811 | CLA  | CAA-C2A-C3A | -2.89 | 104.86      | 112.78   |
| 14  | A     | 803 | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 14  | Y     | 832 | CLA  | C1-O2A-CGA  | 2.89  | 124.03      | 116.44   |
| 14  | B     | 831 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | Z     | 803 | CLA  | CMC-C2C-C1C | 2.89  | 129.44      | 125.04   |
| 15  | B     | 842 | PQN  | C2M-C2-C1   | 2.89  | 121.06      | 116.27   |
| 14  | A     | 806 | CLA  | O2A-C1-C2   | 2.89  | 116.23      | 108.64   |
| 14  | Y     | 814 | CLA  | CMB-C2B-C3B | 2.89  | 130.08      | 124.68   |
| 14  | Z     | 830 | CLA  | O2A-C1-C2   | 2.89  | 116.23      | 108.64   |
| 14  | Z     | 824 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | Q     | 201 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | A     | 821 | CLA  | CMC-C2C-C1C | 2.89  | 129.44      | 125.04   |
| 14  | B     | 809 | CLA  | CMA-C3A-C4A | 2.89  | 119.53      | 111.77   |
| 14  | A     | 815 | CLA  | CMC-C2C-C1C | 2.89  | 129.43      | 125.04   |
| 14  | Z     | 815 | CLA  | CMC-C2C-C1C | 2.88  | 129.43      | 125.04   |
| 14  | B     | 826 | CLA  | C4-C3-C5    | 2.88  | 120.12      | 115.27   |
| 14  | A     | 813 | CLA  | C1-C2-C3    | -2.88 | 121.06      | 126.04   |
| 14  | G     | 813 | CLA  | CMC-C2C-C1C | 2.88  | 129.43      | 125.04   |
| 14  | H     | 822 | CLA  | OBD-CAD-C3D | -2.88 | 123.19      | 127.98   |
| 14  | B     | 805 | CLA  | CMC-C2C-C1C | 2.88  | 129.43      | 125.04   |
| 14  | Y     | 810 | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 14  | A     | 812 | CLA  | CMA-C3A-C4A | 2.88  | 119.52      | 111.77   |
| 14  | B     | 825 | CLA  | OBD-CAD-CBD | -2.88 | 121.78      | 125.89   |
| 17  | B     | 848 | BCR  | C39-C30-C25 | -2.88 | 105.63      | 110.30   |
| 14  | J     | 101 | CLA  | CMA-C3A-C4A | 2.88  | 119.52      | 111.77   |
| 14  | A     | 822 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 14  | G     | 820 | CLA  | C1-O2A-CGA  | 2.88  | 124.00      | 116.44   |
| 14  | A     | 820 | CLA  | O1D-CGD-CBD | -2.88 | 118.59      | 124.48   |
| 14  | A     | 808 | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 14  | Y     | 804 | CLA  | OBD-CAD-C3D | -2.88 | 123.20      | 127.98   |
| 14  | B     | 833 | CLA  | CAA-CBA-CGA | -2.88 | 104.84      | 113.25   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 855  | CLA  | CED-O2D-CGD | 2.88  | 122.45      | 115.94   |
| 14  | Z     | 827  | CLA  | C1-O2A-CGA  | 2.88  | 123.99      | 116.44   |
| 14  | A     | 824  | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 14  | L     | 202  | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.81   |
| 14  | B     | 803  | CLA  | CMC-C2C-C1C | 2.87  | 129.42      | 125.04   |
| 17  | B     | 844  | BCR  | C39-C30-C25 | -2.87 | 105.64      | 110.30   |
| 14  | B     | 816  | CLA  | O2A-C1-C2   | 2.87  | 116.19      | 108.64   |
| 14  | H     | 823  | CLA  | O2D-CGD-O1D | -2.87 | 118.22      | 123.84   |
| 14  | H     | 826  | CLA  | C6-C5-C3    | -2.87 | 105.93      | 113.45   |
| 14  | Z     | 805  | CLA  | CHB-C4A-NA  | 2.87  | 128.48      | 124.51   |
| 17  | f     | 103  | BCR  | C1-C6-C5    | -2.87 | 118.57      | 122.61   |
| 13  | A     | 801  | CL0  | C5-C3-C2    | -2.87 | 115.32      | 121.12   |
| 17  | G     | 854  | BCR  | C29-C30-C25 | -2.87 | 106.07      | 110.48   |
| 14  | A     | 834  | CLA  | OBD-CAD-C3D | -2.87 | 123.22      | 127.98   |
| 14  | G     | 814  | CLA  | CHB-C4A-NA  | 2.87  | 128.47      | 124.51   |
| 14  | G     | 837  | CLA  | C3C-C4C-NC  | 2.86  | 113.78      | 110.57   |
| 14  | G     | 839  | CLA  | CMB-C2B-C3B | 2.86  | 130.04      | 124.68   |
| 14  | Y     | 843  | CLA  | CMC-C2C-C1C | 2.86  | 129.40      | 125.04   |
| 14  | G     | 818  | CLA  | C1-O2A-CGA  | 2.86  | 123.96      | 116.44   |
| 14  | A     | 815  | CLA  | CMA-C3A-C4A | 2.86  | 119.47      | 111.77   |
| 14  | H     | 812  | CLA  | CMA-C3A-C4A | 2.86  | 119.47      | 111.77   |
| 14  | Y     | 814  | CLA  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 14  | B     | 824  | CLA  | C1-C2-C3    | -2.86 | 121.09      | 126.04   |
| 14  | B     | 825  | CLA  | O2A-C1-C2   | 2.86  | 116.16      | 108.64   |
| 14  | U     | 1003 | CLA  | CMB-C2B-C3B | 2.86  | 130.03      | 124.68   |
| 14  | Z     | 829  | CLA  | CMA-C3A-C4A | 2.86  | 119.46      | 111.77   |
| 14  | A     | 839  | CLA  | O2D-CGD-O1D | -2.86 | 118.25      | 123.84   |
| 14  | A     | 831  | CLA  | O1D-CGD-CBD | -2.86 | 118.63      | 124.48   |
| 14  | G     | 806  | CLA  | C1-O2A-CGA  | 2.86  | 123.94      | 116.44   |
| 14  | H     | 819  | CLA  | CMB-C2B-C3B | 2.86  | 130.03      | 124.68   |
| 17  | f     | 104  | BCR  | C30-C25-C26 | -2.86 | 118.59      | 122.61   |
| 14  | Y     | 815  | CLA  | CMC-C2C-C1C | 2.86  | 129.39      | 125.04   |
| 14  | B     | 839  | CLA  | CMC-C2C-C1C | 2.86  | 129.39      | 125.04   |
| 14  | Z     | 836  | CLA  | OBD-CAD-CBD | -2.86 | 121.81      | 125.89   |
| 14  | B     | 823  | CLA  | O2D-CGD-CBD | 2.85  | 116.34      | 111.27   |
| 14  | Y     | 831  | CLA  | CED-O2D-CGD | 2.85  | 122.39      | 115.94   |
| 17  | Y     | 856  | BCR  | C37-C22-C23 | 2.85  | 122.57      | 118.08   |
| 14  | H     | 811  | CLA  | CMC-C2C-C1C | 2.85  | 129.38      | 125.04   |
| 14  | Z     | 825  | CLA  | CED-O2D-CGD | 2.85  | 122.39      | 115.94   |
| 14  | B     | 804  | CLA  | O2D-CGD-CBD | 2.85  | 116.33      | 111.27   |
| 14  | L     | 201  | CLA  | C1-O2A-CGA  | 2.85  | 123.92      | 116.44   |
| 14  | B     | 826  | CLA  | C3C-C4C-NC  | 2.85  | 113.77      | 110.57   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 840  | CLA  | C3C-C4C-NC  | 2.85  | 113.77      | 110.57   |
| 14  | G     | 814  | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 14  | A     | 817  | CLA  | CMA-C3A-C4A | 2.85  | 119.43      | 111.77   |
| 14  | Y     | 827  | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 17  | H     | 845  | BCR  | C36-C18-C19 | -2.84 | 113.60      | 118.08   |
| 14  | Y     | 841  | CLA  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 14  | B     | 810  | CLA  | CHC-C1C-C2C | -2.84 | 118.86      | 126.72   |
| 14  | H     | 807  | CLA  | CMC-C2C-C1C | 2.84  | 129.37      | 125.04   |
| 14  | H     | 835  | CLA  | O2A-CGA-CBA | 2.84  | 120.82      | 111.91   |
| 17  | H     | 842  | BCR  | C37-C22-C23 | 2.84  | 122.55      | 118.08   |
| 13  | G     | 801  | CL0  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 14  | A     | 805  | CLA  | CHB-C4A-NA  | 2.84  | 128.44      | 124.51   |
| 14  | H     | 811  | CLA  | CAA-C2A-C3A | -2.84 | 105.01      | 112.78   |
| 14  | Y     | 823  | CLA  | CMA-C3A-C4A | 2.84  | 119.40      | 111.77   |
| 14  | K     | 103  | CLA  | CHC-C1C-C2C | -2.84 | 118.87      | 126.72   |
| 14  | Y     | 837  | CLA  | CMA-C3A-C4A | 2.84  | 119.39      | 111.77   |
| 17  | L     | 208  | BCR  | C1-C6-C5    | -2.84 | 118.62      | 122.61   |
| 14  | h     | 205  | CLA  | CMC-C2C-C1C | 2.83  | 129.35      | 125.04   |
| 14  | Y     | 838  | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | G     | 842  | CLA  | O2D-CGD-CBD | 2.83  | 116.30      | 111.27   |
| 14  | Y     | 827  | CLA  | C4A-NA-C1A  | 2.83  | 107.98      | 106.71   |
| 14  | B     | 833  | CLA  | C4D-C3D-CAD | 2.83  | 110.05      | 108.47   |
| 14  | S     | 1103 | CLA  | C4-C3-C5    | 2.83  | 120.04      | 115.27   |
| 14  | H     | 801  | CLA  | C3C-C4C-NC  | 2.83  | 113.75      | 110.57   |
| 14  | B     | 810  | CLA  | O1D-CGD-CBD | -2.83 | 118.69      | 124.48   |
| 14  | H     | 816  | CLA  | C1-O2A-CGA  | 2.83  | 123.87      | 116.44   |
| 14  | W     | 1701 | CLA  | CMA-C3A-C4A | 2.83  | 119.38      | 111.77   |
| 14  | Z     | 823  | CLA  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 14  | A     | 823  | CLA  | CED-O2D-CGD | 2.83  | 122.34      | 115.94   |
| 14  | Y     | 807  | CLA  | CED-O2D-CGD | 2.83  | 122.34      | 115.94   |
| 14  | G     | 839  | CLA  | C6-C5-C3    | -2.83 | 106.03      | 113.45   |
| 14  | Z     | 836  | CLA  | CMA-C3A-C4A | 2.83  | 119.38      | 111.77   |
| 14  | A     | 842  | CLA  | CED-O2D-CGD | 2.83  | 122.33      | 115.94   |
| 14  | Y     | 826  | CLA  | C1-O2A-CGA  | 2.83  | 123.86      | 116.44   |
| 14  | B     | 806  | CLA  | C1-C2-C3    | -2.83 | 121.15      | 126.04   |
| 14  | S     | 1103 | CLA  | O2A-C1-C2   | 2.83  | 116.07      | 108.64   |
| 14  | H     | 804  | CLA  | C1-O2A-CGA  | 2.83  | 123.86      | 116.44   |
| 14  | G     | 807  | CLA  | CAC-C3C-C4C | 2.83  | 128.48      | 124.81   |
| 14  | H     | 810  | CLA  | C4D-C3D-CAD | 2.82  | 110.05      | 108.47   |
| 15  | G     | 844  | PQN  | C2M-C2-C1   | 2.82  | 120.95      | 116.27   |
| 17  | Z     | 842  | BCR  | C12-C13-C14 | 2.82  | 123.27      | 118.94   |
| 14  | G     | 836  | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 815  | CLA  | CMB-C2B-C3B | 2.82  | 129.96      | 124.68   |
| 14  | Y     | 835  | CLA  | C3C-C4C-NC  | 2.82  | 113.73      | 110.57   |
| 14  | B     | 807  | CLA  | CHC-C1C-C2C | -2.82 | 118.92      | 126.72   |
| 14  | G     | 805  | CLA  | CAA-C2A-C1A | -2.82 | 102.73      | 111.97   |
| 14  | H     | 809  | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 14  | H     | 826  | CLA  | CAC-C3C-C4C | 2.82  | 128.47      | 124.81   |
| 14  | H     | 818  | CLA  | C4A-NA-C1A  | 2.82  | 107.97      | 106.71   |
| 14  | B     | 808  | CLA  | OBD-CAD-C3D | -2.82 | 123.30      | 127.98   |
| 14  | Y     | 829  | CLA  | CAC-C3C-C4C | 2.81  | 128.46      | 124.81   |
| 14  | G     | 843  | CLA  | C1-C2-C3    | -2.81 | 122.20      | 126.75   |
| 17  | L     | 203  | BCR  | C38-C26-C25 | -2.81 | 121.37      | 124.53   |
| 17  | G     | 847  | BCR  | C33-C5-C6   | -2.81 | 121.37      | 124.53   |
| 14  | A     | 803  | CLA  | CMA-C3A-C4A | 2.81  | 119.33      | 111.77   |
| 17  | Z     | 843  | BCR  | C37-C22-C23 | 2.81  | 122.51      | 118.08   |
| 14  | Y     | 812  | CLA  | CMA-C3A-C4A | 2.81  | 119.33      | 111.77   |
| 14  | Y     | 834  | CLA  | CHD-C4C-C3C | -2.81 | 120.71      | 124.84   |
| 14  | G     | 823  | CLA  | C3C-C4C-NC  | 2.81  | 113.72      | 110.57   |
| 14  | B     | 813  | CLA  | O1D-CGD-CBD | -2.81 | 118.74      | 124.48   |
| 14  | Y     | 831  | CLA  | O2A-CGA-CBA | 2.81  | 120.72      | 111.91   |
| 17  | Q     | 204  | BCR  | C31-C1-C6   | -2.81 | 105.75      | 110.30   |
| 17  | e     | 101  | BCR  | C40-C30-C25 | 2.81  | 114.85      | 110.30   |
| 14  | G     | 836  | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 14  | Y     | 803  | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 14  | A     | 809  | CLA  | CHC-C1C-C2C | -2.81 | 118.96      | 126.72   |
| 14  | B     | 821  | CLA  | CMC-C2C-C1C | 2.81  | 129.31      | 125.04   |
| 14  | Y     | 808  | CLA  | O2A-C1-C2   | 2.81  | 116.01      | 108.64   |
| 14  | G     | 814  | CLA  | CGD-CBD-CAD | -2.81 | 101.65      | 110.73   |
| 14  | H     | 832  | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 17  | h     | 202  | BCR  | C3-C4-C5    | -2.81 | 109.07      | 114.08   |
| 14  | Y     | 806  | CLA  | CMC-C2C-C1C | 2.81  | 129.31      | 125.04   |
| 15  | H     | 839  | PQN  | C2M-C2-C1   | 2.80  | 120.92      | 116.27   |
| 17  | F     | 203  | BCR  | C31-C1-C6   | -2.80 | 105.75      | 110.30   |
| 14  | B     | 834  | CLA  | CED-O2D-CGD | 2.80  | 122.28      | 115.94   |
| 14  | A     | 813  | CLA  | CMB-C2B-C3B | 2.80  | 129.92      | 124.68   |
| 14  | A     | 814  | CLA  | CBA-CAA-C2A | 2.80  | 122.14      | 113.86   |
| 14  | U     | 1002 | CLA  | CMC-C2C-C1C | 2.80  | 129.30      | 125.04   |
| 14  | Z     | 813  | CLA  | CHC-C1C-C2C | -2.80 | 118.98      | 126.72   |
| 14  | Y     | 834  | CLA  | C3C-C4C-NC  | 2.80  | 113.71      | 110.57   |
| 14  | T     | 103  | CLA  | C4D-C3D-CAD | 2.80  | 110.03      | 108.47   |
| 17  | L     | 203  | BCR  | C34-C9-C10  | -2.80 | 119.00      | 122.92   |
| 14  | Y     | 806  | CLA  | CHB-C4A-NA  | 2.80  | 128.38      | 124.51   |
| 17  | f     | 105  | BCR  | C30-C25-C26 | -2.80 | 118.67      | 122.61   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 834  | CLA  | O2A-CGA-CBA | 2.80  | 120.69      | 111.91   |
| 14  | G     | 818  | CLA  | CMC-C2C-C1C | 2.80  | 129.30      | 125.04   |
| 14  | B     | 837  | CLA  | CMA-C3A-C4A | 2.80  | 119.29      | 111.77   |
| 14  | h     | 206  | CLA  | C3C-C4C-NC  | 2.80  | 113.71      | 110.57   |
| 14  | Y     | 842  | CLA  | CED-O2D-CGD | 2.80  | 122.26      | 115.94   |
| 14  | Y     | 804  | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 17  | Y     | 846  | BCR  | C3-C4-C5    | -2.79 | 109.09      | 114.08   |
| 14  | Z     | 838  | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.90   |
| 14  | B     | 840  | CLA  | C4D-C3D-CAD | 2.79  | 110.03      | 108.47   |
| 14  | Z     | 827  | CLA  | CMA-C3A-C4A | 2.79  | 119.28      | 111.77   |
| 14  | H     | 827  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 14  | h     | 205  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 14  | H     | 825  | CLA  | OBD-CAD-C3D | -2.79 | 123.35      | 127.98   |
| 14  | G     | 811  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 14  | Y     | 855  | CLA  | C1-O2A-CGA  | 2.79  | 123.77      | 116.44   |
| 14  | G     | 819  | CLA  | C1-C2-C3    | -2.79 | 121.22      | 126.04   |
| 14  | G     | 819  | CLA  | CHC-C1C-C2C | -2.79 | 119.00      | 126.72   |
| 14  | A     | 826  | CLA  | C1-O2A-CGA  | 2.79  | 123.76      | 116.44   |
| 14  | Z     | 814  | CLA  | CMA-C3A-C4A | 2.79  | 119.27      | 111.77   |
| 14  | A     | 832  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 14  | Z     | 838  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 14  | G     | 832  | CLA  | CHC-C1C-C2C | -2.79 | 119.01      | 126.72   |
| 14  | B     | 828  | CLA  | OBD-CAD-CBD | -2.79 | 121.91      | 125.89   |
| 14  | B     | 841  | CLA  | CBA-CAA-C2A | 2.79  | 122.09      | 113.86   |
| 14  | Z     | 839  | CLA  | CMB-C2B-C3B | 2.78  | 129.89      | 124.68   |
| 14  | Y     | 825  | CLA  | CAC-C3C-C4C | 2.78  | 128.42      | 124.81   |
| 14  | B     | 807  | CLA  | OBD-CAD-C3D | -2.78 | 123.36      | 127.98   |
| 14  | Y     | 820  | CLA  | C1-O2A-CGA  | 2.78  | 123.75      | 116.44   |
| 14  | S     | 1102 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 17  | A     | 845  | BCR  | C23-C24-C25 | -2.78 | 119.39      | 127.20   |
| 17  | f     | 104  | BCR  | C7-C6-C5    | -2.78 | 114.72      | 121.46   |
| 14  | A     | 820  | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 14  | B     | 841  | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 14  | Y     | 817  | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 14  | Y     | 822  | CLA  | CMA-C3A-C4A | 2.78  | 119.25      | 111.77   |
| 14  | B     | 826  | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 14  | B     | 837  | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 14  | A     | 817  | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 14  | Z     | 819  | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 14  | A     | 832  | CLA  | CHC-C1C-C2C | -2.78 | 119.03      | 126.72   |
| 14  | B     | 833  | CLA  | CMA-C3A-C4A | 2.78  | 119.25      | 111.77   |
| 14  | Y     | 821  | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | V     | 1201 | CLA  | O1D-CGD-CBD | -2.78 | 118.80      | 124.48   |
| 14  | L     | 202  | CLA  | CED-O2D-CGD | 2.78  | 122.22      | 115.94   |
| 14  | A     | 828  | CLA  | CED-O2D-CGD | 2.78  | 122.22      | 115.94   |
| 14  | G     | 839  | CLA  | CHB-C4A-NA  | 2.78  | 128.35      | 124.51   |
| 14  | L     | 202  | CLA  | CMA-C3A-C4A | 2.78  | 119.24      | 111.77   |
| 17  | Q     | 202  | BCR  | C30-C25-C26 | -2.78 | 118.70      | 122.61   |
| 14  | H     | 814  | CLA  | OBD-CAD-C3D | -2.78 | 123.37      | 127.98   |
| 14  | L     | 201  | CLA  | CHD-C4C-C3C | -2.78 | 120.76      | 124.84   |
| 17  | Z     | 843  | BCR  | C23-C24-C25 | -2.77 | 119.41      | 127.20   |
| 14  | Y     | 833  | CLA  | O2A-CGA-CBA | 2.77  | 120.61      | 111.91   |
| 14  | A     | 838  | CLA  | C3C-C4C-NC  | 2.77  | 113.68      | 110.57   |
| 14  | Z     | 824  | CLA  | OBD-CAD-CBD | -2.77 | 121.93      | 125.89   |
| 17  | M     | 101  | BCR  | C7-C6-C5    | -2.77 | 114.74      | 121.46   |
| 14  | H     | 822  | CLA  | C1-C2-C3    | -2.77 | 121.25      | 126.04   |
| 17  | G     | 850  | BCR  | C36-C18-C19 | -2.77 | 113.71      | 118.08   |
| 14  | B     | 826  | CLA  | C1-O2A-CGA  | 2.77  | 123.72      | 116.44   |
| 14  | H     | 831  | CLA  | OBD-CAD-CBD | -2.77 | 121.93      | 125.89   |
| 14  | B     | 832  | CLA  | O1D-CGD-CBD | -2.77 | 118.81      | 124.48   |
| 14  | Z     | 831  | CLA  | CED-O2D-CGD | 2.77  | 122.21      | 115.94   |
| 17  | H     | 841  | BCR  | C27-C26-C25 | -2.77 | 118.71      | 122.73   |
| 17  | i     | 101  | BCR  | C4-C5-C6    | -2.77 | 118.71      | 122.73   |
| 14  | A     | 841  | CLA  | C4-C3-C5    | 2.77  | 119.93      | 115.27   |
| 14  | G     | 833  | CLA  | CMA-C3A-C4A | 2.77  | 119.22      | 111.77   |
| 14  | G     | 822  | CLA  | CGD-CBD-CAD | -2.77 | 101.76      | 110.73   |
| 14  | H     | 812  | CLA  | O1D-CGD-CBD | -2.77 | 118.81      | 124.48   |
| 14  | L     | 206  | CLA  | O1D-CGD-CBD | -2.77 | 118.82      | 124.48   |
| 14  | B     | 827  | CLA  | O2A-C1-C2   | 2.77  | 115.92      | 108.64   |
| 17  | G     | 848  | BCR  | C37-C22-C21 | -2.77 | 119.04      | 122.92   |
| 19  | B     | 849  | LMG  | O1-C1-C2    | 2.77  | 112.63      | 108.30   |
| 14  | H     | 831  | CLA  | CMC-C2C-C1C | 2.77  | 129.25      | 125.04   |
| 14  | Y     | 805  | CLA  | O2A-CGA-CBA | 2.77  | 120.59      | 111.91   |
| 17  | Z     | 842  | BCR  | C38-C26-C27 | 2.77  | 118.93      | 113.62   |
| 14  | Y     | 820  | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 14  | Z     | 823  | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 17  | B     | 845  | BCR  | C3-C4-C5    | -2.77 | 109.14      | 114.08   |
| 14  | A     | 802  | CLA  | CAC-C3C-C4C | 2.77  | 128.40      | 124.81   |
| 14  | A     | 825  | CLA  | CMA-C3A-C4A | 2.76  | 119.20      | 111.77   |
| 14  | Z     | 813  | CLA  | CAA-C2A-C3A | -2.76 | 105.21      | 112.78   |
| 17  | Z     | 844  | BCR  | C36-C18-C19 | -2.76 | 113.73      | 118.08   |
| 14  | Y     | 824  | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.90   |
| 14  | G     | 841  | CLA  | C1-O2A-CGA  | 2.76  | 123.69      | 116.44   |
| 14  | G     | 837  | CLA  | C4-C3-C5    | 2.76  | 119.91      | 115.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 842  | CLA  | CHC-C1C-C2C | -2.76 | 119.09      | 126.72   |
| 17  | B     | 847  | BCR  | C33-C5-C6   | -2.76 | 121.43      | 124.53   |
| 14  | H     | 829  | CLA  | CMC-C2C-C1C | 2.76  | 129.24      | 125.04   |
| 14  | Z     | 806  | CLA  | CMC-C2C-C1C | 2.76  | 129.24      | 125.04   |
| 14  | Z     | 804  | CLA  | OBD-CAD-C3D | -2.76 | 123.40      | 127.98   |
| 14  | Z     | 803  | CLA  | CAC-C3C-C4C | 2.76  | 128.39      | 124.81   |
| 17  | G     | 849  | BCR  | C31-C1-C6   | 2.76  | 114.77      | 110.30   |
| 14  | S     | 1103 | CLA  | CMB-C2B-C3B | 2.76  | 129.84      | 124.68   |
| 14  | G     | 821  | CLA  | CMB-C2B-C3B | 2.76  | 129.84      | 124.68   |
| 18  | B     | 850  | LHG  | O8-C23-C24  | 2.76  | 120.56      | 111.91   |
| 14  | A     | 803  | CLA  | C6-C5-C3    | -2.76 | 106.23      | 113.45   |
| 14  | H     | 825  | CLA  | OBD-CAD-CBD | -2.76 | 121.96      | 125.89   |
| 17  | f     | 104  | BCR  | C33-C5-C6   | -2.76 | 121.43      | 124.53   |
| 14  | H     | 828  | CLA  | O1D-CGD-CBD | -2.75 | 118.85      | 124.48   |
| 17  | A     | 845  | BCR  | C33-C5-C6   | -2.75 | 121.44      | 124.53   |
| 14  | G     | 837  | CLA  | CAC-C3C-C4C | 2.75  | 128.38      | 124.81   |
| 14  | K     | 103  | CLA  | CAC-C3C-C4C | 2.75  | 128.38      | 124.81   |
| 14  | Y     | 803  | CLA  | O1D-CGD-CBD | -2.75 | 118.85      | 124.48   |
| 17  | i     | 101  | BCR  | C27-C26-C25 | -2.75 | 118.73      | 122.73   |
| 18  | Y     | 852  | LHG  | O7-C7-C8    | 2.75  | 117.43      | 111.50   |
| 14  | Z     | 812  | CLA  | OBD-CAD-CBD | -2.75 | 121.97      | 125.89   |
| 17  | B     | 851  | BCR  | C38-C26-C27 | 2.75  | 118.90      | 113.62   |
| 17  | A     | 847  | BCR  | C34-C9-C8   | 2.75  | 122.41      | 118.08   |
| 14  | B     | 818  | CLA  | CHC-C1C-C2C | -2.75 | 119.12      | 126.72   |
| 17  | S     | 1104 | BCR  | C31-C1-C6   | -2.75 | 105.84      | 110.30   |
| 14  | T     | 103  | CLA  | C3C-C4C-NC  | 2.75  | 113.65      | 110.57   |
| 14  | B     | 834  | CLA  | CMD-C2D-C3D | -2.75 | 119.54      | 124.68   |
| 14  | B     | 828  | CLA  | C1-O2A-CGA  | 2.75  | 123.65      | 116.44   |
| 14  | G     | 808  | CLA  | O1D-CGD-CBD | -2.75 | 118.86      | 124.48   |
| 14  | H     | 817  | CLA  | C4-C3-C5    | 2.75  | 119.89      | 115.27   |
| 14  | G     | 808  | CLA  | CHB-C4A-NA  | 2.75  | 128.31      | 124.51   |
| 14  | B     | 821  | CLA  | C3C-C4C-NC  | 2.75  | 113.65      | 110.57   |
| 14  | Z     | 820  | CLA  | CGD-CBD-CAD | 2.74  | 119.62      | 110.73   |
| 17  | i     | 101  | BCR  | C30-C25-C26 | -2.74 | 118.75      | 122.61   |
| 14  | B     | 808  | CLA  | C5-C3-C2    | -2.74 | 115.57      | 121.12   |
| 14  | T     | 103  | CLA  | CED-O2D-CGD | 2.74  | 122.14      | 115.94   |
| 14  | H     | 832  | CLA  | CHC-C1C-C2C | -2.74 | 119.14      | 126.72   |
| 14  | Y     | 826  | CLA  | C3C-C4C-NC  | 2.74  | 113.65      | 110.57   |
| 14  | H     | 805  | CLA  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 14  | G     | 822  | CLA  | C1-C2-C3    | -2.74 | 121.30      | 126.04   |
| 14  | B     | 816  | CLA  | CED-O2D-CGD | 2.74  | 122.14      | 115.94   |
| 17  | L     | 208  | BCR  | C7-C8-C9    | -2.74 | 122.09      | 126.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 830  | CLA  | CHC-C1C-C2C | -2.74 | 119.14      | 126.72   |
| 14  | Z     | 820  | CLA  | CED-O2D-CGD | 2.74  | 122.13      | 115.94   |
| 14  | Y     | 821  | CLA  | CAC-C3C-C4C | 2.74  | 128.36      | 124.81   |
| 14  | B     | 835  | CLA  | CED-O2D-CGD | 2.74  | 122.13      | 115.94   |
| 14  | B     | 829  | CLA  | CHC-C1C-C2C | -2.74 | 119.15      | 126.72   |
| 14  | G     | 825  | CLA  | CED-O2D-CGD | 2.74  | 122.13      | 115.94   |
| 14  | H     | 825  | CLA  | C1-C2-C3    | -2.74 | 121.31      | 126.04   |
| 14  | A     | 830  | CLA  | OBD-CAD-C3D | -2.74 | 123.44      | 127.98   |
| 14  | X     | 1701 | CLA  | CMB-C2B-C3B | 2.74  | 129.80      | 124.68   |
| 18  | A     | 851  | LHG  | O8-C23-C24  | 2.74  | 120.49      | 111.91   |
| 14  | B     | 820  | CLA  | CHC-C1C-C2C | -2.73 | 119.16      | 126.72   |
| 14  | H     | 825  | CLA  | CAC-C3C-C4C | 2.73  | 128.36      | 124.81   |
| 14  | Z     | 820  | CLA  | CMB-C2B-C3B | 2.73  | 129.79      | 124.68   |
| 17  | B     | 847  | BCR  | C23-C22-C21 | 2.73  | 123.14      | 118.94   |
| 14  | L     | 205  | CLA  | C4A-NA-C1A  | 2.73  | 107.94      | 106.71   |
| 14  | H     | 823  | CLA  | CED-O2D-CGD | 2.73  | 122.12      | 115.94   |
| 14  | G     | 813  | CLA  | C1-C2-C3    | -2.73 | 121.32      | 126.04   |
| 14  | A     | 807  | CLA  | C1-C2-C3    | -2.73 | 121.32      | 126.04   |
| 14  | B     | 802  | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 14  | H     | 815  | CLA  | CMC-C2C-C1C | 2.73  | 129.20      | 125.04   |
| 14  | Z     | 830  | CLA  | OBD-CAD-C3D | -2.73 | 123.45      | 127.98   |
| 14  | A     | 841  | CLA  | CHC-C1C-C2C | -2.73 | 119.17      | 126.72   |
| 17  | h     | 202  | BCR  | C12-C13-C14 | 2.73  | 123.13      | 118.94   |
| 14  | g     | 101  | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 14  | H     | 807  | CLA  | CAA-C2A-C3A | -2.73 | 105.30      | 112.78   |
| 14  | A     | 811  | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 17  | Z     | 841  | BCR  | C37-C22-C21 | -2.73 | 119.10      | 122.92   |
| 14  | B     | 828  | CLA  | C5-C3-C2    | -2.73 | 115.59      | 121.12   |
| 14  | A     | 852  | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 14  | f     | 102  | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 17  | F     | 201  | BCR  | C8-C9-C10   | -2.73 | 114.76      | 118.94   |
| 15  | G     | 844  | PQN  | C21-C20-C18 | -2.73 | 107.11      | 115.92   |
| 14  | G     | 804  | CLA  | CMC-C2C-C1C | 2.72  | 129.19      | 125.04   |
| 14  | Y     | 854  | CLA  | C3C-C4C-NC  | 2.72  | 113.62      | 110.57   |
| 17  | d     | 203  | BCR  | C33-C5-C6   | -2.72 | 121.47      | 124.53   |
| 14  | H     | 835  | CLA  | O2A-C1-C2   | 2.72  | 115.79      | 108.64   |
| 14  | Y     | 834  | CLA  | CHB-C4A-NA  | 2.72  | 128.28      | 124.51   |
| 14  | S     | 1102 | CLA  | CHC-C1C-C2C | -2.72 | 119.20      | 126.72   |
| 14  | Z     | 823  | CLA  | CMA-C3A-C4A | 2.72  | 119.08      | 111.77   |
| 17  | G     | 846  | BCR  | C37-C22-C23 | 2.72  | 122.36      | 118.08   |
| 14  | G     | 807  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | B     | 822  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 830  | CLA  | CED-O2D-CGD | 2.72  | 122.09      | 115.94   |
| 14  | Z     | 821  | CLA  | C4-C3-C5    | 2.72  | 119.84      | 115.27   |
| 17  | Z     | 842  | BCR  | C30-C25-C26 | -2.72 | 118.78      | 122.61   |
| 14  | d     | 201  | CLA  | OBD-CAD-CBD | -2.72 | 122.01      | 125.89   |
| 17  | e     | 101  | BCR  | C38-C26-C25 | -2.72 | 121.48      | 124.53   |
| 14  | H     | 817  | CLA  | CHB-C4A-NA  | 2.71  | 128.27      | 124.51   |
| 14  | Z     | 823  | CLA  | CAA-C2A-C1A | -2.71 | 103.08      | 111.97   |
| 14  | A     | 830  | CLA  | CHC-C1C-C2C | -2.71 | 119.22      | 126.72   |
| 14  | Z     | 823  | CLA  | OBD-CAD-C3D | -2.71 | 123.48      | 127.98   |
| 14  | Z     | 802  | CLA  | C5-C3-C2    | -2.71 | 115.63      | 121.12   |
| 14  | Z     | 802  | CLA  | OBD-CAD-CBD | -2.71 | 122.02      | 125.89   |
| 14  | B     | 809  | CLA  | O2A-C1-C2   | 2.71  | 115.76      | 108.64   |
| 14  | B     | 815  | CLA  | CAA-C2A-C3A | -2.71 | 105.35      | 112.78   |
| 14  | A     | 828  | CLA  | CMA-C3A-C4A | 2.71  | 119.06      | 111.77   |
| 14  | H     | 828  | CLA  | CMC-C2C-C1C | 2.71  | 129.17      | 125.04   |
| 14  | G     | 829  | CLA  | C1-C2-C3    | -2.71 | 121.36      | 126.04   |
| 14  | A     | 804  | CLA  | C1-O2A-CGA  | 2.71  | 123.55      | 116.44   |
| 14  | G     | 814  | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 17  | J     | 103  | BCR  | C12-C13-C14 | 2.71  | 123.10      | 118.94   |
| 17  | L     | 209  | BCR  | C33-C5-C4   | 2.71  | 118.82      | 113.62   |
| 14  | H     | 829  | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 17  | A     | 848  | BCR  | C28-C27-C26 | -2.71 | 109.24      | 114.08   |
| 14  | Z     | 805  | CLA  | CAA-C2A-C3A | -2.71 | 105.36      | 112.78   |
| 14  | S     | 1103 | CLA  | C4-C3-C2    | -2.71 | 116.73      | 123.68   |
| 14  | Z     | 811  | CLA  | CMA-C3A-C4A | 2.71  | 119.05      | 111.77   |
| 14  | H     | 826  | CLA  | OBD-CAD-C3D | -2.71 | 123.49      | 127.98   |
| 14  | H     | 827  | CLA  | CED-O2D-CGD | 2.71  | 122.06      | 115.94   |
| 17  | i     | 101  | BCR  | C2-C1-C6    | 2.71  | 114.65      | 110.48   |
| 14  | F     | 202  | CLA  | CHC-C1C-C2C | -2.71 | 119.24      | 126.72   |
| 14  | H     | 824  | CLA  | CBC-CAC-C3C | -2.71 | 104.97      | 112.43   |
| 14  | A     | 823  | CLA  | C1-C2-C3    | -2.70 | 122.38      | 126.75   |
| 14  | G     | 812  | CLA  | C4-C3-C5    | 2.70  | 119.82      | 115.27   |
| 14  | Z     | 828  | CLA  | CMA-C3A-C4A | 2.70  | 119.04      | 111.77   |
| 14  | A     | 814  | CLA  | CHC-C1C-C2C | -2.70 | 119.25      | 126.72   |
| 14  | A     | 802  | CLA  | CBC-CAC-C3C | -2.70 | 104.98      | 112.43   |
| 14  | B     | 815  | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 14  | G     | 842  | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 14  | A     | 833  | CLA  | C1-O2A-CGA  | -2.70 | 109.36      | 116.44   |
| 17  | G     | 848  | BCR  | C34-C9-C8   | 2.70  | 122.33      | 118.08   |
| 14  | B     | 810  | CLA  | CBC-CAC-C3C | -2.70 | 104.99      | 112.43   |
| 14  | L     | 202  | CLA  | CMC-C2C-C1C | 2.70  | 129.15      | 125.04   |
| 14  | H     | 823  | CLA  | CAC-C3C-C4C | 2.70  | 128.31      | 124.81   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 819  | CLA  | CMA-C3A-C4A | 2.70  | 119.03      | 111.77   |
| 14  | G     | 815  | CLA  | CMA-C3A-C4A | 2.70  | 119.03      | 111.77   |
| 14  | G     | 832  | CLA  | O2D-CGD-O1D | -2.70 | 118.56      | 123.84   |
| 14  | G     | 841  | CLA  | CAC-C3C-C4C | 2.70  | 128.31      | 124.81   |
| 14  | A     | 812  | CLA  | CHC-C1C-C2C | -2.70 | 119.26      | 126.72   |
| 14  | A     | 813  | CLA  | CHC-C1C-C2C | -2.70 | 119.26      | 126.72   |
| 17  | H     | 844  | BCR  | C7-C6-C5    | -2.70 | 114.93      | 121.46   |
| 14  | Z     | 832  | CLA  | C3C-C4C-NC  | 2.70  | 113.59      | 110.57   |
| 14  | Z     | 809  | CLA  | C1-O2A-CGA  | 2.70  | 123.52      | 116.44   |
| 14  | Z     | 823  | CLA  | C4-C3-C2    | -2.69 | 116.77      | 123.68   |
| 14  | B     | 801  | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 17  | R     | 102  | BCR  | C32-C1-C6   | -2.69 | 105.93      | 110.30   |
| 14  | Z     | 817  | CLA  | O1D-CGD-CBD | -2.69 | 118.97      | 124.48   |
| 14  | A     | 808  | CLA  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 14  | G     | 827  | CLA  | C4D-C3D-CAD | 2.69  | 109.97      | 108.47   |
| 14  | B     | 802  | CLA  | CHB-C4A-NA  | 2.69  | 128.24      | 124.51   |
| 14  | G     | 807  | CLA  | C3C-C4C-NC  | 2.69  | 113.59      | 110.57   |
| 14  | B     | 826  | CLA  | CHC-C1C-C2C | -2.69 | 119.27      | 126.72   |
| 14  | A     | 852  | CLA  | CMA-C3A-C4A | 2.69  | 119.01      | 111.77   |
| 14  | H     | 818  | CLA  | CED-O2D-CGD | 2.69  | 122.03      | 115.94   |
| 17  | G     | 847  | BCR  | C37-C22-C23 | 2.69  | 122.32      | 118.08   |
| 14  | Z     | 803  | CLA  | CHB-C4A-NA  | 2.69  | 128.24      | 124.51   |
| 14  | Z     | 833  | CLA  | CMA-C3A-C4A | 2.69  | 119.01      | 111.77   |
| 14  | G     | 843  | CLA  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 14  | B     | 820  | CLA  | CMA-C3A-C4A | 2.69  | 119.01      | 111.77   |
| 14  | Y     | 826  | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | G     | 817  | CLA  | CED-O2D-CGD | 2.69  | 122.03      | 115.94   |
| 17  | G     | 849  | BCR  | C37-C22-C23 | 2.69  | 122.32      | 118.08   |
| 14  | Y     | 840  | CLA  | CAC-C3C-C4C | 2.69  | 128.30      | 124.81   |
| 17  | I     | 101  | BCR  | C34-C9-C8   | 2.69  | 122.31      | 118.08   |
| 14  | Y     | 843  | CLA  | CMA-C3A-C4A | 2.69  | 119.00      | 111.77   |
| 14  | H     | 825  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 17  | Z     | 843  | BCR  | C15-C14-C13 | -2.69 | 123.47      | 127.31   |
| 17  | S     | 1104 | BCR  | C7-C8-C9    | -2.69 | 122.17      | 126.23   |
| 17  | L     | 203  | BCR  | C8-C7-C6    | -2.69 | 119.65      | 127.20   |
| 14  | A     | 823  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | Y     | 835  | CLA  | CMA-C3A-C4A | 2.69  | 119.00      | 111.77   |
| 14  | Y     | 826  | CLA  | O1D-CGD-CBD | -2.69 | 118.99      | 124.48   |
| 14  | Z     | 801  | CLA  | CMB-C2B-C3B | 2.69  | 129.70      | 124.68   |
| 14  | A     | 819  | CLA  | O2D-CGD-O1D | -2.69 | 118.59      | 123.84   |
| 14  | H     | 812  | CLA  | CMC-C2C-C1C | 2.69  | 129.13      | 125.04   |
| 14  | Z     | 835  | CLA  | CMC-C2C-C1C | 2.69  | 129.13      | 125.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 842  | CLA  | CMA-C3A-C4A | 2.68  | 118.99      | 111.77   |
| 14  | G     | 808  | CLA  | CED-O2D-CGD | 2.68  | 122.01      | 115.94   |
| 14  | h     | 201  | CLA  | CMA-C3A-C4A | 2.68  | 118.98      | 111.77   |
| 14  | B     | 833  | CLA  | O2A-C1-C2   | 2.68  | 115.69      | 108.64   |
| 17  | Y     | 849  | BCR  | C7-C8-C9    | -2.68 | 122.18      | 126.23   |
| 14  | h     | 206  | CLA  | C1-O2A-CGA  | 2.68  | 123.48      | 116.44   |
| 14  | Z     | 834  | CLA  | C3C-C4C-NC  | 2.68  | 113.58      | 110.57   |
| 14  | Y     | 820  | CLA  | CHC-C1C-C2C | -2.68 | 119.31      | 126.72   |
| 14  | A     | 834  | CLA  | CMC-C2C-C1C | 2.68  | 129.12      | 125.04   |
| 14  | Z     | 804  | CLA  | CHC-C1C-C2C | -2.68 | 119.31      | 126.72   |
| 14  | G     | 841  | CLA  | CMA-C3A-C4A | 2.68  | 118.97      | 111.77   |
| 14  | j     | 102  | CLA  | CED-O2D-CGD | 2.68  | 122.00      | 115.94   |
| 14  | G     | 823  | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 14  | S     | 1103 | CLA  | OBD-CAD-CBD | -2.68 | 122.07      | 125.89   |
| 14  | Y     | 802  | CLA  | CMC-C2C-C1C | 2.68  | 129.12      | 125.04   |
| 14  | Y     | 828  | CLA  | C4-C3-C5    | 2.68  | 119.77      | 115.27   |
| 14  | Y     | 823  | CLA  | C3C-C4C-NC  | 2.68  | 113.57      | 110.57   |
| 14  | H     | 831  | CLA  | CAC-C3C-C4C | 2.68  | 128.28      | 124.81   |
| 14  | A     | 841  | CLA  | O2D-CGD-CBD | 2.68  | 116.02      | 111.27   |
| 17  | H     | 848  | BCR  | C29-C30-C25 | -2.68 | 106.36      | 110.48   |
| 14  | Z     | 815  | CLA  | CAC-C3C-C4C | 2.68  | 128.28      | 124.81   |
| 14  | B     | 820  | CLA  | O1D-CGD-CBD | -2.68 | 119.01      | 124.48   |
| 14  | B     | 831  | CLA  | CHC-C1C-C2C | -2.67 | 119.33      | 126.72   |
| 14  | H     | 827  | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 14  | G     | 816  | CLA  | C1-O2A-CGA  | 2.67  | 123.46      | 116.44   |
| 14  | H     | 832  | CLA  | CMB-C2B-C3B | 2.67  | 129.68      | 124.68   |
| 14  | A     | 809  | CLA  | CMD-C2D-C3D | -2.67 | 119.68      | 124.68   |
| 14  | A     | 837  | CLA  | C3C-C4C-NC  | 2.67  | 113.57      | 110.57   |
| 17  | G     | 848  | BCR  | C30-C25-C24 | 2.67  | 123.34      | 115.78   |
| 14  | G     | 811  | CLA  | C3C-C4C-NC  | 2.67  | 113.57      | 110.57   |
| 14  | Y     | 831  | CLA  | CHC-C1C-C2C | -2.67 | 119.33      | 126.72   |
| 14  | A     | 831  | CLA  | CMA-C3A-C4A | 2.67  | 118.95      | 111.77   |
| 14  | H     | 806  | CLA  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 13  | Y     | 801  | CL0  | C1-O2A-CGA  | 2.67  | 123.45      | 116.44   |
| 17  | Y     | 846  | BCR  | C32-C1-C6   | -2.67 | 105.97      | 110.30   |
| 17  | A     | 847  | BCR  | C3-C4-C5    | -2.67 | 109.31      | 114.08   |
| 17  | B     | 844  | BCR  | C3-C4-C5    | -2.67 | 109.31      | 114.08   |
| 14  | Z     | 811  | CLA  | OBD-CAD-C3D | -2.67 | 123.55      | 127.98   |
| 14  | G     | 840  | CLA  | C1-C2-C3    | -2.67 | 122.43      | 126.75   |
| 14  | Z     | 818  | CLA  | CED-O2D-CGD | 2.67  | 121.97      | 115.94   |
| 14  | B     | 837  | CLA  | CHC-C1C-C2C | -2.67 | 119.34      | 126.72   |
| 14  | Z     | 826  | CLA  | C7-C6-C5    | -2.67 | 106.11      | 113.36   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 808  | CLA  | CHC-C1C-C2C | -2.67 | 119.34      | 126.72   |
| 14  | G     | 811  | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 14  | H     | 828  | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 14  | B     | 835  | CLA  | C3C-C4C-NC  | 2.67  | 113.56      | 110.57   |
| 14  | Z     | 820  | CLA  | C4A-NA-C1A  | 2.67  | 107.91      | 106.71   |
| 14  | h     | 205  | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 14  | H     | 807  | CLA  | C3A-C2A-C1A | 2.67  | 105.33      | 101.34   |
| 14  | Z     | 822  | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 14  | W     | 1701 | CLA  | CMC-C2C-C1C | 2.67  | 129.10      | 125.04   |
| 14  | B     | 828  | CLA  | CAC-C3C-C4C | 2.67  | 128.27      | 124.81   |
| 14  | H     | 801  | CLA  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 14  | H     | 834  | CLA  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 14  | A     | 819  | CLA  | CMC-C2C-C1C | 2.66  | 129.10      | 125.04   |
| 17  | f     | 105  | BCR  | C38-C26-C25 | -2.66 | 121.54      | 124.53   |
| 14  | Y     | 812  | CLA  | OBD-CAD-C3D | -2.66 | 123.56      | 127.98   |
| 14  | G     | 820  | CLA  | OBD-CAD-C3D | -2.66 | 123.56      | 127.98   |
| 17  | S     | 1104 | BCR  | C7-C6-C5    | -2.66 | 115.01      | 121.46   |
| 14  | B     | 808  | CLA  | O1D-CGD-CBD | -2.66 | 119.04      | 124.48   |
| 14  | G     | 811  | CLA  | CMC-C2C-C1C | 2.66  | 129.09      | 125.04   |
| 14  | A     | 805  | CLA  | CHC-C1C-C2C | -2.66 | 119.36      | 126.72   |
| 13  | Y     | 801  | CL0  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 14  | H     | 822  | CLA  | CAA-CBA-CGA | -2.66 | 105.48      | 113.25   |
| 14  | B     | 821  | CLA  | CMA-C3A-C4A | 2.66  | 118.92      | 111.77   |
| 14  | A     | 812  | CLA  | C4-C3-C5    | 2.66  | 119.75      | 115.27   |
| 14  | Y     | 802  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 14  | G     | 804  | CLA  | CHC-C1C-C2C | -2.66 | 119.37      | 126.72   |
| 14  | Q     | 201  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 18  | j     | 101  | LHG  | O8-C23-C24  | 2.66  | 120.24      | 111.91   |
| 17  | R     | 102  | BCR  | C38-C26-C25 | -2.65 | 121.55      | 124.53   |
| 17  | e     | 101  | BCR  | C31-C1-C6   | 2.65  | 114.60      | 110.30   |
| 14  | Z     | 814  | CLA  | CAC-C3C-C4C | 2.65  | 128.25      | 124.81   |
| 14  | G     | 825  | CLA  | C11-C10-C8  | -2.65 | 107.34      | 115.92   |
| 14  | A     | 807  | CLA  | CMC-C2C-C1C | 2.65  | 129.08      | 125.04   |
| 17  | R     | 102  | BCR  | C2-C1-C6    | 2.65  | 114.56      | 110.48   |
| 17  | G     | 854  | BCR  | C40-C30-C25 | 2.65  | 114.60      | 110.30   |
| 18  | Y     | 853  | LHG  | C5-O7-C7    | -2.65 | 112.96      | 117.90   |
| 17  | G     | 849  | BCR  | C7-C8-C9    | -2.65 | 122.23      | 126.23   |
| 14  | G     | 839  | CLA  | OBD-CAD-CBD | -2.65 | 122.11      | 125.89   |
| 14  | H     | 838  | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 17  | J     | 103  | BCR  | C30-C25-C26 | -2.65 | 118.89      | 122.61   |
| 14  | T     | 101  | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 14  | G     | 815  | CLA  | O1D-CGD-CBD | -2.65 | 119.07      | 124.48   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 833  | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 17  | G     | 849  | BCR  | C30-C25-C26 | -2.65 | 118.89      | 122.61   |
| 14  | Z     | 826  | CLA  | CBC-CAC-C3C | -2.65 | 105.14      | 112.43   |
| 14  | Z     | 823  | CLA  | CHC-C1C-C2C | -2.64 | 119.41      | 126.72   |
| 14  | B     | 809  | CLA  | CED-O2D-CGD | 2.64  | 121.92      | 115.94   |
| 17  | Z     | 845  | BCR  | C4-C5-C6    | -2.64 | 118.89      | 122.73   |
| 14  | A     | 838  | CLA  | CMA-C3A-C4A | 2.64  | 118.88      | 111.77   |
| 17  | f     | 104  | BCR  | C30-C25-C24 | 2.64  | 123.25      | 115.78   |
| 14  | A     | 820  | CLA  | C3C-C4C-NC  | 2.64  | 113.53      | 110.57   |
| 17  | f     | 103  | BCR  | C31-C1-C6   | -2.64 | 106.02      | 110.30   |
| 17  | I     | 101  | BCR  | C37-C22-C21 | -2.64 | 119.23      | 122.92   |
| 14  | A     | 833  | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 14  | H     | 820  | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 14  | Z     | 808  | CLA  | C6-C5-C3    | -2.64 | 106.54      | 113.45   |
| 14  | Z     | 804  | CLA  | CMD-C2D-C3D | -2.64 | 119.74      | 124.68   |
| 14  | A     | 807  | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 14  | Z     | 835  | CLA  | CMA-C3A-C4A | 2.64  | 118.86      | 111.77   |
| 14  | T     | 101  | CLA  | CHC-C1C-C2C | -2.64 | 119.43      | 126.72   |
| 14  | Q     | 203  | CLA  | CHC-C1C-C2C | -2.63 | 119.43      | 126.72   |
| 14  | Y     | 809  | CLA  | CMD-C2D-C3D | -2.63 | 119.75      | 124.68   |
| 17  | B     | 848  | BCR  | C3-C4-C5    | -2.63 | 109.37      | 114.08   |
| 14  | G     | 818  | CLA  | CAC-C3C-C4C | 2.63  | 128.23      | 124.81   |
| 14  | Y     | 806  | CLA  | CBC-CAC-C3C | -2.63 | 105.17      | 112.43   |
| 14  | G     | 837  | CLA  | CMB-C2B-C3B | 2.63  | 129.60      | 124.68   |
| 17  | L     | 208  | BCR  | C37-C22-C23 | 2.63  | 122.22      | 118.08   |
| 14  | H     | 809  | CLA  | CAC-C3C-C4C | 2.63  | 128.22      | 124.81   |
| 14  | g     | 102  | CLA  | CMA-C3A-C4A | 2.63  | 118.84      | 111.77   |
| 17  | Z     | 843  | BCR  | C31-C1-C6   | -2.63 | 106.03      | 110.30   |
| 14  | H     | 810  | CLA  | CED-O2D-CGD | 2.63  | 121.89      | 115.94   |
| 14  | U     | 1002 | CLA  | CHD-C4C-C3C | -2.63 | 120.97      | 124.84   |
| 17  | A     | 847  | BCR  | C38-C26-C25 | -2.63 | 121.58      | 124.53   |
| 14  | A     | 833  | CLA  | C3C-C4C-NC  | 2.63  | 113.52      | 110.57   |
| 14  | U     | 1004 | CLA  | CHC-C1C-C2C | -2.63 | 119.45      | 126.72   |
| 14  | A     | 841  | CLA  | OBD-CAD-C3D | -2.63 | 123.62      | 127.98   |
| 14  | B     | 803  | CLA  | O2A-C1-C2   | 2.63  | 115.54      | 108.64   |
| 14  | H     | 802  | CLA  | C5-C3-C2    | -2.63 | 115.80      | 121.12   |
| 14  | Z     | 809  | CLA  | CED-O2D-CGD | 2.63  | 121.88      | 115.94   |
| 14  | Z     | 802  | CLA  | C4-C3-C5    | 2.63  | 119.69      | 115.27   |
| 14  | A     | 835  | CLA  | CMB-C2B-C3B | 2.63  | 129.59      | 124.68   |
| 17  | L     | 203  | BCR  | C37-C22-C23 | 2.63  | 122.22      | 118.08   |
| 14  | G     | 838  | CLA  | CHC-C1C-C2C | -2.63 | 119.46      | 126.72   |
| 14  | h     | 207  | CLA  | C4-C3-C5    | 2.63  | 119.69      | 115.27   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | H     | 848  | BCR  | C35-C13-C12 | 2.63  | 122.21      | 118.08   |
| 14  | Y     | 821  | CLA  | C1-O2A-CGA  | 2.62  | 123.33      | 116.44   |
| 17  | B     | 848  | BCR  | C30-C25-C26 | -2.62 | 118.92      | 122.61   |
| 14  | H     | 810  | CLA  | CMC-C2C-C1C | 2.62  | 129.03      | 125.04   |
| 14  | Z     | 808  | CLA  | O2D-CGD-CBD | 2.62  | 115.93      | 111.27   |
| 14  | H     | 822  | CLA  | O2A-C1-C2   | 2.62  | 115.53      | 108.64   |
| 14  | Y     | 836  | CLA  | CMB-C2B-C3B | 2.62  | 129.59      | 124.68   |
| 14  | H     | 837  | CLA  | CED-O2D-CGD | 2.62  | 121.87      | 115.94   |
| 14  | U     | 1003 | CLA  | C1-C2-C3    | -2.62 | 121.51      | 126.04   |
| 14  | f     | 102  | CLA  | CMA-C3A-C4A | 2.62  | 118.81      | 111.77   |
| 14  | H     | 829  | CLA  | CMB-C2B-C3B | 2.62  | 129.58      | 124.68   |
| 14  | H     | 829  | CLA  | C3C-C4C-NC  | 2.62  | 113.51      | 110.57   |
| 14  | B     | 828  | CLA  | CHC-C1C-C2C | -2.62 | 119.49      | 126.72   |
| 17  | B     | 847  | BCR  | C1-C6-C5    | -2.62 | 118.93      | 122.61   |
| 14  | H     | 812  | CLA  | CHC-C1C-C2C | -2.61 | 119.49      | 126.72   |
| 17  | G     | 848  | BCR  | C29-C30-C25 | -2.61 | 106.46      | 110.48   |
| 14  | Y     | 821  | CLA  | OBD-CAD-C3D | -2.61 | 123.64      | 127.98   |
| 14  | A     | 824  | CLA  | C4C-C3C-C2C | -2.61 | 103.09      | 106.90   |
| 17  | H     | 844  | BCR  | C4-C5-C6    | -2.61 | 118.94      | 122.73   |
| 14  | H     | 830  | CLA  | CMC-C2C-C1C | 2.61  | 129.02      | 125.04   |
| 17  | F     | 201  | BCR  | C37-C22-C23 | 2.61  | 122.19      | 118.08   |
| 14  | G     | 836  | CLA  | CHC-C1C-C2C | -2.61 | 119.50      | 126.72   |
| 17  | Y     | 848  | BCR  | C3-C4-C5    | -2.61 | 109.42      | 114.08   |
| 14  | B     | 811  | CLA  | CMA-C3A-C4A | 2.61  | 118.79      | 111.77   |
| 14  | G     | 820  | CLA  | CHC-C1C-C2C | -2.61 | 119.50      | 126.72   |
| 14  | G     | 804  | CLA  | C1-O2A-CGA  | 2.61  | 123.29      | 116.44   |
| 14  | Q     | 201  | CLA  | CHC-C1C-C2C | -2.61 | 119.50      | 126.72   |
| 13  | Y     | 801  | CL0  | C4D-C3D-CAD | 2.61  | 109.92      | 108.47   |
| 14  | h     | 205  | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 17  | G     | 847  | BCR  | C36-C18-C19 | -2.61 | 113.97      | 118.08   |
| 14  | Y     | 840  | CLA  | CMA-C3A-C4A | 2.61  | 118.78      | 111.77   |
| 17  | L     | 203  | BCR  | C1-C6-C5    | -2.61 | 118.94      | 122.61   |
| 14  | A     | 827  | CLA  | O2A-C1-C2   | 2.61  | 115.48      | 108.64   |
| 14  | G     | 826  | CLA  | OBD-CAD-C3D | -2.60 | 123.66      | 127.98   |
| 17  | G     | 848  | BCR  | C40-C30-C25 | 2.60  | 114.52      | 110.30   |
| 17  | Y     | 847  | BCR  | C15-C14-C13 | -2.60 | 123.59      | 127.31   |
| 14  | Z     | 817  | CLA  | C3C-C4C-NC  | 2.60  | 113.49      | 110.57   |
| 14  | H     | 834  | CLA  | CHD-C4C-C3C | -2.60 | 121.01      | 124.84   |
| 14  | H     | 805  | CLA  | CAA-C2A-C3A | -2.60 | 105.66      | 112.78   |
| 14  | G     | 815  | CLA  | CHC-C1C-C2C | -2.60 | 119.53      | 126.72   |
| 14  | H     | 804  | CLA  | CMA-C3A-C4A | 2.60  | 118.76      | 111.77   |
| 14  | A     | 822  | CLA  | CHC-C1C-C2C | -2.60 | 119.53      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | Z     | 843 | BCR  | C12-C13-C14 | 2.60  | 122.93      | 118.94   |
| 14  | Z     | 834 | CLA  | OBD-CAD-CBD | -2.60 | 122.18      | 125.89   |
| 17  | Z     | 845 | BCR  | C7-C6-C5    | -2.60 | 115.17      | 121.46   |
| 14  | Y     | 823 | CLA  | CMB-C2B-C3B | 2.60  | 129.54      | 124.68   |
| 17  | I     | 101 | BCR  | C39-C30-C25 | -2.60 | 106.09      | 110.30   |
| 14  | H     | 838 | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.90   |
| 14  | Z     | 813 | CLA  | CHB-C4A-NA  | 2.60  | 128.10      | 124.51   |
| 14  | Z     | 802 | CLA  | C1-O2A-CGA  | 2.60  | 123.26      | 116.44   |
| 14  | Z     | 806 | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 14  | B     | 812 | CLA  | CHC-C1C-C2C | -2.60 | 119.54      | 126.72   |
| 14  | H     | 805 | CLA  | CHB-C4A-NA  | 2.60  | 128.10      | 124.51   |
| 14  | H     | 805 | CLA  | CED-O2D-CGD | 2.60  | 121.81      | 115.94   |
| 14  | B     | 822 | CLA  | CED-O2D-CGD | 2.60  | 121.81      | 115.94   |
| 17  | Y     | 850 | BCR  | C15-C14-C13 | -2.59 | 123.61      | 127.31   |
| 14  | Z     | 828 | CLA  | CMC-C2C-C1C | 2.59  | 128.99      | 125.04   |
| 14  | H     | 820 | CLA  | CAC-C3C-C4C | 2.59  | 128.18      | 124.81   |
| 14  | B     | 811 | CLA  | CMB-C2B-C3B | 2.59  | 129.53      | 124.68   |
| 14  | B     | 830 | CLA  | CHC-C1C-C2C | -2.59 | 119.55      | 126.72   |
| 17  | Y     | 848 | BCR  | C36-C18-C19 | -2.59 | 113.99      | 118.08   |
| 14  | Z     | 820 | CLA  | CMC-C2C-C1C | 2.59  | 128.99      | 125.04   |
| 14  | G     | 826 | CLA  | CMB-C2B-C3B | 2.59  | 129.53      | 124.68   |
| 14  | H     | 827 | CLA  | C4-C3-C5    | 2.59  | 119.63      | 115.27   |
| 17  | Z     | 841 | BCR  | C8-C9-C10   | -2.59 | 114.97      | 118.94   |
| 14  | B     | 808 | CLA  | CMB-C2B-C3B | 2.59  | 129.52      | 124.68   |
| 14  | Z     | 810 | CLA  | CMA-C3A-C4A | 2.59  | 118.73      | 111.77   |
| 14  | Z     | 834 | CLA  | CMA-C3A-C4A | 2.59  | 118.73      | 111.77   |
| 14  | G     | 815 | CLA  | C1-C2-C3    | -2.59 | 122.56      | 126.75   |
| 14  | K     | 101 | CLA  | CMA-C3A-C4A | 2.59  | 118.73      | 111.77   |
| 14  | Z     | 837 | CLA  | OBD-CAD-CBD | -2.59 | 122.20      | 125.89   |
| 17  | Y     | 846 | BCR  | C37-C22-C23 | 2.59  | 122.15      | 118.08   |
| 14  | Y     | 817 | CLA  | CHC-C1C-C2C | -2.59 | 119.57      | 126.72   |
| 14  | B     | 826 | CLA  | OBD-CAD-CBD | -2.59 | 122.20      | 125.89   |
| 17  | L     | 203 | BCR  | C37-C22-C21 | -2.59 | 119.30      | 122.92   |
| 17  | h     | 202 | BCR  | C28-C27-C26 | -2.58 | 109.46      | 114.08   |
| 14  | A     | 852 | CLA  | CMB-C2B-C3B | 2.58  | 129.51      | 124.68   |
| 14  | H     | 804 | CLA  | OBD-CAD-C3D | -2.58 | 123.69      | 127.98   |
| 14  | B     | 828 | CLA  | O2D-CGD-O1D | -2.58 | 118.79      | 123.84   |
| 14  | B     | 838 | CLA  | CMA-C3A-C4A | 2.58  | 118.71      | 111.77   |
| 14  | G     | 836 | CLA  | C1-O2A-CGA  | 2.58  | 123.22      | 116.44   |
| 14  | H     | 805 | CLA  | CAA-CBA-CGA | -2.58 | 105.71      | 113.25   |
| 14  | A     | 834 | CLA  | C1-C2-C3    | -2.58 | 121.58      | 126.04   |
| 17  | K     | 102 | BCR  | C8-C7-C6    | -2.58 | 119.96      | 127.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 846  | BCR  | C36-C18-C17 | -2.58 | 119.31      | 122.92   |
| 14  | H     | 802  | CLA  | O2D-CGD-CBD | 2.58  | 115.85      | 111.27   |
| 17  | S     | 1104 | BCR  | C37-C22-C21 | -2.58 | 119.31      | 122.92   |
| 14  | T     | 101  | CLA  | CMB-C2B-C3B | 2.58  | 129.50      | 124.68   |
| 14  | Z     | 812  | CLA  | CED-O2D-CGD | 2.58  | 121.77      | 115.94   |
| 14  | H     | 815  | CLA  | O1D-CGD-CBD | -2.58 | 119.21      | 124.48   |
| 14  | Z     | 811  | CLA  | O1D-CGD-CBD | -2.58 | 119.21      | 124.48   |
| 14  | Z     | 839  | CLA  | C3C-C4C-NC  | 2.58  | 113.46      | 110.57   |
| 17  | Z     | 842  | BCR  | C32-C1-C6   | -2.58 | 106.12      | 110.30   |
| 14  | H     | 803  | CLA  | C4C-C3C-C2C | -2.58 | 103.14      | 106.90   |
| 14  | Z     | 801  | CLA  | C3C-C4C-NC  | 2.58  | 113.46      | 110.57   |
| 14  | G     | 832  | CLA  | C4-C3-C5    | 2.58  | 119.60      | 115.27   |
| 14  | H     | 820  | CLA  | O2D-CGD-O1D | -2.57 | 118.80      | 123.84   |
| 14  | Y     | 822  | CLA  | C1-O2A-CGA  | 2.57  | 123.20      | 116.44   |
| 14  | H     | 813  | CLA  | C3C-C4C-NC  | 2.57  | 113.46      | 110.57   |
| 14  | A     | 839  | CLA  | C3C-C4C-NC  | 2.57  | 113.46      | 110.57   |
| 17  | Y     | 856  | BCR  | C12-C13-C14 | 2.57  | 122.89      | 118.94   |
| 17  | Y     | 849  | BCR  | C37-C22-C23 | 2.57  | 122.13      | 118.08   |
| 14  | f     | 101  | CLA  | CMC-C2C-C1C | 2.57  | 128.96      | 125.04   |
| 14  | G     | 809  | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 14  | A     | 815  | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 14  | G     | 839  | CLA  | CED-O2D-CGD | 2.57  | 121.75      | 115.94   |
| 17  | A     | 848  | BCR  | C38-C26-C27 | 2.57  | 118.56      | 113.62   |
| 14  | H     | 808  | CLA  | CMB-C2B-C3B | 2.57  | 129.49      | 124.68   |
| 14  | K     | 103  | CLA  | CED-O2D-CGD | 2.57  | 121.75      | 115.94   |
| 14  | B     | 816  | CLA  | O2D-CGD-CBD | 2.57  | 115.84      | 111.27   |
| 17  | G     | 849  | BCR  | C23-C22-C21 | 2.57  | 122.89      | 118.94   |
| 14  | Y     | 811  | CLA  | CHC-C1C-C2C | -2.57 | 119.61      | 126.72   |
| 17  | A     | 845  | BCR  | C32-C1-C6   | 2.57  | 114.47      | 110.30   |
| 14  | H     | 807  | CLA  | C6-C5-C3    | -2.57 | 106.72      | 113.45   |
| 14  | A     | 802  | CLA  | CMC-C2C-C1C | 2.57  | 128.95      | 125.04   |
| 14  | Y     | 805  | CLA  | CGD-CBD-CAD | -2.57 | 102.42      | 110.73   |
| 14  | B     | 827  | CLA  | CAC-C3C-C4C | 2.56  | 128.14      | 124.81   |
| 14  | A     | 811  | CLA  | CHC-C1C-C2C | -2.56 | 119.63      | 126.72   |
| 14  | Y     | 855  | CLA  | CGD-CBD-CAD | 2.56  | 119.04      | 110.73   |
| 14  | G     | 812  | CLA  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 14  | Z     | 825  | CLA  | CAC-C3C-C4C | 2.56  | 128.14      | 124.81   |
| 14  | H     | 801  | CLA  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 14  | H     | 825  | CLA  | O1D-CGD-CBD | -2.56 | 119.25      | 124.48   |
| 14  | Y     | 834  | CLA  | C4D-C3D-CAD | 2.56  | 109.90      | 108.47   |
| 14  | Y     | 816  | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 14  | A     | 839  | CLA  | C1-O2A-CGA  | 2.56  | 123.16      | 116.44   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | Y     | 856 | BCR  | C15-C14-C13 | -2.56 | 123.66      | 127.31   |
| 14  | H     | 809 | CLA  | OBD-CAD-CBD | -2.56 | 122.24      | 125.89   |
| 17  | G     | 847 | BCR  | C7-C6-C5    | -2.56 | 115.27      | 121.46   |
| 14  | L     | 205 | CLA  | C3C-C4C-NC  | 2.56  | 113.44      | 110.57   |
| 17  | J     | 104 | BCR  | C3-C4-C5    | -2.56 | 109.51      | 114.08   |
| 14  | G     | 835 | CLA  | O2D-CGD-O1D | -2.56 | 118.84      | 123.84   |
| 14  | Z     | 815 | CLA  | C4-C3-C2    | -2.56 | 117.12      | 123.68   |
| 14  | Y     | 820 | CLA  | CBC-CAC-C3C | -2.56 | 105.39      | 112.43   |
| 14  | B     | 815 | CLA  | O1D-CGD-CBD | -2.55 | 119.26      | 124.48   |
| 14  | A     | 802 | CLA  | CHC-C1C-C2C | -2.55 | 119.66      | 126.72   |
| 18  | B     | 850 | LHG  | O7-C7-O9    | -2.55 | 117.53      | 123.70   |
| 14  | B     | 801 | CLA  | CMB-C2B-C3B | 2.55  | 129.46      | 124.68   |
| 14  | Y     | 803 | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 14  | H     | 819 | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 14  | Y     | 818 | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |
| 14  | B     | 840 | CLA  | CMB-C2B-C3B | 2.55  | 129.45      | 124.68   |
| 14  | Y     | 827 | CLA  | C4C-C3C-C2C | -2.55 | 103.18      | 106.90   |
| 14  | Z     | 836 | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 14  | Y     | 826 | CLA  | CAA-C2A-C1A | -2.55 | 103.62      | 111.97   |
| 14  | Z     | 829 | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 14  | A     | 813 | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 14  | B     | 831 | CLA  | O1D-CGD-CBD | -2.55 | 119.27      | 124.48   |
| 14  | Y     | 820 | CLA  | O2D-CGD-O1D | -2.55 | 118.86      | 123.84   |
| 14  | B     | 817 | CLA  | CMC-C2C-C1C | 2.55  | 128.92      | 125.04   |
| 14  | Z     | 811 | CLA  | CED-O2D-CGD | 2.55  | 121.70      | 115.94   |
| 14  | G     | 807 | CLA  | CMB-C2B-C3B | 2.55  | 129.44      | 124.68   |
| 14  | A     | 812 | CLA  | O2D-CGD-O1D | -2.55 | 118.86      | 123.84   |
| 14  | Y     | 807 | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 17  | e     | 101 | BCR  | C7-C8-C9    | -2.55 | 122.39      | 126.23   |
| 14  | B     | 807 | CLA  | O2A-C1-C2   | 2.55  | 115.33      | 108.64   |
| 14  | Y     | 828 | CLA  | CHD-C4C-C3C | -2.55 | 121.10      | 124.84   |
| 14  | G     | 823 | CLA  | CMA-C3A-C4A | 2.55  | 118.61      | 111.77   |
| 14  | Y     | 816 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 14  | H     | 830 | CLA  | C4D-C3D-CAD | 2.54  | 109.89      | 108.47   |
| 14  | H     | 824 | CLA  | CMA-C3A-C4A | 2.54  | 118.61      | 111.77   |
| 14  | B     | 811 | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 14  | A     | 816 | CLA  | CHC-C1C-C2C | -2.54 | 119.69      | 126.72   |
| 14  | A     | 833 | CLA  | CMA-C3A-C4A | 2.54  | 118.61      | 111.77   |
| 14  | H     | 831 | CLA  | CAA-CBA-CGA | -2.54 | 108.12      | 113.59   |
| 14  | Y     | 828 | CLA  | C5-C3-C2    | -2.54 | 115.97      | 121.12   |
| 14  | B     | 822 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 14  | Z     | 818 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 819 | CLA  | CHC-C1C-C2C | -2.54 | 119.70      | 126.72   |
| 14  | B     | 836 | CLA  | CED-O2D-CGD | 2.54  | 121.68      | 115.94   |
| 14  | B     | 818 | CLA  | C3C-C4C-NC  | 2.54  | 113.42      | 110.57   |
| 14  | A     | 817 | CLA  | CAC-C3C-C4C | 2.54  | 128.10      | 124.81   |
| 17  | f     | 103 | BCR  | C35-C13-C14 | -2.54 | 119.37      | 122.92   |
| 14  | A     | 812 | CLA  | C3C-C4C-NC  | 2.54  | 113.42      | 110.57   |
| 14  | B     | 804 | CLA  | C4C-C3C-C2C | -2.54 | 103.20      | 106.90   |
| 14  | A     | 813 | CLA  | O1D-CGD-CBD | -2.54 | 119.29      | 124.48   |
| 14  | H     | 803 | CLA  | O2D-CGD-O1D | -2.54 | 118.88      | 123.84   |
| 14  | H     | 831 | CLA  | CHC-C1C-C2C | -2.54 | 119.71      | 126.72   |
| 17  | Y     | 851 | BCR  | C15-C14-C13 | -2.54 | 123.69      | 127.31   |
| 14  | H     | 834 | CLA  | O1D-CGD-CBD | -2.54 | 119.30      | 124.48   |
| 14  | B     | 819 | CLA  | C1-C2-C3    | -2.53 | 121.66      | 126.04   |
| 14  | Y     | 838 | CLA  | C1-O2A-CGA  | 2.53  | 123.09      | 116.44   |
| 14  | B     | 801 | CLA  | CAC-C3C-C4C | 2.53  | 128.10      | 124.81   |
| 14  | H     | 819 | CLA  | CHB-C4A-NA  | 2.53  | 128.02      | 124.51   |
| 14  | A     | 831 | CLA  | CMC-C2C-C1C | 2.53  | 128.90      | 125.04   |
| 14  | G     | 807 | CLA  | OBD-CAD-C3D | -2.53 | 123.78      | 127.98   |
| 14  | B     | 806 | CLA  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 17  | Y     | 851 | BCR  | C28-C27-C26 | -2.53 | 109.56      | 114.08   |
| 14  | K     | 103 | CLA  | C3C-C4C-NC  | 2.53  | 113.41      | 110.57   |
| 14  | H     | 814 | CLA  | CMB-C2B-C3B | 2.53  | 129.41      | 124.68   |
| 14  | G     | 842 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 14  | B     | 832 | CLA  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 14  | A     | 803 | CLA  | C1-C2-C3    | -2.53 | 121.67      | 126.04   |
| 14  | G     | 843 | CLA  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 14  | K     | 101 | CLA  | CHC-C1C-C2C | -2.53 | 119.73      | 126.72   |
| 17  | A     | 847 | BCR  | C27-C26-C25 | -2.53 | 119.06      | 122.73   |
| 14  | G     | 804 | CLA  | O1D-CGD-CBD | -2.53 | 119.31      | 124.48   |
| 14  | H     | 828 | CLA  | C1-O2A-CGA  | 2.53  | 123.08      | 116.44   |
| 14  | B     | 827 | CLA  | C6-C5-C3    | -2.53 | 106.83      | 113.45   |
| 14  | B     | 814 | CLA  | C4-C3-C5    | 2.53  | 119.52      | 115.27   |
| 14  | Y     | 839 | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.81   |
| 17  | H     | 844 | BCR  | C23-C24-C25 | -2.53 | 120.11      | 127.20   |
| 14  | h     | 205 | CLA  | C3C-C4C-NC  | 2.53  | 113.40      | 110.57   |
| 14  | H     | 816 | CLA  | C1-C2-C3    | -2.53 | 121.67      | 126.04   |
| 14  | A     | 852 | CLA  | O2A-CGA-CBA | 2.53  | 119.83      | 111.91   |
| 14  | H     | 833 | CLA  | CHC-C1C-C2C | -2.52 | 119.74      | 126.72   |
| 14  | Y     | 830 | CLA  | CMA-C3A-C4A | 2.52  | 118.56      | 111.77   |
| 13  | A     | 801 | CL0  | C3C-C4C-NC  | 2.52  | 113.40      | 110.57   |
| 14  | Y     | 842 | CLA  | C1-C2-C3    | -2.52 | 121.68      | 126.04   |
| 17  | L     | 209 | BCR  | C38-C26-C25 | 2.52  | 127.36      | 124.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | B     | 839 | CLA  | O1D-CGD-CBD | -2.52 | 119.32      | 124.48   |
| 14  | d     | 202 | CLA  | OBD-CAD-C3D | -2.52 | 123.79      | 127.98   |
| 17  | J     | 104 | BCR  | C23-C24-C25 | -2.52 | 120.12      | 127.20   |
| 14  | Y     | 811 | CLA  | CAA-CBA-CGA | 2.52  | 120.62      | 113.25   |
| 14  | B     | 834 | CLA  | OBD-CAD-CBD | -2.52 | 122.30      | 125.89   |
| 14  | G     | 841 | CLA  | OBD-CAD-C3D | -2.52 | 123.80      | 127.98   |
| 14  | B     | 828 | CLA  | C3C-C4C-NC  | 2.52  | 113.40      | 110.57   |
| 14  | Y     | 807 | CLA  | CMA-C3A-C4A | 2.52  | 118.54      | 111.77   |
| 14  | A     | 852 | CLA  | C1-O2A-CGA  | 2.52  | 123.05      | 116.44   |
| 14  | Y     | 802 | CLA  | CHC-C1C-C2C | -2.52 | 119.75      | 126.72   |
| 14  | G     | 803 | CLA  | CED-O2D-CGD | 2.52  | 121.63      | 115.94   |
| 14  | A     | 827 | CLA  | CAC-C3C-C4C | 2.52  | 128.08      | 124.81   |
| 14  | K     | 101 | CLA  | CAA-C2A-C1A | -2.52 | 103.73      | 111.97   |
| 14  | H     | 824 | CLA  | CHB-C4A-NA  | 2.52  | 127.99      | 124.51   |
| 17  | f     | 105 | BCR  | C29-C30-C25 | -2.52 | 106.61      | 110.48   |
| 14  | h     | 206 | CLA  | CAC-C3C-C2C | 2.52  | 131.83      | 127.53   |
| 14  | B     | 826 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 14  | Y     | 838 | CLA  | CMC-C2C-C1C | 2.51  | 128.87      | 125.04   |
| 14  | H     | 807 | CLA  | CAA-C2A-C1A | -2.51 | 103.74      | 111.97   |
| 14  | B     | 832 | CLA  | CHC-C1C-C2C | -2.51 | 119.77      | 126.72   |
| 14  | B     | 808 | CLA  | C1-O2A-CGA  | 2.51  | 123.04      | 116.44   |
| 17  | Y     | 847 | BCR  | C36-C18-C19 | -2.51 | 114.12      | 118.08   |
| 14  | A     | 832 | CLA  | C11-C10-C8  | -2.51 | 107.80      | 115.92   |
| 14  | G     | 803 | CLA  | CMB-C2B-C1B | 2.51  | 132.32      | 128.46   |
| 14  | Z     | 823 | CLA  | O1D-CGD-CBD | -2.51 | 119.35      | 124.48   |
| 14  | f     | 102 | CLA  | CMC-C2C-C1C | 2.51  | 128.86      | 125.04   |
| 14  | B     | 838 | CLA  | CHC-C1C-C2C | -2.51 | 119.78      | 126.72   |
| 17  | H     | 841 | BCR  | C37-C22-C23 | 2.51  | 122.03      | 118.08   |
| 14  | Z     | 832 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 14  | A     | 814 | CLA  | CAA-C2A-C1A | -2.51 | 103.76      | 111.97   |
| 14  | Y     | 804 | CLA  | C1-O2A-CGA  | 2.51  | 123.02      | 116.44   |
| 17  | H     | 844 | BCR  | C15-C14-C13 | -2.51 | 123.73      | 127.31   |
| 14  | B     | 841 | CLA  | CHC-C1C-C2C | -2.51 | 119.79      | 126.72   |
| 17  | F     | 203 | BCR  | C8-C7-C6    | -2.51 | 120.17      | 127.20   |
| 14  | G     | 813 | CLA  | O2D-CGD-O1D | -2.51 | 118.94      | 123.84   |
| 14  | Z     | 807 | CLA  | CED-O2D-CGD | 2.51  | 121.60      | 115.94   |
| 14  | H     | 832 | CLA  | CMD-C2D-C3D | -2.50 | 119.99      | 124.68   |
| 14  | Y     | 835 | CLA  | C1-O2A-CGA  | 2.50  | 123.02      | 116.44   |
| 14  | H     | 816 | CLA  | C6-C5-C3    | -2.50 | 106.89      | 113.45   |
| 14  | B     | 826 | CLA  | C4C-C3C-C2C | -2.50 | 103.25      | 106.90   |
| 14  | Z     | 831 | CLA  | O2D-CGD-O1D | -2.50 | 118.94      | 123.84   |
| 14  | A     | 841 | CLA  | CAC-C3C-C4C | 2.50  | 128.06      | 124.81   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 842  | CLA  | CAC-C3C-C4C | 2.50  | 128.06      | 124.81   |
| 14  | Z     | 813  | CLA  | C4C-C3C-C2C | -2.50 | 103.25      | 106.90   |
| 14  | Z     | 816  | CLA  | O2D-CGD-O1D | -2.50 | 118.94      | 123.84   |
| 14  | H     | 801  | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 14  | Y     | 804  | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 14  | H     | 825  | CLA  | CMA-C3A-C4A | 2.50  | 118.50      | 111.77   |
| 14  | G     | 835  | CLA  | CED-O2D-CGD | 2.50  | 121.59      | 115.94   |
| 14  | A     | 804  | CLA  | O2D-CGD-O1D | -2.50 | 118.95      | 123.84   |
| 14  | d     | 202  | CLA  | C3C-C4C-NC  | 2.50  | 113.38      | 110.57   |
| 14  | H     | 820  | CLA  | CMA-C3A-C4A | 2.50  | 118.49      | 111.77   |
| 14  | U     | 1002 | CLA  | C6-C7-C8    | -2.50 | 107.84      | 115.92   |
| 17  | H     | 841  | BCR  | C3-C4-C5    | -2.50 | 109.61      | 114.08   |
| 14  | Y     | 812  | CLA  | O2D-CGD-O1D | -2.50 | 118.95      | 123.84   |
| 14  | B     | 836  | CLA  | C3C-C4C-NC  | 2.50  | 113.37      | 110.57   |
| 15  | Z     | 840  | PQN  | C2M-C2-C3   | -2.50 | 120.32      | 124.40   |
| 14  | Z     | 833  | CLA  | CED-O2D-CGD | 2.50  | 121.59      | 115.94   |
| 14  | B     | 803  | CLA  | O2D-CGD-CBD | 2.50  | 115.71      | 111.27   |
| 14  | H     | 821  | CLA  | CHC-C1C-C2C | -2.50 | 119.81      | 126.72   |
| 14  | G     | 831  | CLA  | C3C-C4C-NC  | 2.50  | 113.37      | 110.57   |
| 14  | Z     | 811  | CLA  | CHC-C1C-C2C | -2.50 | 119.82      | 126.72   |
| 17  | L     | 203  | BCR  | C36-C18-C19 | -2.50 | 114.14      | 118.08   |
| 14  | L     | 207  | CLA  | CMA-C3A-C4A | 2.50  | 118.48      | 111.77   |
| 14  | Y     | 820  | CLA  | O1D-CGD-CBD | -2.50 | 119.38      | 124.48   |
| 14  | H     | 806  | CLA  | C4C-C3C-C2C | -2.50 | 103.26      | 106.90   |
| 14  | Z     | 819  | CLA  | O1D-CGD-CBD | -2.49 | 119.38      | 124.48   |
| 14  | g     | 101  | CLA  | CHC-C1C-C2C | -2.49 | 119.82      | 126.72   |
| 14  | H     | 807  | CLA  | C2A-C3A-C4A | -2.49 | 97.84       | 101.87   |
| 14  | G     | 830  | CLA  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 17  | B     | 847  | BCR  | C8-C9-C10   | 2.49  | 122.77      | 118.94   |
| 14  | A     | 814  | CLA  | CAC-C3C-C4C | 2.49  | 128.04      | 124.81   |
| 14  | G     | 824  | CLA  | O2D-CGD-CBD | 2.49  | 115.70      | 111.27   |
| 14  | Y     | 803  | CLA  | CHC-C1C-C2C | -2.49 | 119.83      | 126.72   |
| 14  | H     | 807  | CLA  | CHC-C1C-C2C | -2.49 | 119.83      | 126.72   |
| 14  | Z     | 816  | CLA  | CHC-C1C-C2C | -2.49 | 119.83      | 126.72   |
| 14  | g     | 102  | CLA  | CHC-C1C-C2C | -2.49 | 119.83      | 126.72   |
| 14  | Y     | 803  | CLA  | C1-O2A-CGA  | 2.49  | 122.98      | 116.44   |
| 14  | H     | 824  | CLA  | CED-O2D-CGD | 2.49  | 121.57      | 115.94   |
| 14  | G     | 838  | CLA  | CED-O2D-CGD | 2.49  | 121.57      | 115.94   |
| 14  | A     | 817  | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 14  | H     | 808  | CLA  | C7-C6-C5    | -2.49 | 106.60      | 113.36   |
| 14  | Y     | 802  | CLA  | C1-O2A-CGA  | 2.49  | 122.98      | 116.44   |
| 14  | A     | 808  | CLA  | C4D-C3D-CAD | 2.49  | 109.86      | 108.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 830 | CLA  | C1-O2A-CGA  | 2.49  | 122.97      | 116.44   |
| 17  | Y     | 850 | BCR  | C33-C5-C6   | -2.49 | 121.73      | 124.53   |
| 14  | G     | 808 | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 14  | Z     | 810 | CLA  | OBD-CAD-CBD | -2.49 | 122.34      | 125.89   |
| 14  | A     | 821 | CLA  | OBD-CAD-C3D | -2.49 | 123.85      | 127.98   |
| 14  | Z     | 837 | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 14  | Z     | 820 | CLA  | O1D-CGD-CBD | -2.49 | 119.40      | 124.48   |
| 14  | Y     | 816 | CLA  | C3C-C4C-NC  | 2.49  | 113.36      | 110.57   |
| 14  | G     | 827 | CLA  | CHD-C4C-C3C | -2.49 | 121.19      | 124.84   |
| 14  | G     | 814 | CLA  | C1-C2-C3    | -2.49 | 122.73      | 126.75   |
| 14  | Z     | 819 | CLA  | CBC-CAC-C3C | -2.48 | 105.58      | 112.43   |
| 14  | G     | 825 | CLA  | O2D-CGD-O1D | -2.48 | 118.98      | 123.84   |
| 14  | G     | 808 | CLA  | C1-O2A-CGA  | 2.48  | 122.96      | 116.44   |
| 14  | Z     | 814 | CLA  | CMB-C2B-C3B | 2.48  | 129.33      | 124.68   |
| 14  | Y     | 807 | CLA  | C4-C3-C5    | 2.48  | 118.82      | 115.98   |
| 14  | Z     | 810 | CLA  | CMC-C2C-C1C | 2.48  | 128.82      | 125.04   |
| 14  | A     | 813 | CLA  | CMA-C3A-C4A | 2.48  | 118.45      | 111.77   |
| 17  | L     | 209 | BCR  | C31-C1-C6   | -2.48 | 106.27      | 110.30   |
| 14  | A     | 834 | CLA  | CAC-C3C-C4C | 2.48  | 128.03      | 124.81   |
| 17  | L     | 208 | BCR  | C33-C5-C4   | 2.48  | 118.39      | 113.62   |
| 14  | G     | 826 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 14  | Y     | 811 | CLA  | CED-O2D-CGD | 2.48  | 121.55      | 115.94   |
| 14  | B     | 839 | CLA  | O2D-CGD-O1D | -2.48 | 118.98      | 123.84   |
| 14  | B     | 814 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 14  | G     | 820 | CLA  | C4-C3-C5    | 2.48  | 119.45      | 115.27   |
| 14  | Y     | 814 | CLA  | CMC-C2C-C1C | 2.48  | 128.82      | 125.04   |
| 14  | B     | 812 | CLA  | C1-C2-C3    | -2.48 | 122.74      | 126.75   |
| 17  | G     | 846 | BCR  | C23-C24-C25 | -2.48 | 120.23      | 127.20   |
| 14  | L     | 206 | CLA  | CED-O2D-CGD | 2.48  | 121.55      | 115.94   |
| 14  | G     | 807 | CLA  | CED-O2D-CGD | 2.48  | 121.55      | 115.94   |
| 14  | B     | 809 | CLA  | CMB-C2B-C3B | 2.48  | 129.32      | 124.68   |
| 14  | Z     | 802 | CLA  | O2D-CGD-CBD | 2.48  | 115.67      | 111.27   |
| 14  | G     | 825 | CLA  | CHD-C4C-C3C | -2.48 | 121.19      | 124.84   |
| 14  | L     | 201 | CLA  | C7-C6-C5    | -2.48 | 106.63      | 113.36   |
| 17  | Y     | 851 | BCR  | C33-C5-C6   | -2.48 | 121.75      | 124.53   |
| 14  | B     | 832 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 14  | Y     | 815 | CLA  | C3C-C4C-NC  | 2.48  | 113.35      | 110.57   |
| 14  | h     | 207 | CLA  | C3C-C4C-NC  | 2.48  | 113.35      | 110.57   |
| 17  | G     | 847 | BCR  | C15-C14-C13 | -2.48 | 123.77      | 127.31   |
| 17  | Y     | 849 | BCR  | C38-C26-C27 | 2.48  | 118.37      | 113.62   |
| 14  | Z     | 833 | CLA  | CHC-C1C-C2C | -2.48 | 119.87      | 126.72   |
| 14  | B     | 823 | CLA  | CHC-C1C-C2C | -2.47 | 119.88      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 828  | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 14  | A     | 822  | CLA  | CMC-C2C-C1C | 2.47  | 128.81      | 125.04   |
| 14  | B     | 841  | CLA  | CMC-C2C-C3C | 2.47  | 132.83      | 126.12   |
| 14  | V     | 1201 | CLA  | CAC-C3C-C4C | 2.47  | 128.02      | 124.81   |
| 17  | Y     | 850  | BCR  | C28-C27-C26 | -2.47 | 109.66      | 114.08   |
| 17  | G     | 850  | BCR  | C29-C28-C27 | -2.47 | 105.85      | 111.38   |
| 14  | G     | 853  | CLA  | CMA-C3A-C4A | 2.47  | 118.42      | 111.77   |
| 14  | H     | 813  | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 14  | G     | 832  | CLA  | CED-O2D-CGD | 2.47  | 121.53      | 115.94   |
| 14  | Y     | 834  | CLA  | CMA-C3A-C4A | 2.47  | 118.42      | 111.77   |
| 14  | H     | 838  | CLA  | CMC-C2C-C3C | 2.47  | 132.83      | 126.12   |
| 14  | H     | 835  | CLA  | O2D-CGD-O1D | -2.47 | 119.01      | 123.84   |
| 14  | H     | 830  | CLA  | OBD-CAD-CBD | -2.47 | 122.36      | 125.89   |
| 17  | G     | 848  | BCR  | C3-C4-C5    | -2.47 | 109.67      | 114.08   |
| 14  | Y     | 812  | CLA  | C3C-C4C-NC  | 2.47  | 113.34      | 110.57   |
| 14  | G     | 817  | CLA  | O1D-CGD-CBD | -2.47 | 119.43      | 124.48   |
| 14  | A     | 830  | CLA  | CMA-C3A-C4A | 2.47  | 118.41      | 111.77   |
| 14  | B     | 833  | CLA  | C3C-C4C-NC  | 2.47  | 113.34      | 110.57   |
| 17  | B     | 848  | BCR  | C33-C5-C4   | 2.47  | 118.35      | 113.62   |
| 17  | J     | 104  | BCR  | C38-C26-C25 | -2.47 | 121.76      | 124.53   |
| 14  | Y     | 809  | CLA  | CMC-C2C-C1C | 2.47  | 128.79      | 125.04   |
| 14  | A     | 825  | CLA  | CHC-C1C-C2C | -2.47 | 119.90      | 126.72   |
| 14  | Z     | 805  | CLA  | OBD-CAD-CBD | -2.47 | 122.37      | 125.89   |
| 14  | G     | 813  | CLA  | C3C-C4C-NC  | 2.46  | 113.33      | 110.57   |
| 17  | B     | 847  | BCR  | C39-C30-C25 | -2.46 | 106.30      | 110.30   |
| 14  | Y     | 825  | CLA  | CHC-C1C-C2C | -2.46 | 119.91      | 126.72   |
| 14  | G     | 825  | CLA  | CMB-C2B-C3B | 2.46  | 129.29      | 124.68   |
| 17  | A     | 846  | BCR  | C7-C8-C9    | -2.46 | 122.51      | 126.23   |
| 14  | Y     | 838  | CLA  | C3C-C4C-NC  | 2.46  | 113.33      | 110.57   |
| 14  | Z     | 827  | CLA  | O1D-CGD-CBD | -2.46 | 119.44      | 124.48   |
| 17  | U     | 1005 | BCR  | C7-C8-C9    | -2.46 | 122.51      | 126.23   |
| 14  | B     | 831  | CLA  | CAC-C3C-C4C | 2.46  | 128.00      | 124.81   |
| 14  | H     | 808  | CLA  | O2A-C1-C2   | 2.46  | 115.11      | 108.64   |
| 17  | Z     | 844  | BCR  | C29-C28-C27 | -2.46 | 105.88      | 111.38   |
| 14  | L     | 201  | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 14  | A     | 833  | CLA  | CED-O2D-CGD | 2.46  | 121.50      | 115.94   |
| 14  | Y     | 811  | CLA  | CMC-C2C-C1C | 2.46  | 128.79      | 125.04   |
| 18  | A     | 851  | LHG  | O7-C7-O9    | -2.46 | 117.76      | 123.70   |
| 14  | A     | 826  | CLA  | CAA-C2A-C1A | -2.46 | 103.91      | 111.97   |
| 14  | Y     | 819  | CLA  | CHC-C1C-C2C | -2.46 | 119.92      | 126.72   |
| 14  | Y     | 823  | CLA  | CMC-C2C-C1C | 2.46  | 128.78      | 125.04   |
| 14  | Z     | 826  | CLA  | CED-O2D-CGD | 2.46  | 121.50      | 115.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | K     | 101 | CLA  | CMC-C2C-C1C | 2.46  | 128.78      | 125.04   |
| 13  | G     | 801 | CL0  | CAA-C2A-C3A | -2.46 | 106.04      | 112.78   |
| 14  | H     | 838 | CLA  | CHC-C1C-C2C | -2.46 | 119.92      | 126.72   |
| 14  | G     | 819 | CLA  | CAA-C2A-C1A | -2.46 | 103.92      | 111.97   |
| 14  | H     | 807 | CLA  | C1-O2A-CGA  | 2.46  | 122.89      | 116.44   |
| 14  | G     | 818 | CLA  | OBD-CAD-C3D | -2.46 | 123.90      | 127.98   |
| 17  | B     | 848 | BCR  | C37-C22-C23 | 2.46  | 121.95      | 118.08   |
| 14  | f     | 102 | CLA  | C3C-C4C-NC  | 2.46  | 113.33      | 110.57   |
| 14  | A     | 825 | CLA  | OBD-CAD-C3D | -2.46 | 123.90      | 127.98   |
| 14  | Y     | 819 | CLA  | CAC-C3C-C4C | 2.46  | 128.00      | 124.81   |
| 14  | Z     | 836 | CLA  | C1-O2A-CGA  | 2.46  | 122.89      | 116.44   |
| 14  | H     | 807 | CLA  | O2A-C1-C2   | 2.46  | 115.09      | 108.64   |
| 14  | A     | 824 | CLA  | CAC-C3C-C4C | 2.46  | 128.00      | 124.81   |
| 17  | A     | 845 | BCR  | C36-C18-C19 | -2.46 | 114.21      | 118.08   |
| 14  | G     | 824 | CLA  | CMC-C2C-C1C | 2.46  | 128.78      | 125.04   |
| 14  | H     | 833 | CLA  | O1D-CGD-CBD | -2.46 | 119.46      | 124.48   |
| 14  | B     | 812 | CLA  | CMA-C3A-C4A | 2.46  | 118.37      | 111.77   |
| 14  | Z     | 823 | CLA  | CAA-C2A-C3A | -2.46 | 106.05      | 112.78   |
| 14  | A     | 840 | CLA  | CHC-C1C-C2C | -2.46 | 119.93      | 126.72   |
| 14  | Y     | 812 | CLA  | C1-C2-C3    | -2.46 | 121.80      | 126.04   |
| 17  | B     | 844 | BCR  | C31-C1-C6   | -2.45 | 106.32      | 110.30   |
| 17  | Y     | 846 | BCR  | C2-C3-C4    | -2.45 | 105.89      | 111.38   |
| 17  | G     | 848 | BCR  | C27-C26-C25 | -2.45 | 119.17      | 122.73   |
| 14  | Z     | 816 | CLA  | CAC-C3C-C4C | 2.45  | 127.99      | 124.81   |
| 14  | B     | 840 | CLA  | CMA-C3A-C2A | 2.45  | 123.73      | 113.83   |
| 14  | Y     | 813 | CLA  | C1-C2-C3    | -2.45 | 121.80      | 126.04   |
| 17  | Z     | 843 | BCR  | C35-C13-C14 | -2.45 | 119.49      | 122.92   |
| 14  | G     | 808 | CLA  | CMB-C2B-C3B | 2.45  | 129.27      | 124.68   |
| 14  | H     | 804 | CLA  | CED-O2D-CGD | 2.45  | 121.48      | 115.94   |
| 14  | H     | 837 | CLA  | CMC-C2C-C1C | 2.45  | 128.77      | 125.04   |
| 17  | i     | 101 | BCR  | C31-C1-C6   | -2.45 | 106.32      | 110.30   |
| 14  | Y     | 831 | CLA  | CMC-C2C-C1C | 2.45  | 128.77      | 125.04   |
| 14  | B     | 833 | CLA  | CBA-CAA-C2A | 2.45  | 121.10      | 113.86   |
| 14  | Z     | 829 | CLA  | CED-O2D-CGD | 2.45  | 121.48      | 115.94   |
| 17  | B     | 848 | BCR  | C23-C22-C21 | 2.45  | 122.70      | 118.94   |
| 14  | d     | 202 | CLA  | CED-O2D-CGD | 2.45  | 121.48      | 115.94   |
| 14  | h     | 206 | CLA  | CMA-C3A-C4A | 2.45  | 118.35      | 111.77   |
| 14  | h     | 206 | CLA  | CAA-C2A-C1A | -2.45 | 103.95      | 111.97   |
| 14  | G     | 839 | CLA  | CBC-CAC-C3C | -2.45 | 105.68      | 112.43   |
| 14  | Y     | 825 | CLA  | CMA-C3A-C4A | 2.45  | 118.35      | 111.77   |
| 14  | H     | 838 | CLA  | C6-C5-C3    | -2.45 | 107.04      | 113.45   |
| 14  | A     | 818 | CLA  | C4C-C3C-C2C | -2.45 | 103.33      | 106.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 823  | CLA  | CAC-C3C-C4C | 2.45  | 127.98      | 124.81   |
| 14  | G     | 853  | CLA  | CHC-C1C-C2C | -2.45 | 119.95      | 126.72   |
| 14  | B     | 812  | CLA  | C1-O2A-CGA  | 2.45  | 122.86      | 116.44   |
| 14  | Z     | 825  | CLA  | CMC-C2C-C1C | 2.45  | 128.76      | 125.04   |
| 14  | A     | 816  | CLA  | CMA-C3A-C4A | 2.45  | 118.34      | 111.77   |
| 14  | G     | 803  | CLA  | C11-C12-C13 | -2.44 | 108.02      | 115.92   |
| 17  | G     | 847  | BCR  | C1-C6-C7    | 2.44  | 122.69      | 115.78   |
| 14  | G     | 826  | CLA  | C5-C3-C2    | -2.44 | 116.17      | 121.12   |
| 14  | G     | 834  | CLA  | CED-O2D-CGD | 2.44  | 121.47      | 115.94   |
| 14  | A     | 804  | CLA  | OBD-CAD-C3D | -2.44 | 123.92      | 127.98   |
| 14  | Y     | 813  | CLA  | O2D-CGD-O1D | -2.44 | 119.06      | 123.84   |
| 14  | G     | 815  | CLA  | CGD-CBD-CAD | -2.44 | 102.82      | 110.73   |
| 14  | A     | 818  | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 14  | Z     | 827  | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 14  | Q     | 201  | CLA  | CED-O2D-CGD | 2.44  | 121.46      | 115.94   |
| 14  | Z     | 831  | CLA  | C4-C3-C5    | 2.44  | 119.38      | 115.27   |
| 14  | Y     | 832  | CLA  | O2D-CGD-O1D | -2.44 | 119.07      | 123.84   |
| 14  | H     | 836  | CLA  | CED-O2D-CGD | 2.44  | 121.45      | 115.94   |
| 14  | Y     | 805  | CLA  | CAA-C2A-C1A | -2.44 | 103.98      | 111.97   |
| 14  | B     | 803  | CLA  | CHD-C4C-C3C | -2.44 | 121.25      | 124.84   |
| 17  | B     | 845  | BCR  | C15-C14-C13 | -2.44 | 123.83      | 127.31   |
| 14  | f     | 102  | CLA  | CAA-CBA-CGA | -2.44 | 106.13      | 113.25   |
| 14  | A     | 831  | CLA  | CMD-C2D-C3D | -2.44 | 120.12      | 124.68   |
| 14  | B     | 841  | CLA  | CHB-C4A-NA  | 2.44  | 127.88      | 124.51   |
| 17  | U     | 1007 | BCR  | C23-C22-C21 | -2.44 | 115.20      | 118.94   |
| 14  | A     | 837  | CLA  | C1-C2-C3    | -2.44 | 121.83      | 126.04   |
| 17  | R     | 101  | BCR  | C39-C30-C25 | -2.44 | 106.35      | 110.30   |
| 14  | W     | 1701 | CLA  | CHC-C1C-C2C | -2.44 | 119.98      | 126.72   |
| 17  | Y     | 850  | BCR  | C23-C22-C21 | 2.44  | 122.68      | 118.94   |
| 17  | B     | 845  | BCR  | C36-C18-C19 | -2.44 | 114.24      | 118.08   |
| 14  | Y     | 806  | CLA  | CHC-C1C-C2C | -2.44 | 119.98      | 126.72   |
| 14  | B     | 812  | CLA  | CMB-C2B-C3B | 2.44  | 129.24      | 124.68   |
| 14  | H     | 818  | CLA  | CMC-C2C-C1C | 2.43  | 128.75      | 125.04   |
| 14  | Z     | 808  | CLA  | CMA-C3A-C4A | 2.43  | 118.32      | 111.77   |
| 14  | Z     | 803  | CLA  | CMA-C3A-C4A | 2.43  | 118.32      | 111.77   |
| 14  | B     | 815  | CLA  | CMA-C3A-C4A | 2.43  | 118.31      | 111.77   |
| 14  | Y     | 831  | CLA  | CAC-C3C-C4C | 2.43  | 127.97      | 124.81   |
| 14  | H     | 829  | CLA  | CAA-C2A-C3A | -2.43 | 106.11      | 112.78   |
| 14  | H     | 804  | CLA  | C3C-C4C-NC  | 2.43  | 113.30      | 110.57   |
| 14  | g     | 102  | CLA  | C3C-C4C-NC  | 2.43  | 113.30      | 110.57   |
| 17  | R     | 101  | BCR  | C31-C1-C6   | -2.43 | 106.35      | 110.30   |
| 14  | G     | 839  | CLA  | C5-C3-C2    | -2.43 | 116.19      | 121.12   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | f     | 104  | BCR  | C36-C18-C19 | -2.43 | 114.24      | 118.08   |
| 14  | B     | 825  | CLA  | C3C-C4C-NC  | 2.43  | 113.30      | 110.57   |
| 13  | A     | 801  | CL0  | CHB-C4A-NA  | 2.43  | 127.88      | 124.51   |
| 19  | H     | 846  | LMG  | O4-C4-C3    | -2.43 | 104.73      | 110.35   |
| 14  | G     | 806  | CLA  | CMC-C2C-C1C | 2.43  | 128.74      | 125.04   |
| 14  | A     | 802  | CLA  | CAA-CBA-CGA | 2.43  | 120.36      | 113.25   |
| 14  | G     | 806  | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 14  | A     | 812  | CLA  | CAC-C3C-C4C | 2.43  | 127.96      | 124.81   |
| 17  | d     | 203  | BCR  | C38-C26-C25 | -2.43 | 121.80      | 124.53   |
| 14  | U     | 1006 | CLA  | CMC-C2C-C1C | 2.43  | 128.74      | 125.04   |
| 14  | Y     | 834  | CLA  | CBC-CAC-C3C | -2.43 | 105.74      | 112.43   |
| 14  | Z     | 821  | CLA  | CHC-C1C-C2C | -2.43 | 120.01      | 126.72   |
| 14  | S     | 1101 | CLA  | CHC-C1C-C2C | -2.43 | 120.01      | 126.72   |
| 14  | G     | 842  | CLA  | C4D-C3D-CAD | 2.43  | 109.82      | 108.47   |
| 14  | A     | 829  | CLA  | CMA-C3A-C4A | 2.43  | 118.29      | 111.77   |
| 17  | H     | 848  | BCR  | C7-C8-C9    | -2.43 | 122.57      | 126.23   |
| 14  | Y     | 833  | CLA  | CHC-C1C-C2C | -2.43 | 120.01      | 126.72   |
| 14  | G     | 813  | CLA  | O2A-CGA-CBA | 2.43  | 119.52      | 111.91   |
| 14  | G     | 839  | CLA  | O1D-CGD-CBD | -2.43 | 119.52      | 124.48   |
| 14  | Z     | 837  | CLA  | CBC-CAC-C3C | -2.42 | 105.75      | 112.43   |
| 15  | G     | 844  | PQN  | C2M-C2-C3   | -2.42 | 120.44      | 124.40   |
| 14  | A     | 803  | CLA  | OBD-CAD-CBD | -2.42 | 122.43      | 125.89   |
| 14  | B     | 806  | CLA  | O1D-CGD-CBD | -2.42 | 119.52      | 124.48   |
| 14  | G     | 843  | CLA  | O1D-CGD-CBD | -2.42 | 119.53      | 124.48   |
| 17  | L     | 209  | BCR  | C30-C25-C26 | -2.42 | 119.20      | 122.61   |
| 14  | B     | 809  | CLA  | CHC-C1C-C2C | -2.42 | 120.02      | 126.72   |
| 14  | Z     | 832  | CLA  | O2D-CGD-O1D | -2.42 | 119.10      | 123.84   |
| 14  | A     | 838  | CLA  | C4D-C3D-CAD | 2.42  | 109.82      | 108.47   |
| 14  | H     | 834  | CLA  | C3C-C4C-NC  | 2.42  | 113.29      | 110.57   |
| 14  | G     | 831  | CLA  | CHD-C4C-C3C | -2.42 | 121.28      | 124.84   |
| 17  | Y     | 848  | BCR  | C7-C8-C9    | -2.42 | 122.58      | 126.23   |
| 14  | S     | 1103 | CLA  | C3C-C4C-NC  | 2.42  | 113.29      | 110.57   |
| 17  | U     | 1008 | BCR  | C35-C13-C14 | -2.42 | 119.53      | 122.92   |
| 14  | G     | 805  | CLA  | CAA-C2A-C3A | -2.42 | 106.15      | 112.78   |
| 14  | J     | 101  | CLA  | CED-O2D-CGD | 2.42  | 121.41      | 115.94   |
| 14  | Z     | 818  | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 14  | A     | 803  | CLA  | CED-O2D-CGD | 2.42  | 121.41      | 115.94   |
| 14  | Y     | 827  | CLA  | CMB-C2B-C3B | 2.42  | 129.21      | 124.68   |
| 14  | B     | 816  | CLA  | C4-C3-C5    | 2.42  | 119.34      | 115.27   |
| 17  | Q     | 202  | BCR  | C37-C22-C23 | 2.42  | 121.89      | 118.08   |
| 14  | F     | 202  | CLA  | C3C-C4C-NC  | 2.42  | 113.28      | 110.57   |
| 14  | Z     | 820  | CLA  | C3C-C4C-NC  | 2.42  | 113.28      | 110.57   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 843  | CLA  | OBD-CAD-C3D | -2.42 | 123.96      | 127.98   |
| 14  | Z     | 824  | CLA  | C3C-C4C-NC  | 2.42  | 113.28      | 110.57   |
| 17  | Z     | 845  | BCR  | C8-C9-C10   | 2.42  | 122.65      | 118.94   |
| 17  | H     | 845  | BCR  | C4-C5-C6    | -2.42 | 119.22      | 122.73   |
| 17  | H     | 842  | BCR  | C33-C5-C6   | -2.42 | 121.81      | 124.53   |
| 14  | d     | 201  | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 14  | A     | 822  | CLA  | CAA-C2A-C3A | -2.42 | 106.16      | 112.78   |
| 14  | H     | 824  | CLA  | C4-C3-C2    | -2.42 | 117.48      | 123.68   |
| 14  | A     | 811  | CLA  | CMC-C2C-C1C | 2.42  | 128.72      | 125.04   |
| 14  | B     | 813  | CLA  | C3C-C4C-NC  | 2.42  | 113.28      | 110.57   |
| 14  | A     | 832  | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 14  | h     | 206  | CLA  | CHB-C4A-NA  | 2.42  | 127.85      | 124.51   |
| 17  | T     | 102  | BCR  | C12-C13-C14 | 2.42  | 122.65      | 118.94   |
| 14  | G     | 821  | CLA  | C1-O2A-CGA  | 2.42  | 122.78      | 116.44   |
| 14  | Y     | 817  | CLA  | CMC-C2C-C3C | 2.42  | 132.67      | 126.12   |
| 14  | S     | 1102 | CLA  | CMA-C3A-C4A | 2.41  | 118.26      | 111.77   |
| 17  | G     | 850  | BCR  | C7-C8-C9    | -2.41 | 122.59      | 126.23   |
| 14  | Y     | 825  | CLA  | O2D-CGD-O1D | -2.41 | 119.12      | 123.84   |
| 14  | B     | 825  | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 17  | f     | 103  | BCR  | C24-C23-C22 | -2.41 | 122.59      | 126.23   |
| 14  | H     | 838  | CLA  | CMA-C3A-C4A | 2.41  | 118.25      | 111.77   |
| 14  | G     | 833  | CLA  | C3C-C4C-NC  | 2.41  | 113.27      | 110.57   |
| 17  | J     | 103  | BCR  | C7-C6-C5    | -2.41 | 115.62      | 121.46   |
| 14  | H     | 815  | CLA  | C1-O2A-CGA  | 2.41  | 122.77      | 116.44   |
| 14  | B     | 805  | CLA  | CHC-C1C-C2C | -2.41 | 120.06      | 126.72   |
| 14  | B     | 834  | CLA  | CHC-C1C-C2C | -2.41 | 120.06      | 126.72   |
| 14  | Y     | 834  | CLA  | C1-O2A-CGA  | 2.41  | 122.76      | 116.44   |
| 19  | Z     | 847  | LMG  | O8-C28-C29  | 2.41  | 119.46      | 111.91   |
| 17  | H     | 844  | BCR  | C7-C8-C9    | -2.41 | 122.60      | 126.23   |
| 14  | A     | 834  | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 17  | T     | 102  | BCR  | C30-C25-C26 | -2.41 | 119.22      | 122.61   |
| 14  | Y     | 806  | CLA  | C1-C2-C3    | -2.41 | 121.88      | 126.04   |
| 14  | B     | 812  | CLA  | CMD-C2D-C3D | -2.41 | 120.18      | 124.68   |
| 14  | B     | 803  | CLA  | CHC-C1C-C2C | -2.41 | 120.07      | 126.72   |
| 14  | G     | 838  | CLA  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 14  | H     | 827  | CLA  | OBD-CAD-C3D | -2.41 | 123.99      | 127.98   |
| 17  | H     | 841  | BCR  | C38-C26-C27 | 2.41  | 118.24      | 113.62   |
| 14  | Z     | 837  | CLA  | O1D-CGD-CBD | -2.40 | 119.56      | 124.48   |
| 17  | Z     | 846  | BCR  | C37-C22-C21 | -2.40 | 119.56      | 122.92   |
| 14  | B     | 814  | CLA  | CAC-C3C-C4C | 2.40  | 127.93      | 124.81   |
| 14  | G     | 819  | CLA  | CHB-C4A-NA  | 2.40  | 127.84      | 124.51   |
| 14  | A     | 824  | CLA  | CMA-C3A-C4A | 2.40  | 118.23      | 111.77   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 807  | CLA  | CAC-C3C-C4C | 2.40  | 127.93      | 124.81   |
| 14  | B     | 803  | CLA  | C3A-C2A-C1A | -2.40 | 97.74       | 101.34   |
| 14  | B     | 819  | CLA  | CED-O2D-CGD | 2.40  | 121.37      | 115.94   |
| 14  | Z     | 820  | CLA  | CAC-C3C-C4C | 2.40  | 127.92      | 124.81   |
| 14  | H     | 817  | CLA  | CMA-C3A-C4A | 2.40  | 118.22      | 111.77   |
| 14  | B     | 822  | CLA  | CHC-C1C-C2C | -2.40 | 120.08      | 126.72   |
| 14  | B     | 815  | CLA  | CHC-C1C-C2C | -2.40 | 120.08      | 126.72   |
| 18  | j     | 101  | LHG  | O8-C23-O10  | -2.40 | 117.54      | 123.59   |
| 14  | A     | 815  | CLA  | CHD-C4C-C3C | -2.40 | 121.31      | 124.84   |
| 14  | G     | 822  | CLA  | CHC-C1C-C2C | -2.40 | 120.09      | 126.72   |
| 14  | Y     | 825  | CLA  | CED-O2D-CGD | 2.40  | 121.36      | 115.94   |
| 14  | H     | 836  | CLA  | CAC-C3C-C4C | 2.40  | 127.92      | 124.81   |
| 14  | B     | 818  | CLA  | C4C-C3C-C2C | -2.40 | 103.40      | 106.90   |
| 14  | Y     | 818  | CLA  | CMA-C3A-C4A | 2.40  | 118.22      | 111.77   |
| 14  | B     | 832  | CLA  | C3C-C4C-NC  | 2.40  | 113.26      | 110.57   |
| 15  | G     | 844  | PQN  | C14-C13-C15 | 2.40  | 119.30      | 115.27   |
| 14  | B     | 816  | CLA  | CGD-CBD-CAD | 2.40  | 118.50      | 110.73   |
| 14  | U     | 1006 | CLA  | C1-C2-C3    | -2.40 | 121.90      | 126.04   |
| 14  | B     | 817  | CLA  | CED-O2D-CGD | 2.40  | 121.36      | 115.94   |
| 14  | A     | 826  | CLA  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 14  | Z     | 804  | CLA  | C1-C2-C3    | -2.40 | 121.90      | 126.04   |
| 14  | Z     | 819  | CLA  | CHC-C1C-C2C | -2.40 | 120.09      | 126.72   |
| 14  | A     | 828  | CLA  | C3C-C4C-NC  | 2.40  | 113.26      | 110.57   |
| 14  | Y     | 804  | CLA  | O1D-CGD-CBD | -2.40 | 119.58      | 124.48   |
| 19  | B     | 849  | LMG  | O6-C1-O1    | -2.40 | 104.30      | 109.97   |
| 14  | Y     | 834  | CLA  | CED-O2D-CGD | 2.40  | 121.36      | 115.94   |
| 14  | B     | 810  | CLA  | CAC-C3C-C4C | 2.40  | 127.92      | 124.81   |
| 14  | A     | 838  | CLA  | CMB-C2B-C3B | 2.40  | 129.16      | 124.68   |
| 14  | G     | 834  | CLA  | CHD-C4C-C3C | -2.39 | 121.32      | 124.84   |
| 17  | K     | 102  | BCR  | C29-C28-C27 | 2.39  | 116.73      | 111.38   |
| 17  | d     | 203  | BCR  | C34-C9-C8   | 2.39  | 121.85      | 118.08   |
| 14  | B     | 819  | CLA  | C4-C3-C5    | 2.39  | 119.30      | 115.27   |
| 17  | M     | 101  | BCR  | C28-C27-C26 | -2.39 | 109.80      | 114.08   |
| 14  | B     | 812  | CLA  | CED-O2D-CGD | 2.39  | 121.35      | 115.94   |
| 17  | B     | 851  | BCR  | C33-C5-C4   | 2.39  | 118.21      | 113.62   |
| 14  | H     | 830  | CLA  | C3C-C4C-NC  | 2.39  | 113.25      | 110.57   |
| 14  | G     | 822  | CLA  | C4-C3-C5    | 2.39  | 119.30      | 115.27   |
| 14  | L     | 201  | CLA  | CMB-C2B-C3B | 2.39  | 129.15      | 124.68   |
| 14  | L     | 207  | CLA  | C3C-C4C-NC  | 2.39  | 113.25      | 110.57   |
| 14  | Z     | 829  | CLA  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 14  | Y     | 839  | CLA  | CMB-C2B-C3B | 2.39  | 129.15      | 124.68   |
| 14  | B     | 827  | CLA  | CHC-C1C-C2C | -2.39 | 120.11      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 826  | CLA  | O1D-CGD-CBD | -2.39 | 119.60      | 124.48   |
| 17  | Z     | 841  | BCR  | C23-C22-C21 | -2.39 | 115.28      | 118.94   |
| 14  | d     | 201  | CLA  | CHC-C1C-C2C | -2.39 | 120.12      | 126.72   |
| 14  | A     | 813  | CLA  | CAC-C3C-C4C | 2.39  | 127.91      | 124.81   |
| 14  | G     | 828  | CLA  | C4C-C3C-C2C | -2.39 | 103.42      | 106.90   |
| 14  | Z     | 834  | CLA  | CAA-CBA-CGA | -2.39 | 108.46      | 113.59   |
| 14  | H     | 830  | CLA  | CED-O2D-CGD | 2.39  | 121.34      | 115.94   |
| 14  | f     | 101  | CLA  | CAC-C3C-C4C | 2.39  | 127.91      | 124.81   |
| 14  | A     | 805  | CLA  | CAA-C2A-C3A | -2.39 | 106.24      | 112.78   |
| 14  | K     | 101  | CLA  | CAD-CBD-CHA | -2.39 | 102.11      | 105.08   |
| 14  | H     | 814  | CLA  | O1D-CGD-CBD | -2.39 | 119.60      | 124.48   |
| 14  | H     | 810  | CLA  | CHC-C1C-C2C | -2.39 | 120.12      | 126.72   |
| 14  | G     | 828  | CLA  | CED-O2D-CGD | 2.39  | 121.33      | 115.94   |
| 14  | A     | 802  | CLA  | CHB-C4A-NA  | 2.39  | 127.81      | 124.51   |
| 14  | B     | 829  | CLA  | CMC-C2C-C1C | 2.39  | 128.67      | 125.04   |
| 14  | H     | 835  | CLA  | OBD-CAD-CBD | -2.38 | 122.49      | 125.89   |
| 14  | G     | 808  | CLA  | CAA-C2A-C1A | -2.38 | 104.16      | 111.97   |
| 14  | G     | 823  | CLA  | CMB-C2B-C3B | 2.38  | 129.14      | 124.68   |
| 14  | Y     | 829  | CLA  | CHC-C1C-C2C | -2.38 | 120.13      | 126.72   |
| 14  | U     | 1006 | CLA  | CAA-C2A-C1A | 2.38  | 119.79      | 111.97   |
| 14  | H     | 809  | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 13  | Y     | 801  | CL0  | C4-C3-C5    | 2.38  | 119.28      | 115.27   |
| 14  | A     | 808  | CLA  | CMA-C3A-C4A | 2.38  | 118.18      | 111.77   |
| 14  | H     | 804  | CLA  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 14  | B     | 817  | CLA  | CHC-C1C-C2C | -2.38 | 120.13      | 126.72   |
| 14  | A     | 829  | CLA  | CAC-C3C-C4C | 2.38  | 127.90      | 124.81   |
| 14  | G     | 843  | CLA  | CMC-C2C-C1C | 2.38  | 128.66      | 125.04   |
| 14  | G     | 838  | CLA  | OBD-CAD-C3D | -2.38 | 124.03      | 127.98   |
| 14  | B     | 813  | CLA  | C4C-C3C-C2C | -2.38 | 103.43      | 106.90   |
| 14  | Y     | 843  | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 14  | Y     | 842  | CLA  | OBD-CAD-C3D | -2.38 | 124.03      | 127.98   |
| 14  | j     | 102  | CLA  | CHC-C1C-C2C | -2.38 | 120.14      | 126.72   |
| 14  | H     | 824  | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 14  | U     | 1006 | CLA  | C4C-C3C-C2C | -2.38 | 103.43      | 106.90   |
| 17  | H     | 842  | BCR  | C12-C13-C14 | 2.38  | 122.59      | 118.94   |
| 14  | G     | 821  | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 14  | G     | 838  | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.81   |
| 14  | B     | 829  | CLA  | CBC-CAC-C3C | -2.38 | 105.88      | 112.43   |
| 14  | B     | 816  | CLA  | C3C-C4C-NC  | 2.38  | 113.24      | 110.57   |
| 17  | H     | 841  | BCR  | C31-C1-C6   | -2.38 | 106.44      | 110.30   |
| 14  | G     | 812  | CLA  | OBD-CAD-C3D | -2.38 | 124.04      | 127.98   |
| 14  | Z     | 809  | CLA  | C4-C3-C2    | -2.38 | 117.58      | 123.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 830  | CLA  | CAA-C2A-C3A | -2.38 | 106.27      | 112.78   |
| 17  | L     | 208  | BCR  | C33-C5-C6   | -2.38 | 121.86      | 124.53   |
| 17  | H     | 842  | BCR  | C31-C1-C6   | -2.37 | 106.45      | 110.30   |
| 14  | J     | 101  | CLA  | CMC-C2C-C1C | 2.37  | 128.65      | 125.04   |
| 14  | Y     | 829  | CLA  | CMA-C3A-C4A | 2.37  | 118.15      | 111.77   |
| 14  | L     | 202  | CLA  | CMB-C2B-C1B | 2.37  | 132.11      | 128.46   |
| 14  | G     | 841  | CLA  | C5-C3-C2    | -2.37 | 116.32      | 121.12   |
| 14  | B     | 830  | CLA  | C3C-C4C-NC  | 2.37  | 113.23      | 110.57   |
| 14  | Y     | 835  | CLA  | OBD-CAD-C3D | -2.37 | 124.04      | 127.98   |
| 14  | Z     | 831  | CLA  | C4C-C3C-C2C | -2.37 | 103.44      | 106.90   |
| 14  | G     | 829  | CLA  | C11-C10-C8  | -2.37 | 108.25      | 115.92   |
| 18  | H     | 847  | LHG  | O8-C23-C24  | 2.37  | 119.35      | 111.91   |
| 14  | B     | 827  | CLA  | CHB-C4A-NA  | 2.37  | 127.79      | 124.51   |
| 14  | Z     | 839  | CLA  | CMC-C2C-C1C | 2.37  | 128.65      | 125.04   |
| 14  | S     | 1101 | CLA  | CMA-C3A-C4A | 2.37  | 118.14      | 111.77   |
| 14  | A     | 824  | CLA  | CHD-C4C-C3C | -2.37 | 121.36      | 124.84   |
| 14  | Y     | 817  | CLA  | OBD-CAD-C3D | -2.37 | 124.05      | 127.98   |
| 14  | Z     | 834  | CLA  | CMB-C2B-C3B | 2.37  | 129.11      | 124.68   |
| 14  | L     | 207  | CLA  | CAA-C2A-C3A | -2.37 | 106.29      | 112.78   |
| 14  | G     | 820  | CLA  | CAC-C3C-C4C | 2.37  | 127.88      | 124.81   |
| 14  | L     | 206  | CLA  | C3C-C4C-NC  | 2.37  | 113.23      | 110.57   |
| 17  | I     | 101  | BCR  | C33-C5-C4   | 2.37  | 118.16      | 113.62   |
| 17  | f     | 103  | BCR  | C33-C5-C4   | 2.37  | 118.16      | 113.62   |
| 14  | Z     | 830  | CLA  | CHC-C1C-C2C | -2.37 | 120.18      | 126.72   |
| 14  | d     | 201  | CLA  | OBD-CAD-C3D | -2.36 | 124.06      | 127.98   |
| 14  | B     | 815  | CLA  | CMC-C2C-C1C | 2.36  | 128.64      | 125.04   |
| 14  | j     | 102  | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 14  | H     | 817  | CLA  | CHC-C1C-C2C | -2.36 | 120.19      | 126.72   |
| 14  | J     | 101  | CLA  | CHC-C1C-C2C | -2.36 | 120.19      | 126.72   |
| 14  | B     | 825  | CLA  | OBD-CAD-C3D | -2.36 | 124.06      | 127.98   |
| 14  | G     | 829  | CLA  | OBD-CAD-C3D | -2.36 | 124.06      | 127.98   |
| 13  | Y     | 801  | CL0  | CHC-C1C-C2C | -2.36 | 120.19      | 126.72   |
| 14  | B     | 824  | CLA  | CED-O2D-CGD | 2.36  | 121.28      | 115.94   |
| 14  | Y     | 833  | CLA  | C16-C15-C13 | -2.36 | 108.29      | 115.92   |
| 14  | A     | 825  | CLA  | C3C-C4C-NC  | 2.36  | 113.22      | 110.57   |
| 14  | H     | 813  | CLA  | CMC-C2C-C1C | 2.36  | 128.63      | 125.04   |
| 14  | Y     | 812  | CLA  | CHC-C1C-C2C | -2.36 | 120.19      | 126.72   |
| 14  | G     | 812  | CLA  | CHC-C1C-C2C | -2.36 | 120.19      | 126.72   |
| 14  | Z     | 826  | CLA  | CHC-C1C-C2C | -2.36 | 120.19      | 126.72   |
| 17  | Q     | 202  | BCR  | C33-C5-C4   | 2.36  | 118.15      | 113.62   |
| 14  | Y     | 832  | CLA  | CMA-C3A-C4A | 2.36  | 118.11      | 111.77   |
| 14  | H     | 808  | CLA  | C1-C2-C3    | -2.36 | 121.96      | 126.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 836  | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 14  | J     | 101  | CLA  | CMB-C2B-C3B | 2.36  | 129.09      | 124.68   |
| 14  | Z     | 821  | CLA  | C3C-C4C-NC  | 2.36  | 113.22      | 110.57   |
| 17  | R     | 102  | BCR  | C7-C6-C5    | 2.36  | 127.17      | 121.46   |
| 14  | H     | 802  | CLA  | CAC-C3C-C4C | 2.36  | 127.87      | 124.81   |
| 14  | A     | 809  | CLA  | CAC-C3C-C4C | 2.36  | 127.87      | 124.81   |
| 14  | Y     | 808  | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 14  | B     | 822  | CLA  | CMA-C3A-C4A | 2.36  | 118.11      | 111.77   |
| 14  | Z     | 835  | CLA  | CHC-C1C-C2C | -2.36 | 120.20      | 126.72   |
| 14  | Z     | 814  | CLA  | C3C-C4C-NC  | 2.36  | 113.22      | 110.57   |
| 14  | Y     | 837  | CLA  | C1-O2A-CGA  | 2.36  | 122.63      | 116.44   |
| 14  | H     | 826  | CLA  | CHC-C1C-C2C | -2.36 | 120.20      | 126.72   |
| 14  | A     | 809  | CLA  | C1-C2-C3    | -2.36 | 121.97      | 126.04   |
| 14  | Z     | 830  | CLA  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 14  | Y     | 809  | CLA  | CHC-C1C-C2C | -2.36 | 120.20      | 126.72   |
| 14  | H     | 823  | CLA  | O1D-CGD-CBD | -2.36 | 119.66      | 124.48   |
| 14  | A     | 838  | CLA  | CAC-C3C-C4C | 2.36  | 127.87      | 124.81   |
| 14  | A     | 804  | CLA  | CHC-C1C-C2C | -2.36 | 120.21      | 126.72   |
| 14  | H     | 826  | CLA  | C4C-C3C-C2C | -2.35 | 103.47      | 106.90   |
| 17  | Z     | 844  | BCR  | C23-C24-C25 | -2.35 | 120.59      | 127.20   |
| 17  | U     | 1005 | BCR  | C33-C5-C6   | -2.35 | 121.88      | 124.53   |
| 14  | Z     | 836  | CLA  | C6-C5-C3    | -2.35 | 107.28      | 113.45   |
| 14  | B     | 818  | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 14  | A     | 825  | CLA  | O2D-CGD-O1D | -2.35 | 119.24      | 123.84   |
| 17  | f     | 105  | BCR  | C37-C22-C23 | 2.35  | 121.78      | 118.08   |
| 14  | B     | 830  | CLA  | CED-O2D-CGD | 2.35  | 121.26      | 115.94   |
| 14  | L     | 207  | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 14  | U     | 1004 | CLA  | C3C-C4C-NC  | 2.35  | 113.21      | 110.57   |
| 17  | Y     | 849  | BCR  | C27-C26-C25 | -2.35 | 119.32      | 122.73   |
| 14  | B     | 814  | CLA  | CMC-C2C-C1C | 2.35  | 128.62      | 125.04   |
| 14  | G     | 802  | CLA  | CHC-C1C-C2C | -2.35 | 120.22      | 126.72   |
| 14  | H     | 834  | CLA  | O2A-C1-C2   | 2.35  | 114.82      | 108.64   |
| 17  | G     | 846  | BCR  | C2-C1-C6    | -2.35 | 106.86      | 110.48   |
| 14  | Z     | 818  | CLA  | C3C-C4C-NC  | 2.35  | 113.21      | 110.57   |
| 14  | Z     | 821  | CLA  | C4-C3-C2    | -2.35 | 117.65      | 123.68   |
| 14  | G     | 817  | CLA  | OBD-CAD-CBD | -2.35 | 122.54      | 125.89   |
| 17  | Z     | 846  | BCR  | C33-C5-C6   | -2.35 | 121.89      | 124.53   |
| 14  | H     | 806  | CLA  | CAC-C3C-C4C | 2.35  | 127.86      | 124.81   |
| 14  | Z     | 824  | CLA  | CMC-C2C-C1C | 2.35  | 128.62      | 125.04   |
| 14  | Y     | 805  | CLA  | CHC-C1C-C2C | -2.35 | 120.22      | 126.72   |
| 17  | M     | 101  | BCR  | C7-C8-C9    | -2.35 | 122.69      | 126.23   |
| 15  | Y     | 844  | PQN  | C2M-C2-C3   | -2.35 | 120.57      | 124.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Z     | 839  | CLA  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |
| 14  | G     | 831  | CLA  | CMA-C3A-C4A | 2.35  | 118.08      | 111.77   |
| 14  | H     | 824  | CLA  | CAA-C2A-C3A | -2.35 | 106.35      | 112.78   |
| 14  | Y     | 807  | CLA  | CMB-C2B-C3B | 2.35  | 129.07      | 124.68   |
| 14  | B     | 830  | CLA  | CMC-C2C-C1C | 2.35  | 128.61      | 125.04   |
| 14  | U     | 1003 | CLA  | CHC-C1C-C2C | -2.34 | 120.24      | 126.72   |
| 19  | H     | 846  | LMG  | C7-O1-C1    | 2.34  | 118.32      | 113.74   |
| 14  | B     | 822  | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 14  | U     | 1002 | CLA  | CGD-CBD-CAD | -2.34 | 103.15      | 110.73   |
| 14  | G     | 821  | CLA  | O2D-CGD-O1D | -2.34 | 119.26      | 123.84   |
| 14  | B     | 840  | CLA  | C4C-C3C-C2C | -2.34 | 103.48      | 106.90   |
| 14  | H     | 824  | CLA  | CAA-C2A-C1A | -2.34 | 104.30      | 111.97   |
| 14  | G     | 832  | CLA  | C16-C15-C13 | -2.34 | 108.35      | 115.92   |
| 17  | B     | 847  | BCR  | C32-C1-C6   | -2.34 | 106.50      | 110.30   |
| 17  | G     | 850  | BCR  | C36-C18-C17 | 2.34  | 126.20      | 122.92   |
| 14  | Z     | 821  | CLA  | CMB-C2B-C3B | 2.34  | 129.06      | 124.68   |
| 14  | Z     | 824  | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 14  | B     | 819  | CLA  | C4C-C3C-C2C | -2.34 | 103.49      | 106.90   |
| 14  | T     | 103  | CLA  | CHC-C1C-C2C | -2.34 | 120.25      | 126.72   |
| 14  | G     | 820  | CLA  | C3C-C4C-NC  | 2.34  | 113.19      | 110.57   |
| 14  | H     | 821  | CLA  | OBD-CAD-CBD | -2.34 | 122.56      | 125.89   |
| 14  | L     | 201  | CLA  | CMA-C3A-C4A | 2.34  | 118.06      | 111.77   |
| 17  | H     | 845  | BCR  | C32-C1-C6   | -2.34 | 106.51      | 110.30   |
| 14  | h     | 206  | CLA  | CAA-C2A-C3A | -2.34 | 106.38      | 112.78   |
| 14  | L     | 202  | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |
| 14  | B     | 802  | CLA  | CMD-C2D-C3D | -2.34 | 120.31      | 124.68   |
| 17  | f     | 104  | BCR  | C12-C13-C14 | 2.34  | 122.53      | 118.94   |
| 14  | G     | 828  | CLA  | CHD-C4C-C3C | -2.34 | 121.41      | 124.84   |
| 14  | H     | 837  | CLA  | CHC-C1C-C2C | -2.33 | 120.27      | 126.72   |
| 14  | Y     | 835  | CLA  | CAC-C3C-C4C | 2.33  | 127.84      | 124.81   |
| 14  | A     | 806  | CLA  | CAC-C3C-C4C | 2.33  | 127.84      | 124.81   |
| 14  | A     | 820  | CLA  | C5-C3-C2    | -2.33 | 116.40      | 121.12   |
| 14  | Z     | 829  | CLA  | C4C-C3C-C2C | -2.33 | 103.50      | 106.90   |
| 14  | H     | 835  | CLA  | C3C-C4C-NC  | 2.33  | 113.19      | 110.57   |
| 17  | Z     | 843  | BCR  | C23-C22-C21 | -2.33 | 115.36      | 118.94   |
| 14  | j     | 102  | CLA  | CMC-C2C-C1C | 2.33  | 128.59      | 125.04   |
| 14  | Y     | 811  | CLA  | C1-O2A-CGA  | 2.33  | 122.56      | 116.44   |
| 14  | B     | 814  | CLA  | C1-O2A-CGA  | 2.33  | 122.55      | 116.44   |
| 14  | B     | 809  | CLA  | C4-C3-C5    | 2.33  | 119.19      | 115.27   |
| 14  | Y     | 813  | CLA  | C3C-C4C-NC  | 2.33  | 113.18      | 110.57   |
| 14  | G     | 824  | CLA  | C4C-C3C-C2C | -2.33 | 103.50      | 106.90   |
| 17  | J     | 103  | BCR  | C33-C5-C6   | -2.33 | 121.91      | 124.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | G     | 852 | LHG  | C6-C5-C4    | -2.33 | 106.28      | 111.79   |
| 14  | H     | 815 | CLA  | OBD-CAD-C3D | -2.33 | 124.12      | 127.98   |
| 14  | B     | 811 | CLA  | C3C-C4C-NC  | 2.33  | 113.18      | 110.57   |
| 14  | Z     | 825 | CLA  | C4C-C3C-C2C | -2.33 | 103.51      | 106.90   |
| 14  | H     | 802 | CLA  | CHA-C1A-NA  | -2.33 | 121.07      | 126.40   |
| 14  | B     | 809 | CLA  | CMC-C2C-C1C | 2.33  | 128.58      | 125.04   |
| 14  | Y     | 830 | CLA  | CHB-C4A-NA  | 2.32  | 127.73      | 124.51   |
| 17  | H     | 841 | BCR  | C4-C5-C6    | -2.32 | 119.36      | 122.73   |
| 14  | G     | 842 | CLA  | C3C-C4C-NC  | 2.32  | 113.18      | 110.57   |
| 15  | H     | 839 | PQN  | C16-C15-C13 | -2.32 | 107.36      | 113.45   |
| 14  | J     | 102 | CLA  | CED-O2D-CGD | 2.32  | 121.19      | 115.94   |
| 14  | G     | 840 | CLA  | CED-O2D-CGD | 2.32  | 121.19      | 115.94   |
| 17  | A     | 846 | BCR  | C38-C26-C27 | 2.32  | 118.08      | 113.62   |
| 14  | Z     | 834 | CLA  | CHC-C1C-C2C | -2.32 | 120.30      | 126.72   |
| 14  | H     | 821 | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |
| 14  | G     | 826 | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |
| 14  | g     | 101 | CLA  | OBD-CAD-C3D | -2.32 | 124.82      | 127.19   |
| 14  | G     | 804 | CLA  | CMB-C2B-C3B | 2.32  | 129.02      | 124.68   |
| 14  | Y     | 843 | CLA  | CHC-C1C-C2C | -2.32 | 120.30      | 126.72   |
| 14  | A     | 841 | CLA  | OBD-CAD-CBD | -2.32 | 122.58      | 125.89   |
| 14  | A     | 807 | CLA  | C3C-C4C-NC  | 2.32  | 113.17      | 110.57   |
| 14  | B     | 823 | CLA  | C4-C3-C2    | -2.32 | 117.73      | 123.68   |
| 14  | Z     | 829 | CLA  | O1D-CGD-CBD | -2.32 | 119.74      | 124.48   |
| 14  | Z     | 809 | CLA  | C3C-C4C-NC  | 2.32  | 113.17      | 110.57   |
| 14  | B     | 811 | CLA  | CHC-C1C-C2C | -2.32 | 120.31      | 126.72   |
| 14  | B     | 816 | CLA  | CHC-C1C-C2C | -2.32 | 120.31      | 126.72   |
| 14  | A     | 806 | CLA  | C3C-C4C-NC  | 2.32  | 113.17      | 110.57   |
| 14  | Y     | 803 | CLA  | CMA-C3A-C4A | 2.32  | 118.00      | 111.77   |
| 14  | Z     | 811 | CLA  | CAC-C3C-C4C | 2.32  | 127.82      | 124.81   |
| 14  | A     | 818 | CLA  | OBD-CAD-C3D | -2.32 | 124.13      | 127.98   |
| 14  | H     | 833 | CLA  | CBC-CAC-C3C | -2.32 | 106.04      | 112.43   |
| 17  | h     | 203 | BCR  | C30-C25-C24 | 2.32  | 122.33      | 115.78   |
| 14  | B     | 808 | CLA  | CHC-C1C-C2C | -2.32 | 120.31      | 126.72   |
| 14  | Y     | 842 | CLA  | C3C-C4C-NC  | 2.32  | 113.17      | 110.57   |
| 14  | Z     | 805 | CLA  | C1-C2-C3    | -2.32 | 122.04      | 126.04   |
| 14  | Z     | 820 | CLA  | CHC-C1C-C2C | -2.32 | 120.32      | 126.72   |
| 14  | G     | 810 | CLA  | CHD-C4C-C3C | -2.31 | 121.44      | 124.84   |
| 14  | A     | 809 | CLA  | C11-C12-C13 | -2.31 | 108.44      | 115.92   |
| 14  | Y     | 854 | CLA  | CHB-C4A-NA  | 2.31  | 127.71      | 124.51   |
| 14  | Z     | 838 | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 14  | B     | 833 | CLA  | CHC-C1C-C2C | -2.31 | 120.32      | 126.72   |
| 17  | d     | 203 | BCR  | C29-C28-C27 | -2.31 | 106.21      | 111.38   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | H     | 840  | BCR  | C30-C25-C26 | -2.31 | 119.36      | 122.61   |
| 14  | Z     | 803  | CLA  | CHC-C1C-C2C | -2.31 | 120.33      | 126.72   |
| 14  | A     | 811  | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 14  | Y     | 855  | CLA  | C3C-C4C-NC  | 2.31  | 113.16      | 110.57   |
| 14  | B     | 841  | CLA  | C4C-C3C-C2C | -2.31 | 103.53      | 106.90   |
| 13  | G     | 801  | CL0  | C4-C3-C2    | -2.31 | 117.75      | 123.68   |
| 14  | V     | 1201 | CLA  | CMA-C3A-C4A | 2.31  | 117.98      | 111.77   |
| 17  | U     | 1007 | BCR  | C29-C30-C25 | -2.31 | 106.93      | 110.48   |
| 14  | G     | 803  | CLA  | CGD-CBD-CAD | -2.31 | 103.26      | 110.73   |
| 14  | G     | 835  | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 14  | A     | 822  | CLA  | O2D-CGD-O1D | -2.31 | 119.33      | 123.84   |
| 14  | G     | 838  | CLA  | C3C-C4C-NC  | 2.31  | 113.16      | 110.57   |
| 14  | H     | 804  | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 14  | A     | 835  | CLA  | C3C-C4C-NC  | 2.31  | 113.16      | 110.57   |
| 14  | Y     | 838  | CLA  | CMB-C2B-C3B | 2.31  | 128.99      | 124.68   |
| 14  | H     | 830  | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 14  | G     | 823  | CLA  | C1-O2A-CGA  | 2.31  | 122.49      | 116.44   |
| 14  | G     | 838  | CLA  | CBC-CAC-C3C | -2.31 | 106.08      | 112.43   |
| 14  | Y     | 818  | CLA  | CMD-C2D-C3D | -2.31 | 120.36      | 124.68   |
| 14  | A     | 829  | CLA  | O2D-CGD-O1D | -2.30 | 119.33      | 123.84   |
| 14  | Y     | 843  | CLA  | CAC-C3C-C4C | 2.30  | 127.80      | 124.81   |
| 14  | Y     | 830  | CLA  | CED-O2D-CGD | 2.30  | 121.15      | 115.94   |
| 14  | G     | 826  | CLA  | CHC-C1C-C2C | -2.30 | 120.35      | 126.72   |
| 14  | B     | 827  | CLA  | CMA-C3A-C4A | 2.30  | 117.97      | 111.77   |
| 14  | H     | 834  | CLA  | CMA-C3A-C4A | 2.30  | 117.97      | 111.77   |
| 14  | Z     | 827  | CLA  | O2D-CGD-O1D | -2.30 | 119.33      | 123.84   |
| 14  | G     | 809  | CLA  | C16-C15-C13 | -2.30 | 108.47      | 115.92   |
| 14  | A     | 816  | CLA  | CMC-C2C-C1C | 2.30  | 128.55      | 125.04   |
| 14  | Z     | 829  | CLA  | CHC-C1C-C2C | -2.30 | 120.35      | 126.72   |
| 14  | Z     | 806  | CLA  | CHC-C1C-C2C | -2.30 | 120.35      | 126.72   |
| 14  | Y     | 836  | CLA  | CED-O2D-CGD | 2.30  | 121.15      | 115.94   |
| 14  | Z     | 816  | CLA  | CMC-C2C-C1C | 2.30  | 128.55      | 125.04   |
| 17  | Z     | 844  | BCR  | C40-C30-C25 | 2.30  | 114.03      | 110.30   |
| 14  | f     | 102  | CLA  | C1-O2A-CGA  | 2.30  | 122.48      | 116.44   |
| 14  | Z     | 810  | CLA  | C3C-C4C-NC  | 2.30  | 113.15      | 110.57   |
| 14  | Y     | 854  | CLA  | CHC-C1C-C2C | -2.30 | 120.36      | 126.72   |
| 14  | B     | 838  | CLA  | C1-O2A-CGA  | 2.30  | 122.48      | 116.44   |
| 14  | L     | 207  | CLA  | C1-C2-C3    | -2.30 | 122.07      | 126.04   |
| 14  | H     | 816  | CLA  | CAA-C2A-C3A | -2.30 | 106.49      | 112.78   |
| 14  | H     | 828  | CLA  | CED-O2D-CGD | 2.30  | 121.13      | 115.94   |
| 14  | A     | 840  | CLA  | CMC-C2C-C1C | 2.30  | 128.54      | 125.04   |
| 14  | H     | 820  | CLA  | CHB-C4A-NA  | 2.30  | 127.69      | 124.51   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 838  | CLA  | C5-C3-C2    | -2.30 | 116.47      | 121.12   |
| 17  | U     | 1005 | BCR  | C37-C22-C23 | 2.30  | 121.69      | 118.08   |
| 14  | A     | 840  | CLA  | CAC-C3C-C4C | 2.30  | 127.79      | 124.81   |
| 14  | h     | 205  | CLA  | OBD-CAD-C3D | -2.30 | 124.17      | 127.98   |
| 15  | A     | 843  | PQN  | C11-C12-C13 | -2.30 | 122.97      | 126.79   |
| 17  | F     | 203  | BCR  | C28-C27-C26 | -2.29 | 109.98      | 114.08   |
| 14  | H     | 819  | CLA  | CHD-C4C-C3C | -2.29 | 121.47      | 124.84   |
| 14  | Y     | 841  | CLA  | OBD-CAD-CBD | -2.29 | 122.62      | 125.89   |
| 14  | G     | 824  | CLA  | C1-C2-C3    | -2.29 | 122.08      | 126.04   |
| 14  | Z     | 814  | CLA  | CHC-C1C-C2C | -2.29 | 120.38      | 126.72   |
| 14  | Y     | 812  | CLA  | C1-O2A-CGA  | 2.29  | 122.46      | 116.44   |
| 14  | Z     | 837  | CLA  | C3C-C4C-NC  | 2.29  | 113.14      | 110.57   |
| 14  | H     | 811  | CLA  | O2D-CGD-O1D | -2.29 | 119.36      | 123.84   |
| 14  | Z     | 816  | CLA  | CMB-C2B-C3B | 2.29  | 128.97      | 124.68   |
| 14  | Z     | 829  | CLA  | OBD-CAD-CBD | -2.29 | 122.62      | 125.89   |
| 14  | G     | 842  | CLA  | CHC-C1C-C2C | -2.29 | 120.39      | 126.72   |
| 14  | G     | 803  | CLA  | CMA-C3A-C4A | 2.29  | 117.93      | 111.77   |
| 14  | Z     | 808  | CLA  | OBD-CAD-C3D | -2.29 | 124.18      | 127.98   |
| 14  | Z     | 803  | CLA  | CAA-C2A-C3A | -2.29 | 106.51      | 112.78   |
| 14  | H     | 836  | CLA  | CHD-C4C-C3C | -2.29 | 121.47      | 124.84   |
| 14  | G     | 829  | CLA  | O1D-CGD-CBD | -2.29 | 119.80      | 124.48   |
| 14  | H     | 831  | CLA  | OBD-CAD-C3D | -2.29 | 124.18      | 127.98   |
| 14  | G     | 841  | CLA  | CHC-C1C-C2C | -2.29 | 120.39      | 126.72   |
| 17  | M     | 101  | BCR  | C38-C26-C25 | -2.29 | 121.96      | 124.53   |
| 14  | Y     | 838  | CLA  | CHB-C4A-NA  | 2.29  | 127.68      | 124.51   |
| 17  | Y     | 850  | BCR  | C30-C25-C26 | -2.29 | 119.39      | 122.61   |
| 14  | Z     | 815  | CLA  | O1D-CGD-CBD | -2.29 | 119.80      | 124.48   |
| 17  | G     | 847  | BCR  | C23-C22-C21 | 2.29  | 122.45      | 118.94   |
| 14  | H     | 837  | CLA  | O2A-CGA-CBA | 2.29  | 119.08      | 111.91   |
| 14  | Z     | 804  | CLA  | O2D-CGD-O1D | -2.29 | 119.37      | 123.84   |
| 14  | Y     | 817  | CLA  | CMB-C2B-C3B | 2.29  | 128.95      | 124.68   |
| 14  | G     | 843  | CLA  | C3C-C4C-NC  | 2.29  | 113.13      | 110.57   |
| 17  | G     | 854  | BCR  | C27-C26-C25 | -2.28 | 119.41      | 122.73   |
| 17  | B     | 848  | BCR  | C8-C7-C6    | -2.28 | 120.79      | 127.20   |
| 14  | H     | 821  | CLA  | C3C-C4C-NC  | 2.28  | 113.13      | 110.57   |
| 14  | Y     | 817  | CLA  | O2D-CGD-O1D | -2.28 | 119.37      | 123.84   |
| 17  | M     | 101  | BCR  | C8-C9-C10   | -2.28 | 115.44      | 118.94   |
| 14  | Y     | 827  | CLA  | CHD-C4C-C3C | -2.28 | 121.48      | 124.84   |
| 14  | A     | 852  | CLA  | CHC-C1C-C2C | -2.28 | 120.41      | 126.72   |
| 14  | B     | 804  | CLA  | CHC-C1C-C2C | -2.28 | 120.41      | 126.72   |
| 14  | Y     | 828  | CLA  | CHB-C4A-NA  | 2.28  | 127.67      | 124.51   |
| 17  | e     | 101  | BCR  | C15-C14-C13 | -2.28 | 124.05      | 127.31   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | R     | 101  | BCR  | C33-C5-C6   | -2.28 | 121.97      | 124.53   |
| 14  | F     | 202  | CLA  | O2D-CGD-O1D | -2.28 | 119.38      | 123.84   |
| 14  | Z     | 813  | CLA  | O2D-CGD-O1D | -2.28 | 119.38      | 123.84   |
| 14  | h     | 201  | CLA  | OBD-CAD-CBD | -2.28 | 122.64      | 125.89   |
| 17  | Y     | 846  | BCR  | C36-C18-C19 | -2.28 | 114.48      | 118.08   |
| 14  | Y     | 854  | CLA  | CMA-C3A-C4A | 2.28  | 117.90      | 111.77   |
| 14  | A     | 839  | CLA  | CED-O2D-CGD | 2.28  | 121.09      | 115.94   |
| 14  | G     | 830  | CLA  | CMC-C2C-C1C | 2.28  | 128.51      | 125.04   |
| 14  | A     | 832  | CLA  | O1D-CGD-CBD | -2.28 | 119.83      | 124.48   |
| 14  | T     | 101  | CLA  | CMC-C2C-C1C | 2.28  | 128.51      | 125.04   |
| 14  | A     | 833  | CLA  | O1D-CGD-CBD | -2.28 | 119.83      | 124.48   |
| 14  | Z     | 825  | CLA  | C3C-C4C-NC  | 2.28  | 113.12      | 110.57   |
| 14  | A     | 807  | CLA  | CHC-C1C-C2C | -2.28 | 120.42      | 126.72   |
| 14  | A     | 802  | CLA  | C1-O2A-CGA  | 2.28  | 122.42      | 116.44   |
| 14  | B     | 825  | CLA  | CED-O2D-CGD | 2.28  | 121.08      | 115.94   |
| 14  | Z     | 836  | CLA  | CHC-C1C-C2C | -2.28 | 120.43      | 126.72   |
| 14  | A     | 813  | CLA  | CMC-C2C-C3C | 2.28  | 132.29      | 126.12   |
| 17  | B     | 844  | BCR  | C8-C7-C6    | -2.28 | 120.81      | 127.20   |
| 17  | h     | 203  | BCR  | C24-C25-C26 | -2.28 | 115.95      | 121.46   |
| 17  | F     | 203  | BCR  | C38-C26-C27 | 2.28  | 117.99      | 113.62   |
| 18  | Y     | 853  | LHG  | O8-C23-C24  | 2.28  | 119.05      | 111.91   |
| 14  | A     | 802  | CLA  | C11-C12-C13 | -2.28 | 108.56      | 115.92   |
| 14  | Y     | 803  | CLA  | CMC-C2C-C1C | 2.27  | 128.50      | 125.04   |
| 17  | Y     | 850  | BCR  | C38-C26-C25 | -2.27 | 121.97      | 124.53   |
| 14  | A     | 836  | CLA  | CHC-C1C-C2C | -2.27 | 120.43      | 126.72   |
| 17  | Q     | 202  | BCR  | C23-C22-C21 | 2.27  | 122.43      | 118.94   |
| 14  | H     | 801  | CLA  | C6-C5-C3    | -2.27 | 107.50      | 113.45   |
| 14  | L     | 201  | CLA  | C4C-C3C-C2C | -2.27 | 103.58      | 106.90   |
| 14  | G     | 840  | CLA  | OBD-CAD-CBD | -2.27 | 122.65      | 125.89   |
| 14  | A     | 816  | CLA  | CED-O2D-CGD | 2.27  | 121.07      | 115.94   |
| 17  | J     | 103  | BCR  | C31-C1-C6   | -2.27 | 106.62      | 110.30   |
| 14  | H     | 830  | CLA  | CMA-C3A-C4A | 2.27  | 117.87      | 111.77   |
| 17  | U     | 1007 | BCR  | C30-C25-C26 | -2.27 | 119.42      | 122.61   |
| 14  | Z     | 822  | CLA  | CHB-C4A-NA  | 2.27  | 127.65      | 124.51   |
| 14  | Z     | 804  | CLA  | OBD-CAD-CBD | 2.27  | 129.14      | 125.89   |
| 14  | A     | 818  | CLA  | C4-C3-C5    | 2.27  | 119.09      | 115.27   |
| 14  | G     | 832  | CLA  | CMB-C2B-C3B | 2.27  | 128.92      | 124.68   |
| 17  | f     | 104  | BCR  | C33-C5-C4   | 2.27  | 117.97      | 113.62   |
| 14  | H     | 811  | CLA  | C3C-C4C-NC  | 2.27  | 113.11      | 110.57   |
| 14  | B     | 807  | CLA  | CBC-CAC-C3C | -2.27 | 106.18      | 112.43   |
| 14  | A     | 836  | CLA  | CED-O2D-CGD | 2.27  | 121.07      | 115.94   |
| 14  | A     | 823  | CLA  | C3C-C4C-NC  | 2.27  | 113.11      | 110.57   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 810  | CLA  | CHC-C1C-C2C | -2.27 | 120.45      | 126.72   |
| 14  | G     | 839  | CLA  | O2D-CGD-O1D | -2.27 | 119.41      | 123.84   |
| 14  | H     | 815  | CLA  | C4-C3-C5    | 2.27  | 119.08      | 115.27   |
| 17  | H     | 845  | BCR  | C30-C25-C26 | -2.27 | 119.42      | 122.61   |
| 14  | J     | 101  | CLA  | OBD-CAD-C3D | -2.27 | 124.22      | 127.98   |
| 14  | B     | 827  | CLA  | CED-O2D-CGD | 2.27  | 121.06      | 115.94   |
| 14  | G     | 843  | CLA  | CMA-C3A-C4A | 2.27  | 117.86      | 111.77   |
| 14  | B     | 811  | CLA  | C4-C3-C2    | -2.27 | 117.86      | 123.68   |
| 14  | A     | 838  | CLA  | O2A-C1-C2   | 2.27  | 114.59      | 108.64   |
| 14  | G     | 814  | CLA  | C3C-C4C-NC  | 2.27  | 113.11      | 110.57   |
| 14  | d     | 202  | CLA  | CHC-C1C-C2C | -2.27 | 120.45      | 126.72   |
| 14  | Y     | 826  | CLA  | CHB-C4A-NA  | 2.26  | 127.64      | 124.51   |
| 14  | G     | 822  | CLA  | C3C-C4C-NC  | 2.26  | 113.11      | 110.57   |
| 17  | B     | 844  | BCR  | C33-C5-C4   | 2.26  | 117.97      | 113.62   |
| 17  | A     | 847  | BCR  | C37-C22-C23 | 2.26  | 121.64      | 118.08   |
| 17  | L     | 209  | BCR  | C34-C9-C8   | 2.26  | 121.64      | 118.08   |
| 14  | Z     | 805  | CLA  | CAC-C3C-C4C | 2.26  | 127.75      | 124.81   |
| 14  | U     | 1002 | CLA  | CMA-C3A-C4A | 2.26  | 117.86      | 111.77   |
| 14  | H     | 802  | CLA  | CHC-C1C-C2C | -2.26 | 120.46      | 126.72   |
| 14  | B     | 833  | CLA  | CAA-C2A-C3A | -2.26 | 106.58      | 112.78   |
| 14  | Y     | 840  | CLA  | CHB-C4A-NA  | 2.26  | 127.64      | 124.51   |
| 14  | A     | 802  | CLA  | C7-C6-C5    | -2.26 | 107.22      | 113.36   |
| 14  | G     | 835  | CLA  | CMD-C2D-C3D | -2.26 | 120.45      | 124.68   |
| 14  | H     | 814  | CLA  | CMC-C2C-C1C | 2.26  | 128.48      | 125.04   |
| 14  | B     | 823  | CLA  | CAC-C3C-C4C | 2.26  | 127.74      | 124.81   |
| 14  | B     | 827  | CLA  | O2D-CGD-O1D | -2.26 | 119.42      | 123.84   |
| 14  | A     | 834  | CLA  | O2D-CGD-O1D | -2.26 | 119.42      | 123.84   |
| 14  | G     | 830  | CLA  | O2D-CGD-O1D | -2.26 | 119.42      | 123.84   |
| 14  | G     | 828  | CLA  | CAC-C3C-C4C | 2.26  | 127.74      | 124.81   |
| 14  | B     | 811  | CLA  | C6-C5-C3    | -2.26 | 107.53      | 113.45   |
| 14  | A     | 842  | CLA  | CHD-C4C-C3C | -2.26 | 121.52      | 124.84   |
| 14  | G     | 835  | CLA  | CAC-C3C-C4C | 2.26  | 127.74      | 124.81   |
| 17  | H     | 848  | BCR  | C38-C26-C27 | 2.26  | 117.95      | 113.62   |
| 17  | Q     | 204  | BCR  | C36-C18-C19 | -2.26 | 114.52      | 118.08   |
| 14  | B     | 815  | CLA  | OBD-CAD-CBD | -2.26 | 122.67      | 125.89   |
| 14  | H     | 809  | CLA  | CED-O2D-CGD | 2.26  | 121.04      | 115.94   |
| 14  | G     | 809  | CLA  | CBC-CAC-C3C | -2.26 | 106.21      | 112.43   |
| 14  | B     | 813  | CLA  | C1-O2A-CGA  | 2.26  | 122.36      | 116.44   |
| 14  | G     | 813  | CLA  | O1D-CGD-CBD | -2.26 | 119.87      | 124.48   |
| 14  | G     | 818  | CLA  | C4C-C3C-C2C | -2.26 | 103.61      | 106.90   |
| 17  | J     | 104  | BCR  | C30-C25-C24 | 2.26  | 122.16      | 115.78   |
| 14  | G     | 831  | CLA  | O1D-CGD-CBD | -2.25 | 119.87      | 124.48   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 814  | CLA  | C4C-C3C-C2C | -2.25 | 103.61      | 106.90   |
| 14  | G     | 809  | CLA  | CMD-C2D-C3D | -2.25 | 120.46      | 124.68   |
| 14  | Y     | 817  | CLA  | CED-O2D-CGD | 2.25  | 121.04      | 115.94   |
| 14  | A     | 822  | CLA  | C3C-C4C-NC  | 2.25  | 113.10      | 110.57   |
| 14  | A     | 817  | CLA  | C1-O2A-CGA  | 2.25  | 122.36      | 116.44   |
| 14  | G     | 822  | CLA  | C1-O2A-CGA  | 2.25  | 122.36      | 116.44   |
| 17  | Y     | 847  | BCR  | C27-C26-C25 | -2.25 | 119.46      | 122.73   |
| 14  | B     | 826  | CLA  | CHA-C1A-NA  | -2.25 | 121.24      | 126.40   |
| 17  | f     | 105  | BCR  | C7-C8-C9    | -2.25 | 122.83      | 126.23   |
| 14  | A     | 832  | CLA  | C4C-C3C-C2C | -2.25 | 103.61      | 106.90   |
| 14  | Y     | 816  | CLA  | CAC-C3C-C4C | 2.25  | 127.73      | 124.81   |
| 17  | H     | 848  | BCR  | C33-C5-C6   | -2.25 | 122.00      | 124.53   |
| 14  | Z     | 806  | CLA  | OBD-CAD-C3D | -2.25 | 124.24      | 127.98   |
| 14  | A     | 815  | CLA  | C1-O2A-CGA  | 2.25  | 122.35      | 116.44   |
| 14  | A     | 806  | CLA  | CED-O2D-CGD | 2.25  | 121.03      | 115.94   |
| 14  | G     | 810  | CLA  | C4C-C3C-C2C | -2.25 | 103.62      | 106.90   |
| 14  | B     | 817  | CLA  | CHA-C1A-NA  | -2.25 | 121.24      | 126.40   |
| 14  | B     | 811  | CLA  | CED-O2D-CGD | 2.25  | 121.03      | 115.94   |
| 14  | Y     | 817  | CLA  | C1-O2A-CGA  | 2.25  | 122.35      | 116.44   |
| 17  | Y     | 856  | BCR  | C38-C26-C27 | 2.25  | 117.94      | 113.62   |
| 14  | B     | 837  | CLA  | C4C-C3C-C2C | -2.25 | 103.62      | 106.90   |
| 14  | B     | 803  | CLA  | CBC-CAC-C3C | -2.25 | 106.23      | 112.43   |
| 14  | Z     | 824  | CLA  | CHC-C1C-C2C | -2.25 | 120.50      | 126.72   |
| 14  | A     | 809  | CLA  | CMA-C3A-C4A | 2.25  | 117.81      | 111.77   |
| 17  | h     | 203  | BCR  | C8-C7-C6    | -2.25 | 120.89      | 127.20   |
| 14  | Z     | 838  | CLA  | CHD-C4C-C3C | -2.25 | 121.54      | 124.84   |
| 14  | G     | 811  | CLA  | CHC-C1C-C2C | -2.25 | 120.51      | 126.72   |
| 17  | S     | 1104 | BCR  | C39-C30-C25 | -2.25 | 106.66      | 110.30   |
| 17  | B     | 845  | BCR  | C32-C1-C6   | 2.25  | 113.94      | 110.30   |
| 14  | G     | 832  | CLA  | CMA-C3A-C4A | 2.25  | 117.81      | 111.77   |
| 14  | A     | 841  | CLA  | CED-O2D-CGD | 2.25  | 121.02      | 115.94   |
| 14  | A     | 805  | CLA  | C1-C2-C3    | -2.25 | 122.16      | 126.04   |
| 17  | G     | 849  | BCR  | C29-C30-C25 | -2.25 | 107.02      | 110.48   |
| 14  | A     | 817  | CLA  | C3C-C4C-NC  | 2.25  | 113.09      | 110.57   |
| 14  | H     | 835  | CLA  | CED-O2D-CGD | 2.25  | 121.02      | 115.94   |
| 17  | B     | 844  | BCR  | C24-C25-C26 | 2.25  | 126.90      | 121.46   |
| 14  | Z     | 820  | CLA  | C1-O2A-CGA  | 2.25  | 122.33      | 116.44   |
| 14  | Z     | 821  | CLA  | C1-O2A-CGA  | 2.25  | 122.33      | 116.44   |
| 17  | A     | 849  | BCR  | C3-C4-C5    | -2.25 | 110.07      | 114.08   |
| 17  | Y     | 849  | BCR  | C33-C5-C4   | 2.25  | 117.93      | 113.62   |
| 14  | Z     | 834  | CLA  | CED-O2D-CGD | 2.24  | 121.01      | 115.94   |
| 17  | F     | 201  | BCR  | C39-C30-C25 | -2.24 | 106.66      | 110.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | Y     | 838  | CLA  | OBD-CAD-C3D | -2.24 | 124.26      | 127.98   |
| 14  | G     | 836  | CLA  | CMA-C3A-C4A | 2.24  | 117.80      | 111.77   |
| 14  | Y     | 855  | CLA  | CHC-C1C-C2C | -2.24 | 120.52      | 126.72   |
| 14  | H     | 822  | CLA  | CHC-C1C-C2C | -2.24 | 120.52      | 126.72   |
| 14  | Y     | 823  | CLA  | C1-O2A-CGA  | 2.24  | 122.33      | 116.44   |
| 17  | A     | 847  | BCR  | C28-C27-C26 | -2.24 | 110.07      | 114.08   |
| 14  | Y     | 837  | CLA  | CED-O2D-CGD | 2.24  | 121.01      | 115.94   |
| 14  | Y     | 834  | CLA  | C1B-CHB-C4A | -2.24 | 125.67      | 130.12   |
| 17  | Y     | 847  | BCR  | C32-C1-C6   | -2.24 | 106.66      | 110.30   |
| 14  | H     | 802  | CLA  | CED-O2D-CGD | 2.24  | 121.00      | 115.94   |
| 14  | Z     | 817  | CLA  | CMA-C3A-C4A | 2.24  | 117.80      | 111.77   |
| 14  | A     | 852  | CLA  | C1-C2-C3    | -2.24 | 122.17      | 126.04   |
| 14  | A     | 805  | CLA  | OBD-CAD-C3D | -2.24 | 124.26      | 127.98   |
| 17  | J     | 103  | BCR  | C24-C25-C26 | 2.24  | 126.89      | 121.46   |
| 14  | Y     | 815  | CLA  | O1D-CGD-CBD | -2.24 | 119.90      | 124.48   |
| 14  | Z     | 805  | CLA  | C4-C3-C5    | 2.24  | 119.04      | 115.27   |
| 17  | J     | 103  | BCR  | C23-C22-C21 | 2.24  | 122.38      | 118.94   |
| 14  | B     | 833  | CLA  | C1-C2-C3    | -2.24 | 122.17      | 126.04   |
| 17  | Q     | 202  | BCR  | C1-C6-C5    | -2.24 | 119.46      | 122.61   |
| 14  | A     | 817  | CLA  | C4-C3-C2    | -2.24 | 117.94      | 123.68   |
| 14  | A     | 804  | CLA  | CHD-C4C-C3C | -2.24 | 121.55      | 124.84   |
| 14  | A     | 810  | CLA  | CMA-C3A-C4A | 2.24  | 117.79      | 111.77   |
| 17  | A     | 849  | BCR  | C29-C28-C27 | -2.24 | 106.38      | 111.38   |
| 17  | A     | 849  | BCR  | C39-C30-C25 | -2.24 | 106.67      | 110.30   |
| 14  | Z     | 838  | CLA  | CAC-C3C-C4C | 2.24  | 127.71      | 124.81   |
| 14  | Y     | 812  | CLA  | C4-C3-C2    | -2.24 | 117.94      | 123.68   |
| 14  | A     | 817  | CLA  | CHC-C1C-C2C | -2.23 | 120.54      | 126.72   |
| 14  | B     | 840  | CLA  | O2A-CGA-CBA | 2.23  | 118.92      | 111.91   |
| 14  | Y     | 816  | CLA  | CHC-C1C-C2C | -2.23 | 120.54      | 126.72   |
| 17  | B     | 845  | BCR  | C7-C8-C9    | -2.23 | 122.86      | 126.23   |
| 14  | W     | 1701 | CLA  | OBD-CAD-C3D | -2.23 | 124.27      | 127.98   |
| 14  | Y     | 839  | CLA  | O1D-CGD-CBD | -2.23 | 119.91      | 124.48   |
| 14  | Z     | 815  | CLA  | CHC-C1C-C2C | -2.23 | 120.55      | 126.72   |
| 14  | Y     | 811  | CLA  | O2D-CGD-O1D | -2.23 | 119.47      | 123.84   |
| 14  | h     | 201  | CLA  | CHC-C1C-C2C | -2.23 | 120.55      | 126.72   |
| 14  | H     | 814  | CLA  | CHC-C1C-C2C | -2.23 | 120.55      | 126.72   |
| 14  | B     | 822  | CLA  | C3C-C4C-NC  | 2.23  | 113.07      | 110.57   |
| 17  | Q     | 202  | BCR  | C15-C14-C13 | -2.23 | 124.12      | 127.31   |
| 14  | U     | 1006 | CLA  | CHC-C1C-C2C | -2.23 | 120.55      | 126.72   |
| 14  | Z     | 832  | CLA  | CAA-C2A-C3A | -2.23 | 106.67      | 112.78   |
| 14  | B     | 814  | CLA  | CAA-C2A-C3A | -2.23 | 106.67      | 112.78   |
| 14  | B     | 815  | CLA  | O2D-CGD-O1D | -2.23 | 119.48      | 123.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 810  | CLA  | CHA-C1A-NA  | -2.23 | 121.29      | 126.40   |
| 18  | Y     | 853  | LHG  | O7-C7-O9    | -2.23 | 118.53      | 122.96   |
| 17  | Y     | 846  | BCR  | C35-C13-C14 | -2.23 | 119.80      | 122.92   |
| 14  | G     | 823  | CLA  | CBC-CAC-C3C | -2.23 | 106.28      | 112.43   |
| 14  | G     | 834  | CLA  | CMC-C2C-C1C | 2.23  | 128.43      | 125.04   |
| 14  | Z     | 822  | CLA  | C4C-C3C-C2C | -2.23 | 103.65      | 106.90   |
| 17  | G     | 847  | BCR  | C3-C4-C5    | -2.23 | 110.10      | 114.08   |
| 17  | V     | 1202 | BCR  | C2-C3-C4    | -2.23 | 106.40      | 111.38   |
| 14  | B     | 810  | CLA  | C11-C12-C13 | -2.23 | 108.72      | 115.92   |
| 17  | G     | 848  | BCR  | C12-C13-C14 | 2.23  | 122.36      | 118.94   |
| 14  | B     | 833  | CLA  | CED-O2D-CGD | 2.23  | 120.97      | 115.94   |
| 14  | B     | 802  | CLA  | CAC-C3C-C4C | 2.23  | 127.70      | 124.81   |
| 14  | B     | 820  | CLA  | CMD-C2D-C3D | -2.23 | 120.51      | 124.68   |
| 14  | Z     | 807  | CLA  | CHD-C4C-C3C | -2.23 | 121.56      | 124.84   |
| 14  | B     | 808  | CLA  | CAC-C3C-C4C | 2.23  | 127.70      | 124.81   |
| 14  | G     | 840  | CLA  | O2D-CGD-O1D | -2.23 | 119.48      | 123.84   |
| 17  | U     | 1007 | BCR  | C40-C30-C25 | -2.23 | 106.69      | 110.30   |
| 14  | B     | 839  | CLA  | C3C-C4C-NC  | 2.23  | 113.07      | 110.57   |
| 14  | Y     | 804  | CLA  | CED-O2D-CGD | 2.23  | 120.97      | 115.94   |
| 14  | A     | 810  | CLA  | CED-O2D-CGD | 2.23  | 120.97      | 115.94   |
| 14  | Z     | 805  | CLA  | CBC-CAC-C3C | -2.23 | 106.30      | 112.43   |
| 14  | Z     | 828  | CLA  | CHC-C1C-C2C | -2.22 | 120.57      | 126.72   |
| 14  | L     | 202  | CLA  | CHC-C1C-C2C | -2.22 | 120.57      | 126.72   |
| 14  | h     | 205  | CLA  | CHC-C1C-C2C | -2.22 | 120.57      | 126.72   |
| 14  | W     | 1701 | CLA  | CMB-C2B-C3B | 2.22  | 128.84      | 124.68   |
| 14  | H     | 803  | CLA  | CAA-C2A-C3A | -2.22 | 106.69      | 112.78   |
| 14  | d     | 201  | CLA  | CHB-C4A-NA  | 2.22  | 127.59      | 124.51   |
| 14  | Z     | 835  | CLA  | C1-C2-C3    | -2.22 | 122.20      | 126.04   |
| 14  | Y     | 824  | CLA  | O1D-CGD-CBD | -2.22 | 119.94      | 124.48   |
| 14  | Z     | 831  | CLA  | CAA-CBA-CGA | -2.22 | 106.76      | 113.25   |
| 14  | B     | 841  | CLA  | C6-C5-C3    | -2.22 | 107.63      | 113.45   |
| 17  | G     | 854  | BCR  | C23-C22-C21 | 2.22  | 122.35      | 118.94   |
| 14  | Y     | 838  | CLA  | C1-C2-C3    | -2.22 | 122.20      | 126.04   |
| 14  | G     | 803  | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 14  | A     | 835  | CLA  | CED-O2D-CGD | 2.22  | 120.96      | 115.94   |
| 14  | H     | 834  | CLA  | CHC-C1C-C2C | -2.22 | 120.58      | 126.72   |
| 17  | Y     | 850  | BCR  | C38-C26-C27 | 2.22  | 117.88      | 113.62   |
| 14  | B     | 824  | CLA  | C4C-C3C-C2C | -2.22 | 103.66      | 106.90   |
| 14  | Y     | 834  | CLA  | C2A-C3A-C4A | -2.22 | 98.28       | 101.87   |
| 14  | A     | 809  | CLA  | CMB-C2B-C3B | 2.22  | 128.83      | 124.68   |
| 14  | f     | 101  | CLA  | C4C-C3C-C2C | -2.22 | 103.66      | 106.90   |
| 14  | A     | 808  | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | R     | 101  | BCR  | C24-C25-C26 | 2.22  | 126.84      | 121.46   |
| 17  | M     | 101  | BCR  | C34-C9-C10  | -2.22 | 119.81      | 122.92   |
| 17  | T     | 102  | BCR  | C35-C13-C14 | -2.22 | 119.81      | 122.92   |
| 14  | f     | 102  | CLA  | CMB-C2B-C3B | 2.22  | 128.83      | 124.68   |
| 14  | G     | 809  | CLA  | CHC-C1C-C2C | -2.22 | 120.58      | 126.72   |
| 14  | Y     | 840  | CLA  | CHC-C1C-C2C | -2.22 | 120.59      | 126.72   |
| 14  | H     | 837  | CLA  | C4C-C3C-C2C | -2.22 | 103.66      | 106.90   |
| 18  | G     | 851  | LHG  | C5-O7-C7    | -2.22 | 112.33      | 117.79   |
| 14  | Y     | 821  | CLA  | CMA-C3A-C4A | 2.22  | 117.73      | 111.77   |
| 14  | Z     | 816  | CLA  | C3C-C4C-NC  | 2.22  | 113.06      | 110.57   |
| 14  | H     | 816  | CLA  | C3A-C2A-C1A | 2.22  | 104.66      | 101.34   |
| 17  | L     | 208  | BCR  | C38-C26-C25 | -2.22 | 122.04      | 124.53   |
| 14  | Z     | 811  | CLA  | C3C-C4C-NC  | 2.22  | 113.06      | 110.57   |
| 17  | Y     | 851  | BCR  | C1-C6-C5    | -2.22 | 119.49      | 122.61   |
| 17  | A     | 849  | BCR  | C33-C5-C4   | 2.22  | 117.87      | 113.62   |
| 14  | H     | 820  | CLA  | CGD-CBD-CAD | -2.22 | 103.56      | 110.73   |
| 14  | H     | 831  | CLA  | CMD-C2D-C3D | -2.21 | 120.53      | 124.68   |
| 14  | Z     | 817  | CLA  | CHC-C1C-C2C | -2.21 | 120.60      | 126.72   |
| 14  | B     | 838  | CLA  | CHB-C4A-NA  | 2.21  | 127.57      | 124.51   |
| 14  | W     | 1701 | CLA  | CAC-C3C-C4C | 2.21  | 127.68      | 124.81   |
| 14  | G     | 840  | CLA  | C1-O2A-CGA  | 2.21  | 122.25      | 116.44   |
| 14  | Z     | 812  | CLA  | C1-O2A-CGA  | 2.21  | 122.25      | 116.44   |
| 14  | T     | 101  | CLA  | CMA-C3A-C4A | 2.21  | 117.72      | 111.77   |
| 14  | H     | 806  | CLA  | C4D-C3D-CAD | 2.21  | 109.70      | 108.47   |
| 14  | Z     | 810  | CLA  | CHC-C1C-C2C | -2.21 | 120.60      | 126.72   |
| 14  | B     | 821  | CLA  | CMB-C2B-C3B | 2.21  | 128.82      | 124.68   |
| 14  | B     | 819  | CLA  | CAC-C3C-C4C | 2.21  | 127.68      | 124.81   |
| 14  | G     | 843  | CLA  | C1-O2A-CGA  | 2.21  | 122.24      | 116.44   |
| 17  | J     | 104  | BCR  | C37-C22-C23 | 2.21  | 121.56      | 118.08   |
| 14  | A     | 838  | CLA  | OBD-CAD-C3D | -2.21 | 124.31      | 127.98   |
| 14  | F     | 202  | CLA  | CHA-C1A-NA  | -2.21 | 121.34      | 126.40   |
| 14  | Y     | 802  | CLA  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 14  | G     | 803  | CLA  | CAC-C3C-C4C | 2.21  | 127.68      | 124.81   |
| 14  | d     | 201  | CLA  | CED-O2D-CGD | 2.21  | 120.93      | 115.94   |
| 14  | Z     | 829  | CLA  | CHB-C4A-NA  | 2.21  | 127.57      | 124.51   |
| 14  | H     | 818  | CLA  | CHC-C1C-C2C | -2.21 | 120.61      | 126.72   |
| 17  | h     | 203  | BCR  | C39-C30-C25 | 2.21  | 113.88      | 110.30   |
| 14  | A     | 814  | CLA  | C1-O2A-CGA  | 2.21  | 122.24      | 116.44   |
| 14  | H     | 807  | CLA  | C4D-C3D-CAD | 2.21  | 109.70      | 108.47   |
| 17  | Z     | 844  | BCR  | C29-C30-C25 | 2.21  | 113.88      | 110.48   |
| 17  | H     | 848  | BCR  | C23-C22-C21 | 2.21  | 122.33      | 118.94   |
| 14  | Y     | 813  | CLA  | C4-C3-C5    | 2.21  | 118.98      | 115.27   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | H     | 827  | CLA  | O1D-CGD-CBD | -2.21 | 119.97      | 124.48   |
| 17  | S     | 1104 | BCR  | C30-C25-C24 | 2.21  | 122.02      | 115.78   |
| 14  | Y     | 805  | CLA  | CHB-C4A-NA  | 2.21  | 127.56      | 124.51   |
| 14  | Z     | 812  | CLA  | CMA-C3A-C4A | 2.21  | 117.70      | 111.77   |
| 14  | G     | 821  | CLA  | C3C-C4C-NC  | 2.21  | 113.04      | 110.57   |
| 14  | L     | 207  | CLA  | OBD-CAD-C3D | -2.20 | 124.32      | 127.98   |
| 14  | g     | 101  | CLA  | CAD-CBD-CHA | -2.20 | 102.34      | 105.08   |
| 14  | H     | 837  | CLA  | O2D-CGD-O1D | -2.20 | 119.53      | 123.84   |
| 14  | S     | 1103 | CLA  | C1-O2A-CGA  | 2.20  | 122.22      | 116.44   |
| 14  | A     | 837  | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 17  | h     | 203  | BCR  | C35-C13-C12 | 2.20  | 121.55      | 118.08   |
| 14  | T     | 101  | CLA  | C3C-C4C-NC  | 2.20  | 113.04      | 110.57   |
| 14  | H     | 814  | CLA  | C3C-C4C-NC  | 2.20  | 113.04      | 110.57   |
| 14  | U     | 1002 | CLA  | CHB-C4A-NA  | 2.20  | 127.56      | 124.51   |
| 17  | f     | 105  | BCR  | C33-C5-C6   | -2.20 | 122.06      | 124.53   |
| 14  | Z     | 824  | CLA  | C7-C6-C5    | -2.20 | 107.38      | 113.36   |
| 14  | H     | 820  | CLA  | O1D-CGD-CBD | -2.20 | 119.98      | 124.48   |
| 14  | Z     | 820  | CLA  | CMA-C3A-C4A | 2.20  | 117.69      | 111.77   |
| 14  | B     | 826  | CLA  | CAC-C3C-C4C | 2.20  | 127.66      | 124.81   |
| 14  | B     | 813  | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.94   |
| 14  | B     | 821  | CLA  | CAC-C3C-C4C | 2.20  | 127.66      | 124.81   |
| 14  | Z     | 808  | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.94   |
| 14  | Z     | 814  | CLA  | CGD-CBD-CAD | -2.20 | 103.61      | 110.73   |
| 14  | A     | 831  | CLA  | OBD-CAD-C3D | -2.20 | 124.33      | 127.98   |
| 14  | A     | 819  | CLA  | C3C-C4C-NC  | 2.20  | 113.04      | 110.57   |
| 14  | A     | 810  | CLA  | CHC-C1C-C2C | -2.20 | 120.64      | 126.72   |
| 14  | H     | 835  | CLA  | CAC-C3C-C4C | 2.20  | 127.66      | 124.81   |
| 17  | H     | 845  | BCR  | C33-C5-C4   | 2.20  | 117.84      | 113.62   |
| 14  | G     | 837  | CLA  | CHC-C1C-C2C | -2.20 | 120.64      | 126.72   |
| 14  | G     | 834  | CLA  | CHB-C4A-NA  | 2.20  | 127.55      | 124.51   |
| 14  | G     | 842  | CLA  | C5-C3-C2    | -2.20 | 116.67      | 121.12   |
| 14  | A     | 819  | CLA  | CHB-C4A-NA  | 2.20  | 127.55      | 124.51   |
| 14  | Z     | 839  | CLA  | C14-C13-C12 | 2.19  | 119.24      | 111.29   |
| 14  | H     | 838  | CLA  | CMB-C2B-C3B | 2.19  | 128.78      | 124.68   |
| 19  | B     | 849  | LMG  | O7-C10-C11  | 2.19  | 116.23      | 111.50   |
| 14  | H     | 802  | CLA  | C3C-C4C-NC  | 2.19  | 113.03      | 110.57   |
| 14  | G     | 837  | CLA  | CMC-C2C-C1C | 2.19  | 128.38      | 125.04   |
| 14  | Z     | 809  | CLA  | CHC-C1C-C2C | -2.19 | 120.66      | 126.72   |
| 14  | Y     | 831  | CLA  | O1D-CGD-CBD | -2.19 | 120.00      | 124.48   |
| 17  | H     | 844  | BCR  | C39-C30-C25 | -2.19 | 106.74      | 110.30   |
| 14  | Y     | 823  | CLA  | CHC-C1C-C2C | -2.19 | 120.66      | 126.72   |
| 14  | H     | 825  | CLA  | CHC-C1C-C2C | -2.19 | 120.66      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Z     | 843  | BCR  | C30-C25-C26 | -2.19 | 119.53      | 122.61   |
| 13  | Y     | 801  | CL0  | C4-C3-C2    | -2.19 | 118.06      | 123.68   |
| 14  | B     | 804  | CLA  | C3C-C4C-NC  | 2.19  | 113.03      | 110.57   |
| 14  | H     | 813  | CLA  | CAA-C2A-C3A | -2.19 | 106.78      | 112.78   |
| 14  | j     | 102  | CLA  | CMA-C3A-C4A | 2.19  | 117.66      | 111.77   |
| 14  | Z     | 807  | CLA  | C1-C2-C3    | -2.19 | 122.25      | 126.04   |
| 14  | W     | 1701 | CLA  | C3C-C4C-NC  | 2.19  | 113.03      | 110.57   |
| 18  | j     | 101  | LHG  | O7-C7-O9    | -2.19 | 118.41      | 123.70   |
| 14  | Z     | 804  | CLA  | C1-O2A-CGA  | 2.19  | 122.19      | 116.44   |
| 14  | G     | 807  | CLA  | C1-O2A-CGA  | 2.19  | 122.19      | 116.44   |
| 14  | H     | 838  | CLA  | CHD-C4C-C3C | -2.19 | 121.62      | 124.84   |
| 14  | Z     | 836  | CLA  | O2D-CGD-O1D | -2.19 | 119.56      | 123.84   |
| 14  | B     | 821  | CLA  | CHC-C1C-C2C | -2.19 | 120.67      | 126.72   |
| 17  | G     | 848  | BCR  | C35-C13-C14 | -2.19 | 119.86      | 122.92   |
| 14  | Z     | 824  | CLA  | CED-O2D-CGD | 2.19  | 120.89      | 115.94   |
| 14  | F     | 202  | CLA  | CAA-C2A-C1A | 2.19  | 119.14      | 111.97   |
| 14  | A     | 836  | CLA  | CHA-C1A-NA  | -2.19 | 121.39      | 126.40   |
| 14  | H     | 823  | CLA  | CHC-C1C-C2C | -2.19 | 120.68      | 126.72   |
| 14  | L     | 206  | CLA  | CAA-CBA-CGA | 2.18  | 119.64      | 113.25   |
| 14  | G     | 808  | CLA  | CBC-CAC-C3C | -2.18 | 106.41      | 112.43   |
| 14  | j     | 102  | CLA  | O2D-CGD-CBD | 2.18  | 115.15      | 111.27   |
| 14  | A     | 821  | CLA  | C1-O2A-CGA  | 2.18  | 122.17      | 116.44   |
| 14  | B     | 810  | CLA  | CED-O2D-CGD | 2.18  | 120.88      | 115.94   |
| 14  | g     | 101  | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 14  | A     | 809  | CLA  | O2D-CGD-O1D | -2.18 | 119.57      | 123.84   |
| 14  | G     | 837  | CLA  | C1-O2A-CGA  | 2.18  | 122.17      | 116.44   |
| 14  | L     | 205  | CLA  | CED-O2D-CGD | 2.18  | 120.87      | 115.94   |
| 14  | S     | 1101 | CLA  | C16-C15-C13 | -2.18 | 108.87      | 115.92   |
| 17  | f     | 105  | BCR  | C31-C1-C6   | -2.18 | 106.76      | 110.30   |
| 14  | Z     | 802  | CLA  | CAA-C2A-C3A | -2.18 | 106.80      | 112.78   |
| 14  | B     | 819  | CLA  | C11-C10-C8  | -2.18 | 108.87      | 115.92   |
| 14  | H     | 819  | CLA  | CHC-C1C-C2C | -2.18 | 120.69      | 126.72   |
| 14  | G     | 833  | CLA  | CMB-C2B-C3B | 2.18  | 128.76      | 124.68   |
| 14  | Y     | 837  | CLA  | CHC-C1C-C2C | -2.18 | 120.69      | 126.72   |
| 17  | H     | 842  | BCR  | C35-C13-C14 | -2.18 | 119.87      | 122.92   |
| 14  | G     | 843  | CLA  | CHC-C1C-C2C | -2.18 | 120.69      | 126.72   |
| 17  | I     | 101  | BCR  | C8-C9-C10   | 2.18  | 122.29      | 118.94   |
| 14  | B     | 825  | CLA  | CMA-C3A-C4A | 2.18  | 117.63      | 111.77   |
| 14  | H     | 822  | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 14  | A     | 833  | CLA  | C16-C15-C13 | -2.18 | 108.88      | 115.92   |
| 14  | Z     | 804  | CLA  | CAC-C3C-C2C | -2.18 | 123.80      | 127.53   |
| 14  | G     | 808  | CLA  | C6-C5-C3    | -2.18 | 107.74      | 113.45   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 846  | BCR  | C36-C18-C19 | -2.18 | 114.65      | 118.08   |
| 17  | Y     | 856  | BCR  | C38-C26-C25 | -2.18 | 122.08      | 124.53   |
| 14  | B     | 802  | CLA  | CMA-C3A-C4A | 2.18  | 117.62      | 111.77   |
| 14  | d     | 201  | CLA  | C4C-C3C-C2C | -2.18 | 103.72      | 106.90   |
| 14  | Y     | 833  | CLA  | CMB-C2B-C3B | 2.18  | 128.75      | 124.68   |
| 14  | H     | 823  | CLA  | CHA-C1A-NA  | -2.18 | 121.41      | 126.40   |
| 14  | Y     | 810  | CLA  | OBD-CAD-C3D | -2.18 | 124.37      | 127.98   |
| 14  | Y     | 813  | CLA  | OBD-CAD-C3D | -2.18 | 124.37      | 127.98   |
| 14  | B     | 811  | CLA  | C4-C3-C5    | 2.18  | 118.93      | 115.27   |
| 14  | G     | 814  | CLA  | CHA-C1A-NA  | -2.18 | 121.42      | 126.40   |
| 17  | d     | 203  | BCR  | C8-C9-C10   | 2.18  | 122.28      | 118.94   |
| 15  | G     | 844  | PQN  | C15-C13-C12 | -2.17 | 116.72      | 121.12   |
| 14  | Y     | 826  | CLA  | CHD-C4C-C3C | -2.17 | 121.64      | 124.84   |
| 17  | J     | 104  | BCR  | C7-C6-C5    | -2.17 | 116.20      | 121.46   |
| 14  | H     | 836  | CLA  | CMA-C3A-C4A | 2.17  | 117.61      | 111.77   |
| 17  | K     | 102  | BCR  | C27-C26-C25 | -2.17 | 119.58      | 122.73   |
| 14  | Y     | 813  | CLA  | CHC-C1C-C2C | -2.17 | 120.71      | 126.72   |
| 14  | H     | 818  | CLA  | C4C-C3C-C2C | -2.17 | 103.73      | 106.90   |
| 14  | H     | 834  | CLA  | C4C-C3C-C2C | -2.17 | 103.73      | 106.90   |
| 14  | H     | 802  | CLA  | CMC-C2C-C1C | 2.17  | 128.35      | 125.04   |
| 14  | Y     | 843  | CLA  | CED-O2D-CGD | 2.17  | 120.85      | 115.94   |
| 14  | H     | 807  | CLA  | C3C-C4C-NC  | 2.17  | 113.01      | 110.57   |
| 14  | G     | 837  | CLA  | O2A-C1-C2   | 2.17  | 114.34      | 108.64   |
| 14  | Z     | 839  | CLA  | CHC-C1C-C2C | -2.17 | 120.72      | 126.72   |
| 14  | Z     | 820  | CLA  | OBD-CAD-CBD | -2.17 | 122.79      | 125.89   |
| 14  | Y     | 818  | CLA  | CHC-C1C-C2C | -2.17 | 120.72      | 126.72   |
| 14  | G     | 832  | CLA  | OBD-CAD-C3D | -2.17 | 124.38      | 127.98   |
| 14  | G     | 827  | CLA  | CHB-C4A-NA  | 2.17  | 127.51      | 124.51   |
| 17  | B     | 843  | BCR  | C33-C5-C4   | 2.17  | 117.78      | 113.62   |
| 14  | H     | 809  | CLA  | CAA-C2A-C1A | 2.17  | 119.08      | 111.97   |
| 17  | Y     | 847  | BCR  | C3-C4-C5    | -2.17 | 110.20      | 114.08   |
| 14  | B     | 808  | CLA  | C4-C3-C5    | 2.17  | 118.92      | 115.27   |
| 17  | f     | 103  | BCR  | C4-C5-C6    | -2.17 | 119.58      | 122.73   |
| 14  | A     | 822  | CLA  | C3B-C4B-NB  | 2.17  | 112.01      | 109.21   |
| 14  | G     | 806  | CLA  | CHC-C1C-C2C | -2.17 | 120.73      | 126.72   |
| 14  | H     | 836  | CLA  | CGD-CBD-CAD | -2.17 | 103.72      | 110.73   |
| 14  | G     | 805  | CLA  | CHD-C4C-C3C | -2.17 | 121.66      | 124.84   |
| 17  | Z     | 845  | BCR  | C28-C27-C26 | -2.17 | 110.21      | 114.08   |
| 14  | G     | 818  | CLA  | O1D-CGD-CBD | -2.17 | 120.05      | 124.48   |
| 17  | T     | 102  | BCR  | C27-C26-C25 | -2.17 | 119.59      | 122.73   |
| 14  | H     | 826  | CLA  | C1-C2-C3    | -2.17 | 122.30      | 126.04   |
| 17  | V     | 1202 | BCR  | C3-C4-C5    | -2.17 | 110.21      | 114.08   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 815  | CLA  | O1D-CGD-CBD | -2.17 | 120.05      | 124.48   |
| 14  | Y     | 819  | CLA  | O1D-CGD-CBD | -2.17 | 120.05      | 124.48   |
| 14  | B     | 814  | CLA  | C3C-C4C-NC  | 2.16  | 113.00      | 110.57   |
| 14  | B     | 825  | CLA  | O1D-CGD-CBD | -2.16 | 120.06      | 124.48   |
| 14  | Q     | 203  | CLA  | CMC-C2C-C1C | 2.16  | 128.34      | 125.04   |
| 14  | A     | 823  | CLA  | CMC-C2C-C1C | 2.16  | 128.34      | 125.04   |
| 14  | A     | 802  | CLA  | CAA-C2A-C3A | -2.16 | 106.85      | 112.78   |
| 14  | U     | 1004 | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 14  | U     | 1002 | CLA  | C4C-C3C-C2C | -2.16 | 103.74      | 106.90   |
| 14  | G     | 840  | CLA  | CMA-C3A-C4A | 2.16  | 117.59      | 111.77   |
| 14  | B     | 834  | CLA  | C3C-C4C-NC  | 2.16  | 113.00      | 110.57   |
| 17  | f     | 103  | BCR  | C23-C22-C21 | 2.16  | 122.26      | 118.94   |
| 14  | Y     | 809  | CLA  | O2D-CGD-O1D | -2.16 | 119.61      | 123.84   |
| 14  | Y     | 818  | CLA  | O2D-CGD-O1D | -2.16 | 119.61      | 123.84   |
| 14  | J     | 102  | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 14  | Y     | 841  | CLA  | C5-C3-C2    | -2.16 | 116.75      | 121.12   |
| 17  | B     | 847  | BCR  | C1-C6-C7    | 2.16  | 121.89      | 115.78   |
| 14  | Z     | 816  | CLA  | OBD-CAD-C3D | -2.16 | 124.39      | 127.98   |
| 14  | G     | 832  | CLA  | C3C-C4C-NC  | 2.16  | 112.99      | 110.57   |
| 14  | G     | 841  | CLA  | CMB-C2B-C3B | 2.16  | 128.72      | 124.68   |
| 14  | Y     | 808  | CLA  | O1D-CGD-CBD | -2.16 | 120.07      | 124.48   |
| 14  | G     | 819  | CLA  | CMC-C2C-C3C | 2.16  | 131.98      | 126.12   |
| 14  | B     | 810  | CLA  | C11-C10-C8  | -2.16 | 108.94      | 115.92   |
| 14  | H     | 820  | CLA  | CHC-C1C-C2C | -2.16 | 120.75      | 126.72   |
| 14  | A     | 823  | CLA  | CMD-C2D-C3D | -2.16 | 120.64      | 124.68   |
| 14  | Y     | 809  | CLA  | C1-O2A-CGA  | 2.16  | 122.10      | 116.44   |
| 17  | G     | 850  | BCR  | C30-C25-C24 | 2.16  | 121.88      | 115.78   |
| 14  | H     | 809  | CLA  | CHB-C4A-NA  | 2.16  | 127.49      | 124.51   |
| 14  | A     | 829  | CLA  | C4-C3-C5    | 2.16  | 118.90      | 115.27   |
| 14  | L     | 201  | CLA  | O2D-CGD-O1D | -2.15 | 119.62      | 123.84   |
| 17  | B     | 844  | BCR  | C30-C25-C26 | -2.15 | 119.58      | 122.61   |
| 14  | Y     | 839  | CLA  | C4C-C3C-C2C | -2.15 | 103.76      | 106.90   |
| 14  | B     | 822  | CLA  | CAC-C3C-C4C | 2.15  | 127.61      | 124.81   |
| 14  | A     | 822  | CLA  | OBD-CAD-C3D | -2.15 | 124.41      | 127.98   |
| 14  | H     | 821  | CLA  | CHB-C4A-NA  | 2.15  | 127.49      | 124.51   |
| 14  | G     | 830  | CLA  | C3C-C4C-NC  | 2.15  | 112.99      | 110.57   |
| 14  | G     | 805  | CLA  | C6-C5-C3    | -2.15 | 107.81      | 113.45   |
| 14  | Z     | 802  | CLA  | CHA-C1A-NA  | -2.15 | 121.47      | 126.40   |
| 14  | L     | 201  | CLA  | CAA-C2A-C3A | -2.15 | 106.88      | 112.78   |
| 14  | G     | 812  | CLA  | O2D-CGD-O1D | -2.15 | 119.63      | 123.84   |
| 14  | B     | 805  | CLA  | C3C-C4C-NC  | 2.15  | 112.98      | 110.57   |
| 14  | A     | 831  | CLA  | CHC-C1C-C2C | -2.15 | 120.77      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 837  | CLA  | CHD-C4C-C3C | -2.15 | 121.67      | 124.84   |
| 14  | G     | 817  | CLA  | C3C-C4C-NC  | 2.15  | 112.98      | 110.57   |
| 17  | Q     | 202  | BCR  | C7-C8-C9    | -2.15 | 122.98      | 126.23   |
| 14  | B     | 802  | CLA  | CHC-C1C-C2C | -2.15 | 120.77      | 126.72   |
| 14  | A     | 813  | CLA  | C4C-C3C-C2C | -2.15 | 103.76      | 106.90   |
| 14  | H     | 803  | CLA  | CMC-C2C-C3C | 2.15  | 131.95      | 126.12   |
| 14  | B     | 822  | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 17  | A     | 849  | BCR  | C30-C25-C24 | 2.15  | 121.86      | 115.78   |
| 14  | U     | 1006 | CLA  | CMB-C2B-C3B | 2.15  | 128.70      | 124.68   |
| 14  | Z     | 834  | CLA  | CMC-C2C-C1C | 2.15  | 128.31      | 125.04   |
| 14  | Y     | 839  | CLA  | CMA-C3A-C4A | 2.15  | 117.55      | 111.77   |
| 14  | B     | 831  | CLA  | CMB-C2B-C3B | 2.15  | 128.70      | 124.68   |
| 17  | F     | 201  | BCR  | C33-C5-C4   | 2.15  | 117.74      | 113.62   |
| 14  | B     | 820  | CLA  | CMC-C2C-C3C | 2.15  | 131.94      | 126.12   |
| 14  | A     | 813  | CLA  | OBD-CAD-C3D | -2.15 | 124.42      | 127.98   |
| 14  | G     | 833  | CLA  | CHD-C4C-C3C | -2.15 | 121.68      | 124.84   |
| 17  | Y     | 848  | BCR  | C23-C24-C25 | -2.15 | 121.18      | 127.20   |
| 14  | A     | 827  | CLA  | OBD-CAD-CBD | -2.15 | 122.83      | 125.89   |
| 17  | J     | 104  | BCR  | C33-C5-C4   | 2.15  | 117.74      | 113.62   |
| 14  | Z     | 828  | CLA  | CGD-CBD-CAD | -2.15 | 103.79      | 110.73   |
| 17  | R     | 102  | BCR  | C2-C3-C4    | -2.14 | 106.58      | 111.38   |
| 14  | B     | 834  | CLA  | CAA-C2A-C3A | -2.14 | 106.91      | 112.78   |
| 14  | G     | 842  | CLA  | CHD-C4C-C3C | -2.14 | 121.69      | 124.84   |
| 14  | A     | 805  | CLA  | CAA-C2A-C1A | -2.14 | 104.95      | 111.97   |
| 17  | H     | 843  | BCR  | C38-C26-C25 | -2.14 | 122.12      | 124.53   |
| 14  | Z     | 827  | CLA  | CMC-C2C-C3C | 2.14  | 131.93      | 126.12   |
| 14  | B     | 830  | CLA  | O2D-CGD-O1D | -2.14 | 119.65      | 123.84   |
| 14  | H     | 820  | CLA  | C3C-C4C-NC  | 2.14  | 112.97      | 110.57   |
| 14  | B     | 836  | CLA  | CHC-C1C-C2C | -2.14 | 120.80      | 126.72   |
| 14  | A     | 817  | CLA  | OBD-CAD-C3D | -2.14 | 124.43      | 127.98   |
| 15  | B     | 842  | PQN  | C16-C15-C13 | -2.14 | 107.84      | 113.45   |
| 14  | G     | 831  | CLA  | CHC-C1C-C2C | -2.14 | 120.80      | 126.72   |
| 17  | B     | 844  | BCR  | C1-C6-C5    | -2.14 | 119.60      | 122.61   |
| 14  | B     | 816  | CLA  | O2D-CGD-O1D | -2.14 | 119.66      | 123.84   |
| 14  | B     | 806  | CLA  | CMD-C2D-C3D | -2.14 | 120.68      | 124.68   |
| 17  | Y     | 849  | BCR  | C1-C6-C5    | -2.14 | 119.60      | 122.61   |
| 14  | B     | 804  | CLA  | C6-C7-C8    | -2.14 | 109.01      | 115.92   |
| 14  | G     | 832  | CLA  | CMC-C2C-C3C | 2.14  | 131.92      | 126.12   |
| 14  | A     | 827  | CLA  | CED-O2D-CGD | 2.14  | 120.77      | 115.94   |
| 14  | G     | 827  | CLA  | C4C-C3C-C2C | -2.14 | 103.78      | 106.90   |
| 14  | Y     | 836  | CLA  | CHB-C4A-NA  | 2.13  | 127.46      | 124.51   |
| 14  | Z     | 831  | CLA  | CHC-C1C-C2C | -2.13 | 120.82      | 126.72   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 833  | CLA  | C1-C2-C3    | -2.13 | 122.35      | 126.04   |
| 14  | Y     | 805  | CLA  | C6-C5-C3    | -2.13 | 107.86      | 113.45   |
| 14  | K     | 101  | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 14  | G     | 815  | CLA  | CMC-C2C-C3C | 2.13  | 131.91      | 126.12   |
| 14  | A     | 812  | CLA  | C4C-C3C-C2C | -2.13 | 103.79      | 106.90   |
| 14  | B     | 824  | CLA  | CGD-CBD-CAD | -2.13 | 103.83      | 110.73   |
| 14  | Z     | 828  | CLA  | CHB-C4A-NA  | 2.13  | 127.46      | 124.51   |
| 14  | G     | 824  | CLA  | CHC-C1C-C2C | -2.13 | 120.82      | 126.72   |
| 17  | B     | 846  | BCR  | C27-C26-C25 | -2.13 | 119.64      | 122.73   |
| 14  | Z     | 815  | CLA  | C4-C3-C5    | 2.13  | 118.86      | 115.27   |
| 14  | B     | 817  | CLA  | C1-C2-C3    | -2.13 | 122.36      | 126.04   |
| 14  | G     | 818  | CLA  | CMA-C3A-C4A | 2.13  | 117.50      | 111.77   |
| 14  | G     | 832  | CLA  | CAA-C2A-C3A | -2.13 | 106.94      | 112.78   |
| 14  | Z     | 828  | CLA  | CHD-C4C-C3C | -2.13 | 121.71      | 124.84   |
| 14  | h     | 207  | CLA  | CHD-C4C-C3C | -2.13 | 121.71      | 124.84   |
| 14  | U     | 1003 | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 14  | A     | 814  | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 14  | G     | 827  | CLA  | C6-C7-C8    | -2.13 | 109.03      | 115.92   |
| 17  | Z     | 841  | BCR  | C15-C14-C13 | -2.13 | 124.27      | 127.31   |
| 14  | Y     | 804  | CLA  | CHC-C1C-C2C | -2.13 | 120.83      | 126.72   |
| 14  | Y     | 813  | CLA  | CAC-C3C-C4C | 2.13  | 127.57      | 124.81   |
| 14  | Z     | 822  | CLA  | C1-C2-C3    | -2.13 | 122.36      | 126.04   |
| 19  | H     | 846  | LMG  | O1-C7-C8    | -2.13 | 105.76      | 110.90   |
| 14  | A     | 812  | CLA  | CMB-C2B-C3B | 2.13  | 128.66      | 124.68   |
| 14  | B     | 805  | CLA  | CHB-C4A-NA  | 2.13  | 127.45      | 124.51   |
| 14  | L     | 206  | CLA  | C4-C3-C5    | 2.13  | 118.85      | 115.27   |
| 14  | B     | 809  | CLA  | C3A-C2A-C1A | 2.13  | 104.53      | 101.34   |
| 14  | Z     | 806  | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 14  | B     | 802  | CLA  | CAA-CBA-CGA | -2.13 | 107.04      | 113.25   |
| 14  | A     | 836  | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 17  | B     | 845  | BCR  | C29-C30-C25 | 2.13  | 113.75      | 110.48   |
| 14  | B     | 804  | CLA  | C6-C5-C3    | -2.13 | 107.88      | 113.45   |
| 14  | G     | 819  | CLA  | CMA-C3A-C4A | 2.13  | 117.49      | 111.77   |
| 17  | H     | 848  | BCR  | C2-C1-C6    | 2.13  | 113.75      | 110.48   |
| 14  | G     | 825  | CLA  | C1-C2-C3    | -2.13 | 122.37      | 126.04   |
| 14  | Y     | 831  | CLA  | CAA-C2A-C3A | -2.13 | 106.96      | 112.78   |
| 17  | F     | 201  | BCR  | C34-C9-C10  | -2.13 | 119.95      | 122.92   |
| 17  | Y     | 850  | BCR  | C7-C8-C9    | -2.13 | 123.02      | 126.23   |
| 14  | G     | 829  | CLA  | CMC-C2C-C1C | 2.12  | 128.28      | 125.04   |
| 17  | M     | 101  | BCR  | C31-C1-C6   | -2.12 | 106.85      | 110.30   |
| 14  | A     | 802  | CLA  | CHA-C1A-NA  | -2.12 | 121.53      | 126.40   |
| 14  | G     | 839  | CLA  | CAA-C2A-C3A | -2.12 | 106.96      | 112.78   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 817  | CLA  | CMB-C2B-C3B | 2.12  | 128.65      | 124.68   |
| 14  | Y     | 815  | CLA  | CGD-CBD-CAD | -2.12 | 103.86      | 110.73   |
| 14  | Q     | 201  | CLA  | O2A-C1-C2   | 2.12  | 114.21      | 108.64   |
| 14  | G     | 803  | CLA  | C3C-C4C-NC  | 2.12  | 112.95      | 110.57   |
| 14  | Y     | 813  | CLA  | C4C-C3C-C2C | -2.12 | 103.80      | 106.90   |
| 14  | H     | 804  | CLA  | CHC-C1C-C2C | -2.12 | 120.85      | 126.72   |
| 14  | Z     | 815  | CLA  | C3C-C4C-NC  | 2.12  | 112.95      | 110.57   |
| 17  | J     | 103  | BCR  | C1-C6-C7    | 2.12  | 121.78      | 115.78   |
| 14  | Z     | 807  | CLA  | C11-C10-C8  | -2.12 | 109.06      | 115.92   |
| 14  | H     | 818  | CLA  | CMA-C3A-C4A | 2.12  | 117.47      | 111.77   |
| 17  | e     | 101  | BCR  | C30-C25-C26 | -2.12 | 119.63      | 122.61   |
| 17  | A     | 845  | BCR  | C2-C3-C4    | -2.12 | 106.64      | 111.38   |
| 14  | H     | 836  | CLA  | CHC-C1C-C2C | -2.12 | 120.86      | 126.72   |
| 14  | Y     | 805  | CLA  | C1-O2A-CGA  | 2.12  | 122.01      | 116.44   |
| 14  | B     | 818  | CLA  | CMC-C2C-C1C | 2.12  | 128.27      | 125.04   |
| 14  | G     | 828  | CLA  | C6-C7-C8    | -2.12 | 109.07      | 115.92   |
| 14  | L     | 206  | CLA  | OBD-CAD-C3D | -2.12 | 124.46      | 127.98   |
| 14  | A     | 830  | CLA  | C16-C15-C13 | -2.12 | 109.07      | 115.92   |
| 14  | T     | 101  | CLA  | CMD-C2D-C3D | -2.12 | 120.71      | 124.68   |
| 17  | V     | 1202 | BCR  | C38-C26-C27 | 2.12  | 117.69      | 113.62   |
| 14  | H     | 822  | CLA  | C3C-C4C-NC  | 2.12  | 112.95      | 110.57   |
| 17  | Z     | 843  | BCR  | C34-C9-C8   | 2.12  | 121.42      | 118.08   |
| 14  | Y     | 842  | CLA  | CBC-CAC-C3C | -2.12 | 106.59      | 112.43   |
| 14  | Q     | 203  | CLA  | CED-O2D-CGD | 2.12  | 120.73      | 115.94   |
| 14  | U     | 1002 | CLA  | CHC-C1C-C2C | -2.12 | 120.86      | 126.72   |
| 17  | H     | 843  | BCR  | C15-C14-C13 | -2.12 | 124.26      | 127.30   |
| 15  | H     | 839  | PQN  | C11-C12-C13 | -2.12 | 123.27      | 126.79   |
| 14  | H     | 808  | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 14  | H     | 827  | CLA  | CHC-C1C-C2C | -2.12 | 120.87      | 126.72   |
| 14  | Z     | 826  | CLA  | OBD-CAD-CBD | -2.12 | 122.87      | 125.89   |
| 14  | Y     | 808  | CLA  | C4-C3-C5    | 2.12  | 118.83      | 115.27   |
| 14  | G     | 825  | CLA  | C4C-C3C-C2C | -2.12 | 103.81      | 106.90   |
| 13  | G     | 801  | CL0  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 14  | H     | 816  | CLA  | O1D-CGD-CBD | -2.12 | 120.16      | 124.48   |
| 14  | J     | 102  | CLA  | C3C-C4C-NC  | 2.12  | 112.94      | 110.57   |
| 14  | G     | 840  | CLA  | CHC-C1C-C2C | -2.11 | 120.87      | 126.72   |
| 14  | G     | 808  | CLA  | C3C-C4C-NC  | 2.11  | 112.94      | 110.57   |
| 14  | B     | 817  | CLA  | CMA-C3A-C4A | 2.11  | 117.45      | 111.77   |
| 17  | H     | 845  | BCR  | C24-C25-C26 | 2.11  | 126.58      | 121.46   |
| 14  | H     | 824  | CLA  | CHD-C4C-C3C | -2.11 | 121.73      | 124.84   |
| 17  | U     | 1008 | BCR  | C30-C25-C26 | -2.11 | 119.64      | 122.61   |
| 17  | F     | 203  | BCR  | C1-C6-C5    | -2.11 | 119.64      | 122.61   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 833  | CLA  | CHA-C1A-NA  | -2.11 | 121.56      | 126.40   |
| 14  | B     | 813  | CLA  | C16-C15-C13 | -2.11 | 109.09      | 115.92   |
| 14  | Y     | 808  | CLA  | C5-C3-C2    | -2.11 | 116.84      | 121.12   |
| 14  | G     | 837  | CLA  | C4C-C3C-C2C | -2.11 | 103.82      | 106.90   |
| 14  | A     | 812  | CLA  | C5-C3-C2    | -2.11 | 116.84      | 121.12   |
| 14  | G     | 803  | CLA  | CHC-C1C-C2C | -2.11 | 120.88      | 126.72   |
| 14  | B     | 802  | CLA  | CBC-CAC-C3C | -2.11 | 106.61      | 112.43   |
| 17  | R     | 101  | BCR  | C2-C1-C6    | -2.11 | 107.23      | 110.48   |
| 14  | Z     | 818  | CLA  | CHC-C1C-C2C | -2.11 | 120.89      | 126.72   |
| 14  | Y     | 824  | CLA  | CHC-C1C-C2C | -2.11 | 120.89      | 126.72   |
| 14  | Y     | 810  | CLA  | C3C-C4C-NC  | 2.11  | 112.94      | 110.57   |
| 17  | Y     | 848  | BCR  | C32-C1-C6   | 2.11  | 113.72      | 110.30   |
| 14  | Y     | 816  | CLA  | CAA-CBA-CGA | -2.11 | 107.09      | 113.25   |
| 14  | H     | 829  | CLA  | CAC-C3C-C4C | 2.11  | 127.55      | 124.81   |
| 17  | Q     | 204  | BCR  | C28-C27-C26 | -2.11 | 110.31      | 114.08   |
| 14  | B     | 841  | CLA  | CMB-C2B-C3B | 2.11  | 128.62      | 124.68   |
| 14  | Y     | 832  | CLA  | CAA-C2A-C3A | -2.11 | 107.00      | 112.78   |
| 14  | Z     | 832  | CLA  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 14  | Z     | 813  | CLA  | CAC-C3C-C2C | 2.11  | 131.13      | 127.53   |
| 17  | T     | 102  | BCR  | C32-C1-C6   | -2.11 | 106.88      | 110.30   |
| 17  | Q     | 204  | BCR  | C30-C25-C26 | -2.11 | 119.65      | 122.61   |
| 14  | B     | 803  | CLA  | OBD-CAD-CBD | -2.11 | 122.89      | 125.89   |
| 14  | S     | 1101 | CLA  | C3C-C4C-NC  | 2.11  | 112.93      | 110.57   |
| 14  | Q     | 201  | CLA  | CMA-C3A-C4A | 2.11  | 117.43      | 111.77   |
| 14  | j     | 102  | CLA  | CGD-CBD-CAD | -2.10 | 103.92      | 110.73   |
| 17  | H     | 844  | BCR  | C37-C22-C23 | 2.10  | 121.39      | 118.08   |
| 14  | G     | 823  | CLA  | CHD-C4C-C3C | -2.10 | 121.75      | 124.84   |
| 14  | G     | 828  | CLA  | O1D-CGD-CBD | -2.10 | 120.18      | 124.48   |
| 17  | Y     | 851  | BCR  | C30-C25-C24 | 2.10  | 121.73      | 115.78   |
| 14  | Y     | 824  | CLA  | OBD-CAD-C3D | -2.10 | 124.49      | 127.98   |
| 14  | H     | 815  | CLA  | CHC-C1C-C2C | -2.10 | 120.90      | 126.72   |
| 14  | Z     | 831  | CLA  | CAC-C3C-C4C | 2.10  | 127.54      | 124.81   |
| 14  | U     | 1006 | CLA  | C4-C3-C5    | 2.10  | 118.81      | 115.27   |
| 14  | G     | 822  | CLA  | OBD-CAD-CBD | -2.10 | 122.89      | 125.89   |
| 14  | B     | 815  | CLA  | CBC-CAC-C3C | -2.10 | 106.64      | 112.43   |
| 14  | H     | 837  | CLA  | CMB-C2B-C3B | 2.10  | 128.61      | 124.68   |
| 14  | G     | 835  | CLA  | CHC-C1C-C2C | -2.10 | 120.91      | 126.72   |
| 14  | H     | 813  | CLA  | O2D-CGD-O1D | -2.10 | 119.73      | 123.84   |
| 17  | H     | 845  | BCR  | C35-C13-C14 | -2.10 | 119.98      | 122.92   |
| 14  | Z     | 814  | CLA  | C4C-C3C-C2C | -2.10 | 103.84      | 106.90   |
| 14  | g     | 102  | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 14  | Y     | 823  | CLA  | C1-C2-C3    | -2.10 | 123.36      | 126.75   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 838  | CLA  | C4C-C3C-C2C | -2.10 | 103.84      | 106.90   |
| 14  | G     | 808  | CLA  | CHC-C1C-C2C | -2.10 | 120.92      | 126.72   |
| 15  | H     | 839  | PQN  | C11-C3-C4   | 2.10  | 120.75      | 118.50   |
| 14  | Z     | 811  | CLA  | CMC-C2C-C1C | 2.10  | 128.23      | 125.04   |
| 17  | L     | 208  | BCR  | C4-C5-C6    | -2.10 | 119.69      | 122.73   |
| 14  | A     | 839  | CLA  | OBD-CAD-C3D | -2.10 | 124.50      | 127.98   |
| 17  | H     | 844  | BCR  | C23-C22-C21 | 2.10  | 122.16      | 118.94   |
| 14  | A     | 852  | CLA  | C3C-C4C-NC  | 2.10  | 112.92      | 110.57   |
| 14  | H     | 808  | CLA  | O1D-CGD-CBD | -2.10 | 120.20      | 124.48   |
| 14  | A     | 833  | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.51   |
| 14  | H     | 816  | CLA  | C2A-C3A-C4A | -2.09 | 98.48       | 101.87   |
| 14  | H     | 813  | CLA  | CHC-C1C-C2C | -2.09 | 120.93      | 126.72   |
| 15  | B     | 842  | PQN  | C16-C17-C18 | -2.09 | 109.15      | 115.92   |
| 14  | Z     | 831  | CLA  | OBD-CAD-CBD | -2.09 | 122.90      | 125.89   |
| 14  | J     | 101  | CLA  | OBD-CAD-CBD | -2.09 | 122.90      | 125.89   |
| 14  | A     | 834  | CLA  | C3C-C4C-NC  | 2.09  | 112.92      | 110.57   |
| 14  | H     | 825  | CLA  | CED-O2D-CGD | 2.09  | 120.67      | 115.94   |
| 14  | A     | 826  | CLA  | CMD-C2D-C3D | -2.09 | 120.76      | 124.68   |
| 17  | Z     | 844  | BCR  | C24-C23-C22 | -2.09 | 123.07      | 126.23   |
| 14  | h     | 206  | CLA  | C2A-C3A-C4A | -2.09 | 98.49       | 101.87   |
| 14  | Y     | 806  | CLA  | CHA-C1A-NA  | -2.09 | 121.61      | 126.40   |
| 17  | Z     | 845  | BCR  | C35-C13-C14 | -2.09 | 119.99      | 122.92   |
| 14  | A     | 815  | CLA  | CAC-C3C-C2C | 2.09  | 131.10      | 127.53   |
| 14  | Z     | 810  | CLA  | CGD-CBD-CAD | 2.09  | 117.50      | 110.73   |
| 14  | Y     | 812  | CLA  | CMB-C2B-C3B | 2.09  | 128.59      | 124.68   |
| 14  | G     | 825  | CLA  | O2A-C1-C2   | 2.09  | 114.13      | 108.64   |
| 14  | A     | 814  | CLA  | C1-C2-C3    | -2.09 | 123.37      | 126.75   |
| 14  | Y     | 808  | CLA  | C1-O2A-CGA  | 2.09  | 121.92      | 116.44   |
| 14  | V     | 1201 | CLA  | C4C-C3C-C2C | -2.09 | 103.85      | 106.90   |
| 14  | Y     | 834  | CLA  | C3A-C2A-C1A | 2.09  | 104.47      | 101.34   |
| 14  | Y     | 842  | CLA  | C6-C5-C3    | -2.09 | 107.98      | 113.45   |
| 14  | S     | 1102 | CLA  | CBC-CAC-C3C | -2.09 | 106.68      | 112.43   |
| 14  | H     | 829  | CLA  | CHC-C1C-C2C | -2.09 | 120.95      | 126.72   |
| 14  | G     | 816  | CLA  | CED-O2D-CGD | 2.09  | 120.66      | 115.94   |
| 14  | A     | 841  | CLA  | CMB-C2B-C3B | 2.09  | 128.58      | 124.68   |
| 14  | Z     | 802  | CLA  | C3C-C4C-NC  | 2.08  | 112.91      | 110.57   |
| 14  | Y     | 803  | CLA  | OBD-CAD-C3D | -2.08 | 124.52      | 127.98   |
| 14  | G     | 822  | CLA  | CMD-C2D-C3D | -2.08 | 120.78      | 124.68   |
| 14  | H     | 807  | CLA  | C4-C3-C5    | 2.08  | 118.78      | 115.27   |
| 14  | Z     | 838  | CLA  | C7-C6-C5    | -2.08 | 107.70      | 113.36   |
| 14  | G     | 833  | CLA  | CHB-C4A-NA  | 2.08  | 127.39      | 124.51   |
| 14  | Z     | 839  | CLA  | CHB-C4A-NA  | 2.08  | 127.39      | 124.51   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | K     | 102  | BCR  | C23-C22-C21 | -2.08 | 115.74      | 118.94   |
| 14  | Z     | 838  | CLA  | C1-O2A-CGA  | 2.08  | 121.91      | 116.44   |
| 14  | Y     | 822  | CLA  | CED-O2D-CGD | 2.08  | 120.65      | 115.94   |
| 14  | Z     | 822  | CLA  | CGD-CBD-CAD | -2.08 | 103.99      | 110.73   |
| 14  | Y     | 808  | CLA  | C4C-C3C-C2C | -2.08 | 103.86      | 106.90   |
| 15  | H     | 839  | PQN  | C21-C20-C18 | -2.08 | 109.19      | 115.92   |
| 13  | G     | 801  | CL0  | CED-O2D-CGD | 2.08  | 120.65      | 115.94   |
| 14  | Z     | 826  | CLA  | C5-C3-C2    | -2.08 | 116.90      | 121.12   |
| 14  | B     | 824  | CLA  | CHC-C1C-C2C | -2.08 | 120.97      | 126.72   |
| 14  | S     | 1102 | CLA  | O2D-CGD-O1D | -2.08 | 119.77      | 123.84   |
| 14  | Z     | 801  | CLA  | CAA-CBA-CGA | 2.08  | 119.33      | 113.25   |
| 14  | G     | 829  | CLA  | C4C-C3C-C2C | -2.08 | 103.86      | 106.90   |
| 14  | Z     | 823  | CLA  | CMD-C2D-C3D | -2.08 | 120.79      | 124.68   |
| 14  | A     | 823  | CLA  | OBD-CAD-C3D | -2.08 | 124.53      | 127.98   |
| 17  | U     | 1008 | BCR  | C33-C5-C4   | 2.08  | 117.61      | 113.62   |
| 14  | B     | 831  | CLA  | C3C-C4C-NC  | 2.08  | 112.90      | 110.57   |
| 14  | Z     | 833  | CLA  | CAC-C3C-C4C | 2.08  | 127.51      | 124.81   |
| 14  | B     | 801  | CLA  | CED-O2D-CGD | 2.08  | 120.64      | 115.94   |
| 17  | Y     | 856  | BCR  | C31-C1-C6   | -2.08 | 106.93      | 110.30   |
| 14  | Q     | 201  | CLA  | C1-O2A-CGA  | 2.08  | 121.89      | 116.44   |
| 14  | Z     | 819  | CLA  | CMB-C2B-C1B | -2.08 | 125.27      | 128.46   |
| 14  | B     | 832  | CLA  | CMC-C2C-C3C | 2.08  | 131.75      | 126.12   |
| 14  | B     | 807  | CLA  | CMC-C2C-C1C | 2.08  | 128.20      | 125.04   |
| 17  | G     | 846  | BCR  | C12-C13-C14 | 2.08  | 122.13      | 118.94   |
| 14  | Z     | 810  | CLA  | CAA-C2A-C3A | -2.08 | 107.09      | 112.78   |
| 17  | J     | 103  | BCR  | C23-C24-C25 | -2.08 | 121.37      | 127.20   |
| 18  | A     | 850  | LHG  | O8-C23-O10  | -2.08 | 118.35      | 123.59   |
| 14  | Z     | 801  | CLA  | CHC-C1C-C2C | -2.08 | 120.98      | 126.72   |
| 14  | H     | 821  | CLA  | CMA-C3A-C4A | 2.08  | 117.35      | 111.77   |
| 14  | f     | 102  | CLA  | C4-C3-C2    | -2.08 | 118.35      | 123.68   |
| 14  | A     | 824  | CLA  | CED-O2D-CGD | 2.08  | 120.63      | 115.94   |
| 14  | H     | 805  | CLA  | CBC-CAC-C3C | -2.08 | 106.71      | 112.43   |
| 14  | A     | 837  | CLA  | CED-O2D-CGD | 2.07  | 120.63      | 115.94   |
| 14  | G     | 853  | CLA  | CMC-C2C-C3C | 2.07  | 131.75      | 126.12   |
| 14  | f     | 102  | CLA  | C4-C3-C5    | 2.07  | 118.76      | 115.27   |
| 14  | G     | 836  | CLA  | C3C-C4C-NC  | 2.07  | 112.90      | 110.57   |
| 17  | A     | 849  | BCR  | C24-C25-C26 | -2.07 | 116.44      | 121.46   |
| 14  | Z     | 803  | CLA  | C1-O2A-CGA  | 2.07  | 121.89      | 116.44   |
| 14  | B     | 803  | CLA  | CHA-C1A-NA  | -2.07 | 121.65      | 126.40   |
| 14  | H     | 833  | CLA  | CHA-C1A-NA  | -2.07 | 121.65      | 126.40   |
| 14  | G     | 837  | CLA  | C5-C3-C2    | -2.07 | 116.92      | 121.12   |
| 14  | A     | 837  | CLA  | CHD-C4C-C3C | -2.07 | 121.79      | 124.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 819  | CLA  | CHB-C4A-NA  | 2.07  | 127.38      | 124.51   |
| 14  | B     | 818  | CLA  | C1-C2-C3    | -2.07 | 122.46      | 126.04   |
| 14  | U     | 1006 | CLA  | O2D-CGD-O1D | -2.07 | 119.79      | 123.84   |
| 17  | h     | 203  | BCR  | C3-C4-C5    | -2.07 | 110.38      | 114.08   |
| 14  | Z     | 805  | CLA  | CMC-C2C-C3C | 2.07  | 131.74      | 126.12   |
| 14  | G     | 818  | CLA  | CHC-C1C-C2C | -2.07 | 121.00      | 126.72   |
| 14  | A     | 837  | CLA  | C4-C3-C5    | 2.07  | 118.75      | 115.27   |
| 14  | B     | 810  | CLA  | O2D-CGD-O1D | -2.07 | 119.79      | 123.84   |
| 14  | G     | 819  | CLA  | CMB-C2B-C1B | -2.07 | 125.28      | 128.46   |
| 14  | Y     | 832  | CLA  | CHC-C1C-C2C | -2.07 | 121.00      | 126.72   |
| 17  | B     | 851  | BCR  | C30-C25-C26 | -2.07 | 119.70      | 122.61   |
| 14  | A     | 831  | CLA  | C3C-C4C-NC  | 2.07  | 112.89      | 110.57   |
| 14  | B     | 827  | CLA  | CMD-C2D-C3D | -2.07 | 120.81      | 124.68   |
| 14  | B     | 805  | CLA  | CMD-C2D-C3D | -2.07 | 120.81      | 124.68   |
| 14  | B     | 820  | CLA  | CHA-C1A-NA  | -2.07 | 121.67      | 126.40   |
| 17  | M     | 101  | BCR  | C37-C22-C23 | 2.07  | 121.33      | 118.08   |
| 14  | A     | 827  | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.51   |
| 14  | B     | 819  | CLA  | O1D-CGD-CBD | -2.06 | 120.26      | 124.48   |
| 14  | H     | 811  | CLA  | CMB-C2B-C3B | 2.06  | 128.54      | 124.68   |
| 14  | H     | 809  | CLA  | C5-C3-C2    | -2.06 | 116.94      | 121.12   |
| 17  | H     | 848  | BCR  | C35-C13-C14 | -2.06 | 120.03      | 122.92   |
| 14  | B     | 838  | CLA  | CHD-C4C-C3C | -2.06 | 121.81      | 124.84   |
| 14  | G     | 809  | CLA  | C3C-C4C-NC  | 2.06  | 112.89      | 110.57   |
| 14  | A     | 835  | CLA  | CHC-C1C-C2C | -2.06 | 121.02      | 126.72   |
| 14  | H     | 801  | CLA  | CED-O2D-CGD | 2.06  | 120.60      | 115.94   |
| 15  | B     | 842  | PQN  | C11-C3-C4   | 2.06  | 120.71      | 118.50   |
| 14  | F     | 202  | CLA  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 17  | M     | 101  | BCR  | C36-C18-C19 | -2.06 | 114.83      | 118.08   |
| 14  | H     | 808  | CLA  | CMA-C3A-C4A | 2.06  | 117.31      | 111.77   |
| 17  | T     | 102  | BCR  | C15-C14-C13 | -2.06 | 124.37      | 127.31   |
| 14  | Z     | 807  | CLA  | CHC-C1C-C2C | -2.06 | 121.02      | 126.72   |
| 14  | Z     | 817  | CLA  | CHD-C4C-C3C | -2.06 | 121.81      | 124.84   |
| 14  | B     | 840  | CLA  | CHB-C4A-NA  | 2.06  | 127.36      | 124.51   |
| 14  | A     | 806  | CLA  | O2D-CGD-O1D | -2.06 | 119.81      | 123.84   |
| 14  | A     | 815  | CLA  | C3D-CAD-CBD | -2.06 | 104.89      | 107.61   |
| 14  | B     | 831  | CLA  | C4C-C3C-C2C | -2.06 | 103.90      | 106.90   |
| 14  | H     | 815  | CLA  | C3C-C4C-NC  | 2.06  | 112.88      | 110.57   |
| 14  | f     | 101  | CLA  | CMA-C3A-C4A | 2.06  | 117.31      | 111.77   |
| 14  | Z     | 839  | CLA  | C16-C15-C13 | -2.06 | 109.27      | 115.92   |
| 14  | B     | 818  | CLA  | CHA-C1A-NA  | -2.06 | 121.69      | 126.40   |
| 14  | U     | 1002 | CLA  | CMB-C2B-C3B | 2.06  | 128.53      | 124.68   |
| 14  | B     | 841  | CLA  | CAA-CBA-CGA | -2.06 | 107.24      | 113.25   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 811  | CLA  | O2A-C1-C2   | 2.06  | 114.04      | 108.64   |
| 14  | Z     | 821  | CLA  | C4C-C3C-C2C | -2.06 | 103.90      | 106.90   |
| 14  | Y     | 805  | CLA  | CAA-C2A-C3A | -2.06 | 107.15      | 112.78   |
| 14  | A     | 835  | CLA  | CMA-C3A-C4A | 2.05  | 117.30      | 111.77   |
| 14  | A     | 821  | CLA  | O1D-CGD-CBD | -2.05 | 120.28      | 124.48   |
| 14  | G     | 802  | CLA  | CMC-C2C-C1C | 2.05  | 128.17      | 125.04   |
| 14  | Z     | 838  | CLA  | OBD-CAD-CBD | -2.05 | 122.96      | 125.89   |
| 14  | Y     | 827  | CLA  | CHA-C1A-NA  | -2.05 | 121.69      | 126.40   |
| 14  | H     | 837  | CLA  | C2A-C3A-C4A | -2.05 | 98.55       | 101.87   |
| 17  | U     | 1007 | BCR  | C39-C30-C25 | 2.05  | 113.63      | 110.30   |
| 14  | B     | 824  | CLA  | CHD-C4C-C3C | -2.05 | 121.82      | 124.84   |
| 15  | Z     | 840  | PQN  | C16-C15-C13 | -2.05 | 108.07      | 113.45   |
| 17  | Y     | 848  | BCR  | C32-C1-C31  | 2.05  | 114.83      | 108.53   |
| 14  | d     | 202  | CLA  | O1D-CGD-CBD | -2.05 | 120.29      | 124.48   |
| 14  | G     | 803  | CLA  | C6-C5-C3    | -2.05 | 108.08      | 113.45   |
| 14  | G     | 805  | CLA  | CBC-CAC-C3C | -2.05 | 106.78      | 112.43   |
| 14  | H     | 814  | CLA  | CAA-C2A-C3A | -2.05 | 107.16      | 112.78   |
| 14  | A     | 823  | CLA  | CHC-C1C-C2C | -2.05 | 121.05      | 126.72   |
| 14  | B     | 832  | CLA  | O2A-C1-C2   | 2.05  | 114.02      | 108.64   |
| 17  | H     | 840  | BCR  | C37-C22-C21 | -2.05 | 120.05      | 122.92   |
| 14  | B     | 814  | CLA  | CHC-C1C-C2C | -2.05 | 121.05      | 126.72   |
| 14  | g     | 102  | CLA  | O2D-CGD-O1D | -2.05 | 119.83      | 123.84   |
| 14  | Y     | 815  | CLA  | CED-O2D-CGD | 2.05  | 120.57      | 115.94   |
| 17  | F     | 201  | BCR  | C4-C5-C6    | -2.05 | 119.76      | 122.73   |
| 14  | G     | 842  | CLA  | C16-C15-C13 | -2.05 | 109.30      | 115.92   |
| 14  | A     | 822  | CLA  | CHB-C4A-NA  | 2.05  | 127.34      | 124.51   |
| 14  | Y     | 820  | CLA  | CMC-C2C-C1C | 2.05  | 128.16      | 125.04   |
| 14  | Y     | 804  | CLA  | C3C-C4C-NC  | 2.05  | 112.87      | 110.57   |
| 17  | G     | 846  | BCR  | C7-C8-C9    | -2.05 | 123.14      | 126.23   |
| 14  | Y     | 830  | CLA  | CAA-C2A-C3A | -2.05 | 107.17      | 112.78   |
| 14  | Z     | 818  | CLA  | CBC-CAC-C3C | -2.05 | 106.79      | 112.43   |
| 14  | G     | 818  | CLA  | CHB-C4A-NA  | 2.05  | 127.34      | 124.51   |
| 14  | U     | 1003 | CLA  | CMD-C2D-C3D | -2.05 | 120.85      | 124.68   |
| 14  | G     | 830  | CLA  | C4D-C3D-CAD | 2.05  | 109.61      | 108.47   |
| 14  | B     | 802  | CLA  | C3C-C4C-NC  | 2.05  | 112.86      | 110.57   |
| 14  | Z     | 808  | CLA  | CAA-C2A-C1A | 2.05  | 118.68      | 111.97   |
| 14  | Z     | 831  | CLA  | C5-C3-C2    | -2.05 | 116.98      | 121.12   |
| 18  | H     | 847  | LHG  | O8-C23-O10  | -2.05 | 118.43      | 123.59   |
| 14  | B     | 808  | CLA  | C16-C15-C13 | -2.05 | 109.31      | 115.92   |
| 17  | G     | 850  | BCR  | C39-C30-C25 | -2.05 | 106.98      | 110.30   |
| 14  | Z     | 816  | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.51   |
| 14  | S     | 1102 | CLA  | C3C-C4C-NC  | 2.04  | 112.86      | 110.57   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 815  | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.51   |
| 14  | B     | 823  | CLA  | CMC-C2C-C1C | 2.04  | 128.15      | 125.04   |
| 17  | f     | 105  | BCR  | C8-C7-C6    | -2.04 | 121.46      | 127.20   |
| 17  | B     | 847  | BCR  | C30-C25-C24 | 2.04  | 121.56      | 115.78   |
| 14  | d     | 201  | CLA  | CAC-C3C-C4C | 2.04  | 127.46      | 124.81   |
| 14  | Y     | 828  | CLA  | C4C-C3C-C2C | -2.04 | 103.92      | 106.90   |
| 14  | B     | 828  | CLA  | C4C-C3C-C2C | -2.04 | 103.92      | 106.90   |
| 14  | h     | 206  | CLA  | C3D-CAD-CBD | -2.04 | 104.92      | 107.61   |
| 14  | B     | 814  | CLA  | OBD-CAD-CBD | -2.04 | 122.98      | 125.89   |
| 14  | Z     | 826  | CLA  | CMC-C2C-C1C | 2.04  | 128.15      | 125.04   |
| 17  | Z     | 843  | BCR  | C24-C25-C26 | 2.04  | 126.41      | 121.46   |
| 14  | T     | 103  | CLA  | CMB-C2B-C3B | 2.04  | 128.50      | 124.68   |
| 14  | A     | 827  | CLA  | C6-C5-C3    | -2.04 | 108.10      | 113.45   |
| 14  | L     | 202  | CLA  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 14  | B     | 818  | CLA  | CMA-C3A-C4A | 2.04  | 117.26      | 111.77   |
| 14  | Z     | 815  | CLA  | CHB-C4A-NA  | 2.04  | 127.33      | 124.51   |
| 14  | h     | 206  | CLA  | OBD-CAD-C3D | -2.04 | 124.59      | 127.98   |
| 14  | B     | 821  | CLA  | C4C-C3C-C2C | -2.04 | 103.92      | 106.90   |
| 14  | G     | 829  | CLA  | C4-C3-C5    | 2.04  | 118.70      | 115.27   |
| 14  | Y     | 854  | CLA  | CMC-C2C-C1C | 2.04  | 128.15      | 125.04   |
| 14  | Z     | 832  | CLA  | C4C-C3C-C2C | -2.04 | 103.92      | 106.90   |
| 14  | U     | 1003 | CLA  | OBD-CAD-C3D | -2.04 | 124.60      | 127.98   |
| 14  | Z     | 807  | CLA  | O2D-CGD-O1D | -2.04 | 119.85      | 123.84   |
| 14  | L     | 205  | CLA  | CAC-C3C-C4C | 2.04  | 127.45      | 124.81   |
| 14  | Y     | 840  | CLA  | C1-O2A-CGA  | 2.04  | 121.79      | 116.44   |
| 14  | Z     | 828  | CLA  | CMB-C2B-C3B | 2.04  | 128.49      | 124.68   |
| 14  | A     | 821  | CLA  | CMA-C3A-C4A | 2.04  | 117.25      | 111.77   |
| 14  | Y     | 812  | CLA  | CED-O2D-CGD | 2.04  | 120.54      | 115.94   |
| 14  | H     | 822  | CLA  | O2D-CGD-O1D | -2.04 | 119.86      | 123.84   |
| 14  | A     | 812  | CLA  | OBD-CAD-C3D | -2.04 | 124.60      | 127.98   |
| 14  | B     | 828  | CLA  | CHB-C4A-NA  | 2.04  | 127.33      | 124.51   |
| 14  | A     | 819  | CLA  | O1D-CGD-CBD | -2.04 | 120.32      | 124.48   |
| 14  | h     | 207  | CLA  | C16-C15-C13 | -2.03 | 109.34      | 115.92   |
| 14  | G     | 839  | CLA  | CAA-CBA-CGA | -2.03 | 107.31      | 113.25   |
| 14  | H     | 814  | CLA  | CHB-C4A-NA  | 2.03  | 127.33      | 124.51   |
| 17  | Z     | 842  | BCR  | C35-C13-C12 | -2.03 | 114.87      | 118.08   |
| 14  | Y     | 829  | CLA  | C3C-C4C-NC  | 2.03  | 112.85      | 110.57   |
| 14  | A     | 840  | CLA  | CMD-C2D-C3D | -2.03 | 120.87      | 124.68   |
| 14  | B     | 833  | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 14  | H     | 811  | CLA  | CHC-C1C-C2C | -2.03 | 121.10      | 126.72   |
| 14  | A     | 809  | CLA  | CMC-C2C-C1C | 2.03  | 128.13      | 125.04   |
| 14  | A     | 808  | CLA  | C1-O2A-CGA  | 2.03  | 121.78      | 116.44   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | f     | 103  | BCR  | C33-C5-C6   | -2.03 | 122.25      | 124.53   |
| 14  | H     | 803  | CLA  | C3C-C4C-NC  | 2.03  | 112.85      | 110.57   |
| 14  | B     | 812  | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 14  | A     | 838  | CLA  | CHC-C1C-C2C | -2.03 | 121.10      | 126.72   |
| 14  | H     | 810  | CLA  | CMB-C2B-C1B | 2.03  | 131.59      | 128.46   |
| 17  | H     | 840  | BCR  | C27-C26-C25 | -2.03 | 119.78      | 122.73   |
| 14  | U     | 1003 | CLA  | O1D-CGD-CBD | -2.03 | 120.33      | 124.48   |
| 14  | B     | 830  | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 14  | H     | 816  | CLA  | CGD-CBD-CAD | -2.03 | 104.16      | 110.73   |
| 14  | H     | 816  | CLA  | CHD-C4C-C3C | -2.03 | 121.85      | 124.84   |
| 14  | G     | 817  | CLA  | CAC-C3C-C4C | 2.03  | 127.44      | 124.81   |
| 14  | A     | 825  | CLA  | CAA-CBA-CGA | -2.03 | 107.32      | 113.25   |
| 14  | H     | 801  | CLA  | CHC-C1C-C2C | -2.03 | 121.11      | 126.72   |
| 14  | H     | 822  | CLA  | OBD-CAD-CBD | 2.03  | 128.79      | 125.89   |
| 14  | H     | 827  | CLA  | C1-O2A-CGA  | 2.03  | 121.77      | 116.44   |
| 14  | G     | 817  | CLA  | C4-C3-C2    | -2.03 | 118.47      | 123.68   |
| 14  | h     | 206  | CLA  | CED-O2D-CGD | 2.03  | 120.53      | 115.94   |
| 14  | Z     | 814  | CLA  | CMC-C2C-C1C | 2.03  | 128.13      | 125.04   |
| 14  | A     | 837  | CLA  | CMD-C2D-C3D | -2.03 | 120.88      | 124.68   |
| 14  | A     | 839  | CLA  | CHC-C1C-C2C | -2.03 | 121.11      | 126.72   |
| 14  | B     | 803  | CLA  | C2A-C3A-C4A | 2.03  | 105.15      | 101.87   |
| 14  | A     | 837  | CLA  | O2D-CGD-O1D | -2.03 | 119.87      | 123.84   |
| 17  | V     | 1202 | BCR  | C15-C14-C13 | -2.03 | 124.42      | 127.31   |
| 14  | B     | 807  | CLA  | CHA-C1A-NA  | -2.03 | 121.75      | 126.40   |
| 14  | B     | 833  | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 13  | G     | 801  | CL0  | CHC-C1C-C2C | -2.03 | 121.11      | 126.72   |
| 14  | B     | 833  | CLA  | CAC-C3C-C4C | 2.03  | 127.44      | 124.81   |
| 14  | L     | 202  | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 14  | H     | 806  | CLA  | CHC-C1C-C2C | -2.03 | 121.12      | 126.72   |
| 17  | Y     | 847  | BCR  | C24-C25-C26 | -2.03 | 116.55      | 121.46   |
| 14  | Z     | 828  | CLA  | O1D-CGD-CBD | -2.03 | 120.34      | 124.48   |
| 17  | A     | 846  | BCR  | C1-C6-C7    | 2.03  | 121.51      | 115.78   |
| 14  | G     | 817  | CLA  | CHC-C1C-C2C | -2.03 | 121.12      | 126.72   |
| 14  | B     | 825  | CLA  | O2D-CGD-O1D | -2.02 | 119.88      | 123.84   |
| 14  | Y     | 812  | CLA  | CHB-C4A-NA  | 2.02  | 127.31      | 124.51   |
| 14  | Y     | 823  | CLA  | O1D-CGD-CBD | -2.02 | 120.34      | 124.48   |
| 13  | G     | 801  | CL0  | CAA-CBA-CGA | 2.02  | 119.17      | 113.25   |
| 13  | Y     | 801  | CL0  | C3C-C4C-NC  | 2.02  | 112.84      | 110.57   |
| 17  | Y     | 846  | BCR  | C30-C25-C26 | -2.02 | 119.76      | 122.61   |
| 14  | A     | 837  | CLA  | C6-C5-C3    | -2.02 | 108.15      | 113.45   |
| 14  | A     | 820  | CLA  | CHC-C1C-C2C | -2.02 | 121.13      | 126.72   |
| 14  | F     | 202  | CLA  | CMC-C2C-C3C | 2.02  | 131.61      | 126.12   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 810 | CLA  | CHC-C1C-C2C | -2.02 | 121.13      | 126.72   |
| 14  | B     | 835 | CLA  | CHC-C1C-C2C | -2.02 | 121.13      | 126.72   |
| 14  | A     | 808 | CLA  | C3C-C4C-NC  | 2.02  | 112.84      | 110.57   |
| 14  | K     | 101 | CLA  | CHB-C4A-NA  | 2.02  | 127.31      | 124.51   |
| 17  | L     | 208 | BCR  | C28-C27-C26 | -2.02 | 110.47      | 114.08   |
| 14  | Y     | 808 | CLA  | CAA-C2A-C1A | -2.02 | 105.35      | 111.97   |
| 14  | A     | 811 | CLA  | C3C-C4C-NC  | 2.02  | 112.84      | 110.57   |
| 14  | L     | 202 | CLA  | CHA-C1A-NA  | -2.02 | 121.77      | 126.40   |
| 14  | B     | 822 | CLA  | CMD-C2D-C3D | -2.02 | 120.90      | 124.68   |
| 14  | G     | 810 | CLA  | CHB-C4A-NA  | 2.02  | 127.31      | 124.51   |
| 14  | H     | 832 | CLA  | C3C-C4C-NC  | 2.02  | 112.84      | 110.57   |
| 14  | H     | 827 | CLA  | CAC-C3C-C4C | 2.02  | 127.43      | 124.81   |
| 14  | Y     | 832 | CLA  | CHB-C4A-NA  | 2.02  | 127.30      | 124.51   |
| 14  | h     | 206 | CLA  | CHD-C4C-C3C | -2.02 | 121.87      | 124.84   |
| 17  | H     | 841 | BCR  | C8-C7-C6    | -2.02 | 121.53      | 127.20   |
| 14  | A     | 832 | CLA  | CMC-C2C-C3C | 2.02  | 131.60      | 126.12   |
| 17  | d     | 203 | BCR  | C31-C1-C6   | -2.02 | 107.03      | 110.30   |
| 13  | Y     | 801 | CL0  | C4C-C3C-C2C | -2.02 | 103.95      | 106.90   |
| 14  | Y     | 818 | CLA  | CED-O2D-CGD | 2.02  | 120.50      | 115.94   |
| 14  | A     | 833 | CLA  | CAA-C2A-C3A | -2.02 | 107.25      | 112.78   |
| 14  | G     | 836 | CLA  | CAC-C3C-C4C | 2.02  | 127.43      | 124.81   |
| 14  | H     | 823 | CLA  | C4-C3-C5    | 2.02  | 118.67      | 115.27   |
| 14  | G     | 813 | CLA  | C4C-C3C-C2C | -2.02 | 103.96      | 106.90   |
| 14  | H     | 824 | CLA  | C3A-C2A-C1A | 2.02  | 104.36      | 101.34   |
| 14  | B     | 821 | CLA  | CMD-C2D-C3D | -2.02 | 120.91      | 124.68   |
| 14  | G     | 824 | CLA  | CMA-C3A-C4A | 2.02  | 117.19      | 111.77   |
| 14  | Z     | 821 | CLA  | OBD-CAD-C3D | -2.02 | 124.63      | 127.98   |
| 17  | i     | 101 | BCR  | C38-C26-C27 | 2.02  | 117.49      | 113.62   |
| 14  | G     | 838 | CLA  | CMD-C2D-C3D | -2.02 | 120.91      | 124.68   |
| 17  | Z     | 844 | BCR  | C30-C25-C26 | -2.02 | 119.77      | 122.61   |
| 14  | H     | 814 | CLA  | CAC-C3C-C4C | 2.02  | 127.42      | 124.81   |
| 17  | Z     | 843 | BCR  | C40-C30-C25 | -2.02 | 107.03      | 110.30   |
| 14  | G     | 843 | CLA  | CED-O2D-CGD | 2.01  | 120.49      | 115.94   |
| 14  | h     | 207 | CLA  | CHB-C4A-NA  | 2.01  | 127.30      | 124.51   |
| 14  | G     | 823 | CLA  | CHC-C1C-C2C | -2.01 | 121.15      | 126.72   |
| 17  | L     | 203 | BCR  | C12-C13-C14 | 2.01  | 122.03      | 118.94   |
| 14  | G     | 825 | CLA  | CHC-C1C-C2C | -2.01 | 121.15      | 126.72   |
| 14  | G     | 814 | CLA  | CHC-C1C-C2C | -2.01 | 121.15      | 126.72   |
| 14  | Y     | 839 | CLA  | CED-O2D-CGD | 2.01  | 120.49      | 115.94   |
| 14  | Y     | 822 | CLA  | C3C-C4C-NC  | 2.01  | 112.83      | 110.57   |
| 14  | A     | 807 | CLA  | CAA-C2A-C3A | -2.01 | 107.26      | 112.78   |
| 14  | G     | 809 | CLA  | C1-C2-C3    | -2.01 | 122.56      | 126.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 806  | CLA  | C3C-C4C-NC  | 2.01  | 112.83      | 110.57   |
| 14  | S     | 1101 | CLA  | CHB-C4A-NA  | 2.01  | 127.30      | 124.51   |
| 14  | G     | 842  | CLA  | CED-O2D-CGD | 2.01  | 120.49      | 115.94   |
| 14  | A     | 826  | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 14  | Y     | 815  | CLA  | CHC-C1C-C2C | -2.01 | 121.16      | 126.72   |
| 14  | Y     | 829  | CLA  | C4-C3-C5    | 2.01  | 118.66      | 115.27   |
| 17  | Z     | 846  | BCR  | C37-C22-C23 | 2.01  | 121.25      | 118.08   |
| 14  | H     | 826  | CLA  | O2D-CGD-O1D | -2.01 | 119.91      | 123.84   |
| 14  | Z     | 801  | CLA  | CHD-C4C-C3C | -2.01 | 121.88      | 124.84   |
| 17  | Y     | 848  | BCR  | C7-C6-C5    | -2.01 | 116.59      | 121.46   |
| 14  | H     | 821  | CLA  | CMD-C2D-C3D | -2.01 | 120.92      | 124.68   |
| 14  | Z     | 839  | CLA  | CMD-C2D-C3D | -2.01 | 120.92      | 124.68   |
| 14  | B     | 812  | CLA  | CAA-C2A-C3A | -2.01 | 107.28      | 112.78   |
| 14  | d     | 201  | CLA  | CMC-C2C-C1C | 2.01  | 128.10      | 125.04   |
| 14  | H     | 818  | CLA  | CHA-C1A-NA  | -2.01 | 121.80      | 126.40   |
| 14  | H     | 805  | CLA  | CHC-C1C-C2C | -2.01 | 121.17      | 126.72   |
| 14  | B     | 811  | CLA  | CBA-CAA-C2A | 2.01  | 119.79      | 113.86   |
| 14  | Z     | 807  | CLA  | CMC-C2C-C1C | 2.01  | 128.10      | 125.04   |
| 18  | G     | 852  | LHG  | O8-C23-O10  | -2.01 | 118.53      | 123.59   |
| 17  | L     | 203  | BCR  | C30-C25-C24 | 2.01  | 121.45      | 115.78   |
| 14  | H     | 808  | CLA  | OBD-CAD-CBD | -2.01 | 123.03      | 125.89   |
| 14  | B     | 823  | CLA  | OBD-CAD-CBD | -2.01 | 123.03      | 125.89   |
| 14  | B     | 806  | CLA  | C6-C5-C3    | -2.01 | 108.20      | 113.45   |
| 14  | A     | 829  | CLA  | C4C-C3C-C2C | -2.00 | 103.97      | 106.90   |
| 14  | A     | 821  | CLA  | C3C-C4C-NC  | 2.00  | 112.82      | 110.57   |
| 14  | A     | 809  | CLA  | OBD-CAD-C3D | -2.00 | 124.65      | 127.98   |
| 14  | Z     | 814  | CLA  | O1D-CGD-CBD | -2.00 | 120.38      | 124.48   |
| 14  | L     | 205  | CLA  | CGD-CBD-CAD | -2.00 | 104.24      | 110.73   |
| 14  | G     | 811  | CLA  | CBA-CAA-C2A | 2.00  | 119.78      | 113.86   |
| 14  | H     | 818  | CLA  | C11-C10-C8  | -2.00 | 109.44      | 115.92   |
| 14  | B     | 826  | CLA  | CMC-C2C-C3C | 2.00  | 131.56      | 126.12   |
| 14  | Y     | 825  | CLA  | C11-C10-C8  | -2.00 | 109.44      | 115.92   |
| 14  | H     | 822  | CLA  | CMB-C2B-C3B | 2.00  | 128.43      | 124.68   |
| 14  | Y     | 839  | CLA  | CHD-C4C-C3C | -2.00 | 121.89      | 124.84   |
| 14  | Z     | 822  | CLA  | CHC-C1C-C2C | -2.00 | 121.18      | 126.72   |
| 14  | A     | 837  | CLA  | O1D-CGD-CBD | -2.00 | 120.39      | 124.48   |
| 14  | A     | 817  | CLA  | O1D-CGD-CBD | -2.00 | 120.39      | 124.48   |
| 14  | B     | 832  | CLA  | C16-C15-C13 | -2.00 | 109.45      | 115.92   |
| 14  | H     | 825  | CLA  | C4-C3-C5    | 2.00  | 118.64      | 115.27   |
| 17  | Y     | 856  | BCR  | C32-C1-C6   | -2.00 | 107.05      | 110.30   |
| 15  | B     | 842  | PQN  | O1-C1-C10   | -2.00 | 118.32      | 121.56   |
| 14  | H     | 809  | CLA  | CBC-CAC-C3C | -2.00 | 106.91      | 112.43   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | H     | 801 | CLA  | C4C-C3C-C2C | -2.00 | 103.98      | 106.90   |
| 14  | A     | 838 | CLA  | CHA-C1A-NA  | -2.00 | 121.81      | 126.40   |
| 15  | A     | 843 | PQN  | O4-C4-C5    | -2.00 | 118.32      | 121.56   |
| 14  | H     | 834 | CLA  | C4-C3-C5    | 2.00  | 118.64      | 115.27   |

All (855) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | B     | 811 | CLA  | NC   |
| 14  | B     | 811 | CLA  | ND   |
| 14  | B     | 811 | CLA  | NA   |
| 14  | B     | 817 | CLA  | NC   |
| 14  | B     | 817 | CLA  | ND   |
| 14  | B     | 817 | CLA  | NA   |
| 14  | B     | 833 | CLA  | NC   |
| 14  | B     | 833 | CLA  | ND   |
| 14  | B     | 833 | CLA  | NA   |
| 14  | H     | 820 | CLA  | NC   |
| 14  | H     | 820 | CLA  | ND   |
| 14  | H     | 820 | CLA  | NA   |
| 14  | Y     | 810 | CLA  | NC   |
| 14  | Y     | 810 | CLA  | ND   |
| 14  | Y     | 810 | CLA  | NA   |
| 14  | Y     | 827 | CLA  | NC   |
| 14  | Y     | 827 | CLA  | ND   |
| 14  | Y     | 827 | CLA  | NA   |
| 14  | A     | 852 | CLA  | NC   |
| 14  | A     | 852 | CLA  | ND   |
| 14  | A     | 852 | CLA  | NA   |
| 14  | A     | 826 | CLA  | NC   |
| 14  | A     | 826 | CLA  | ND   |
| 14  | A     | 826 | CLA  | NA   |
| 14  | Y     | 835 | CLA  | NC   |
| 14  | Y     | 835 | CLA  | ND   |
| 14  | Y     | 835 | CLA  | NA   |
| 14  | Z     | 808 | CLA  | NC   |
| 14  | Z     | 808 | CLA  | ND   |
| 14  | Z     | 808 | CLA  | NA   |
| 14  | B     | 841 | CLA  | NC   |
| 14  | B     | 841 | CLA  | ND   |
| 14  | B     | 841 | CLA  | NA   |
| 14  | H     | 817 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | H     | 817 | CLA  | ND   |
| 14  | H     | 817 | CLA  | NA   |
| 14  | H     | 818 | CLA  | NC   |
| 14  | H     | 818 | CLA  | ND   |
| 14  | H     | 818 | CLA  | NA   |
| 14  | H     | 831 | CLA  | NC   |
| 14  | H     | 831 | CLA  | ND   |
| 14  | H     | 831 | CLA  | NA   |
| 14  | A     | 832 | CLA  | NC   |
| 14  | A     | 832 | CLA  | ND   |
| 14  | A     | 832 | CLA  | NA   |
| 14  | G     | 824 | CLA  | NC   |
| 14  | G     | 824 | CLA  | ND   |
| 14  | G     | 824 | CLA  | NA   |
| 14  | d     | 202 | CLA  | NC   |
| 14  | d     | 202 | CLA  | ND   |
| 14  | d     | 202 | CLA  | NA   |
| 14  | B     | 802 | CLA  | NC   |
| 14  | B     | 802 | CLA  | ND   |
| 14  | B     | 802 | CLA  | NA   |
| 14  | Z     | 831 | CLA  | NC   |
| 14  | Z     | 831 | CLA  | ND   |
| 14  | Z     | 831 | CLA  | NA   |
| 14  | B     | 838 | CLA  | NC   |
| 14  | B     | 838 | CLA  | ND   |
| 14  | B     | 838 | CLA  | NA   |
| 14  | H     | 804 | CLA  | NC   |
| 14  | H     | 804 | CLA  | ND   |
| 14  | H     | 804 | CLA  | NA   |
| 14  | Y     | 855 | CLA  | NC   |
| 14  | Y     | 855 | CLA  | ND   |
| 14  | Y     | 855 | CLA  | NA   |
| 14  | G     | 839 | CLA  | NC   |
| 14  | G     | 839 | CLA  | ND   |
| 14  | G     | 839 | CLA  | NA   |
| 14  | H     | 813 | CLA  | NC   |
| 14  | H     | 813 | CLA  | ND   |
| 14  | H     | 813 | CLA  | NA   |
| 14  | A     | 822 | CLA  | NC   |
| 14  | A     | 822 | CLA  | ND   |
| 14  | A     | 822 | CLA  | NA   |
| 14  | H     | 837 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | H     | 837  | CLA  | ND   |
| 14  | H     | 837  | CLA  | NA   |
| 14  | L     | 205  | CLA  | NC   |
| 14  | L     | 205  | CLA  | ND   |
| 14  | L     | 205  | CLA  | NA   |
| 14  | F     | 202  | CLA  | NC   |
| 14  | F     | 202  | CLA  | ND   |
| 14  | F     | 202  | CLA  | NA   |
| 14  | Y     | 830  | CLA  | NC   |
| 14  | Y     | 830  | CLA  | ND   |
| 14  | Y     | 830  | CLA  | NA   |
| 14  | Y     | 825  | CLA  | NC   |
| 14  | Y     | 825  | CLA  | ND   |
| 14  | Y     | 825  | CLA  | NA   |
| 14  | Y     | 809  | CLA  | NC   |
| 14  | Y     | 809  | CLA  | ND   |
| 14  | Y     | 809  | CLA  | NA   |
| 14  | W     | 1701 | CLA  | NC   |
| 14  | W     | 1701 | CLA  | ND   |
| 14  | W     | 1701 | CLA  | NA   |
| 14  | G     | 813  | CLA  | NC   |
| 14  | G     | 813  | CLA  | ND   |
| 14  | G     | 813  | CLA  | NA   |
| 14  | Y     | 840  | CLA  | NC   |
| 14  | Y     | 840  | CLA  | ND   |
| 14  | Y     | 840  | CLA  | NA   |
| 14  | B     | 837  | CLA  | NC   |
| 14  | B     | 837  | CLA  | ND   |
| 14  | B     | 837  | CLA  | NA   |
| 14  | U     | 1003 | CLA  | NC   |
| 14  | U     | 1003 | CLA  | ND   |
| 14  | U     | 1003 | CLA  | NA   |
| 14  | B     | 834  | CLA  | NC   |
| 14  | B     | 834  | CLA  | ND   |
| 14  | B     | 834  | CLA  | NA   |
| 14  | A     | 836  | CLA  | NC   |
| 14  | A     | 836  | CLA  | ND   |
| 14  | A     | 836  | CLA  | NA   |
| 14  | U     | 1002 | CLA  | NC   |
| 14  | U     | 1002 | CLA  | ND   |
| 14  | U     | 1002 | CLA  | NA   |
| 14  | A     | 812  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | A     | 812  | CLA  | ND   |
| 14  | A     | 812  | CLA  | NA   |
| 14  | H     | 805  | CLA  | NC   |
| 14  | H     | 805  | CLA  | ND   |
| 14  | H     | 805  | CLA  | NA   |
| 14  | G     | 816  | CLA  | NC   |
| 14  | G     | 816  | CLA  | ND   |
| 14  | G     | 816  | CLA  | NA   |
| 14  | G     | 836  | CLA  | NC   |
| 14  | G     | 836  | CLA  | ND   |
| 14  | G     | 836  | CLA  | NA   |
| 14  | A     | 820  | CLA  | NC   |
| 14  | A     | 820  | CLA  | ND   |
| 14  | A     | 820  | CLA  | NA   |
| 14  | G     | 817  | CLA  | NC   |
| 14  | G     | 817  | CLA  | ND   |
| 14  | G     | 817  | CLA  | NA   |
| 14  | H     | 807  | CLA  | NC   |
| 14  | H     | 807  | CLA  | ND   |
| 14  | H     | 807  | CLA  | NA   |
| 14  | Y     | 811  | CLA  | NC   |
| 14  | Y     | 811  | CLA  | ND   |
| 14  | Y     | 811  | CLA  | NA   |
| 14  | Y     | 838  | CLA  | NC   |
| 14  | Y     | 838  | CLA  | ND   |
| 14  | Y     | 838  | CLA  | NA   |
| 14  | H     | 815  | CLA  | NC   |
| 14  | H     | 815  | CLA  | ND   |
| 14  | H     | 815  | CLA  | NA   |
| 14  | B     | 825  | CLA  | NC   |
| 14  | B     | 825  | CLA  | ND   |
| 14  | B     | 825  | CLA  | NA   |
| 14  | Y     | 812  | CLA  | NC   |
| 14  | Y     | 812  | CLA  | ND   |
| 14  | Y     | 812  | CLA  | NA   |
| 14  | J     | 102  | CLA  | NC   |
| 14  | J     | 102  | CLA  | ND   |
| 14  | J     | 102  | CLA  | NA   |
| 14  | S     | 1102 | CLA  | NC   |
| 14  | S     | 1102 | CLA  | ND   |
| 14  | S     | 1102 | CLA  | NA   |
| 14  | A     | 807  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | A     | 807  | CLA  | ND   |
| 14  | A     | 807  | CLA  | NA   |
| 14  | Z     | 815  | CLA  | NC   |
| 14  | Z     | 815  | CLA  | ND   |
| 14  | Z     | 815  | CLA  | NA   |
| 14  | H     | 810  | CLA  | NC   |
| 14  | H     | 810  | CLA  | ND   |
| 14  | H     | 810  | CLA  | NA   |
| 14  | H     | 802  | CLA  | NC   |
| 14  | H     | 802  | CLA  | ND   |
| 14  | H     | 802  | CLA  | NA   |
| 14  | Y     | 820  | CLA  | NC   |
| 14  | Y     | 820  | CLA  | ND   |
| 14  | Y     | 820  | CLA  | NA   |
| 14  | T     | 101  | CLA  | NC   |
| 14  | T     | 101  | CLA  | ND   |
| 14  | T     | 101  | CLA  | NA   |
| 14  | U     | 1006 | CLA  | NC   |
| 14  | U     | 1006 | CLA  | ND   |
| 14  | U     | 1006 | CLA  | NA   |
| 14  | Y     | 834  | CLA  | NC   |
| 14  | Y     | 834  | CLA  | ND   |
| 14  | Y     | 834  | CLA  | NA   |
| 14  | Z     | 832  | CLA  | NC   |
| 14  | Z     | 832  | CLA  | ND   |
| 14  | Z     | 832  | CLA  | NA   |
| 14  | Z     | 833  | CLA  | NC   |
| 14  | Z     | 833  | CLA  | ND   |
| 14  | Z     | 833  | CLA  | NA   |
| 14  | A     | 825  | CLA  | NC   |
| 14  | A     | 825  | CLA  | ND   |
| 14  | A     | 825  | CLA  | NA   |
| 14  | H     | 821  | CLA  | NC   |
| 14  | H     | 821  | CLA  | ND   |
| 14  | H     | 821  | CLA  | NA   |
| 14  | L     | 207  | CLA  | NC   |
| 14  | L     | 207  | CLA  | ND   |
| 14  | L     | 207  | CLA  | NA   |
| 14  | B     | 819  | CLA  | NC   |
| 14  | B     | 819  | CLA  | ND   |
| 14  | B     | 819  | CLA  | NA   |
| 14  | G     | 809  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | G     | 809 | CLA  | ND   |
| 14  | G     | 809 | CLA  | NA   |
| 14  | A     | 841 | CLA  | NC   |
| 14  | A     | 841 | CLA  | ND   |
| 14  | A     | 841 | CLA  | NA   |
| 14  | G     | 834 | CLA  | NC   |
| 14  | G     | 834 | CLA  | ND   |
| 14  | G     | 834 | CLA  | NA   |
| 14  | A     | 816 | CLA  | NC   |
| 14  | A     | 816 | CLA  | ND   |
| 14  | A     | 816 | CLA  | NA   |
| 14  | Z     | 837 | CLA  | NC   |
| 14  | Z     | 837 | CLA  | ND   |
| 14  | Z     | 837 | CLA  | NA   |
| 14  | A     | 815 | CLA  | NC   |
| 14  | A     | 815 | CLA  | ND   |
| 14  | A     | 815 | CLA  | NA   |
| 14  | H     | 823 | CLA  | NC   |
| 14  | H     | 823 | CLA  | ND   |
| 14  | H     | 823 | CLA  | NA   |
| 14  | B     | 801 | CLA  | NC   |
| 14  | B     | 801 | CLA  | ND   |
| 14  | B     | 801 | CLA  | NA   |
| 14  | H     | 824 | CLA  | NC   |
| 14  | H     | 824 | CLA  | ND   |
| 14  | H     | 824 | CLA  | NA   |
| 14  | Y     | 833 | CLA  | NC   |
| 14  | Y     | 833 | CLA  | ND   |
| 14  | Y     | 833 | CLA  | NA   |
| 14  | H     | 835 | CLA  | NC   |
| 14  | H     | 835 | CLA  | ND   |
| 14  | H     | 835 | CLA  | NA   |
| 14  | G     | 806 | CLA  | NC   |
| 14  | G     | 806 | CLA  | ND   |
| 14  | G     | 806 | CLA  | NA   |
| 14  | Z     | 814 | CLA  | NC   |
| 14  | Z     | 814 | CLA  | ND   |
| 14  | Z     | 814 | CLA  | NA   |
| 14  | A     | 804 | CLA  | NC   |
| 14  | A     | 804 | CLA  | ND   |
| 14  | A     | 804 | CLA  | NA   |
| 14  | A     | 829 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | A     | 829  | CLA  | ND   |
| 14  | A     | 829  | CLA  | NA   |
| 14  | G     | 812  | CLA  | NC   |
| 14  | G     | 812  | CLA  | ND   |
| 14  | G     | 812  | CLA  | NA   |
| 14  | Y     | 808  | CLA  | NC   |
| 14  | Y     | 808  | CLA  | ND   |
| 14  | Y     | 808  | CLA  | NA   |
| 14  | H     | 832  | CLA  | NC   |
| 14  | H     | 832  | CLA  | ND   |
| 14  | H     | 832  | CLA  | NA   |
| 14  | Z     | 801  | CLA  | NC   |
| 14  | Z     | 801  | CLA  | ND   |
| 14  | Z     | 801  | CLA  | NA   |
| 14  | Z     | 807  | CLA  | NC   |
| 14  | Z     | 807  | CLA  | ND   |
| 14  | Z     | 807  | CLA  | NA   |
| 14  | U     | 1004 | CLA  | NC   |
| 14  | U     | 1004 | CLA  | ND   |
| 14  | U     | 1004 | CLA  | NA   |
| 14  | H     | 827  | CLA  | NC   |
| 14  | H     | 827  | CLA  | ND   |
| 14  | H     | 827  | CLA  | NA   |
| 14  | G     | 804  | CLA  | NC   |
| 14  | G     | 804  | CLA  | ND   |
| 14  | G     | 804  | CLA  | NA   |
| 14  | Y     | 802  | CLA  | NC   |
| 14  | Y     | 802  | CLA  | ND   |
| 14  | Y     | 802  | CLA  | NA   |
| 14  | G     | 811  | CLA  | NC   |
| 14  | G     | 811  | CLA  | ND   |
| 14  | G     | 811  | CLA  | NA   |
| 14  | H     | 808  | CLA  | NC   |
| 14  | H     | 808  | CLA  | ND   |
| 14  | H     | 808  | CLA  | NA   |
| 14  | H     | 838  | CLA  | NC   |
| 14  | H     | 838  | CLA  | ND   |
| 14  | H     | 838  | CLA  | NA   |
| 13  | G     | 801  | CL0  | NC   |
| 13  | G     | 801  | CL0  | ND   |
| 13  | G     | 801  | CL0  | NA   |
| 14  | B     | 804  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | B     | 804  | CLA  | ND   |
| 14  | B     | 804  | CLA  | NA   |
| 14  | Z     | 812  | CLA  | NC   |
| 14  | Z     | 812  | CLA  | ND   |
| 14  | Z     | 812  | CLA  | NA   |
| 14  | j     | 102  | CLA  | NC   |
| 14  | j     | 102  | CLA  | ND   |
| 14  | j     | 102  | CLA  | NA   |
| 14  | L     | 206  | CLA  | NC   |
| 14  | L     | 206  | CLA  | ND   |
| 14  | L     | 206  | CLA  | NA   |
| 14  | A     | 838  | CLA  | NC   |
| 14  | A     | 838  | CLA  | ND   |
| 14  | A     | 838  | CLA  | NA   |
| 14  | Z     | 830  | CLA  | NC   |
| 14  | Z     | 830  | CLA  | ND   |
| 14  | Z     | 830  | CLA  | NA   |
| 14  | B     | 832  | CLA  | NC   |
| 14  | B     | 832  | CLA  | ND   |
| 14  | B     | 832  | CLA  | NA   |
| 14  | B     | 810  | CLA  | NC   |
| 14  | B     | 810  | CLA  | ND   |
| 14  | B     | 810  | CLA  | NA   |
| 14  | S     | 1103 | CLA  | NC   |
| 14  | S     | 1103 | CLA  | ND   |
| 14  | S     | 1103 | CLA  | NA   |
| 14  | T     | 103  | CLA  | NC   |
| 14  | T     | 103  | CLA  | ND   |
| 14  | T     | 103  | CLA  | NA   |
| 14  | H     | 833  | CLA  | NC   |
| 14  | H     | 833  | CLA  | ND   |
| 14  | H     | 833  | CLA  | NA   |
| 14  | H     | 809  | CLA  | NC   |
| 14  | H     | 809  | CLA  | ND   |
| 14  | H     | 809  | CLA  | NA   |
| 14  | Y     | 822  | CLA  | NC   |
| 14  | Y     | 822  | CLA  | ND   |
| 14  | Y     | 822  | CLA  | NA   |
| 14  | H     | 803  | CLA  | NC   |
| 14  | H     | 803  | CLA  | ND   |
| 14  | H     | 803  | CLA  | NA   |
| 14  | G     | 837  | CLA  | NC   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | G     | 837 | CLA  | ND   |
| 14  | G     | 837 | CLA  | NA   |
| 14  | J     | 101 | CLA  | NC   |
| 14  | J     | 101 | CLA  | ND   |
| 14  | J     | 101 | CLA  | NA   |
| 14  | Y     | 832 | CLA  | NC   |
| 14  | Y     | 832 | CLA  | ND   |
| 14  | Y     | 832 | CLA  | NA   |
| 14  | A     | 827 | CLA  | NC   |
| 14  | A     | 827 | CLA  | ND   |
| 14  | A     | 827 | CLA  | NA   |
| 14  | H     | 830 | CLA  | NC   |
| 14  | H     | 830 | CLA  | ND   |
| 14  | H     | 830 | CLA  | NA   |
| 14  | Y     | 818 | CLA  | NC   |
| 14  | Y     | 818 | CLA  | ND   |
| 14  | Y     | 818 | CLA  | NA   |
| 14  | A     | 809 | CLA  | NC   |
| 14  | A     | 809 | CLA  | ND   |
| 14  | A     | 809 | CLA  | NA   |
| 14  | B     | 813 | CLA  | NC   |
| 14  | B     | 813 | CLA  | ND   |
| 14  | B     | 813 | CLA  | NA   |
| 14  | G     | 840 | CLA  | NC   |
| 14  | G     | 840 | CLA  | ND   |
| 14  | G     | 840 | CLA  | NA   |
| 14  | Z     | 806 | CLA  | NC   |
| 14  | Z     | 806 | CLA  | ND   |
| 14  | Z     | 806 | CLA  | NA   |
| 14  | Z     | 834 | CLA  | NC   |
| 14  | Z     | 834 | CLA  | ND   |
| 14  | Z     | 834 | CLA  | NA   |
| 14  | B     | 806 | CLA  | NC   |
| 14  | B     | 806 | CLA  | ND   |
| 14  | B     | 806 | CLA  | NA   |
| 14  | Z     | 809 | CLA  | NC   |
| 14  | Z     | 809 | CLA  | ND   |
| 14  | Z     | 809 | CLA  | NA   |
| 14  | G     | 808 | CLA  | NC   |
| 14  | G     | 808 | CLA  | ND   |
| 14  | G     | 808 | CLA  | NA   |
| 14  | G     | 832 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | G     | 832 | CLA  | ND   |
| 14  | G     | 832 | CLA  | NA   |
| 14  | H     | 801 | CLA  | NC   |
| 14  | H     | 801 | CLA  | ND   |
| 14  | H     | 801 | CLA  | NA   |
| 14  | Y     | 821 | CLA  | NC   |
| 14  | Y     | 821 | CLA  | ND   |
| 14  | Y     | 821 | CLA  | NA   |
| 14  | Z     | 828 | CLA  | NC   |
| 14  | Z     | 828 | CLA  | ND   |
| 14  | Z     | 828 | CLA  | NA   |
| 14  | B     | 812 | CLA  | NC   |
| 14  | B     | 812 | CLA  | ND   |
| 14  | B     | 812 | CLA  | NA   |
| 14  | H     | 806 | CLA  | NC   |
| 14  | H     | 806 | CLA  | ND   |
| 14  | H     | 806 | CLA  | NA   |
| 14  | G     | 810 | CLA  | NC   |
| 14  | G     | 810 | CLA  | ND   |
| 14  | G     | 810 | CLA  | NA   |
| 14  | G     | 841 | CLA  | NC   |
| 14  | G     | 841 | CLA  | ND   |
| 14  | G     | 841 | CLA  | NA   |
| 14  | A     | 805 | CLA  | NC   |
| 14  | A     | 805 | CLA  | ND   |
| 14  | A     | 805 | CLA  | NA   |
| 14  | Z     | 817 | CLA  | NC   |
| 14  | Z     | 817 | CLA  | ND   |
| 14  | Z     | 817 | CLA  | NA   |
| 14  | Z     | 803 | CLA  | NC   |
| 14  | Z     | 803 | CLA  | ND   |
| 14  | Z     | 803 | CLA  | NA   |
| 14  | Y     | 814 | CLA  | NC   |
| 14  | Y     | 814 | CLA  | ND   |
| 14  | Y     | 814 | CLA  | NA   |
| 14  | h     | 201 | CLA  | NC   |
| 14  | h     | 201 | CLA  | ND   |
| 14  | h     | 201 | CLA  | NA   |
| 14  | Z     | 819 | CLA  | NC   |
| 14  | Z     | 819 | CLA  | ND   |
| 14  | Z     | 819 | CLA  | NA   |
| 14  | B     | 827 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | B     | 827 | CLA  | ND   |
| 14  | B     | 827 | CLA  | NA   |
| 14  | Y     | 815 | CLA  | NC   |
| 14  | Y     | 815 | CLA  | ND   |
| 14  | Y     | 815 | CLA  | NA   |
| 14  | B     | 803 | CLA  | NC   |
| 14  | B     | 803 | CLA  | ND   |
| 14  | B     | 803 | CLA  | NA   |
| 14  | B     | 824 | CLA  | NC   |
| 14  | B     | 824 | CLA  | ND   |
| 14  | B     | 824 | CLA  | NA   |
| 14  | B     | 821 | CLA  | NC   |
| 14  | B     | 821 | CLA  | ND   |
| 14  | B     | 821 | CLA  | NA   |
| 14  | Z     | 804 | CLA  | NC   |
| 14  | Z     | 804 | CLA  | ND   |
| 14  | Z     | 804 | CLA  | NA   |
| 14  | H     | 812 | CLA  | NC   |
| 14  | H     | 812 | CLA  | ND   |
| 14  | H     | 812 | CLA  | NA   |
| 14  | A     | 821 | CLA  | NC   |
| 14  | A     | 821 | CLA  | ND   |
| 14  | A     | 821 | CLA  | NA   |
| 14  | G     | 830 | CLA  | NC   |
| 14  | G     | 830 | CLA  | ND   |
| 14  | G     | 830 | CLA  | NA   |
| 14  | A     | 842 | CLA  | NC   |
| 14  | A     | 842 | CLA  | ND   |
| 14  | A     | 842 | CLA  | NA   |
| 14  | A     | 802 | CLA  | NC   |
| 14  | A     | 802 | CLA  | ND   |
| 14  | A     | 802 | CLA  | NA   |
| 14  | A     | 831 | CLA  | NC   |
| 14  | A     | 831 | CLA  | ND   |
| 14  | A     | 831 | CLA  | NA   |
| 14  | Y     | 823 | CLA  | NC   |
| 14  | Y     | 823 | CLA  | ND   |
| 14  | Y     | 823 | CLA  | NA   |
| 14  | A     | 839 | CLA  | NC   |
| 14  | A     | 839 | CLA  | ND   |
| 14  | A     | 839 | CLA  | NA   |
| 14  | Y     | 839 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | Y     | 839 | CLA  | ND   |
| 14  | Y     | 839 | CLA  | NA   |
| 14  | G     | 825 | CLA  | NC   |
| 14  | G     | 825 | CLA  | ND   |
| 14  | G     | 825 | CLA  | NA   |
| 14  | Y     | 816 | CLA  | NC   |
| 14  | Y     | 816 | CLA  | ND   |
| 14  | Y     | 816 | CLA  | NA   |
| 14  | Q     | 201 | CLA  | NC   |
| 14  | Q     | 201 | CLA  | ND   |
| 14  | Q     | 201 | CLA  | NA   |
| 14  | K     | 101 | CLA  | NC   |
| 14  | K     | 101 | CLA  | ND   |
| 14  | K     | 101 | CLA  | NA   |
| 14  | L     | 201 | CLA  | NC   |
| 14  | L     | 201 | CLA  | ND   |
| 14  | L     | 201 | CLA  | NA   |
| 14  | A     | 833 | CLA  | NC   |
| 14  | A     | 833 | CLA  | ND   |
| 14  | A     | 833 | CLA  | NA   |
| 14  | H     | 829 | CLA  | NC   |
| 14  | H     | 829 | CLA  | ND   |
| 14  | H     | 829 | CLA  | NA   |
| 14  | A     | 824 | CLA  | NC   |
| 14  | A     | 824 | CLA  | ND   |
| 14  | A     | 824 | CLA  | NA   |
| 14  | L     | 202 | CLA  | NC   |
| 14  | L     | 202 | CLA  | ND   |
| 14  | L     | 202 | CLA  | NA   |
| 14  | G     | 820 | CLA  | NC   |
| 14  | G     | 820 | CLA  | ND   |
| 14  | G     | 820 | CLA  | NA   |
| 14  | G     | 835 | CLA  | NC   |
| 14  | G     | 835 | CLA  | ND   |
| 14  | G     | 835 | CLA  | NA   |
| 14  | Y     | 826 | CLA  | NC   |
| 14  | Y     | 826 | CLA  | ND   |
| 14  | Y     | 826 | CLA  | NA   |
| 14  | Y     | 804 | CLA  | NC   |
| 14  | Y     | 804 | CLA  | ND   |
| 14  | Y     | 804 | CLA  | NA   |
| 14  | d     | 201 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | d     | 201  | CLA  | ND   |
| 14  | d     | 201  | CLA  | NA   |
| 14  | Z     | 825  | CLA  | NC   |
| 14  | Z     | 825  | CLA  | ND   |
| 14  | Z     | 825  | CLA  | NA   |
| 14  | Y     | 837  | CLA  | NC   |
| 14  | Y     | 837  | CLA  | ND   |
| 14  | Y     | 837  | CLA  | NA   |
| 14  | Z     | 818  | CLA  | NC   |
| 14  | Z     | 818  | CLA  | ND   |
| 14  | Z     | 818  | CLA  | NA   |
| 14  | A     | 814  | CLA  | NC   |
| 14  | A     | 814  | CLA  | ND   |
| 14  | A     | 814  | CLA  | NA   |
| 14  | G     | 803  | CLA  | NC   |
| 14  | G     | 803  | CLA  | ND   |
| 14  | G     | 803  | CLA  | NA   |
| 14  | Y     | 813  | CLA  | NC   |
| 14  | Y     | 813  | CLA  | ND   |
| 14  | Y     | 813  | CLA  | NA   |
| 14  | S     | 1101 | CLA  | NC   |
| 14  | S     | 1101 | CLA  | ND   |
| 14  | S     | 1101 | CLA  | NA   |
| 14  | B     | 820  | CLA  | NC   |
| 14  | B     | 820  | CLA  | ND   |
| 14  | B     | 820  | CLA  | NA   |
| 14  | G     | 833  | CLA  | NC   |
| 14  | G     | 833  | CLA  | ND   |
| 14  | G     | 833  | CLA  | NA   |
| 14  | Z     | 838  | CLA  | NC   |
| 14  | Z     | 838  | CLA  | ND   |
| 14  | Z     | 838  | CLA  | NA   |
| 14  | Z     | 811  | CLA  | NC   |
| 14  | Z     | 811  | CLA  | ND   |
| 14  | Z     | 811  | CLA  | NA   |
| 14  | H     | 822  | CLA  | NC   |
| 14  | H     | 822  | CLA  | ND   |
| 14  | H     | 822  | CLA  | NA   |
| 14  | G     | 829  | CLA  | NC   |
| 14  | G     | 829  | CLA  | ND   |
| 14  | G     | 829  | CLA  | NA   |
| 14  | Y     | 806  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | Y     | 806  | CLA  | ND   |
| 14  | Y     | 806  | CLA  | NA   |
| 14  | h     | 207  | CLA  | NC   |
| 14  | h     | 207  | CLA  | ND   |
| 14  | h     | 207  | CLA  | NA   |
| 14  | Y     | 829  | CLA  | NC   |
| 14  | Y     | 829  | CLA  | ND   |
| 14  | Y     | 829  | CLA  | NA   |
| 14  | G     | 853  | CLA  | NC   |
| 14  | G     | 853  | CLA  | ND   |
| 14  | G     | 853  | CLA  | NA   |
| 14  | Z     | 823  | CLA  | NC   |
| 14  | Z     | 823  | CLA  | ND   |
| 14  | Z     | 823  | CLA  | NA   |
| 14  | A     | 828  | CLA  | NC   |
| 14  | A     | 828  | CLA  | ND   |
| 14  | A     | 828  | CLA  | NA   |
| 14  | A     | 803  | CLA  | NC   |
| 14  | A     | 803  | CLA  | ND   |
| 14  | A     | 803  | CLA  | NA   |
| 14  | B     | 830  | CLA  | NC   |
| 14  | B     | 830  | CLA  | ND   |
| 14  | B     | 830  | CLA  | NA   |
| 14  | Z     | 820  | CLA  | NC   |
| 14  | Z     | 820  | CLA  | ND   |
| 14  | Z     | 820  | CLA  | NA   |
| 14  | G     | 838  | CLA  | NC   |
| 14  | G     | 838  | CLA  | ND   |
| 14  | G     | 838  | CLA  | NA   |
| 14  | Y     | 841  | CLA  | NC   |
| 14  | Y     | 841  | CLA  | ND   |
| 14  | Y     | 841  | CLA  | NA   |
| 14  | Z     | 822  | CLA  | NC   |
| 14  | Z     | 822  | CLA  | ND   |
| 14  | Z     | 822  | CLA  | NA   |
| 14  | Y     | 842  | CLA  | NC   |
| 14  | Y     | 842  | CLA  | ND   |
| 14  | Y     | 842  | CLA  | NA   |
| 14  | A     | 819  | CLA  | NC   |
| 14  | A     | 819  | CLA  | ND   |
| 14  | A     | 819  | CLA  | NA   |
| 14  | V     | 1201 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | V     | 1201 | CLA  | ND   |
| 14  | V     | 1201 | CLA  | NA   |
| 14  | A     | 840  | CLA  | NC   |
| 14  | A     | 840  | CLA  | ND   |
| 14  | A     | 840  | CLA  | NA   |
| 14  | Z     | 802  | CLA  | NC   |
| 14  | Z     | 802  | CLA  | ND   |
| 14  | Z     | 802  | CLA  | NA   |
| 14  | H     | 834  | CLA  | NC   |
| 14  | H     | 834  | CLA  | ND   |
| 14  | H     | 834  | CLA  | NA   |
| 14  | B     | 814  | CLA  | NC   |
| 14  | B     | 814  | CLA  | ND   |
| 14  | B     | 814  | CLA  | NA   |
| 14  | Y     | 805  | CLA  | NC   |
| 14  | Y     | 805  | CLA  | ND   |
| 14  | Y     | 805  | CLA  | NA   |
| 14  | Q     | 203  | CLA  | NC   |
| 14  | Q     | 203  | CLA  | ND   |
| 14  | Q     | 203  | CLA  | NA   |
| 14  | Y     | 854  | CLA  | NC   |
| 14  | Y     | 854  | CLA  | ND   |
| 14  | Y     | 854  | CLA  | NA   |
| 14  | G     | 807  | CLA  | NC   |
| 14  | G     | 807  | CLA  | ND   |
| 14  | G     | 807  | CLA  | NA   |
| 14  | Z     | 821  | CLA  | NC   |
| 14  | Z     | 821  | CLA  | ND   |
| 14  | Z     | 821  | CLA  | NA   |
| 14  | A     | 830  | CLA  | NC   |
| 14  | A     | 830  | CLA  | ND   |
| 14  | A     | 830  | CLA  | NA   |
| 14  | G     | 828  | CLA  | NC   |
| 14  | G     | 828  | CLA  | ND   |
| 14  | G     | 828  | CLA  | NA   |
| 14  | H     | 836  | CLA  | NC   |
| 14  | H     | 836  | CLA  | ND   |
| 14  | H     | 836  | CLA  | NA   |
| 14  | B     | 808  | CLA  | NC   |
| 14  | B     | 808  | CLA  | ND   |
| 14  | B     | 808  | CLA  | NA   |
| 14  | B     | 816  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | B     | 816 | CLA  | ND   |
| 14  | B     | 816 | CLA  | NA   |
| 14  | Z     | 839 | CLA  | NC   |
| 14  | Z     | 839 | CLA  | ND   |
| 14  | Z     | 839 | CLA  | NA   |
| 14  | G     | 826 | CLA  | NC   |
| 14  | G     | 826 | CLA  | ND   |
| 14  | G     | 826 | CLA  | NA   |
| 14  | A     | 823 | CLA  | NC   |
| 14  | A     | 823 | CLA  | ND   |
| 14  | A     | 823 | CLA  | NA   |
| 14  | G     | 821 | CLA  | NC   |
| 14  | G     | 821 | CLA  | ND   |
| 14  | G     | 821 | CLA  | NA   |
| 14  | B     | 822 | CLA  | NC   |
| 14  | B     | 822 | CLA  | ND   |
| 14  | B     | 822 | CLA  | NA   |
| 14  | Y     | 843 | CLA  | NC   |
| 14  | Y     | 843 | CLA  | ND   |
| 14  | Y     | 843 | CLA  | NA   |
| 14  | B     | 839 | CLA  | NC   |
| 14  | B     | 839 | CLA  | ND   |
| 14  | B     | 839 | CLA  | NA   |
| 14  | A     | 808 | CLA  | NC   |
| 14  | A     | 808 | CLA  | ND   |
| 14  | A     | 808 | CLA  | NA   |
| 14  | H     | 811 | CLA  | NC   |
| 14  | H     | 811 | CLA  | ND   |
| 14  | H     | 811 | CLA  | NA   |
| 14  | B     | 823 | CLA  | NC   |
| 14  | B     | 823 | CLA  | ND   |
| 14  | B     | 823 | CLA  | NA   |
| 14  | A     | 811 | CLA  | NC   |
| 14  | A     | 811 | CLA  | ND   |
| 14  | A     | 811 | CLA  | NA   |
| 14  | Z     | 810 | CLA  | NC   |
| 14  | Z     | 810 | CLA  | ND   |
| 14  | Z     | 810 | CLA  | NA   |
| 14  | Y     | 803 | CLA  | NC   |
| 14  | Y     | 803 | CLA  | ND   |
| 14  | Y     | 803 | CLA  | NA   |
| 14  | H     | 826 | CLA  | NC   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | H     | 826  | CLA  | ND   |
| 14  | H     | 826  | CLA  | NA   |
| 14  | B     | 807  | CLA  | NC   |
| 14  | B     | 807  | CLA  | ND   |
| 14  | B     | 807  | CLA  | NA   |
| 14  | Z     | 816  | CLA  | NC   |
| 14  | Z     | 816  | CLA  | ND   |
| 14  | Z     | 816  | CLA  | NA   |
| 14  | B     | 836  | CLA  | NC   |
| 14  | B     | 836  | CLA  | ND   |
| 14  | B     | 836  | CLA  | NA   |
| 14  | G     | 805  | CLA  | NC   |
| 14  | G     | 805  | CLA  | ND   |
| 14  | G     | 805  | CLA  | NA   |
| 14  | H     | 828  | CLA  | NC   |
| 14  | H     | 828  | CLA  | ND   |
| 14  | H     | 828  | CLA  | NA   |
| 14  | B     | 831  | CLA  | NC   |
| 14  | B     | 831  | CLA  | ND   |
| 14  | B     | 831  | CLA  | NA   |
| 14  | f     | 102  | CLA  | NC   |
| 14  | f     | 102  | CLA  | ND   |
| 14  | f     | 102  | CLA  | NA   |
| 14  | Z     | 835  | CLA  | NC   |
| 14  | Z     | 835  | CLA  | ND   |
| 14  | Z     | 835  | CLA  | NA   |
| 14  | B     | 826  | CLA  | NC   |
| 14  | B     | 826  | CLA  | ND   |
| 14  | B     | 826  | CLA  | NA   |
| 14  | A     | 835  | CLA  | NC   |
| 14  | A     | 835  | CLA  | ND   |
| 14  | A     | 835  | CLA  | NA   |
| 14  | B     | 815  | CLA  | NC   |
| 14  | B     | 815  | CLA  | ND   |
| 14  | B     | 815  | CLA  | NA   |
| 14  | Z     | 813  | CLA  | NC   |
| 14  | Z     | 813  | CLA  | ND   |
| 14  | Z     | 813  | CLA  | NA   |
| 14  | X     | 1701 | CLA  | NC   |
| 14  | X     | 1701 | CLA  | ND   |
| 14  | X     | 1701 | CLA  | NA   |
| 14  | A     | 806  | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | A     | 806 | CLA  | ND   |
| 14  | A     | 806 | CLA  | NA   |
| 14  | B     | 829 | CLA  | NC   |
| 14  | B     | 829 | CLA  | ND   |
| 14  | B     | 829 | CLA  | NA   |
| 14  | Y     | 828 | CLA  | NC   |
| 14  | Y     | 828 | CLA  | ND   |
| 14  | Y     | 828 | CLA  | NA   |
| 14  | Z     | 826 | CLA  | NC   |
| 14  | Z     | 826 | CLA  | ND   |
| 14  | Z     | 826 | CLA  | NA   |
| 14  | B     | 805 | CLA  | NC   |
| 14  | B     | 805 | CLA  | ND   |
| 14  | B     | 805 | CLA  | NA   |
| 14  | G     | 815 | CLA  | NC   |
| 14  | G     | 815 | CLA  | ND   |
| 14  | G     | 815 | CLA  | NA   |
| 14  | g     | 102 | CLA  | NC   |
| 14  | g     | 102 | CLA  | ND   |
| 14  | g     | 102 | CLA  | NA   |
| 14  | G     | 831 | CLA  | NC   |
| 14  | G     | 831 | CLA  | ND   |
| 14  | G     | 831 | CLA  | NA   |
| 14  | B     | 809 | CLA  | NC   |
| 14  | B     | 809 | CLA  | ND   |
| 14  | B     | 809 | CLA  | NA   |
| 14  | G     | 823 | CLA  | NC   |
| 14  | G     | 823 | CLA  | ND   |
| 14  | G     | 823 | CLA  | NA   |
| 14  | Y     | 807 | CLA  | NC   |
| 14  | Y     | 807 | CLA  | ND   |
| 14  | Y     | 807 | CLA  | NA   |
| 14  | K     | 103 | CLA  | NC   |
| 14  | K     | 103 | CLA  | ND   |
| 14  | K     | 103 | CLA  | NA   |
| 14  | Z     | 829 | CLA  | NC   |
| 14  | Z     | 829 | CLA  | ND   |
| 14  | Z     | 829 | CLA  | NA   |
| 14  | B     | 840 | CLA  | NC   |
| 14  | B     | 840 | CLA  | ND   |
| 14  | B     | 840 | CLA  | NA   |
| 14  | G     | 822 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | G     | 822 | CLA  | ND   |
| 14  | G     | 822 | CLA  | NA   |
| 14  | H     | 814 | CLA  | NC   |
| 14  | H     | 814 | CLA  | ND   |
| 14  | H     | 814 | CLA  | NA   |
| 14  | Y     | 824 | CLA  | NC   |
| 14  | Y     | 824 | CLA  | ND   |
| 14  | Y     | 824 | CLA  | NA   |
| 14  | A     | 837 | CLA  | NC   |
| 14  | A     | 837 | CLA  | ND   |
| 14  | A     | 837 | CLA  | NA   |
| 14  | H     | 819 | CLA  | NC   |
| 14  | H     | 819 | CLA  | ND   |
| 14  | H     | 819 | CLA  | NA   |
| 14  | g     | 101 | CLA  | NC   |
| 14  | g     | 101 | CLA  | ND   |
| 14  | g     | 101 | CLA  | NA   |
| 14  | B     | 818 | CLA  | NC   |
| 14  | B     | 818 | CLA  | ND   |
| 14  | B     | 818 | CLA  | NA   |
| 14  | H     | 816 | CLA  | NC   |
| 14  | H     | 816 | CLA  | ND   |
| 14  | H     | 816 | CLA  | NA   |
| 14  | G     | 802 | CLA  | NC   |
| 14  | G     | 802 | CLA  | ND   |
| 14  | G     | 802 | CLA  | NA   |
| 14  | G     | 818 | CLA  | NC   |
| 14  | G     | 818 | CLA  | ND   |
| 14  | G     | 818 | CLA  | NA   |
| 14  | A     | 818 | CLA  | NC   |
| 14  | A     | 818 | CLA  | ND   |
| 14  | A     | 818 | CLA  | NA   |
| 14  | Z     | 827 | CLA  | NC   |
| 14  | Z     | 827 | CLA  | ND   |
| 14  | Z     | 827 | CLA  | NA   |
| 13  | A     | 801 | CL0  | NC   |
| 13  | A     | 801 | CL0  | ND   |
| 13  | A     | 801 | CL0  | NA   |
| 14  | f     | 101 | CLA  | NC   |
| 14  | f     | 101 | CLA  | ND   |
| 14  | f     | 101 | CLA  | NA   |
| 14  | Y     | 817 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | Y     | 817 | CLA  | ND   |
| 14  | Y     | 817 | CLA  | NA   |
| 13  | Y     | 801 | CL0  | NC   |
| 13  | Y     | 801 | CL0  | ND   |
| 13  | Y     | 801 | CL0  | NA   |
| 14  | A     | 817 | CLA  | NC   |
| 14  | A     | 817 | CLA  | ND   |
| 14  | A     | 817 | CLA  | NA   |
| 14  | Z     | 836 | CLA  | NC   |
| 14  | Z     | 836 | CLA  | ND   |
| 14  | Z     | 836 | CLA  | NA   |
| 14  | G     | 814 | CLA  | NC   |
| 14  | G     | 814 | CLA  | ND   |
| 14  | G     | 814 | CLA  | NA   |
| 14  | A     | 810 | CLA  | NC   |
| 14  | A     | 810 | CLA  | ND   |
| 14  | A     | 810 | CLA  | NA   |
| 14  | h     | 205 | CLA  | NC   |
| 14  | h     | 205 | CLA  | ND   |
| 14  | h     | 205 | CLA  | NA   |
| 14  | Y     | 836 | CLA  | NC   |
| 14  | Y     | 836 | CLA  | ND   |
| 14  | Y     | 836 | CLA  | NA   |
| 14  | h     | 206 | CLA  | NC   |
| 14  | h     | 206 | CLA  | ND   |
| 14  | h     | 206 | CLA  | NA   |
| 14  | H     | 825 | CLA  | NC   |
| 14  | H     | 825 | CLA  | ND   |
| 14  | H     | 825 | CLA  | NA   |
| 14  | A     | 834 | CLA  | NC   |
| 14  | A     | 834 | CLA  | ND   |
| 14  | A     | 834 | CLA  | NA   |
| 14  | Y     | 831 | CLA  | NC   |
| 14  | Y     | 831 | CLA  | ND   |
| 14  | Y     | 831 | CLA  | NA   |
| 14  | Z     | 805 | CLA  | NC   |
| 14  | Z     | 805 | CLA  | ND   |
| 14  | Z     | 805 | CLA  | NA   |
| 14  | Z     | 824 | CLA  | NC   |
| 14  | Z     | 824 | CLA  | ND   |
| 14  | Z     | 824 | CLA  | NA   |
| 14  | B     | 828 | CLA  | NC   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | B     | 828 | CLA  | ND   |
| 14  | B     | 828 | CLA  | NA   |
| 14  | G     | 819 | CLA  | NC   |
| 14  | G     | 819 | CLA  | ND   |
| 14  | G     | 819 | CLA  | NA   |
| 14  | B     | 835 | CLA  | NC   |
| 14  | B     | 835 | CLA  | ND   |
| 14  | B     | 835 | CLA  | NA   |
| 14  | G     | 842 | CLA  | NC   |
| 14  | G     | 842 | CLA  | ND   |
| 14  | G     | 842 | CLA  | NA   |
| 14  | Y     | 819 | CLA  | NC   |
| 14  | Y     | 819 | CLA  | ND   |
| 14  | Y     | 819 | CLA  | NA   |
| 14  | G     | 827 | CLA  | NC   |
| 14  | G     | 827 | CLA  | ND   |
| 14  | G     | 827 | CLA  | NA   |
| 14  | A     | 813 | CLA  | NC   |
| 14  | A     | 813 | CLA  | ND   |
| 14  | A     | 813 | CLA  | NA   |
| 14  | G     | 843 | CLA  | NC   |
| 14  | G     | 843 | CLA  | ND   |
| 14  | G     | 843 | CLA  | NA   |

All (4327) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 811 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 811 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 820 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 820 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 810 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 827 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 852 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 18  | Y     | 852 | LHG  | C1-C2-C3-O3     |
| 18  | Y     | 852 | LHG  | C4-O6-P-O4      |
| 18  | Y     | 852 | LHG  | C4-O6-P-O5      |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Y     | 852  | LHG  | O7-C5-C6-O8     |
| 14  | Z     | 808  | CLA  | CBD-CGD-O2D-CED |
| 17  | M     | 101  | BCR  | C11-C10-C9-C34  |
| 17  | M     | 101  | BCR  | C10-C11-C12-C13 |
| 17  | M     | 101  | BCR  | C15-C16-C17-C18 |
| 14  | H     | 817  | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 818  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 831  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 831  | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 831  | CLA  | CHA-CBD-CGD-O2D |
| 17  | U     | 1005 | BCR  | C11-C10-C9-C8   |
| 17  | U     | 1005 | BCR  | C11-C10-C9-C34  |
| 17  | U     | 1005 | BCR  | C9-C10-C11-C12  |
| 17  | U     | 1005 | BCR  | C10-C11-C12-C13 |
| 17  | U     | 1005 | BCR  | C16-C17-C18-C36 |
| 14  | A     | 832  | CLA  | C12-C13-C15-C16 |
| 17  | G     | 846  | BCR  | C5-C6-C7-C8     |
| 17  | G     | 846  | BCR  | C9-C10-C11-C12  |
| 17  | G     | 846  | BCR  | C10-C11-C12-C13 |
| 17  | G     | 846  | BCR  | C23-C24-C25-C26 |
| 17  | G     | 846  | BCR  | C23-C24-C25-C30 |
| 14  | d     | 202  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 831  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 831  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 831  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 17  | e     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | e     | 101  | BCR  | C5-C6-C7-C8     |
| 17  | e     | 101  | BCR  | C10-C11-C12-C13 |
| 14  | G     | 839  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 839  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 205  | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 205  | CLA  | C3A-C2A-CAA-CBA |
| 14  | L     | 205  | CLA  | CHA-CBD-CGD-O1D |
| 14  | L     | 205  | CLA  | CHA-CBD-CGD-O2D |
| 14  | L     | 205  | CLA  | CAD-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | L     | 205  | CLA  | CAD-CBD-CGD-O2D |
| 14  | Y     | 830  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 830  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 825  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 825  | CLA  | CBD-CGD-O2D-CED |
| 14  | W     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 813  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 840  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 840  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 840  | CLA  | CAD-CBD-CGD-O2D |
| 17  | H     | 845  | BCR  | C10-C11-C12-C13 |
| 17  | H     | 845  | BCR  | C11-C12-C13-C14 |
| 17  | H     | 845  | BCR  | C11-C12-C13-C35 |
| 17  | H     | 845  | BCR  | C14-C15-C16-C17 |
| 14  | B     | 834  | CLA  | CBD-CGD-O2D-CED |
| 18  | G     | 852  | LHG  | C1-C2-C3-O3     |
| 18  | G     | 852  | LHG  | O9-C7-O7-C5     |
| 18  | G     | 852  | LHG  | C8-C7-O7-C5     |
| 17  | J     | 103  | BCR  | C1-C6-C7-C8     |
| 14  | U     | 1002 | CLA  | C1A-C2A-CAA-CBA |
| 14  | U     | 1002 | CLA  | C3A-C2A-CAA-CBA |
| 14  | U     | 1002 | CLA  | CHA-CBD-CGD-O1D |
| 14  | U     | 1002 | CLA  | CHA-CBD-CGD-O2D |
| 14  | U     | 1002 | CLA  | CAD-CBD-CGD-O1D |
| 14  | U     | 1002 | CLA  | CBD-CGD-O2D-CED |
| 17  | A     | 847  | BCR  | C10-C11-C12-C13 |
| 17  | G     | 854  | BCR  | C10-C11-C12-C13 |
| 17  | G     | 854  | BCR  | C23-C24-C25-C26 |
| 17  | Y     | 846  | BCR  | C11-C10-C9-C8   |
| 17  | Y     | 846  | BCR  | C11-C10-C9-C34  |
| 17  | Y     | 846  | BCR  | C9-C10-C11-C12  |
| 17  | Y     | 846  | BCR  | C10-C11-C12-C13 |
| 17  | Y     | 846  | BCR  | C18-C19-C20-C21 |
| 18  | A     | 850  | LHG  | O2-C2-C3-O3     |
| 14  | A     | 820  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 820  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 820  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 820  | CLA  | C4-C3-C5-C6     |
| 17  | d     | 203  | BCR  | C14-C15-C16-C17 |
| 17  | d     | 203  | BCR  | C18-C19-C20-C21 |
| 14  | G     | 817  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 817  | CLA  | C4-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | Y     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 838 | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 838 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 825 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 825 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 825 | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 18  | j     | 101 | LHG  | C3-O3-P-O4      |
| 14  | J     | 102 | CLA  | C1A-C2A-CAA-CBA |
| 14  | J     | 102 | CLA  | C3A-C2A-CAA-CBA |
| 14  | J     | 102 | CLA  | O1A-CGA-O2A-C1  |
| 14  | J     | 102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | J     | 102 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 844 | BCR  | C11-C10-C9-C8   |
| 17  | B     | 844 | BCR  | C11-C10-C9-C34  |
| 17  | B     | 844 | BCR  | C9-C10-C11-C12  |
| 17  | B     | 844 | BCR  | C10-C11-C12-C13 |
| 17  | B     | 844 | BCR  | C23-C24-C25-C26 |
| 17  | H     | 841 | BCR  | C11-C10-C9-C8   |
| 17  | H     | 841 | BCR  | C11-C10-C9-C34  |
| 17  | H     | 841 | BCR  | C9-C10-C11-C12  |
| 17  | H     | 841 | BCR  | C10-C11-C12-C13 |
| 17  | H     | 841 | BCR  | C11-C12-C13-C14 |
| 17  | H     | 841 | BCR  | C11-C12-C13-C35 |
| 17  | H     | 841 | BCR  | C23-C24-C25-C26 |
| 17  | A     | 845 | BCR  | C10-C11-C12-C13 |
| 17  | A     | 845 | BCR  | C11-C12-C13-C14 |
| 17  | A     | 845 | BCR  | C11-C12-C13-C35 |
| 14  | A     | 807 | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 810 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 810 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 851 | LHG  | C3-O3-P-O5      |
| 18  | A     | 851 | LHG  | C8-C7-O7-C5     |
| 14  | H     | 802 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 802 | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | H     | 802 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 802 | CLA  | C4-C3-C5-C6     |
| 17  | G     | 849 | BCR  | C10-C11-C12-C13 |
| 17  | H     | 842 | BCR  | C11-C10-C9-C8   |
| 17  | H     | 842 | BCR  | C11-C10-C9-C34  |
| 17  | H     | 842 | BCR  | C9-C10-C11-C12  |
| 17  | H     | 842 | BCR  | C10-C11-C12-C13 |
| 17  | Y     | 851 | BCR  | C10-C11-C12-C13 |
| 17  | Y     | 851 | BCR  | C11-C12-C13-C14 |
| 17  | Y     | 851 | BCR  | C11-C12-C13-C35 |
| 14  | Y     | 834 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 832 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 833 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 833 | CLA  | O1D-CGD-O2D-CED |
| 17  | A     | 849 | BCR  | C1-C6-C7-C8     |
| 17  | A     | 849 | BCR  | C5-C6-C7-C8     |
| 17  | A     | 849 | BCR  | C10-C11-C12-C13 |
| 17  | B     | 851 | BCR  | C10-C11-C12-C13 |
| 17  | B     | 851 | BCR  | C14-C15-C16-C17 |
| 14  | H     | 821 | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 207 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 819 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 819 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 819 | CLA  | CHA-CBD-CGD-O2D |
| 18  | H     | 847 | LHG  | C4-O6-P-O3      |
| 18  | H     | 847 | LHG  | C4-O6-P-O4      |
| 18  | H     | 847 | LHG  | C4-O6-P-O5      |
| 17  | B     | 848 | BCR  | C11-C10-C9-C8   |
| 17  | B     | 848 | BCR  | C11-C10-C9-C34  |
| 17  | B     | 848 | BCR  | C10-C11-C12-C13 |
| 14  | A     | 841 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 841 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 841 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 816 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 823 | CLA  | C2-C3-C5-C6     |
| 14  | H     | 823 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 801 | CLA  | CBA-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 801 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 801 | CLA  | CBD-CGD-O2D-CED |
| 17  | h     | 202 | BCR  | C11-C10-C9-C34  |
| 17  | h     | 202 | BCR  | C9-C10-C11-C12  |
| 17  | h     | 202 | BCR  | C10-C11-C12-C13 |
| 17  | h     | 202 | BCR  | C11-C12-C13-C14 |
| 17  | h     | 202 | BCR  | C11-C12-C13-C35 |
| 14  | H     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 824 | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 833 | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 833 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 833 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 814 | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 814 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 829 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 829 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 829 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 808 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 832 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 832 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 832 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 801 | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 801 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 801 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 807 | CLA  | CHA-CBD-CGD-O2D |
| 17  | J     | 104 | BCR  | C1-C6-C7-C8     |
| 17  | J     | 104 | BCR  | C5-C6-C7-C8     |
| 17  | J     | 104 | BCR  | C11-C10-C9-C8   |
| 17  | J     | 104 | BCR  | C11-C10-C9-C34  |
| 17  | J     | 104 | BCR  | C9-C10-C11-C12  |
| 17  | J     | 104 | BCR  | C10-C11-C12-C13 |
| 17  | J     | 104 | BCR  | C37-C22-C23-C24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | H     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 827 | CLA  | C4-C3-C5-C6     |
| 17  | Y     | 848 | BCR  | C11-C10-C9-C8   |
| 17  | Y     | 848 | BCR  | C11-C10-C9-C34  |
| 17  | Y     | 848 | BCR  | C10-C11-C12-C13 |
| 17  | Y     | 848 | BCR  | C17-C18-C19-C20 |
| 17  | Y     | 848 | BCR  | C36-C18-C19-C20 |
| 14  | G     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 802 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 811 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 811 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 808 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 17  | L     | 203 | BCR  | C11-C10-C9-C8   |
| 17  | L     | 203 | BCR  | C11-C10-C9-C34  |
| 17  | L     | 203 | BCR  | C10-C11-C12-C13 |
| 17  | L     | 203 | BCR  | C11-C12-C13-C14 |
| 17  | L     | 203 | BCR  | C11-C12-C13-C35 |
| 17  | L     | 203 | BCR  | C23-C24-C25-C26 |
| 17  | L     | 203 | BCR  | C23-C24-C25-C30 |
| 13  | G     | 801 | CL0  | CBD-CGD-O2D-CED |
| 13  | G     | 801 | CL0  | C2-C3-C5-C6     |
| 13  | G     | 801 | CL0  | C4-C3-C5-C6     |
| 14  | B     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 804 | CLA  | CBD-CGD-O2D-CED |
| 17  | f     | 103 | BCR  | C10-C11-C12-C13 |
| 17  | f     | 103 | BCR  | C11-C12-C13-C14 |
| 17  | f     | 103 | BCR  | C11-C12-C13-C35 |
| 18  | Y     | 853 | LHG  | C3-O3-P-O4      |
| 18  | Y     | 853 | LHG  | C3-O3-P-O5      |
| 18  | Y     | 853 | LHG  | C3-O3-P-O6      |
| 18  | Y     | 853 | LHG  | C4-O6-P-O3      |
| 18  | Y     | 853 | LHG  | C4-O6-P-O4      |
| 18  | Y     | 853 | LHG  | C4-O6-P-O5      |
| 14  | A     | 838 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 838 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 830 | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 830  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 830  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 830  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 832  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 832  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | S     | 1103 | CLA  | C1A-C2A-CAA-CBA |
| 14  | S     | 1103 | CLA  | C3A-C2A-CAA-CBA |
| 14  | S     | 1103 | CLA  | CBA-CGA-O2A-C1  |
| 14  | S     | 1103 | CLA  | O1A-CGA-O2A-C1  |
| 14  | S     | 1103 | CLA  | CBD-CGD-O2D-CED |
| 17  | f     | 104  | BCR  | C11-C10-C9-C8   |
| 17  | f     | 104  | BCR  | C11-C10-C9-C34  |
| 17  | f     | 104  | BCR  | C9-C10-C11-C12  |
| 17  | f     | 104  | BCR  | C10-C11-C12-C13 |
| 17  | f     | 104  | BCR  | C17-C18-C19-C20 |
| 14  | T     | 103  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 833  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 833  | CLA  | CBD-CGD-O2D-CED |
| 17  | Y     | 850  | BCR  | C11-C10-C9-C8   |
| 17  | Y     | 850  | BCR  | C11-C10-C9-C34  |
| 17  | R     | 101  | BCR  | C11-C10-C9-C8   |
| 17  | R     | 101  | BCR  | C11-C10-C9-C34  |
| 17  | R     | 101  | BCR  | C10-C11-C12-C13 |
| 17  | R     | 101  | BCR  | C21-C22-C23-C24 |
| 17  | R     | 101  | BCR  | C23-C24-C25-C26 |
| 14  | Y     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 837  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 837  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | J     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 832  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 832  | CLA  | C4-C3-C5-C6     |
| 14  | H     | 830  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 809  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 813  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 813  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 840  | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | Z     | 806 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 834 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 806 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 806 | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 809 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 809 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 809 | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 809 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 801 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 801 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 801 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 821 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 812 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 812 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 812 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 812 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 806 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 810 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 810 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 810 | CLA  | CBD-CGD-O2D-CED |
| 17  | A     | 848 | BCR  | C10-C11-C12-C13 |
| 17  | A     | 848 | BCR  | C11-C12-C13-C14 |
| 17  | A     | 848 | BCR  | C11-C12-C13-C35 |
| 14  | G     | 841 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 805 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 805 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 805 | CLA  | CAD-CBD-CGD-O2D |
| 14  | Z     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 814 | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 17  | B     | 847 | BCR  | C5-C6-C7-C8     |
| 17  | B     | 847 | BCR  | C10-C11-C12-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | G     | 847 | BCR  | C11-C10-C9-C8   |
| 17  | G     | 847 | BCR  | C11-C10-C9-C34  |
| 17  | G     | 847 | BCR  | C10-C11-C12-C13 |
| 17  | G     | 847 | BCR  | C14-C15-C16-C17 |
| 17  | G     | 847 | BCR  | C16-C17-C18-C36 |
| 14  | B     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 803 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 824 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 824 | CLA  | C4-C3-C5-C6     |
| 17  | Z     | 841 | BCR  | C11-C10-C9-C8   |
| 17  | Z     | 841 | BCR  | C11-C10-C9-C34  |
| 17  | Z     | 841 | BCR  | C10-C11-C12-C13 |
| 17  | Z     | 841 | BCR  | C11-C12-C13-C14 |
| 17  | Z     | 841 | BCR  | C11-C12-C13-C35 |
| 17  | Z     | 841 | BCR  | C14-C15-C16-C17 |
| 17  | Z     | 841 | BCR  | C15-C16-C17-C18 |
| 17  | Z     | 841 | BCR  | C21-C22-C23-C24 |
| 17  | Z     | 841 | BCR  | C23-C24-C25-C26 |
| 17  | Z     | 841 | BCR  | C23-C24-C25-C30 |
| 14  | Z     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 812 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 821 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 830 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 830 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 830 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 842 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 842 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 842 | CLA  | O1A-CGA-O2A-C1  |
| 18  | B     | 850 | LHG  | O1-C1-C2-C3     |
| 18  | B     | 850 | LHG  | C1-C2-C3-O3     |
| 18  | B     | 850 | LHG  | C3-O3-P-O4      |
| 18  | B     | 850 | LHG  | O7-C5-C6-O8     |
| 18  | B     | 850 | LHG  | C8-C7-O7-C5     |
| 17  | L     | 208 | BCR  | C11-C10-C9-C8   |
| 17  | L     | 208 | BCR  | C11-C10-C9-C34  |
| 17  | L     | 208 | BCR  | C10-C11-C12-C13 |
| 17  | L     | 208 | BCR  | C11-C12-C13-C14 |
| 17  | L     | 208 | BCR  | C11-C12-C13-C35 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | L     | 208 | BCR  | C14-C15-C16-C17 |
| 17  | L     | 208 | BCR  | C16-C17-C18-C36 |
| 14  | Y     | 823 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 823 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 823 | CLA  | CBD-CGD-O2D-CED |
| 17  | f     | 105 | BCR  | C10-C11-C12-C13 |
| 17  | f     | 105 | BCR  | C15-C16-C17-C18 |
| 17  | Z     | 846 | BCR  | C14-C15-C16-C17 |
| 17  | Z     | 846 | BCR  | C16-C17-C18-C19 |
| 17  | Z     | 846 | BCR  | C16-C17-C18-C36 |
| 17  | Y     | 847 | BCR  | C10-C11-C12-C13 |
| 14  | A     | 839 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 839 | CLA  | O1D-CGD-O2D-CED |
| 17  | Y     | 856 | BCR  | C11-C10-C9-C8   |
| 17  | Y     | 856 | BCR  | C10-C11-C12-C13 |
| 17  | Y     | 856 | BCR  | C11-C12-C13-C14 |
| 17  | Y     | 856 | BCR  | C11-C12-C13-C35 |
| 17  | Y     | 856 | BCR  | C14-C15-C16-C17 |
| 17  | Y     | 856 | BCR  | C15-C16-C17-C18 |
| 17  | Z     | 845 | BCR  | C1-C6-C7-C8     |
| 17  | Z     | 845 | BCR  | C5-C6-C7-C8     |
| 17  | Z     | 845 | BCR  | C10-C11-C12-C13 |
| 14  | Y     | 839 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 839 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 845 | BCR  | C1-C6-C7-C8     |
| 17  | B     | 845 | BCR  | C5-C6-C7-C8     |
| 17  | B     | 845 | BCR  | C11-C10-C9-C8   |
| 17  | B     | 845 | BCR  | C11-C10-C9-C34  |
| 17  | B     | 845 | BCR  | C9-C10-C11-C12  |
| 14  | Q     | 201 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Q     | 201 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Q     | 201 | CLA  | C2A-CAA-CBA-CGA |
| 17  | G     | 850 | BCR  | C1-C6-C7-C8     |
| 17  | G     | 850 | BCR  | C5-C6-C7-C8     |
| 17  | G     | 850 | BCR  | C11-C10-C9-C8   |
| 17  | G     | 850 | BCR  | C11-C10-C9-C34  |
| 17  | G     | 850 | BCR  | C10-C11-C12-C13 |
| 14  | K     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 14  | K     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 14  | K     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | L     | 201 | CLA  | C2-C1-O2A-CGA   |
| 14  | L     | 201 | CLA  | CHA-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | L     | 201  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 833  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 829  | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 829  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 824  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 824  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 820  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 820  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 820  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 835  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 14  | d     | 201  | CLA  | CBD-CGD-O2D-CED |
| 17  | V     | 1202 | BCR  | C10-C11-C12-C13 |
| 17  | V     | 1202 | BCR  | C11-C12-C13-C14 |
| 17  | V     | 1202 | BCR  | C11-C12-C13-C35 |
| 14  | Z     | 825  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 825  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 17  | U     | 1008 | BCR  | C10-C11-C12-C13 |
| 17  | U     | 1008 | BCR  | C11-C12-C13-C14 |
| 17  | U     | 1008 | BCR  | C11-C12-C13-C35 |
| 14  | S     | 1101 | CLA  | C1A-C2A-CAA-CBA |
| 14  | S     | 1101 | CLA  | C3A-C2A-CAA-CBA |
| 14  | S     | 1101 | CLA  | CHA-CBD-CGD-O1D |
| 14  | S     | 1101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | S     | 1101 | CLA  | C6-C7-C8-C9     |
| 17  | F     | 203  | BCR  | C9-C10-C11-C12  |
| 17  | F     | 203  | BCR  | C10-C11-C12-C13 |
| 17  | F     | 203  | BCR  | C18-C19-C20-C21 |
| 17  | U     | 1007 | BCR  | C11-C10-C9-C8   |
| 17  | U     | 1007 | BCR  | C11-C10-C9-C34  |
| 17  | U     | 1007 | BCR  | C11-C12-C13-C14 |
| 17  | U     | 1007 | BCR  | C11-C12-C13-C35 |
| 17  | U     | 1007 | BCR  | C14-C15-C16-C17 |
| 17  | U     | 1007 | BCR  | C21-C22-C23-C24 |
| 17  | U     | 1007 | BCR  | C23-C24-C25-C26 |
| 17  | U     | 1007 | BCR  | C23-C24-C25-C30 |
| 14  | G     | 833  | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | G     | 833 | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 838 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 822 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 822 | CLA  | CHA-CBD-CGD-O2D |
| 17  | G     | 848 | BCR  | C10-C11-C12-C13 |
| 17  | G     | 848 | BCR  | C23-C24-C25-C26 |
| 14  | G     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 829 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 829 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 806 | CLA  | CBD-CGD-O2D-CED |
| 14  | h     | 207 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 829 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 829 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 829 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 17  | A     | 846 | BCR  | C11-C10-C9-C8   |
| 17  | A     | 846 | BCR  | C11-C10-C9-C34  |
| 17  | A     | 846 | BCR  | C10-C11-C12-C13 |
| 17  | A     | 846 | BCR  | C11-C12-C13-C14 |
| 17  | A     | 846 | BCR  | C11-C12-C13-C35 |
| 17  | A     | 846 | BCR  | C14-C15-C16-C17 |
| 17  | A     | 846 | BCR  | C36-C18-C19-C20 |
| 14  | A     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 17  | Z     | 843 | BCR  | C11-C10-C9-C8   |
| 17  | Z     | 843 | BCR  | C11-C10-C9-C34  |
| 14  | B     | 830 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 820 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 841 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 841 | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 841 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 843 | BCR  | C9-C10-C11-C12  |
| 17  | B     | 843 | BCR  | C10-C11-C12-C13 |
| 14  | Z     | 822 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 822 | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 822 | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 842 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 842 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 842 | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 819  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | V     | 1201 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 802  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 802  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Q     | 203  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Q     | 203  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 807  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 807  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 807  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 830  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 830  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 828  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 828  | CLA  | C3A-C2A-CAA-CBA |
| 17  | Z     | 842  | BCR  | C11-C10-C9-C8   |
| 17  | Z     | 842  | BCR  | C11-C10-C9-C34  |
| 17  | Z     | 842  | BCR  | C9-C10-C11-C12  |
| 17  | Z     | 842  | BCR  | C10-C11-C12-C13 |
| 14  | G     | 826  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 823  | CLA  | C3A-C2A-CAA-CBA |
| 17  | h     | 203  | BCR  | C10-C11-C12-C13 |
| 17  | h     | 203  | BCR  | C15-C16-C17-C18 |
| 14  | G     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 843  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 843  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 843  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 843  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 808  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 803  | CLA  | C2-C1-O2A-CGA   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | H     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 826 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 816 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 816 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 805 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 805 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 805 | CLA  | CBD-CGD-O2D-CED |
| 17  | i     | 101 | BCR  | C11-C10-C9-C8   |
| 17  | i     | 101 | BCR  | C11-C10-C9-C34  |
| 17  | i     | 101 | BCR  | C10-C11-C12-C13 |
| 17  | i     | 101 | BCR  | C15-C16-C17-C18 |
| 14  | H     | 828 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 831 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 14  | f     | 102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | f     | 102 | CLA  | CHA-CBD-CGD-O2D |
| 14  | f     | 102 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 17  | L     | 209 | BCR  | C10-C11-C12-C13 |
| 17  | L     | 209 | BCR  | C11-C12-C13-C14 |
| 17  | L     | 209 | BCR  | C11-C12-C13-C35 |
| 14  | B     | 815 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 813 | CLA  | CBD-CGD-O2D-CED |
| 17  | F     | 201 | BCR  | C7-C8-C9-C10    |
| 17  | F     | 201 | BCR  | C10-C11-C12-C13 |
| 17  | F     | 201 | BCR  | C11-C12-C13-C14 |
| 17  | F     | 201 | BCR  | C11-C12-C13-C35 |
| 17  | F     | 201 | BCR  | C23-C24-C25-C26 |
| 17  | F     | 201 | BCR  | C23-C24-C25-C30 |
| 14  | A     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 806 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 829 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 828 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 828 | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | H     | 844  | BCR  | C1-C6-C7-C8     |
| 17  | H     | 844  | BCR  | C7-C8-C9-C10    |
| 17  | H     | 844  | BCR  | C7-C8-C9-C34    |
| 17  | H     | 844  | BCR  | C23-C24-C25-C26 |
| 14  | Z     | 826  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 826  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 826  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 826  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 826  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 815  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 815  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 809  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 809  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 809  | CLA  | C11-C12-C13-C14 |
| 17  | H     | 840  | BCR  | C9-C10-C11-C12  |
| 17  | H     | 840  | BCR  | C10-C11-C12-C13 |
| 17  | H     | 840  | BCR  | C14-C15-C16-C17 |
| 17  | H     | 840  | BCR  | C23-C24-C25-C26 |
| 17  | H     | 840  | BCR  | C23-C24-C25-C30 |
| 14  | G     | 823  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 807  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 807  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 807  | CLA  | C4-C3-C5-C6     |
| 17  | S     | 1104 | BCR  | C1-C6-C7-C8     |
| 17  | S     | 1104 | BCR  | C5-C6-C7-C8     |
| 17  | S     | 1104 | BCR  | C11-C10-C9-C8   |
| 17  | S     | 1104 | BCR  | C11-C10-C9-C34  |
| 17  | S     | 1104 | BCR  | C10-C11-C12-C13 |
| 17  | S     | 1104 | BCR  | C19-C20-C21-C22 |
| 14  | K     | 103  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 822  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 814  | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 824  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 824  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 824  | CLA  | CBD-CGD-O2D-CED |
| 17  | Q     | 202  | BCR  | C11-C10-C9-C8   |
| 17  | Q     | 202  | BCR  | C11-C10-C9-C34  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | Q     | 202 | BCR  | C10-C11-C12-C13 |
| 14  | H     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 819 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 818 | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 816 | CLA  | O1A-CGA-O2A-C1  |
| 17  | T     | 102 | BCR  | C10-C11-C12-C13 |
| 17  | T     | 102 | BCR  | C37-C22-C23-C24 |
| 14  | G     | 802 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 818 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 818 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 818 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 818 | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 827 | CLA  | CBD-CGD-O2D-CED |
| 17  | I     | 101 | BCR  | C10-C11-C12-C13 |
| 17  | I     | 101 | BCR  | C11-C12-C13-C14 |
| 17  | I     | 101 | BCR  | C11-C12-C13-C35 |
| 17  | I     | 101 | BCR  | C19-C20-C21-C22 |
| 13  | Y     | 801 | CL0  | C1A-C2A-CAA-CBA |
| 13  | Y     | 801 | CL0  | C3A-C2A-CAA-CBA |
| 13  | Y     | 801 | CL0  | CBD-CGD-O2D-CED |
| 14  | A     | 817 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 817 | CLA  | CHA-CBD-CGD-O2D |
| 18  | G     | 851 | LHG  | C1-C2-C3-O3     |
| 18  | G     | 851 | LHG  | C4-O6-P-O4      |
| 14  | G     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 810 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 810 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 810 | CLA  | CBD-CGD-O2D-CED |
| 14  | h     | 205 | CLA  | C1A-C2A-CAA-CBA |
| 14  | h     | 205 | CLA  | C3A-C2A-CAA-CBA |
| 14  | h     | 205 | CLA  | CHA-CBD-CGD-O1D |
| 14  | h     | 205 | CLA  | CHA-CBD-CGD-O2D |
| 14  | h     | 205 | CLA  | CAD-CBD-CGD-O1D |
| 14  | h     | 205 | CLA  | CAD-CBD-CGD-O2D |
| 14  | h     | 205 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 836 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 836 | CLA  | CHA-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 834 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 834 | CLA  | CHA-CBD-CGD-O2D |
| 17  | R     | 102 | BCR  | C1-C6-C7-C8     |
| 17  | R     | 102 | BCR  | C5-C6-C7-C8     |
| 17  | R     | 102 | BCR  | C7-C8-C9-C10    |
| 17  | R     | 102 | BCR  | C11-C10-C9-C8   |
| 17  | R     | 102 | BCR  | C11-C10-C9-C34  |
| 17  | R     | 102 | BCR  | C10-C11-C12-C13 |
| 14  | Z     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 17  | Z     | 844 | BCR  | C17-C18-C19-C20 |
| 17  | Z     | 844 | BCR  | C36-C18-C19-C20 |
| 17  | Z     | 844 | BCR  | C18-C19-C20-C21 |
| 17  | Z     | 844 | BCR  | C21-C22-C23-C24 |
| 17  | Z     | 844 | BCR  | C37-C22-C23-C24 |
| 14  | B     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 828 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 819 | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 835 | CLA  | CBD-CGD-O2D-CED |
| 17  | H     | 848 | BCR  | C10-C11-C12-C13 |
| 17  | H     | 848 | BCR  | C11-C12-C13-C14 |
| 17  | H     | 848 | BCR  | C11-C12-C13-C35 |
| 17  | H     | 848 | BCR  | C15-C16-C17-C18 |
| 14  | G     | 842 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 842 | CLA  | C4-C3-C5-C6     |
| 17  | K     | 102 | BCR  | C11-C10-C9-C8   |
| 17  | K     | 102 | BCR  | C11-C10-C9-C34  |
| 17  | K     | 102 | BCR  | C10-C11-C12-C13 |
| 17  | K     | 102 | BCR  | C19-C20-C21-C22 |
| 14  | Y     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 819 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 813 | CLA  | CBD-CGD-O2D-CED |
| 17  | Y     | 849 | BCR  | C10-C11-C12-C13 |
| 17  | Y     | 849 | BCR  | C14-C15-C16-C17 |
| 17  | Y     | 849 | BCR  | C17-C18-C19-C20 |
| 17  | Y     | 849 | BCR  | C36-C18-C19-C20 |
| 14  | G     | 843 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 817 | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 810 | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 839  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | J     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | C4C-C3C-CAC-CBC |
| 18  | Y     | 853  | LHG  | C8-C7-O7-C5     |
| 14  | Z     | 839  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Z     | 839  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 817  | CLA  | C2C-C3C-CAC-CBC |
| 14  | F     | 202  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 840  | CLA  | O1D-CGD-O2D-CED |
| 14  | U     | 1002 | CLA  | O1D-CGD-O2D-CED |
| 14  | S     | 1102 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | d     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 843  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 823  | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 824  | CLA  | O1D-CGD-O2D-CED |
| 13  | Y     | 801  | CL0  | O1D-CGD-O2D-CED |
| 14  | h     | 205  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 833  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 855  | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 205  | CLA  | CBD-CGD-O2D-CED |
| 14  | F     | 202  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 840  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 825  | CLA  | CBD-CGD-O2D-CED |
| 14  | S     | 1102 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 818  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 808  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 802  | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 825  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | Q     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 813  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 853  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 823  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 840  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 854  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 823  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 843  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 808  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | X     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | K     | 103  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | f     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | S     | 1101 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | f     | 102  | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 841  | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 838  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 855  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 853  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 840  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | f     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 838  | CLA  | C4C-C3C-CAC-CBC |
| 14  | d     | 202  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 825  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | L     | 207  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | S     | 1103 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 840  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 838  | CLA  | O1D-CGD-O2D-CED |
| 14  | h     | 207  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | Q     | 203  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 831  | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | f     | 102  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 824  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | f     | 102  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | J     | 102  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | U     | 1004 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | h     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | S     | 1101 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 833  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 102  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 841  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 13  | G     | 801  | CL0  | O1A-CGA-O2A-C1  |
| 14  | Y     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 831  | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 801  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 832  | CLA  | O1D-CGD-O2D-CED |
| 13  | G     | 801  | CL0  | O1D-CGD-O2D-CED |
| 14  | Y     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 843  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | T     | 103  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 825  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 801  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 841  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 812  | CLA  | C8-C10-C11-C12  |
| 15  | Y     | 844  | PQN  | C18-C20-C21-C22 |
| 14  | W     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 801  | CLA  | O1D-CGD-O2D-CED |
| 14  | V     | 1201 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | K     | 103  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 805  | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Y     | 852  | LHG  | O9-C7-O7-C5     |
| 18  | A     | 851  | LHG  | O9-C7-O7-C5     |
| 18  | B     | 850  | LHG  | O9-C7-O7-C5     |
| 14  | B     | 813  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 833  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 838  | CLA  | C3-C5-C6-C7     |
| 14  | L     | 205  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 810  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 814  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 801  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | U     | 1004 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 832  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 813  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 842  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 805  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 816  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 818  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 836  | CLA  | C3-C5-C6-C7     |
| 14  | h     | 206  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 825  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 834  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 805  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 824  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 835  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 841  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 18  | Y     | 853  | LHG  | C24-C23-O8-C6   |
| 14  | Y     | 832  | CLA  | CBA-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | S     | 1101 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | h     | 207  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 842  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | X     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 824  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 810  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 827  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 810  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 824  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 824  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 812  | CLA  | C4-C3-C5-C6     |
| 14  | S     | 1103 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 807  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 816  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 805  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 805  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 852  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 812  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 824  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 827  | CLA  | C2-C3-C5-C6     |
| 14  | S     | 1103 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 807  | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 816  | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 805  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 842  | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 825  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 818  | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 834  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 804  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 805  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 837  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 824  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 842  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 835  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 842  | CLA  | O1D-CGD-O2D-CED |
| 19  | Z     | 847  | LMG  | C35-C36-C37-C38 |
| 19  | B     | 849  | LMG  | C20-C21-C22-C23 |
| 19  | H     | 846  | LMG  | C35-C36-C37-C38 |
| 14  | B     | 817  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 837  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 801  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 808  | CLA  | C3-C5-C6-C7     |
| 14  | L     | 206  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 808  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | U     | 1002 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | J     | 102  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 13  | G     | 801  | CL0  | CBA-CGA-O2A-C1  |
| 14  | A     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | h     | 201  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 803  | CLA  | CBA-CGA-O2A-C1  |
| 19  | B     | 849  | LMG  | C35-C36-C37-C38 |
| 14  | Y     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 804  | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Q     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 832  | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | L     | 205  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 825  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 838  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 825  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 839  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 14  | U     | 1003 | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 207  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 18  | Y     | 853  | LHG  | O10-C23-O8-C6   |
| 14  | h     | 201  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | T     | 101  | CLA  | C2A-CAA-CBA-CGA |
| 14  | T     | 101  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 817  | CLA  | O1D-CGD-O2D-CED |
| 18  | j     | 101  | LHG  | C5-C6-O8-C23    |
| 17  | M     | 101  | BCR  | C9-C10-C11-C12  |
| 17  | G     | 846  | BCR  | C15-C16-C17-C18 |
| 17  | J     | 103  | BCR  | C9-C10-C11-C12  |
| 17  | J     | 103  | BCR  | C15-C16-C17-C18 |
| 17  | d     | 203  | BCR  | C9-C10-C11-C12  |
| 17  | d     | 203  | BCR  | C19-C20-C21-C22 |
| 17  | B     | 844  | BCR  | C19-C20-C21-C22 |
| 17  | H     | 841  | BCR  | C15-C16-C17-C18 |
| 17  | A     | 845  | BCR  | C9-C10-C11-C12  |
| 17  | B     | 851  | BCR  | C15-C16-C17-C18 |
| 17  | f     | 103  | BCR  | C9-C10-C11-C12  |
| 17  | R     | 101  | BCR  | C19-C20-C21-C22 |
| 17  | f     | 105  | BCR  | C9-C10-C11-C12  |
| 17  | Z     | 846  | BCR  | C15-C16-C17-C18 |
| 17  | Y     | 847  | BCR  | C15-C16-C17-C18 |
| 17  | Q     | 204  | BCR  | C9-C10-C11-C12  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | V     | 1202 | BCR  | C9-C10-C11-C12  |
| 17  | U     | 1007 | BCR  | C15-C16-C17-C18 |
| 17  | A     | 846  | BCR  | C9-C10-C11-C12  |
| 17  | A     | 846  | BCR  | C15-C16-C17-C18 |
| 17  | B     | 843  | BCR  | C15-C16-C17-C18 |
| 17  | i     | 101  | BCR  | C9-C10-C11-C12  |
| 17  | H     | 840  | BCR  | C15-C16-C17-C18 |
| 17  | T     | 102  | BCR  | C19-C20-C21-C22 |
| 17  | H     | 848  | BCR  | C9-C10-C11-C12  |
| 17  | Y     | 849  | BCR  | C9-C10-C11-C12  |
| 14  | B     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 806  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 816  | CLA  | O1D-CGD-O2D-CED |
| 18  | Y     | 852  | LHG  | O2-C2-C3-O3     |
| 18  | G     | 852  | LHG  | O2-C2-C3-O3     |
| 18  | B     | 850  | LHG  | O2-C2-C3-O3     |
| 18  | G     | 851  | LHG  | O2-C2-C3-O3     |
| 14  | Y     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | U     | 1002 | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 815  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 837  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 813  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 812  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | L     | 202  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 823  | CLA  | C3-C5-C6-C7     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 828  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 828  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 840  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 824  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 205  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 207  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 814  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 206  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 803  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 835  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | h     | 206  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | U     | 1002 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | h     | 207  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 808  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 830  | CLA  | C13-C15-C16-C17 |
| 18  | Y     | 852  | LHG  | C8-C7-O7-C5     |
| 14  | B     | 841  | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | j     | 102  | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 202  | CLA  | CBD-CGD-O2D-CED |
| 18  | Y     | 852  | LHG  | C13-C14-C15-C16 |
| 14  | Y     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 813  | CLA  | O1D-CGD-O2D-CED |
| 18  | H     | 847  | LHG  | C25-C26-C27-C28 |
| 14  | Y     | 824  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Z     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 852  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 817  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 812  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | V     | 1201 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 808  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | U     | 1003 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 809  | CLA  | O1D-CGD-O2D-CED |
| 19  | Z     | 847  | LMG  | O6-C5-C6-O5     |
| 18  | B     | 850  | LHG  | C2-C3-O3-P      |
| 14  | L     | 205  | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 206  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 19  | B     | 849  | LMG  | O6-C5-C6-O5     |
| 14  | J     | 102  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 841  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 840  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 814  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 818  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 817  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | J     | 102  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 841  | CLA  | C2-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 840  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 814  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 818  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 817  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 836  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 838  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 823  | CLA  | O1D-CGD-O2D-CED |
| 19  | H     | 846  | LMG  | O6-C5-C6-O5     |
| 14  | Z     | 814  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 835  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | h     | 206  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | V     | 1201 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | V     | 1201 | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 814  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 832  | CLA  | C4C-C3C-CAC-CBC |
| 14  | B     | 838  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 102  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 18  | Y     | 853  | LHG  | O9-C7-O7-C5     |
| 14  | S     | 1101 | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 854  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 824  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 850  | LHG  | C1-C2-C3-O3     |
| 14  | Y     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 819  | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 816  | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 818  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 816  | CLA  | C3-C5-C6-C7     |
| 13  | A     | 801  | CL0  | C3-C5-C6-C7     |
| 14  | Z     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 14  | U     | 1004 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 814  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 818  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | C2C-C3C-CAC-CBC |
| 14  | S     | 1102 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 828  | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 836  | CLA  | C2A-CAA-CBA-CGA |
| 17  | U     | 1005 | BCR  | C15-C16-C17-C18 |
| 17  | d     | 203  | BCR  | C15-C16-C17-C18 |
| 17  | L     | 208  | BCR  | C15-C16-C17-C18 |
| 17  | F     | 203  | BCR  | C19-C20-C21-C22 |
| 17  | U     | 1007 | BCR  | C9-C10-C11-C12  |
| 17  | Z     | 844  | BCR  | C19-C20-C21-C22 |
| 17  | K     | 102  | BCR  | C9-C10-C11-C12  |
| 17  | Y     | 849  | BCR  | C15-C16-C17-C18 |
| 14  | A     | 832  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 830  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 829  | CLA  | C5-C6-C7-C8     |
| 19  | H     | 846  | LMG  | C4-C5-C6-O5     |
| 18  | H     | 847  | LHG  | C27-C28-C29-C30 |
| 14  | K     | 101  | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 833  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 804  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 832  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 822  | CLA  | C8-C10-C11-C12  |
| 14  | h     | 201  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 827  | CLA  | C15-C16-C17-C18 |
| 14  | L     | 202  | CLA  | C13-C15-C16-C17 |
| 14  | Z     | 825  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 811  | CLA  | C10-C11-C12-C13 |
| 14  | h     | 207  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 836  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 827  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 813  | CLA  | O1A-CGA-O2A-C1  |
| 14  | V     | 1201 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 812  | CLA  | C4-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | Z     | 847  | LMG  | C4-C5-C6-O5     |
| 14  | G     | 812  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 805  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 826  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 832  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 855  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 839  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 813  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 837  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 830  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 809  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 815  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 802  | CLA  | C11-C12-C13-C14 |
| 14  | L     | 207  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 809  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 801  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 801  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 824  | CLA  | C11-C10-C8-C9   |
| 14  | H     | 824  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 801  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 801  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | L     | 206  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 809  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 803  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 832  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 827  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 806  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 803  | CLA  | C11-C12-C13-C14 |
| 14  | L     | 202  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | S     | 1101 | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 811  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 830  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 839  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 808  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 828  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 818  | CLA  | C11-C12-C13-C14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 818  | CLA  | C11-C12-C13-C14 |
| 14  | h     | 206  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 805  | CLA  | C14-C13-C15-C16 |
| 15  | Z     | 840  | PQN  | C16-C17-C18-C19 |
| 14  | G     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 813  | CLA  | C6-C7-C8-C9     |
| 14  | J     | 102  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | h     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | H     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 838  | CLA  | C2A-CAA-CBA-CGA |
| 17  | M     | 101  | BCR  | C11-C12-C13-C35 |
| 17  | G     | 854  | BCR  | C11-C12-C13-C35 |
| 17  | G     | 849  | BCR  | C11-C12-C13-C35 |
| 17  | f     | 104  | BCR  | C36-C18-C19-C20 |
| 17  | R     | 101  | BCR  | C37-C22-C23-C24 |
| 17  | Z     | 841  | BCR  | C37-C22-C23-C24 |
| 17  | Z     | 845  | BCR  | C7-C8-C9-C34    |
| 17  | G     | 850  | BCR  | C11-C12-C13-C35 |
| 17  | U     | 1007 | BCR  | C37-C22-C23-C24 |
| 17  | K     | 102  | BCR  | C37-C22-C23-C24 |
| 17  | G     | 854  | BCR  | C11-C12-C13-C14 |
| 17  | G     | 849  | BCR  | C11-C12-C13-C14 |
| 17  | J     | 104  | BCR  | C21-C22-C23-C24 |
| 17  | B     | 847  | BCR  | C7-C8-C9-C10    |
| 17  | Z     | 845  | BCR  | C7-C8-C9-C10    |
| 17  | K     | 102  | BCR  | C21-C22-C23-C24 |
| 19  | B     | 849  | LMG  | C4-C5-C6-O5     |
| 14  | H     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 813  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 827  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 802  | CLA  | C10-C11-C12-C13 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 812  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 833  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | Z     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 802  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 818  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 805  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 819  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 18  | H     | 847  | LHG  | C24-C23-O8-C6   |
| 14  | A     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 809  | CLA  | CBA-CGA-O2A-C1  |
| 14  | h     | 205  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 817  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 817  | CLA  | C10-C11-C12-C13 |
| 14  | L     | 205  | CLA  | C13-C15-C16-C17 |
| 14  | H     | 805  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 815  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 801  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 809  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 806  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 806  | CLA  | C13-C15-C16-C17 |
| 15  | H     | 839  | PQN  | C23-C25-C26-C27 |
| 14  | Q     | 201  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 803  | CLA  | C8-C10-C11-C12  |
| 14  | S     | 1101 | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 841  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 842  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 835  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 840  | CLA  | C13-C15-C16-C17 |
| 14  | H     | 816  | CLA  | C13-C15-C16-C17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 818  | CLA  | C10-C11-C12-C13 |
| 13  | Y     | 801  | CL0  | C15-C16-C17-C18 |
| 14  | Z     | 805  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 824  | CLA  | C15-C16-C17-C18 |
| 18  | G     | 852  | LHG  | C23-C24-C25-C26 |
| 14  | H     | 825  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 839  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 802  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 822  | CLA  | C5-C6-C7-C8     |
| 14  | L     | 205  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 825  | CLA  | C5-C6-C7-C8     |
| 14  | U     | 1002 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 820  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 812  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 824  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 806  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 801  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 801  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 811  | CLA  | C13-C15-C16-C17 |
| 14  | H     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 837  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | Z     | 806  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | H     | 822  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | Z     | 802  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 834  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 823  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 807  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 805  | CLA  | C8-C10-C11-C12  |
| 15  | A     | 843  | PQN  | C23-C25-C26-C27 |
| 14  | B     | 829  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 824  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 802  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 827  | CLA  | C13-C15-C16-C17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | Y     | 801  | CL0  | C5-C6-C7-C8     |
| 14  | h     | 205  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 828  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 827  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 832  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 851  | LHG  | O1-C1-C2-O2     |
| 18  | H     | 847  | LHG  | C7-C8-C9-C10    |
| 18  | B     | 850  | LHG  | C23-C24-C25-C26 |
| 14  | H     | 805  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 815  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 818  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 841  | CLA  | C13-C15-C16-C17 |
| 14  | h     | 201  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | L     | 201  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 803  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 823  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 803  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 842  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 840  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 811  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 826  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 822  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 817  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | S     | 1101 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | L     | 205  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 841  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 815  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 823  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 830  | CLA  | C2-C1-O2A-CGA   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 822  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 818  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 804  | CLA  | C2-C1-O2A-CGA   |
| 14  | Q     | 201  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 803  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 838  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 826  | CLA  | C2-C1-O2A-CGA   |
| 14  | h     | 205  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 828  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 839  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 817  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 834  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | U     | 1004 | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 832  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 835  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 819  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 832  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 851  | LHG  | C23-C24-C25-C26 |
| 14  | B     | 806  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 811  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 806  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 823  | CLA  | C8-C10-C11-C12  |
| 15  | B     | 842  | PQN  | C23-C25-C26-C27 |
| 15  | Z     | 840  | PQN  | C18-C20-C21-C22 |
| 14  | A     | 826  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 832  | CLA  | C11-C12-C13-C15 |
| 14  | L     | 205  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 825  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 806  | CLA  | C11-C10-C8-C7   |
| 14  | U     | 1004 | CLA  | C11-C12-C13-C15 |
| 15  | G     | 844  | PQN  | C21-C22-C23-C25 |
| 14  | Y     | 832  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 808  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 808  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 825  | CLA  | C6-C7-C8-C10    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | Z     | 838 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 822 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 826 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 811 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 828 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 826 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 829 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 840 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 837 | CLA  | C11-C10-C8-C7   |
| 13  | A     | 801 | CL0  | C11-C12-C13-C15 |
| 14  | Z     | 805 | CLA  | C11-C10-C8-C7   |
| 15  | Z     | 840 | PQN  | C16-C17-C18-C20 |
| 14  | A     | 813 | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 805 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 842 | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 804 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 822 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 834 | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 843 | CLA  | C2C-C3C-CAC-CBC |
| 17  | H     | 845 | BCR  | C9-C10-C11-C12  |
| 17  | A     | 847 | BCR  | C9-C10-C11-C12  |
| 17  | G     | 854 | BCR  | C9-C10-C11-C12  |
| 17  | B     | 847 | BCR  | C9-C10-C11-C12  |
| 17  | G     | 847 | BCR  | C15-C16-C17-C18 |
| 17  | Z     | 841 | BCR  | C9-C10-C11-C12  |
| 17  | Y     | 856 | BCR  | C9-C10-C11-C12  |
| 17  | Z     | 845 | BCR  | C9-C10-C11-C12  |
| 17  | L     | 209 | BCR  | C9-C10-C11-C12  |
| 17  | F     | 201 | BCR  | C15-C16-C17-C18 |
| 17  | T     | 102 | BCR  | C9-C10-C11-C12  |
| 17  | R     | 102 | BCR  | C15-C16-C17-C18 |
| 14  | G     | 836 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 815 | CLA  | C2A-CAA-CBA-CGA |
| 14  | L     | 201 | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 824  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 843  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 823  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 807  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 824  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 818  | CLA  | C10-C11-C12-C13 |
| 14  | H     | 823  | CLA  | C5-C6-C7-C8     |
| 13  | G     | 801  | CL0  | C5-C6-C7-C8     |
| 14  | Z     | 812  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 803  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 821  | CLA  | C13-C15-C16-C17 |
| 14  | Z     | 811  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 805  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 835  | CLA  | C8-C10-C11-C12  |
| 13  | A     | 801  | CL0  | C13-C15-C16-C17 |
| 14  | A     | 817  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 836  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 813  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 814  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 832  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 810  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 834  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 826  | CLA  | C15-C16-C17-C18 |
| 14  | L     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 836  | CLA  | O1D-CGD-O2D-CED |
| 17  | J     | 104  | BCR  | C18-C19-C20-C21 |
| 17  | f     | 103  | BCR  | C18-C19-C20-C21 |
| 17  | Y     | 850  | BCR  | C18-C19-C20-C21 |
| 17  | Z     | 846  | BCR  | C10-C11-C12-C13 |
| 17  | H     | 843  | BCR  | C18-C19-C20-C21 |
| 17  | h     | 203  | BCR  | C18-C19-C20-C21 |
| 17  | L     | 209  | BCR  | C18-C19-C20-C21 |
| 14  | V     | 1201 | CLA  | C4C-C3C-CAC-CBC |
| 18  | A     | 851  | LHG  | O2-C2-C3-O3     |
| 18  | Y     | 853  | LHG  | O2-C2-C3-O3     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 839  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 811  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 807  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 827  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | H     | 803  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 837  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 841  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 820  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 813  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 823  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 828  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 802  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 807  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 822  | CLA  | C8-C10-C11-C12  |
| 13  | Y     | 801  | CL0  | C10-C11-C12-C13 |
| 15  | Z     | 840  | PQN  | C15-C16-C17-C18 |
| 14  | G     | 827  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 13  | A     | 801  | CL0  | CBA-CGA-O2A-C1  |
| 14  | Y     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | U     | 1004 | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | U     | 1004 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | h     | 205  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 841  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 822  | CLA  | C8-C10-C11-C12  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 837  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 809  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 838  | CLA  | C5-C6-C7-C8     |
| 14  | L     | 207  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 833  | CLA  | C15-C16-C17-C18 |
| 14  | H     | 803  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 833  | CLA  | C10-C11-C12-C13 |
| 15  | B     | 842  | PQN  | C25-C26-C27-C28 |
| 14  | B     | 807  | CLA  | C13-C15-C16-C17 |
| 13  | A     | 801  | CL0  | C8-C10-C11-C12  |
| 14  | h     | 205  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 819  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 829  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 18  | H     | 847  | LHG  | O10-C23-O8-C6   |
| 14  | Y     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 838  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 830  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 813  | CLA  | C10-C11-C12-C13 |
| 14  | H     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 801  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 829  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 830  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 832  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 837  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 802  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | S     | 1101 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 829  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 854  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 806  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 837  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 817  | CLA  | C10-C11-C12-C13 |
| 13  | Y     | 801  | CL0  | C13-C15-C16-C17 |
| 14  | A     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 819  | CLA  | C15-C16-C17-C18 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Y     | 852  | LHG  | C4-O6-P-O3      |
| 18  | G     | 852  | LHG  | C3-O3-P-O6      |
| 18  | A     | 850  | LHG  | C4-O6-P-O3      |
| 18  | j     | 101  | LHG  | C4-O6-P-O3      |
| 18  | B     | 850  | LHG  | C3-O3-P-O6      |
| 18  | G     | 851  | LHG  | C4-O6-P-O3      |
| 14  | G     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | S     | 1103 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 831  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 840  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 832  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 819  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 821  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 851  | LHG  | C1-C2-C3-O3     |
| 18  | Y     | 853  | LHG  | C1-C2-C3-O3     |
| 14  | Z     | 815  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 812  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 826  | CLA  | C4-C3-C5-C6     |
| 14  | T     | 101  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Z     | 808  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 825  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 817  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 837  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 832  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 826  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 837  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 822  | CLA  | C16-C17-C18-C20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 811  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 838  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 820  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 802  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 854  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 805  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 839  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 814  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 202  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 15  | Z     | 840  | PQN  | C23-C25-C26-C27 |
| 17  | H     | 848  | BCR  | C14-C15-C16-C17 |
| 14  | Z     | 818  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 101  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 839  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 821  | CLA  | C13-C15-C16-C17 |
| 17  | e     | 101  | BCR  | C19-C20-C21-C22 |
| 17  | H     | 845  | BCR  | C15-C16-C17-C18 |
| 17  | G     | 849  | BCR  | C9-C10-C11-C12  |
| 17  | B     | 851  | BCR  | C9-C10-C11-C12  |
| 17  | Y     | 848  | BCR  | C15-C16-C17-C18 |
| 17  | G     | 847  | BCR  | C9-C10-C11-C12  |
| 17  | U     | 1008 | BCR  | C9-C10-C11-C12  |
| 18  | G     | 851  | LHG  | C13-C14-C15-C16 |
| 14  | Z     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 838  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | H     | 826  | CLA  | C5-C6-C7-C8     |
| 15  | Y     | 844  | PQN  | C15-C16-C17-C18 |
| 17  | M     | 101  | BCR  | C16-C17-C18-C36 |
| 17  | e     | 101  | BCR  | C11-C10-C9-C34  |
| 17  | d     | 203  | BCR  | C16-C17-C18-C36 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | H     | 841  | BCR  | C16-C17-C18-C36 |
| 17  | A     | 845  | BCR  | C11-C10-C9-C34  |
| 17  | A     | 845  | BCR  | C16-C17-C18-C36 |
| 17  | A     | 849  | BCR  | C11-C10-C9-C34  |
| 17  | B     | 847  | BCR  | C11-C10-C9-C34  |
| 17  | Z     | 841  | BCR  | C16-C17-C18-C36 |
| 17  | Z     | 846  | BCR  | C11-C10-C9-C34  |
| 17  | Y     | 847  | BCR  | C11-C10-C9-C34  |
| 17  | Y     | 856  | BCR  | C11-C10-C9-C34  |
| 17  | U     | 1007 | BCR  | C16-C17-C18-C36 |
| 17  | h     | 203  | BCR  | C16-C17-C18-C36 |
| 17  | L     | 209  | BCR  | C11-C10-C9-C34  |
| 17  | H     | 840  | BCR  | C16-C17-C18-C36 |
| 17  | T     | 102  | BCR  | C11-C10-C9-C34  |
| 14  | Y     | 854  | CLA  | C3-C5-C6-C7     |
| 15  | Z     | 840  | PQN  | C13-C15-C16-C17 |
| 14  | Z     | 801  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 824  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 824  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 803  | CLA  | C16-C17-C18-C20 |
| 15  | H     | 839  | PQN  | C26-C27-C28-C29 |
| 14  | G     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 814  | CLA  | C16-C17-C18-C20 |
| 15  | A     | 843  | PQN  | C26-C27-C28-C29 |
| 14  | G     | 822  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 824  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 816  | CLA  | C16-C17-C18-C19 |
| 14  | h     | 205  | CLA  | C16-C17-C18-C20 |
| 18  | A     | 850  | LHG  | C15-C16-C17-C18 |
| 14  | H     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | U     | 1004 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 805  | CLA  | CBD-CGD-O2D-CED |
| 18  | G     | 851  | LHG  | C16-C17-C18-C19 |
| 14  | Z     | 831  | CLA  | O1D-CGD-O2D-CED |
| 19  | Z     | 847  | LMG  | C11-C12-C13-C14 |
| 14  | Z     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 801  | CLA  | C5-C6-C7-C8     |
| 17  | M     | 101  | BCR  | C11-C10-C9-C8   |
| 17  | U     | 1005 | BCR  | C16-C17-C18-C19 |
| 17  | e     | 101  | BCR  | C11-C10-C9-C8   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | H     | 845  | BCR  | C11-C10-C9-C8   |
| 17  | H     | 841  | BCR  | C16-C17-C18-C19 |
| 17  | A     | 845  | BCR  | C11-C10-C9-C8   |
| 17  | A     | 849  | BCR  | C11-C10-C9-C8   |
| 17  | h     | 202  | BCR  | C11-C10-C9-C8   |
| 17  | B     | 847  | BCR  | C11-C10-C9-C8   |
| 17  | G     | 847  | BCR  | C16-C17-C18-C19 |
| 17  | L     | 208  | BCR  | C16-C17-C18-C19 |
| 17  | Z     | 846  | BCR  | C11-C10-C9-C8   |
| 17  | Y     | 847  | BCR  | C11-C10-C9-C8   |
| 17  | G     | 848  | BCR  | C11-C10-C9-C8   |
| 17  | L     | 209  | BCR  | C11-C10-C9-C8   |
| 17  | H     | 840  | BCR  | C16-C17-C18-C19 |
| 17  | Q     | 202  | BCR  | C16-C17-C18-C19 |
| 17  | T     | 102  | BCR  | C11-C10-C9-C8   |
| 14  | Z     | 801  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 18  | H     | 847  | LHG  | C10-C11-C12-C13 |
| 19  | Z     | 847  | LMG  | C14-C15-C16-C17 |
| 14  | Y     | 821  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 821  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | H     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 832  | CLA  | C16-C17-C18-C20 |
| 14  | U     | 1003 | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 814  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 829  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 813  | CLA  | C16-C17-C18-C20 |
| 15  | B     | 842  | PQN  | C26-C27-C28-C30 |
| 14  | A     | 840  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | C14-C13-C15-C16 |
| 14  | H     | 805  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 825  | CLA  | C11-C10-C8-C9   |
| 14  | U     | 1006 | CLA  | C11-C12-C13-C14 |
| 14  | h     | 201  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 802  | CLA  | C14-C13-C15-C16 |
| 14  | L     | 202  | CLA  | C11-C10-C8-C9   |
| 14  | L     | 202  | CLA  | C14-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 837  | CLA  | C11-C10-C8-C9   |
| 14  | h     | 205  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 842  | CLA  | C6-C7-C8-C9     |
| 14  | L     | 202  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 819  | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 850  | LHG  | C11-C12-C13-C14 |
| 18  | G     | 851  | LHG  | C28-C29-C30-C31 |
| 18  | G     | 851  | LHG  | C29-C30-C31-C32 |
| 14  | U     | 1006 | CLA  | C15-C16-C17-C18 |
| 15  | G     | 844  | PQN  | C23-C25-C26-C27 |
| 14  | B     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | J     | 102  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 801  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 805  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 847  | BCR  | C7-C8-C9-C34    |
| 14  | Y     | 834  | CLA  | C2C-C3C-CAC-CBC |
| 19  | Z     | 847  | LMG  | C31-C32-C33-C34 |
| 18  | G     | 852  | LHG  | O1-C1-C2-C3     |
| 18  | A     | 851  | LHG  | O1-C1-C2-C3     |
| 18  | G     | 851  | LHG  | O1-C1-C2-C3     |
| 17  | M     | 101  | BCR  | C11-C12-C13-C14 |
| 17  | G     | 850  | BCR  | C11-C12-C13-C14 |
| 17  | A     | 846  | BCR  | C17-C18-C19-C20 |
| 17  | F     | 201  | BCR  | C21-C22-C23-C24 |
| 17  | I     | 101  | BCR  | C21-C22-C23-C24 |
| 14  | H     | 801  | CLA  | C3-C5-C6-C7     |
| 15  | G     | 844  | PQN  | C15-C16-C17-C18 |
| 14  | G     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 819  | CLA  | C10-C11-C12-C13 |
| 18  | A     | 850  | LHG  | C28-C29-C30-C31 |
| 18  | Y     | 852  | LHG  | C11-C10-C9-C8   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | Y     | 852 | LHG  | C15-C16-C17-C18 |
| 18  | A     | 850 | LHG  | C11-C10-C9-C8   |
| 18  | A     | 850 | LHG  | C16-C17-C18-C19 |
| 18  | A     | 851 | LHG  | C25-C26-C27-C28 |
| 18  | G     | 851 | LHG  | C25-C26-C27-C28 |
| 14  | Y     | 827 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 852 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 832 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 824 | CLA  | C11-C12-C13-C15 |
| 14  | L     | 205 | CLA  | C16-C17-C18-C19 |
| 14  | J     | 102 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 810 | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 801 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 832 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 832 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 810 | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 832 | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 832 | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 823 | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 842 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 814 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 808 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 808 | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 826 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 816 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 825 | CLA  | C15-C16-C17-C18 |
| 14  | L     | 207 | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 814 | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 804 | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 812 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 814 | CLA  | C4C-C3C-CAC-CBC |
| 18  | A     | 850 | LHG  | C29-C30-C31-C32 |
| 18  | H     | 847 | LHG  | C28-C29-C30-C31 |
| 14  | B     | 837 | CLA  | C5-C6-C7-C8     |
| 14  | H     | 802 | CLA  | C10-C11-C12-C13 |
| 14  | Q     | 201 | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 838 | CLA  | C15-C16-C17-C18 |
| 14  | h     | 205 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 202 | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 13  | A     | 801  | CL0  | O1A-CGA-O2A-C1  |
| 18  | Y     | 853  | LHG  | C24-C25-C26-C27 |
| 14  | X     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 14  | h     | 207  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 836  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 836  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 13  | G     | 801  | CL0  | C3A-C2A-CAA-CBA |
| 14  | j     | 102  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 813  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 840  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 835  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 837  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 814  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 811  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 834  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 835  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 829  | CLA  | C15-C16-C17-C18 |
| 17  | L     | 203  | BCR  | C15-C16-C17-C18 |
| 18  | A     | 850  | LHG  | C30-C31-C32-C33 |
| 18  | H     | 847  | LHG  | C9-C10-C11-C12  |
| 14  | G     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 838  | CLA  | C16-C17-C18-C19 |
| 14  | J     | 102  | CLA  | C6-C7-C8-C9     |
| 14  | L     | 207  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 808  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 810  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 803  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 803  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 842  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 802  | CLA  | C16-C17-C18-C20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 803  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 826  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 824  | CLA  | C11-C12-C13-C14 |
| 18  | A     | 851  | LHG  | C26-C27-C28-C29 |
| 18  | B     | 850  | LHG  | C25-C26-C27-C28 |
| 14  | A     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 821  | CLA  | CBD-CGD-O2D-CED |
| 19  | Z     | 847  | LMG  | C33-C34-C35-C36 |
| 17  | M     | 101  | BCR  | C14-C15-C16-C17 |
| 17  | U     | 1005 | BCR  | C14-C15-C16-C17 |
| 17  | H     | 841  | BCR  | C14-C15-C16-C17 |
| 17  | F     | 201  | BCR  | C14-C15-C16-C17 |
| 14  | B     | 819  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 805  | CLA  | C3-C5-C6-C7     |
| 19  | B     | 849  | LMG  | C11-C12-C13-C14 |
| 18  | G     | 851  | LHG  | C11-C12-C13-C14 |
| 14  | A     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 809  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 832  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 811  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 804  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 832  | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 817  | CLA  | C2-C3-C5-C6     |
| 14  | Q     | 201  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 824  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 18  | G     | 852  | LHG  | O1-C1-C2-O2     |
| 18  | A     | 851  | LHG  | O1-C1-C2-O2     |
| 18  | B     | 850  | LHG  | O1-C1-C2-O2     |
| 18  | Y     | 852  | LHG  | C28-C29-C30-C31 |
| 18  | j     | 101  | LHG  | C23-C24-C25-C26 |
| 14  | Z     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 18  | Y     | 853  | LHG  | C23-C24-C25-C26 |
| 14  | Y     | 808  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 829  | CLA  | C16-C17-C18-C20 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 841  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 819  | CLA  | C13-C15-C16-C17 |
| 19  | Z     | 847  | LMG  | C19-C20-C21-C22 |
| 14  | Y     | 855  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 817  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 813  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 816  | CLA  | C4C-C3C-CAC-CBC |
| 14  | G     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 801  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 824  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 805  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 836  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 817  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 838  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 824  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 839  | CLA  | C2-C1-O2A-CGA   |
| 14  | S     | 1101 | CLA  | C2-C1-O2A-CGA   |
| 14  | h     | 207  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 803  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 841  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 840  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 814  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 823  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 807  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 805  | CLA  | C2-C1-O2A-CGA   |
| 14  | f     | 102  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 825  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 809  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 813  | CLA  | C10-C11-C12-C13 |
| 15  | B     | 842  | PQN  | C20-C21-C22-C23 |
| 18  | j     | 101  | LHG  | C2-C3-O3-P      |
| 14  | Y     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 19  | Z     | 847  | LMG  | C16-C17-C18-C19 |
| 19  | H     | 846  | LMG  | C18-C19-C20-C21 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 809 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 813 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 803 | CLA  | C16-C17-C18-C19 |
| 17  | G     | 846 | BCR  | C1-C6-C7-C8     |
| 17  | e     | 101 | BCR  | C23-C24-C25-C26 |
| 17  | J     | 103 | BCR  | C5-C6-C7-C8     |
| 17  | G     | 854 | BCR  | C5-C6-C7-C8     |
| 17  | G     | 854 | BCR  | C23-C24-C25-C30 |
| 17  | Y     | 846 | BCR  | C23-C24-C25-C26 |
| 17  | Y     | 846 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 844 | BCR  | C23-C24-C25-C30 |
| 17  | H     | 841 | BCR  | C5-C6-C7-C8     |
| 17  | H     | 841 | BCR  | C23-C24-C25-C30 |
| 17  | A     | 845 | BCR  | C1-C6-C7-C8     |
| 17  | G     | 849 | BCR  | C1-C6-C7-C8     |
| 17  | G     | 849 | BCR  | C5-C6-C7-C8     |
| 17  | H     | 842 | BCR  | C1-C6-C7-C8     |
| 17  | H     | 842 | BCR  | C5-C6-C7-C8     |
| 17  | Y     | 851 | BCR  | C1-C6-C7-C8     |
| 17  | Y     | 851 | BCR  | C5-C6-C7-C8     |
| 17  | B     | 851 | BCR  | C5-C6-C7-C8     |
| 17  | B     | 851 | BCR  | C23-C24-C25-C30 |
| 17  | Y     | 848 | BCR  | C5-C6-C7-C8     |
| 17  | L     | 203 | BCR  | C5-C6-C7-C8     |
| 17  | f     | 103 | BCR  | C1-C6-C7-C8     |
| 14  | B     | 832 | CLA  | C3-C5-C6-C7     |
| 17  | Y     | 850 | BCR  | C23-C24-C25-C26 |
| 17  | R     | 101 | BCR  | C23-C24-C25-C30 |
| 17  | A     | 848 | BCR  | C1-C6-C7-C8     |
| 17  | A     | 848 | BCR  | C23-C24-C25-C26 |
| 17  | A     | 848 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 847 | BCR  | C1-C6-C7-C8     |
| 17  | B     | 847 | BCR  | C23-C24-C25-C26 |
| 17  | B     | 847 | BCR  | C23-C24-C25-C30 |
| 17  | L     | 208 | BCR  | C1-C6-C7-C8     |
| 17  | L     | 208 | BCR  | C5-C6-C7-C8     |
| 17  | f     | 105 | BCR  | C23-C24-C25-C30 |
| 17  | Z     | 846 | BCR  | C5-C6-C7-C8     |
| 17  | Z     | 845 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 845 | BCR  | C23-C24-C25-C26 |
| 17  | Q     | 204 | BCR  | C23-C24-C25-C26 |
| 17  | Q     | 204 | BCR  | C23-C24-C25-C30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | V     | 1202 | BCR  | C1-C6-C7-C8     |
| 17  | V     | 1202 | BCR  | C5-C6-C7-C8     |
| 17  | U     | 1007 | BCR  | C5-C6-C7-C8     |
| 17  | G     | 848  | BCR  | C23-C24-C25-C30 |
| 17  | H     | 843  | BCR  | C23-C24-C25-C26 |
| 17  | H     | 843  | BCR  | C23-C24-C25-C30 |
| 14  | Y     | 841  | CLA  | C3-C5-C6-C7     |
| 17  | Z     | 842  | BCR  | C23-C24-C25-C26 |
| 17  | Z     | 842  | BCR  | C23-C24-C25-C30 |
| 17  | h     | 203  | BCR  | C23-C24-C25-C30 |
| 17  | i     | 101  | BCR  | C23-C24-C25-C26 |
| 17  | i     | 101  | BCR  | C23-C24-C25-C30 |
| 17  | F     | 201  | BCR  | C1-C6-C7-C8     |
| 17  | H     | 844  | BCR  | C5-C6-C7-C8     |
| 17  | H     | 844  | BCR  | C23-C24-C25-C30 |
| 17  | Q     | 202  | BCR  | C5-C6-C7-C8     |
| 17  | T     | 102  | BCR  | C23-C24-C25-C30 |
| 17  | B     | 846  | BCR  | C23-C24-C25-C30 |
| 17  | I     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | H     | 848  | BCR  | C5-C6-C7-C8     |
| 17  | Y     | 849  | BCR  | C5-C6-C7-C8     |
| 14  | G     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 833  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 855  | CLA  | C8-C10-C11-C12  |
| 14  | L     | 207  | CLA  | C10-C11-C12-C13 |
| 14  | H     | 812  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 842  | CLA  | C5-C6-C7-C8     |
| 18  | A     | 850  | LHG  | C8-C7-O7-C5     |
| 19  | H     | 846  | LMG  | C14-C15-C16-C17 |
| 18  | G     | 851  | LHG  | C33-C34-C35-C36 |
| 18  | A     | 851  | LHG  | C28-C29-C30-C31 |
| 14  | B     | 831  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 837  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 818  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 832  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 808  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 803  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 828  | CLA  | C5-C6-C7-C8     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 838  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 804  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 817  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 824  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 803  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 817  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 838  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | U     | 1003 | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 811  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 838  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 815  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 802  | CLA  | C11-C12-C13-C15 |
| 14  | U     | 1006 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 829  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 801  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | L     | 206  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 830  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 822  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 822  | CLA  | C11-C12-C13-C15 |
| 14  | h     | 201  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | L     | 201  | CLA  | C12-C13-C15-C16 |
| 14  | L     | 202  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | S     | 1101 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 829  | CLA  | C12-C13-C15-C16 |
| 14  | h     | 207  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 829  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 842  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 814  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 803  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 803  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 807  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 826  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 837  | CLA  | C12-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 818  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 817  | CLA  | C11-C10-C8-C7   |
| 14  | h     | 205  | CLA  | C11-C12-C13-C15 |
| 14  | h     | 205  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | Z     | 824  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 842  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 827  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 805  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 839  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 838  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 806  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 808  | CLA  | C15-C16-C17-C18 |
| 17  | F     | 201  | BCR  | C9-C10-C11-C12  |
| 14  | H     | 813  | CLA  | C16-C17-C18-C19 |
| 14  | L     | 205  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 841  | CLA  | C16-C17-C18-C19 |
| 14  | G     | 841  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 823  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 826  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 815  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 851  | LHG  | C7-C8-C9-C10    |
| 14  | H     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 824  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 843  | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 850  | LHG  | C13-C14-C15-C16 |
| 14  | G     | 812  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 827  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 813  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | U     | 1003 | CLA  | C10-C11-C12-C13 |
| 14  | H     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 832  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 811  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | S     | 1101 | CLA  | C4C-C3C-CAC-CBC |
| 18  | A     | 850  | LHG  | C25-C26-C27-C28 |
| 14  | H     | 804  | CLA  | C15-C16-C17-C18 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 840  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 828  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 840  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 830  | CLA  | O1D-CGD-O2D-CED |
| 19  | Z     | 847  | LMG  | C39-C40-C41-C42 |
| 14  | G     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 837  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 824  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 812  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 823  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 826  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 841  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 851  | LHG  | C23-C24-C25-C26 |
| 17  | d     | 203  | BCR  | C10-C11-C12-C13 |
| 17  | S     | 1104 | BCR  | C18-C19-C20-C21 |
| 17  | B     | 846  | BCR  | C18-C19-C20-C21 |
| 17  | I     | 101  | BCR  | C18-C19-C20-C21 |
| 14  | A     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | U     | 1003 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 810  | CLA  | C10-C11-C12-C13 |
| 14  | h     | 201  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 819  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 839  | CLA  | C13-C15-C16-C17 |
| 18  | j     | 101  | LHG  | O7-C5-C6-O8     |
| 14  | Z     | 814  | CLA  | C6-C7-C8-C9     |
| 14  | Q     | 201  | CLA  | C16-C17-C18-C19 |
| 15  | B     | 842  | PQN  | C26-C27-C28-C29 |
| 14  | A     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 812  | CLA  | C4-C3-C5-C6     |
| 14  | Q     | 201  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 815  | CLA  | C2-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | Z     | 812 | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 811 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 824 | CLA  | C11-C10-C8-C9   |
| 14  | L     | 205 | CLA  | C6-C7-C8-C9     |
| 14  | L     | 205 | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 809 | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 838 | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 838 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 819 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 806 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 829 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 838 | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 830 | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 822 | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 832 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 808 | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 804 | CLA  | C11-C10-C8-C9   |
| 14  | Z     | 838 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 829 | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 806 | CLA  | C14-C13-C15-C16 |
| 14  | h     | 207 | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 842 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 814 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 826 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 823 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 811 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 807 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 826 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 806 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 829 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 840 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 840 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 818 | CLA  | C6-C7-C8-C9     |
| 13  | A     | 801 | CL0  | C11-C12-C13-C14 |
| 14  | h     | 205 | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 824 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 812 | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 817 | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 826 | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 838 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 842 | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | f     | 102  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 818  | CLA  | C2A-CAA-CBA-CGA |
| 17  | J     | 104  | BCR  | C36-C18-C19-C20 |
| 14  | Z     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 830  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | S     | 1101 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | f     | 102  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 827  | CLA  | C5-C6-C7-C8     |
| 17  | J     | 104  | BCR  | C17-C18-C19-C20 |
| 17  | T     | 102  | BCR  | C21-C22-C23-C24 |
| 14  | G     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 811  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 841  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 824  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 831  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 838  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 813  | CLA  | C1A-C2A-CAA-CBA |
| 14  | U     | 1003 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 836  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 836  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 825  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 816  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 808  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 832  | CLA  | C1A-C2A-CAA-CBA |
| 14  | j     | 102  | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 206  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 838  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 832  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 832  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 830  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 840  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 808  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 817  | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | Z     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 822 | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 811 | CLA  | C16-C17-C18-C20 |
| 14  | H     | 810 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 824 | CLA  | C16-C17-C18-C19 |
| 15  | H     | 839 | PQN  | C26-C27-C28-C30 |
| 14  | h     | 205 | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 805 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 842 | CLA  | C16-C17-C18-C19 |
| 18  | A     | 850 | LHG  | O9-C7-O7-C5     |
| 18  | Y     | 852 | LHG  | C25-C26-C27-C28 |
| 18  | B     | 850 | LHG  | C27-C28-C29-C30 |
| 17  | Y     | 850 | BCR  | C9-C10-C11-C12  |
| 17  | H     | 843 | BCR  | C15-C16-C17-C18 |
| 17  | H     | 843 | BCR  | C19-C20-C21-C22 |
| 14  | Y     | 832 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 812 | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 836 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 809 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 803 | CLA  | O1D-CGD-O2D-CED |
| 14  | K     | 101 | CLA  | C4C-C3C-CAC-CBC |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 833  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Z     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 815  | CLA  | C5-C6-C7-C8     |
| 15  | H     | 839  | PQN  | C25-C26-C27-C28 |
| 14  | Q     | 201  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 813  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 18  | H     | 847  | LHG  | O6-C4-C5-C6     |
| 14  | j     | 102  | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 850  | LHG  | C7-C8-C9-C10    |
| 14  | H     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 832  | CLA  | C13-C15-C16-C17 |
| 15  | B     | 842  | PQN  | C15-C16-C17-C18 |
| 14  | A     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 818  | CLA  | C8-C10-C11-C12  |
| 14  | U     | 1003 | CLA  | C16-C17-C18-C19 |
| 14  | H     | 805  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 840  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 854  | CLA  | C16-C17-C18-C19 |
| 15  | A     | 843  | PQN  | C26-C27-C28-C30 |
| 14  | G     | 822  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 818  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 812  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 827  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 843  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 819  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 820  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 821  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | Q     | 201  | CLA  | C3-C5-C6-C7     |
| 18  | j     | 101  | LHG  | C4-C5-C6-O8     |
| 18  | H     | 847  | LHG  | C13-C14-C15-C16 |
| 14  | A     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 803  | CLA  | C8-C10-C11-C12  |
| 14  | h     | 207  | CLA  | C13-C15-C16-C17 |
| 14  | Z     | 839  | CLA  | C8-C10-C11-C12  |
| 18  | G     | 852  | LHG  | C26-C27-C28-C29 |
| 14  | Z     | 829  | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 818  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 833  | CLA  | C10-C11-C12-C13 |
| 17  | H     | 844  | BCR  | C9-C10-C11-C12  |
| 18  | Y     | 852  | LHG  | C19-C20-C21-C22 |
| 14  | A     | 829  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 830  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 827  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 830  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 825  | CLA  | C5-C6-C7-C8     |
| 17  | f     | 105  | BCR  | C11-C10-C9-C34  |
| 17  | Y     | 856  | BCR  | C16-C17-C18-C36 |
| 17  | U     | 1008 | BCR  | C11-C10-C9-C34  |
| 17  | R     | 102  | BCR  | C16-C17-C18-C36 |
| 14  | Y     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 833  | CLA  | C4-C3-C5-C6     |
| 15  | Y     | 844  | PQN  | C14-C13-C15-C16 |
| 14  | Y     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 808  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 841  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Z     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 801  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | S     | 1101 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 829  | CLA  | C15-C16-C17-C18 |
| 18  | A     | 850  | LHG  | C33-C34-C35-C36 |
| 14  | Y     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 822  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 825  | CLA  | C8-C10-C11-C12  |
| 14  | U     | 1002 | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 838  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 815  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 820  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 824  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 839  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 829  | CLA  | C2-C1-O2A-CGA   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 805  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 843  | CLA  | C4C-C3C-CAC-CBC |
| 14  | H     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 811  | CLA  | C13-C15-C16-C17 |
| 18  | G     | 851  | LHG  | C35-C36-C37-C38 |
| 14  | H     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 836  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 824  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 827  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 809  | CLA  | C16-C17-C18-C19 |
| 18  | B     | 850  | LHG  | C9-C10-C11-C12  |
| 14  | Y     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 808  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 828  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 808  | CLA  | C15-C16-C17-C18 |
| 18  | A     | 850  | LHG  | C13-C14-C15-C16 |
| 14  | U     | 1006 | CLA  | O1D-CGD-O2D-CED |
| 14  | Y     | 832  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 807  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 818  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 827  | CLA  | C8-C10-C11-C12  |
| 17  | A     | 845  | BCR  | C16-C17-C18-C19 |
| 17  | h     | 203  | BCR  | C16-C17-C18-C19 |
| 14  | B     | 811  | CLA  | C2C-C3C-CAC-CBC |
| 18  | G     | 851  | LHG  | C11-C10-C9-C8   |
| 14  | A     | 805  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 833  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 822  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 824  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 841  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 841  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 802  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 804  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 813  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 813  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 822  | CLA  | C11-C12-C13-C15 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 837  | CLA  | C12-C13-C15-C16 |
| 14  | L     | 205  | CLA  | C11-C12-C13-C15 |
| 14  | L     | 205  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 809  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 809  | CLA  | C12-C13-C15-C16 |
| 14  | U     | 1002 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 805  | CLA  | C6-C7-C8-C10    |
| 14  | Z     | 815  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 820  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 819  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 801  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 801  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 824  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 835  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | L     | 206  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 832  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 837  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 806  | CLA  | C6-C7-C8-C10    |
| 14  | Z     | 817  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 804  | CLA  | C6-C7-C8-C10    |
| 14  | S     | 1101 | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 819  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 814  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 805  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 854  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 828  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 821  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 808  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 826  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 828  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 840  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 824  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 824  | CLA  | C6-C7-C8-C10    |
| 15  | Y     | 844  | PQN  | C12-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 802  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 818  | CLA  | C11-C12-C13-C15 |
| 13  | Y     | 801  | CL0  | C6-C7-C8-C10    |
| 13  | Y     | 801  | CL0  | C12-C13-C15-C16 |
| 14  | Z     | 836  | CLA  | C12-C13-C15-C16 |
| 14  | h     | 206  | CLA  | C11-C10-C8-C7   |
| 14  | h     | 206  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 825  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 842  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 819  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 817  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 817  | CLA  | C11-C10-C8-C9   |
| 14  | H     | 818  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 832  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 802  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 804  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 822  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 837  | CLA  | C11-C12-C13-C14 |
| 14  | L     | 205  | CLA  | C11-C12-C13-C14 |
| 14  | U     | 1003 | CLA  | C11-C12-C13-C14 |
| 14  | U     | 1002 | CLA  | C6-C7-C8-C9     |
| 14  | U     | 1002 | CLA  | C11-C12-C13-C14 |
| 14  | H     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 807  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 811  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 838  | CLA  | C14-C13-C15-C16 |
| 14  | H     | 824  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 835  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 804  | CLA  | C11-C10-C8-C9   |
| 14  | L     | 206  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 832  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 822  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 837  | CLA  | C14-C13-C15-C16 |
| 15  | G     | 844  | PQN  | C21-C22-C23-C24 |
| 14  | H     | 801  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 817  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 803  | CLA  | C11-C10-C8-C9   |
| 14  | H     | 812  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 825  | CLA  | C11-C10-C8-C9   |
| 14  | Q     | 201  | CLA  | C11-C12-C13-C14 |
| 14  | L     | 201  | CLA  | C14-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 825  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 822  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 829  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 819  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 814  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 854  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 828  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 828  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 824  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 837  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 802  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 818  | CLA  | C11-C10-C8-C9   |
| 13  | Y     | 801  | CL0  | C6-C7-C8-C9     |
| 13  | Y     | 801  | CL0  | C14-C13-C15-C16 |
| 14  | Z     | 836  | CLA  | C14-C13-C15-C16 |
| 14  | h     | 206  | CLA  | C11-C10-C8-C9   |
| 14  | h     | 206  | CLA  | C11-C12-C13-C14 |
| 15  | Z     | 840  | PQN  | C21-C22-C23-C24 |
| 14  | G     | 842  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 819  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 827  | CLA  | C11-C12-C13-C14 |
| 17  | Y     | 846  | BCR  | C19-C20-C21-C22 |
| 17  | Y     | 850  | BCR  | C19-C20-C21-C22 |
| 14  | A     | 831  | CLA  | CBD-CGD-O2D-CED |
| 17  | h     | 203  | BCR  | C14-C15-C16-C17 |
| 18  | Y     | 852  | LHG  | C31-C32-C33-C34 |
| 14  | U     | 1006 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 820  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 813  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 811  | CLA  | C8-C10-C11-C12  |
| 14  | U     | 1004 | CLA  | C2A-CAA-CBA-CGA |
| 18  | H     | 847  | LHG  | C29-C30-C31-C32 |
| 14  | A     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 821  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 820  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 826  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 803  | CLA  | C16-C17-C18-C19 |
| 18  | j     | 101  | LHG  | C11-C10-C9-C8   |
| 17  | A     | 847  | BCR  | C21-C22-C23-C24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 802  | CLA  | C5-C6-C7-C8     |
| 18  | Y     | 852  | LHG  | C33-C34-C35-C36 |
| 18  | B     | 850  | LHG  | C30-C31-C32-C33 |
| 14  | U     | 1006 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 201  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 841  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 824  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 835  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 852  | CLA  | C16-C17-C18-C19 |
| 14  | H     | 813  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 837  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 808  | CLA  | C13-C15-C16-C17 |
| 18  | A     | 850  | LHG  | O6-C4-C5-C6     |
| 14  | B     | 841  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 802  | CLA  | C3-C5-C6-C7     |
| 18  | G     | 851  | LHG  | C31-C32-C33-C34 |
| 14  | B     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 809  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 854  | CLA  | CBA-CGA-O2A-C1  |
| 17  | Y     | 856  | BCR  | C18-C19-C20-C21 |
| 17  | H     | 844  | BCR  | C10-C11-C12-C13 |
| 14  | G     | 841  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 806  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 822  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 827  | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 816  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 819  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 830  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 809  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 820  | CLA  | CAA-CBA-CGA-O2A |
| 18  | Y     | 852  | LHG  | C7-C8-C9-C10    |
| 14  | G     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 826  | CLA  | C3A-C2A-CAA-CBA |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 802 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 14  | H     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 841 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 14  | h     | 207 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 840 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 805 | CLA  | C4C-C3C-CAC-CBC |
| 14  | H     | 811 | CLA  | O1D-CGD-O2D-CED |
| 17  | f     | 103 | BCR  | C19-C20-C21-C22 |
| 14  | G     | 809 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 810 | CLA  | C15-C16-C17-C18 |
| 15  | Z     | 840 | PQN  | C25-C26-C27-C28 |
| 14  | A     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 18  | G     | 851 | LHG  | C15-C16-C17-C18 |
| 14  | L     | 207 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 841 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 841 | CLA  | C16-C17-C18-C20 |
| 14  | B     | 828 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 851 | LHG  | C24-C23-O8-C6   |
| 14  | G     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 802 | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 822 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 841 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 824 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 833 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 829 | CLA  | C8-C10-C11-C12  |
| 18  | Y     | 852 | LHG  | C4-C5-C6-O8     |
| 18  | Y     | 853 | LHG  | C4-C5-C6-O8     |
| 18  | B     | 850 | LHG  | C4-C5-C6-O8     |
| 14  | A     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 805 | CLA  | C16-C17-C18-C19 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 812  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 826  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 811  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Z     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 817  | CLA  | C10-C11-C12-C13 |
| 18  | G     | 852  | LHG  | O6-C4-C5-O7     |
| 18  | A     | 850  | LHG  | O6-C4-C5-O7     |
| 18  | A     | 851  | LHG  | O6-C4-C5-O7     |
| 18  | A     | 850  | LHG  | C26-C27-C28-C29 |
| 14  | Y     | 841  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 825  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 809  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 809  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 841  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 835  | CLA  | C10-C11-C12-C13 |
| 13  | A     | 801  | CL0  | CAA-CBA-CGA-O2A |
| 19  | Z     | 847  | LMG  | O1-C7-C8-O7     |
| 18  | Y     | 853  | LHG  | O7-C5-C6-O8     |
| 14  | U     | 1004 | CLA  | C13-C15-C16-C17 |
| 15  | H     | 839  | PQN  | C15-C16-C17-C18 |
| 14  | A     | 803  | CLA  | C15-C16-C17-C18 |
| 17  | A     | 845  | BCR  | C15-C16-C17-C18 |
| 18  | A     | 850  | LHG  | C35-C36-C37-C38 |
| 14  | G     | 826  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 839  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 835  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 842  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 843  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 806  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 839  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 832  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 840  | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 825  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 829  | CLA  | C6-C7-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 807  | CLA  | C11-C12-C13-C14 |
| 14  | U     | 1004 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 838  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 810  | CLA  | C11-C10-C8-C9   |
| 14  | H     | 809  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 837  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 813  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 801  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 821  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 833  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 839  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 802  | CLA  | C6-C7-C8-C9     |
| 19  | Z     | 847  | LMG  | C12-C13-C14-C15 |
| 14  | H     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 842  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 802  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 818  | CLA  | C16-C17-C18-C20 |
| 17  | A     | 845  | BCR  | C5-C6-C7-C8     |
| 17  | h     | 202  | BCR  | C1-C6-C7-C8     |
| 17  | Y     | 850  | BCR  | C23-C24-C25-C30 |
| 17  | R     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | Z     | 846  | BCR  | C1-C6-C7-C8     |
| 17  | Z     | 845  | BCR  | C23-C24-C25-C26 |
| 17  | V     | 1202 | BCR  | C23-C24-C25-C30 |
| 17  | Z     | 843  | BCR  | C1-C6-C7-C8     |
| 17  | L     | 209  | BCR  | C1-C6-C7-C8     |
| 17  | H     | 848  | BCR  | C23-C24-C25-C30 |
| 14  | L     | 206  | CLA  | C10-C11-C12-C13 |
| 15  | H     | 839  | PQN  | C20-C21-C22-C23 |
| 14  | A     | 833  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 832  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 822  | CLA  | CAA-CBA-CGA-O2A |
| 14  | L     | 207  | CLA  | CAA-CBA-CGA-O2A |
| 17  | U     | 1005 | BCR  | C11-C12-C13-C14 |
| 17  | f     | 103  | BCR  | C17-C18-C19-C20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | R     | 101  | BCR  | C17-C18-C19-C20 |
| 17  | G     | 847  | BCR  | C11-C12-C13-C14 |
| 17  | G     | 848  | BCR  | C7-C8-C9-C10    |
| 17  | G     | 848  | BCR  | C21-C22-C23-C24 |
| 17  | B     | 846  | BCR  | C17-C18-C19-C20 |
| 14  | B     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | L     | 202  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | Z     | 829  | CLA  | C4C-C3C-CAC-CBC |
| 14  | G     | 827  | CLA  | CBD-CGD-O2D-CED |
| 17  | Y     | 848  | BCR  | C14-C15-C16-C17 |
| 14  | G     | 812  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 806  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 828  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 837  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 825  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 838  | CLA  | C8-C10-C11-C12  |
| 18  | j     | 101  | LHG  | O6-C4-C5-C6     |
| 14  | H     | 817  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 818  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 813  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 822  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 840  | CLA  | C11-C10-C8-C7   |
| 14  | U     | 1002 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 820  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 838  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 809  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 833  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 835  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 808  | CLA  | C11-C10-C8-C7   |
| 14  | U     | 1004 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | Z     | 830  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 810  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 809  | CLA  | C12-C13-C15-C16 |
| 14  | H     | 803  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 837  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 809  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 813  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 813  | CLA  | C11-C10-C8-C7   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 806  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 801  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 801  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 821  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 805  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 803  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 812  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 821  | CLA  | C11-C10-C8-C7   |
| 14  | Q     | 201  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 833  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 820  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 833  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 829  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 803  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 842  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 814  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 830  | CLA  | C6-C7-C8-C10    |
| 14  | Z     | 816  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 809  | CLA  | C11-C12-C13-C15 |
| 15  | Y     | 844  | PQN  | C17-C18-C20-C21 |
| 14  | Z     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | h     | 205  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 825  | CLA  | C12-C13-C15-C16 |
| 15  | Z     | 840  | PQN  | C21-C22-C23-C25 |
| 14  | Z     | 824  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 806  | CLA  | C2C-C3C-CAC-CBC |
| 17  | Y     | 851  | BCR  | C9-C10-C11-C12  |
| 17  | J     | 104  | BCR  | C19-C20-C21-C22 |
| 17  | V     | 1202 | BCR  | C15-C16-C17-C18 |
| 17  | G     | 848  | BCR  | C9-C10-C11-C12  |
| 17  | Q     | 202  | BCR  | C19-C20-C21-C22 |
| 14  | A     | 825  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 801  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 821  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 842  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 834  | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 833  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 828  | CLA  | C13-C15-C16-C17 |
| 14  | H     | 828  | CLA  | C13-C15-C16-C17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 806  | CLA  | C2A-CAA-CBA-CGA |
| 17  | H     | 845  | BCR  | C11-C10-C9-C34  |
| 14  | G     | 833  | CLA  | C4C-C3C-CAC-CBC |
| 17  | G     | 848  | BCR  | C11-C10-C9-C34  |
| 17  | A     | 846  | BCR  | C16-C17-C18-C36 |
| 17  | F     | 201  | BCR  | C16-C17-C18-C36 |
| 17  | S     | 1104 | BCR  | C16-C17-C18-C36 |
| 14  | H     | 830  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 838  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 808  | CLA  | C16-C17-C18-C19 |
| 14  | H     | 821  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | Y     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 813  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 824  | CLA  | C4C-C3C-CAC-CBC |
| 18  | Y     | 853  | LHG  | C25-C26-C27-C28 |
| 14  | A     | 852  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 852  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 841  | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 813  | CLA  | CAD-CBD-CGD-O2D |
| 14  | U     | 1002 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 820  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 825  | CLA  | CAD-CBD-CGD-O2D |
| 13  | G     | 801  | CL0  | CAD-CBD-CGD-O2D |
| 14  | Z     | 812  | CLA  | CAD-CBD-CGD-O2D |
| 14  | L     | 202  | CLA  | CAD-CBD-CGD-O2D |
| 14  | Z     | 839  | CLA  | CAD-CBD-CGD-O2D |
| 14  | Y     | 807  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 840  | CLA  | CAD-CBD-CGD-O2D |
| 14  | Y     | 831  | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 827  | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 811  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | Z     | 806  | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 824  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Z     | 807  | CLA  | C13-C15-C16-C17 |
| 14  | H     | 822  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 822  | CLA  | C5-C6-C7-C8     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 802  | CLA  | C10-C11-C12-C13 |
| 14  | U     | 1004 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 207  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 822  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | H     | 826  | CLA  | C16-C17-C18-C20 |
| 14  | L     | 206  | CLA  | CBD-CGD-O2D-CED |
| 14  | Z     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 18  | H     | 847  | LHG  | C12-C13-C14-C15 |
| 18  | H     | 847  | LHG  | O6-C4-C5-O7     |
| 14  | Y     | 821  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | h     | 207  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 809  | CLA  | C2A-CAA-CBA-CGA |
| 17  | H     | 843  | BCR  | C14-C15-C16-C17 |
| 14  | H     | 801  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 817  | CLA  | C10-C11-C12-C13 |
| 14  | Q     | 201  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 820  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 831  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 824  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 824  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 802  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 825  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 825  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 838  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 838  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 815  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 825  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 825  | CLA  | CHA-CBD-CGD-O2D |
| 14  | U     | 1006 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 834  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 815  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 823  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 823  | CLA  | CHA-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 801 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 801 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 807 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 821 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 819 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 819 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 824 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 824 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 821 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 14  | d     | 201 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 833 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 822 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 822 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Q     | 203 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 854 | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 854 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 829 | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 102 | CLA  | CHA-CBD-CGD-O2D |
| 14  | K     | 103 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 827 | CLA  | CHA-CBD-CGD-O1D |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Z     | 827  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 825  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 825  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 812  | CLA  | C2C-C3C-CAC-CBC |
| 15  | A     | 843  | PQN  | C13-C15-C16-C17 |
| 14  | H     | 834  | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 851  | LHG  | O10-C23-O8-C6   |
| 14  | H     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 201  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 854  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 834  | CLA  | C4C-C3C-CAC-CBC |
| 14  | B     | 819  | CLA  | O1D-CGD-O2D-CED |
| 17  | f     | 105  | BCR  | C11-C10-C9-C8   |
| 17  | F     | 201  | BCR  | C16-C17-C18-C19 |
| 17  | Z     | 844  | BCR  | C20-C21-C22-C23 |
| 18  | G     | 851  | LHG  | O7-C5-C6-O8     |
| 14  | B     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 835  | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 830  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 841  | CLA  | C16-C17-C18-C19 |
| 14  | U     | 1006 | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 827  | CLA  | C2-C3-C5-C6     |
| 18  | G     | 852  | LHG  | C29-C30-C31-C32 |
| 14  | A     | 822  | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 834  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 804  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 810  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 809  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 808  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 820  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 840  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 821  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 836  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 825  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 824  | CLA  | C14-C13-C15-C16 |
| 14  | H     | 805  | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 808 | CLA  | C8-C10-C11-C12  |
| 14  | H     | 838 | CLA  | C8-C10-C11-C12  |
| 14  | h     | 206 | CLA  | C13-C15-C16-C17 |
| 14  | H     | 815 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 834 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 806 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 818 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 843 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 810 | CLA  | C8-C10-C11-C12  |
| 14  | f     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Q     | 201 | CLA  | O1A-CGA-O2A-C1  |
| 17  | Z     | 843 | BCR  | C11-C12-C13-C35 |
| 14  | Y     | 839 | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 806 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 814 | CLA  | C13-C15-C16-C17 |
| 15  | A     | 843 | PQN  | C15-C16-C17-C18 |
| 17  | Y     | 847 | BCR  | C21-C22-C23-C24 |
| 17  | Z     | 843 | BCR  | C11-C12-C13-C14 |
| 14  | B     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 802 | CLA  | C1A-C2A-CAA-CBA |
| 13  | G     | 801 | CL0  | C1A-C2A-CAA-CBA |
| 14  | J     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | h     | 207 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 14  | h     | 206 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 832 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 802 | CLA  | C8-C10-C11-C12  |
| 13  | G     | 801 | CL0  | C8-C10-C11-C12  |
| 14  | Z     | 830 | CLA  | C8-C10-C11-C12  |
| 14  | G     | 808 | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 818 | CLA  | C4C-C3C-CAC-CBC |
| 14  | B     | 817 | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 815 | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 827 | CLA  | C2-C1-O2A-CGA   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 835  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 17  | L     | 209  | BCR  | C19-C20-C21-C22 |
| 18  | j     | 101  | LHG  | C3-O3-P-O6      |
| 14  | G     | 816  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 850  | LHG  | C2-C3-O3-P      |
| 14  | G     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 18  | G     | 852  | LHG  | C3-O3-P-O5      |
| 18  | A     | 850  | LHG  | C4-O6-P-O5      |
| 18  | j     | 101  | LHG  | C4-O6-P-O5      |
| 18  | B     | 850  | LHG  | C3-O3-P-O5      |
| 14  | B     | 819  | CLA  | C11-C12-C13-C15 |
| 14  | S     | 1103 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 803  | CLA  | C16-C17-C18-C19 |
| 14  | G     | 833  | CLA  | C16-C17-C18-C20 |
| 18  | A     | 851  | LHG  | C7-C8-C9-C10    |
| 14  | B     | 838  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 840  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 18  | G     | 852  | LHG  | O6-C4-C5-C6     |
| 18  | A     | 851  | LHG  | O6-C4-C5-C6     |
| 19  | B     | 849  | LMG  | C18-C19-C20-C21 |
| 14  | G     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 835  | CLA  | C3-C5-C6-C7     |
| 15  | B     | 842  | PQN  | C13-C15-C16-C17 |
| 14  | B     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 828  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 827  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Y     | 825  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Z     | 804  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 837  | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 825  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Z     | 824  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Y     | 818  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 819  | CLA  | C13-C15-C16-C17 |
| 14  | Y     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 830  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 816  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 840  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 840  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 831  | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 827  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 808  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 841  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 838  | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 855  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | U     | 1002 | CLA  | C11-C10-C8-C7   |
| 14  | H     | 805  | CLA  | C11-C10-C8-C7   |
| 14  | Y     | 811  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 815  | CLA  | C12-C13-C15-C16 |
| 14  | Y     | 834  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 824  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 801  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 809  | CLA  | C11-C12-C13-C15 |
| 15  | G     | 844  | PQN  | C22-C23-C25-C26 |
| 14  | Y     | 832  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 832  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 827  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 832  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | Z     | 817  | CLA  | C11-C10-C8-C7   |
| 14  | Z     | 804  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 825  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 840  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 839  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 808  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 807  | CLA  | C6-C7-C8-C10    |
| 14  | H     | 816  | CLA  | C11-C12-C13-C15 |
| 14  | h     | 206  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 819  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | H     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 17  | G     | 854  | BCR  | C15-C16-C17-C18 |
| 17  | h     | 203  | BCR  | C19-C20-C21-C22 |
| 18  | A     | 850  | LHG  | C31-C32-C33-C34 |
| 14  | G     | 822  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 825  | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 835  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 803  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 835  | CLA  | C6-C7-C8-C9     |
| 13  | A     | 801  | CL0  | C16-C17-C18-C20 |
| 14  | L     | 201  | CLA  | C2C-C3C-CAC-CBC |
| 18  | H     | 847  | LHG  | C23-C24-C25-C26 |
| 19  | H     | 846  | LMG  | C10-C11-C12-C13 |
| 19  | Z     | 847  | LMG  | O1-C7-C8-C9     |
| 14  | G     | 819  | CLA  | C5-C6-C7-C8     |
| 14  | H     | 815  | CLA  | C5-C6-C7-C8     |
| 15  | B     | 842  | PQN  | C18-C20-C21-C22 |
| 14  | A     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 852  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 804  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 832  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 829  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 852  | CLA  | CBA-CGA-O2A-C1  |
| 14  | Y     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 808  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 804  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 822  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 827  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 830  | CLA  | C10-C11-C12-C13 |
| 14  | U     | 1002 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 820  | CLA  | C11-C10-C8-C9   |
| 14  | Z     | 815  | CLA  | C14-C13-C15-C16 |
| 14  | Y     | 820  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 820  | CLA  | C11-C10-C8-C9   |
| 14  | U     | 1006 | CLA  | C14-C13-C15-C16 |
| 14  | H     | 835  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 806  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 808  | CLA  | C11-C10-C8-C9   |
| 14  | U     | 1004 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 813  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 832  | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 821  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 830  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 825  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 803  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 842  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 854  | CLA  | C6-C7-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 803  | CLA  | C11-C10-C8-C9   |
| 14  | Z     | 816  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 828  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 826  | CLA  | C11-C12-C13-C14 |
| 15  | Y     | 844  | PQN  | C19-C18-C20-C21 |
| 14  | A     | 817  | CLA  | C11-C10-C8-C9   |
| 14  | Z     | 821  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | U     | 1006 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 17  | e     | 101  | BCR  | C18-C19-C20-C21 |
| 17  | J     | 103  | BCR  | C10-C11-C12-C13 |
| 17  | B     | 844  | BCR  | C18-C19-C20-C21 |
| 17  | R     | 101  | BCR  | C18-C19-C20-C21 |
| 17  | B     | 845  | BCR  | C10-C11-C12-C13 |
| 17  | Q     | 204  | BCR  | C10-C11-C12-C13 |
| 17  | U     | 1007 | BCR  | C10-C11-C12-C13 |
| 17  | T     | 102  | BCR  | C18-C19-C20-C21 |
| 17  | K     | 102  | BCR  | C18-C19-C20-C21 |
| 14  | B     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 821  | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 829  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 808  | CLA  | C16-C17-C18-C19 |
| 14  | f     | 102  | CLA  | C6-C7-C8-C9     |
| 18  | A     | 850  | LHG  | C27-C28-C29-C30 |
| 14  | U     | 1003 | CLA  | C2C-C3C-CAC-CBC |
| 14  | U     | 1006 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 809  | CLA  | C4-C3-C5-C6     |
| 14  | H     | 806  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 802  | CLA  | CAA-CBA-CGA-O2A |
| 18  | G     | 851  | LHG  | O8-C23-C24-C25  |
| 14  | B     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 823  | CLA  | C6-C7-C8-C10    |
| 14  | f     | 102  | CLA  | C6-C7-C8-C10    |
| 14  | U     | 1004 | CLA  | C2C-C3C-CAC-CBC |
| 14  | h     | 205  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 830  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 809  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 810  | CLA  | C2-C1-O2A-CGA   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 830  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 841  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 831  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 820  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 811  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 822  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 811  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 835  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 824  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 830  | CLA  | C2C-C3C-CAC-CBC |
| 18  | A     | 850  | LHG  | C23-C24-C25-C26 |
| 14  | A     | 824  | CLA  | CBD-CGD-O2D-CED |
| 18  | Y     | 852  | LHG  | O8-C23-C24-C25  |
| 18  | A     | 850  | LHG  | O8-C23-C24-C25  |
| 14  | G     | 829  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 838  | CLA  | C8-C10-C11-C12  |
| 18  | Y     | 852  | LHG  | O6-C4-C5-O7     |
| 18  | j     | 101  | LHG  | O6-C4-C5-O7     |
| 14  | Z     | 804  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 830  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 804  | CLA  | C2C-C3C-CAC-CBC |
| 17  | f     | 103  | BCR  | C5-C6-C7-C8     |
| 14  | L     | 207  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 832  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 824  | CLA  | C10-C11-C12-C13 |
| 18  | Y     | 852  | LHG  | C34-C35-C36-C37 |
| 14  | A     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | H     | 808  | CLA  | C16-C17-C18-C19 |
| 19  | H     | 846  | LMG  | C40-C41-C42-C43 |
| 14  | A     | 806  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 817  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 850  | LHG  | O7-C5-C6-O8     |
| 18  | Y     | 852  | LHG  | C3-O3-P-O6      |
| 18  | A     | 850  | LHG  | C3-O3-P-O6      |
| 18  | A     | 851  | LHG  | C3-O3-P-O6      |
| 18  | H     | 847  | LHG  | C3-O3-P-O6      |
| 18  | G     | 851  | LHG  | C3-O3-P-O6      |
| 13  | A     | 801  | CL0  | C16-C17-C18-C19 |
| 14  | Y     | 835  | CLA  | C2C-C3C-CAC-CBC |
| 14  | U     | 1002 | CLA  | C4-C3-C5-C6     |
| 14  | U     | 1004 | CLA  | C4-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 814  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 825  | CLA  | C12-C13-C15-C16 |
| 14  | H     | 805  | CLA  | C11-C12-C13-C15 |
| 14  | U     | 1006 | CLA  | C12-C13-C15-C16 |
| 14  | L     | 207  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 808  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 807  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 802  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 841  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 838  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 813  | CLA  | C11-C10-C8-C9   |
| 14  | Y     | 809  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 825  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 809  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 832  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 832  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 830  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 807  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 826  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 809  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 816  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 832  | CLA  | C8-C10-C11-C12  |
| 17  | Y     | 846  | BCR  | C15-C16-C17-C18 |
| 17  | A     | 848  | BCR  | C15-C16-C17-C18 |
| 14  | H     | 802  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 15  | H     | 839  | PQN  | C18-C20-C21-C22 |
| 14  | h     | 207  | CLA  | C15-C16-C17-C18 |
| 13  | A     | 801  | CL0  | C5-C6-C7-C8     |
| 14  | H     | 809  | CLA  | C2A-CAA-CBA-CGA |
| 17  | R     | 102  | BCR  | C7-C8-C9-C34    |
| 14  | H     | 816  | CLA  | C15-C16-C17-C18 |
| 14  | H     | 830  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 818  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 838  | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | L     | 207  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 835  | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 806  | CLA  | C4-C3-C5-C6     |
| 14  | f     | 102  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | H     | 806  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 826  | CLA  | C2-C3-C5-C6     |
| 18  | A     | 850  | LHG  | C9-C10-C11-C12  |
| 14  | U     | 1002 | CLA  | C16-C17-C18-C19 |
| 14  | Y     | 809  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 814  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | H     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | S     | 1103 | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 820  | CLA  | C10-C11-C12-C13 |
| 14  | S     | 1101 | CLA  | C15-C16-C17-C18 |
| 17  | A     | 847  | BCR  | C19-C20-C21-C22 |
| 17  | A     | 849  | BCR  | C19-C20-C21-C22 |
| 17  | Z     | 846  | BCR  | C9-C10-C11-C12  |
| 17  | Y     | 847  | BCR  | C19-C20-C21-C22 |
| 17  | Y     | 849  | BCR  | C19-C20-C21-C22 |
| 14  | H     | 813  | CLA  | C2C-C3C-CAC-CBC |
| 13  | G     | 801  | CL0  | CAA-CBA-CGA-O2A |
| 14  | G     | 826  | CLA  | C8-C10-C11-C12  |
| 18  | G     | 851  | LHG  | O6-C4-C5-O7     |
| 17  | Q     | 202  | BCR  | C18-C19-C20-C21 |
| 17  | Y     | 849  | BCR  | C18-C19-C20-C21 |
| 14  | U     | 1006 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 825  | CLA  | C3-C5-C6-C7     |
| 18  | Y     | 852  | LHG  | C11-C12-C13-C14 |
| 14  | B     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 825  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 806  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 825  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 14  | Y     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 205  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 802  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 805  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 839  | CLA  | C4C-C3C-CAC-CBC |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 813  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 837  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 838  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 830  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 834  | CLA  | C2-C1-O2A-CGA   |
| 13  | A     | 801  | CL0  | C2-C1-O2A-CGA   |
| 14  | Y     | 817  | CLA  | C2-C1-O2A-CGA   |
| 14  | H     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 830  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 801  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 816  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | T     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 812  | CLA  | C16-C17-C18-C19 |
| 14  | Z     | 806  | CLA  | C16-C17-C18-C19 |
| 14  | H     | 802  | CLA  | CAA-CBA-CGA-O2A |
| 17  | L     | 203  | BCR  | C9-C10-C11-C12  |
| 17  | S     | 1104 | BCR  | C15-C16-C17-C18 |
| 17  | Q     | 202  | BCR  | C9-C10-C11-C12  |
| 14  | G     | 817  | CLA  | C8-C10-C11-C12  |
| 15  | B     | 842  | PQN  | C14-C13-C15-C16 |
| 14  | U     | 1004 | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 827  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 852  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 841  | CLA  | C11-C12-C13-C14 |
| 14  | U     | 1003 | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 808  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 808  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 812  | CLA  | C11-C12-C13-C14 |
| 15  | G     | 844  | PQN  | C16-C17-C18-C19 |
| 14  | A     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | H     | 801  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 804  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 812  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 823  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 828  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 802  | CLA  | C6-C7-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 808  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 809  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 802  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 808  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 829  | CLA  | C15-C16-C17-C18 |
| 14  | H     | 827  | CLA  | C15-C16-C17-C18 |
| 17  | d     | 203  | BCR  | C35-C13-C14-C15 |
| 17  | H     | 842  | BCR  | C20-C21-C22-C37 |
| 17  | Y     | 851  | BCR  | C11-C10-C9-C34  |
| 17  | Y     | 851  | BCR  | C16-C17-C18-C36 |
| 17  | A     | 849  | BCR  | C16-C17-C18-C36 |
| 17  | B     | 845  | BCR  | C20-C21-C22-C37 |
| 17  | G     | 850  | BCR  | C16-C17-C18-C36 |
| 17  | Q     | 204  | BCR  | C35-C13-C14-C15 |
| 17  | F     | 203  | BCR  | C35-C13-C14-C15 |
| 17  | Z     | 843  | BCR  | C20-C21-C22-C37 |
| 17  | Q     | 202  | BCR  | C16-C17-C18-C36 |
| 18  | G     | 851  | LHG  | C4-C5-C6-O8     |
| 17  | Z     | 844  | BCR  | C20-C21-C22-C37 |
| 14  | B     | 812  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 803  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | Z     | 808  | CLA  | C16-C17-C18-C20 |
| 14  | H     | 803  | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 841  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 801  | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 824  | CLA  | O2A-C1-C2-C3    |
| 14  | Y     | 819  | CLA  | C5-C6-C7-C8     |
| 17  | U     | 1005 | BCR  | C11-C12-C13-C35 |
| 17  | A     | 849  | BCR  | C11-C12-C13-C35 |
| 14  | A     | 835  | CLA  | CBD-CGD-O2D-CED |
| 17  | Q     | 202  | BCR  | C17-C18-C19-C20 |
| 14  | A     | 825  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 801  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | T     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 815  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 813  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 812  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 805  | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | G     | 853 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 102 | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 13  | Y     | 801 | CL0  | CAA-CBA-CGA-O2A |
| 14  | H     | 813 | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 830 | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 825 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 829 | CLA  | C6-C7-C8-C10    |
| 14  | Z     | 801 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 811 | CLA  | C12-C13-C15-C16 |
| 14  | h     | 201 | CLA  | C11-C12-C13-C15 |
| 14  | L     | 202 | CLA  | C6-C7-C8-C10    |
| 15  | B     | 842 | PQN  | C17-C18-C20-C21 |
| 14  | Z     | 802 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 823 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 818 | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 825 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 14  | Z     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 14  | H     | 812 | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 819 | CLA  | C13-C15-C16-C17 |
| 19  | H     | 846 | LMG  | C30-C31-C32-C33 |
| 14  | Y     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 808 | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 801 | CLA  | C15-C16-C17-C18 |
| 14  | Y     | 842 | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 14  | Q     | 201 | CLA  | CBA-CGA-O2A-C1  |
| 18  | Y     | 852 | LHG  | O6-C4-C5-C6     |
| 14  | A     | 826 | CLA  | C11-C12-C13-C15 |
| 14  | Y     | 803 | CLA  | C2C-C3C-CAC-CBC |
| 14  | Z     | 801 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 834 | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 826 | CLA  | C4-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | L     | 201  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Z     | 824  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 827  | CLA  | C2-C3-C5-C6     |
| 15  | B     | 842  | PQN  | C12-C13-C15-C16 |
| 14  | H     | 805  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 828  | CLA  | C16-C17-C18-C20 |
| 17  | d     | 203  | BCR  | C12-C13-C14-C15 |
| 17  | d     | 203  | BCR  | C16-C17-C18-C19 |
| 17  | H     | 842  | BCR  | C20-C21-C22-C23 |
| 17  | Y     | 851  | BCR  | C11-C10-C9-C8   |
| 17  | Y     | 851  | BCR  | C16-C17-C18-C19 |
| 17  | A     | 849  | BCR  | C16-C17-C18-C19 |
| 17  | L     | 203  | BCR  | C20-C21-C22-C23 |
| 17  | Z     | 841  | BCR  | C16-C17-C18-C19 |
| 17  | B     | 845  | BCR  | C20-C21-C22-C23 |
| 17  | G     | 850  | BCR  | C16-C17-C18-C19 |
| 17  | Q     | 204  | BCR  | C12-C13-C14-C15 |
| 17  | F     | 203  | BCR  | C12-C13-C14-C15 |
| 17  | U     | 1007 | BCR  | C20-C21-C22-C23 |
| 17  | Z     | 843  | BCR  | C20-C21-C22-C23 |
| 14  | H     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 206  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 827  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 826  | CLA  | C2C-C3C-CAC-CBC |
| 14  | h     | 206  | CLA  | C8-C10-C11-C12  |
| 18  | Y     | 852  | LHG  | C17-C18-C19-C20 |
| 14  | B     | 803  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 806  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 834  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 829  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 827  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 838  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 808  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 809  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 806  | CLA  | C2-C3-C5-C6     |
| 14  | U     | 1004 | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 802  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 809  | CLA  | C2-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 18  | j     | 101  | LHG  | C7-C8-C9-C10    |
| 14  | Z     | 808  | CLA  | C6-C7-C8-C9     |
| 14  | Y     | 855  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 825  | CLA  | C6-C7-C8-C9     |
| 14  | S     | 1101 | CLA  | C11-C10-C8-C9   |
| 14  | Z     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 18  | G     | 852  | LHG  | O8-C23-C24-C25  |
| 14  | H     | 813  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 841  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 824  | CLA  | C2A-CAA-CBA-CGA |
| 15  | Z     | 840  | PQN  | C26-C27-C28-C30 |
| 18  | A     | 850  | LHG  | C11-C12-C13-C14 |
| 17  | B     | 851  | BCR  | C1-C6-C7-C8     |
| 17  | Y     | 856  | BCR  | C23-C24-C25-C26 |
| 17  | Q     | 202  | BCR  | C1-C6-C7-C8     |
| 17  | I     | 101  | BCR  | C5-C6-C7-C8     |
| 17  | R     | 102  | BCR  | C23-C24-C25-C26 |
| 14  | Y     | 832  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 843  | CLA  | CAA-CBA-CGA-O2A |
| 19  | H     | 846  | LMG  | C32-C33-C34-C35 |
| 18  | G     | 852  | LHG  | C28-C29-C30-C31 |
| 17  | G     | 849  | BCR  | C15-C16-C17-C18 |
| 14  | Z     | 831  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 819  | CLA  | C4-C3-C5-C6     |
| 15  | G     | 844  | PQN  | C14-C13-C15-C16 |
| 14  | G     | 808  | CLA  | C4-C3-C5-C6     |
| 14  | L     | 202  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 808  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 818  | CLA  | C4-C3-C5-C6     |
| 17  | e     | 101  | BCR  | C21-C22-C23-C24 |
| 14  | A     | 837  | CLA  | C15-C16-C17-C18 |
| 14  | U     | 1002 | CLA  | C2-C3-C5-C6     |
| 14  | S     | 1101 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 841  | CLA  | CAA-CBA-CGA-O2A |
| 14  | J     | 102  | CLA  | C3-C5-C6-C7     |
| 14  | H     | 827  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 841  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 833  | CLA  | C6-C7-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 811 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 819 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 837 | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 842 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 812 | CLA  | C3-C5-C6-C7     |
| 14  | H     | 806 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 827 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 827 | CLA  | C8-C10-C11-C12  |
| 18  | G     | 851 | LHG  | O6-C4-C5-C6     |
| 19  | B     | 849 | LMG  | C28-C29-C30-C31 |
| 14  | G     | 824 | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 830 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 813 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 815 | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 834 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 810 | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 814 | CLA  | C4-C3-C5-C6     |
| 14  | H     | 822 | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 823 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 811 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 825 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 806 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 810 | CLA  | C6-C7-C8-C10    |
| 14  | H     | 826 | CLA  | C11-C12-C13-C15 |
| 14  | f     | 102 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 817 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 832 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 809 | CLA  | C15-C16-C17-C18 |
| 14  | G     | 808 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 19  | H     | 846 | LMG  | C33-C34-C35-C36 |
| 14  | G     | 841 | CLA  | CAA-CBA-CGA-O1A |
| 18  | G     | 851 | LHG  | O7-C7-C8-C9     |
| 14  | Z     | 839 | CLA  | C16-C17-C18-C20 |
| 18  | j     | 101 | LHG  | C24-C23-O8-C6   |
| 14  | Y     | 828 | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 811 | CLA  | C15-C16-C17-C18 |
| 14  | H     | 827 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 818 | CLA  | C13-C15-C16-C17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Y     | 853  | LHG  | O8-C23-C24-C25  |
| 14  | U     | 1003 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 807  | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 805  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 825  | CLA  | C4C-C3C-CAC-CBC |
| 17  | Y     | 848  | BCR  | C16-C17-C18-C36 |
| 17  | L     | 203  | BCR  | C20-C21-C22-C37 |
| 17  | U     | 1007 | BCR  | C20-C21-C22-C37 |
| 17  | h     | 203  | BCR  | C20-C21-C22-C37 |
| 17  | Y     | 849  | BCR  | C20-C21-C22-C37 |
| 14  | A     | 816  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 825  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 805  | CLA  | C4-C3-C5-C6     |
| 14  | H     | 807  | CLA  | C4-C3-C5-C6     |
| 14  | U     | 1006 | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 807  | CLA  | C4-C3-C5-C6     |
| 14  | H     | 809  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 804  | CLA  | C4-C3-C5-C6     |
| 14  | Z     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 802  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 801  | CLA  | C2-C3-C5-C6     |
| 15  | G     | 844  | PQN  | C12-C13-C15-C16 |
| 14  | L     | 202  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | Z     | 826  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 835  | CLA  | CAA-CBA-CGA-O2A |
| 19  | B     | 849  | LMG  | O7-C10-C11-C12  |
| 14  | Z     | 808  | CLA  | C11-C10-C8-C9   |
| 14  | H     | 813  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 801  | CLA  | C11-C12-C13-C14 |
| 15  | G     | 844  | PQN  | C24-C23-C25-C26 |
| 14  | G     | 832  | CLA  | C6-C7-C8-C9     |
| 14  | h     | 201  | CLA  | C11-C12-C13-C14 |
| 14  | h     | 207  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 803  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 802  | CLA  | C11-C12-C13-C14 |
| 14  | Y     | 854  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 808  | CLA  | C11-C10-C8-C9   |
| 14  | h     | 205  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 804  | CLA  | C3-C5-C6-C7     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 837 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Y     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 802 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 14  | f     | 102 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 831 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 807 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 812 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 829 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 843 | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 813 | CLA  | CBD-CGD-O2D-CED |
| 14  | Y     | 810 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 826 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 802 | CLA  | CAD-CBD-CGD-O2D |
| 14  | H     | 804 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 834 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 836 | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 836 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 807 | CLA  | CAD-CBD-CGD-O2D |
| 14  | Y     | 820 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 815 | CLA  | CAD-CBD-CGD-O2D |
| 14  | j     | 102 | CLA  | CAD-CBD-CGD-O2D |
| 14  | J     | 101 | CLA  | CAD-CBD-CGD-O2D |
| 14  | Z     | 828 | CLA  | CAD-CBD-CGD-O2D |
| 14  | Y     | 837 | CLA  | CAD-CBD-CGD-O2D |
| 14  | Z     | 811 | CLA  | CAD-CBD-CGD-O2D |
| 14  | Z     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 13  | Y     | 801 | CL0  | CAD-CBD-CGD-O2D |
| 14  | B     | 833 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 817 | CLA  | C11-C12-C13-C14 |
| 17  | J     | 104 | BCR  | C15-C16-C17-C18 |
| 14  | A     | 818 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 803 | CLA  | C4C-C3C-CAC-CBC |
| 14  | B     | 838 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 839 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 816 | CLA  | CAA-CBA-CGA-O2A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | Y     | 833  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 812  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 14  | L     | 207  | CLA  | CAA-CBA-CGA-O1A |
| 14  | h     | 206  | CLA  | O1D-CGD-O2D-CED |
| 13  | G     | 801  | CL0  | C15-C16-C17-C18 |
| 14  | A     | 826  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 835  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 833  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | S     | 1101 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 823  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 822  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 825  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 816  | CLA  | C6-C7-C8-C9     |
| 14  | L     | 207  | CLA  | C4C-C3C-CAC-CBC |
| 19  | Z     | 847  | LMG  | O6-C1-O1-C7     |
| 14  | Z     | 801  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 814  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 829  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 834  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 808  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 811  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 802  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 14  | S     | 1103 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 808  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 17  | J     | 103  | BCR  | C11-C12-C13-C14 |
| 17  | G     | 849  | BCR  | C7-C8-C9-C10    |
| 17  | A     | 849  | BCR  | C11-C12-C13-C14 |
| 17  | i     | 101  | BCR  | C17-C18-C19-C20 |
| 17  | S     | 1104 | BCR  | C11-C12-C13-C14 |
| 17  | S     | 1104 | BCR  | C21-C22-C23-C24 |
| 14  | W     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 18  | Y     | 852  | LHG  | C29-C30-C31-C32 |
| 18  | Y     | 853  | LHG  | O6-C4-C5-O7     |
| 18  | B     | 850  | LHG  | O6-C4-C5-O7     |
| 14  | Z     | 806  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 815  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 823  | CLA  | CAA-CBA-CGA-O2A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 805  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 822  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 852  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 820  | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 810  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 825  | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 850  | LHG  | O7-C7-C8-C9     |
| 14  | U     | 1004 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | H     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | H     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 810  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 810  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 827  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 818  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 818  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 802  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 855  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 855  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 812  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 812  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 807  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 811  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 811  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 812  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Y     | 812  | CLA  | CHA-CBD-CGD-O2D |
| 14  | S     | 1102 | CLA  | CHA-CBD-CGD-O1D |
| 14  | S     | 1102 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 802  | CLA  | CHA-CBD-CGD-O2D |
| 14  | U     | 1006 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 832  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 832  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 833  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 833  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 841  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 841  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 824  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 804  | CLA  | CHA-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 804  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 827  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 827  | CLA  | CHA-CBD-CGD-O2D |
| 14  | L     | 206  | CLA  | CHA-CBD-CGD-O1D |
| 14  | L     | 206  | CLA  | CHA-CBD-CGD-O2D |
| 14  | S     | 1103 | CLA  | CHA-CBD-CGD-O1D |
| 14  | T     | 103  | CLA  | CHA-CBD-CGD-O1D |
| 14  | T     | 103  | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 809  | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 809  | CLA  | CHA-CBD-CGD-O2D |
| 14  | J     | 101  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 813  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 813  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 806  | CLA  | CHA-CBD-CGD-O2D |
| 14  | Y     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 830  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 842  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 842  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 802  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 802  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 839  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 839  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 820  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 835  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 835  | CLA  | CHA-CBD-CGD-O2D |
| 14  | d     | 201  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 814  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 814  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 803  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 830  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 838  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 838  | CLA  | CHA-CBD-CGD-O2D |
| 14  | V     | 1201 | CLA  | CHA-CBD-CGD-O1D |
| 14  | V     | 1201 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 821  | CLA  | CHA-CBD-CGD-O1D |
| 14  | Z     | 821  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 816  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 821  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 821  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 808  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 808  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 823  | CLA  | CHA-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 14  | Z     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 819 | CLA  | CHA-CBD-CGD-O1D |
| 14  | H     | 819 | CLA  | CHA-CBD-CGD-O2D |
| 14  | f     | 101 | CLA  | CHA-CBD-CGD-O1D |
| 14  | f     | 101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 843 | CLA  | CHA-CBD-CGD-O2D |
| 14  | H     | 835 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 806 | CLA  | C4-C3-C5-C6     |
| 13  | A     | 801 | CL0  | C4-C3-C5-C6     |
| 14  | Z     | 807 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 814 | CLA  | C4C-C3C-CAC-CBC |
| 14  | B     | 821 | CLA  | C2C-C3C-CAC-CBC |
| 17  | h     | 203 | BCR  | C20-C21-C22-C23 |
| 14  | Z     | 803 | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 827 | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 828 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 805 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 819 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 807 | CLA  | CAA-CBA-CGA-O2A |
| 18  | j     | 101 | LHG  | O10-C23-O8-C6   |
| 14  | Y     | 835 | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 811 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 837 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 809 | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 814 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 840 | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 821 | CLA  | C13-C15-C16-C17 |
| 14  | G     | 816 | CLA  | C4C-C3C-CAC-CBC |
| 14  | L     | 205 | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 822 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 855 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 838 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 814 | CLA  | CAA-CBA-CGA-O2A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 832  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 813  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 824  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 839  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 837  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 808  | CLA  | C11-C10-C8-C7   |
| 14  | H     | 809  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 841  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 830  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 811  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 823  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 823  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 828  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 826  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 802  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 818  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 842  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 833  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 825  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 813  | CLA  | C11-C10-C8-C9   |
| 14  | U     | 1002 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | H     | 808  | CLA  | C11-C10-C8-C9   |
| 14  | Z     | 830  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 817  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 825  | CLA  | C14-C13-C15-C16 |
| 15  | B     | 842  | PQN  | C19-C18-C20-C21 |
| 14  | A     | 819  | CLA  | C11-C12-C13-C14 |
| 14  | Z     | 802  | CLA  | C11-C10-C8-C9   |
| 14  | H     | 826  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 805  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 819  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 823  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 825  | CLA  | CAA-CBA-CGA-O1A |
| 13  | A     | 801  | CL0  | CAA-CBA-CGA-O1A |
| 14  | Y     | 809  | CLA  | C16-C17-C18-C19 |
| 14  | G     | 802  | CLA  | C16-C17-C18-C20 |
| 19  | B     | 849  | LMG  | C31-C32-C33-C34 |
| 14  | A     | 807  | CLA  | C2A-CAA-CBA-CGA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 828  | CLA  | C2A-CAA-CBA-CGA |
| 18  | Y     | 853  | LHG  | O10-C23-C24-C25 |
| 14  | G     | 805  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 817  | CLA  | C11-C12-C13-C15 |
| 14  | U     | 1002 | CLA  | C16-C17-C18-C20 |
| 14  | Y     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 825  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 817  | CLA  | C11-C12-C13-C15 |
| 19  | B     | 849  | LMG  | C30-C31-C32-C33 |
| 14  | A     | 805  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 817  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 820  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 839  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 812  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 829  | CLA  | CAA-CBA-CGA-O1A |
| 17  | B     | 847  | BCR  | C21-C22-C23-C24 |
| 17  | Q     | 204  | BCR  | C21-C22-C23-C24 |
| 14  | Z     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | U     | 1006 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 801  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Y     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 812  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 824  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 822  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 802  | CLA  | C1A-C2A-CAA-CBA |
| 14  | Z     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 839  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 811  | CLA  | C1A-C2A-CAA-CBA |
| 14  | f     | 102  | CLA  | C1A-C2A-CAA-CBA |
| 14  | K     | 103  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 822  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 813  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 838  | CLA  | CAA-CBA-CGA-O1A |
| 19  | B     | 849  | LMG  | O9-C10-C11-C12  |
| 18  | G     | 851  | LHG  | O9-C7-C8-C9     |
| 14  | Y     | 822  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 827  | CLA  | O1A-CGA-O2A-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 808  | CLA  | C2-C1-O2A-CGA   |
| 14  | Y     | 837  | CLA  | C2-C1-O2A-CGA   |
| 14  | Z     | 803  | CLA  | C4C-C3C-CAC-CBC |
| 14  | G     | 825  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 831  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 833  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Z     | 806  | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 812  | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 850  | LHG  | O9-C7-C8-C9     |
| 14  | B     | 808  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 818  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 813  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 836  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 818  | CLA  | C4C-C3C-CAC-CBC |
| 14  | Y     | 855  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 807  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 814  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 811  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 832  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 816  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Z     | 820  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 807  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 803  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 818  | CLA  | C2-C3-C5-C6     |
| 17  | L     | 203  | BCR  | C14-C15-C16-C17 |
| 14  | A     | 825  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 831  | CLA  | C2C-C3C-CAC-CBC |
| 18  | Y     | 852  | LHG  | C3-O3-P-O5      |
| 18  | j     | 101  | LHG  | C3-O3-P-O5      |
| 18  | G     | 851  | LHG  | C3-O3-P-O5      |
| 14  | Z     | 825  | CLA  | C16-C17-C18-C20 |
| 14  | Z     | 808  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 825  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Z     | 809  | CLA  | CAA-CBA-CGA-O1A |
| 14  | h     | 201  | CLA  | C15-C16-C17-C18 |
| 17  | U     | 1005 | BCR  | C23-C24-C25-C26 |
| 17  | U     | 1005 | BCR  | C23-C24-C25-C30 |
| 17  | h     | 202  | BCR  | C23-C24-C25-C30 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | Y     | 848  | BCR  | C1-C6-C7-C8     |
| 17  | A     | 846  | BCR  | C5-C6-C7-C8     |
| 17  | i     | 101  | BCR  | C5-C6-C7-C8     |
| 17  | Y     | 849  | BCR  | C1-C6-C7-C8     |
| 14  | U     | 1003 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 823  | CLA  | C8-C10-C11-C12  |
| 19  | Z     | 847  | LMG  | C28-C29-C30-C31 |
| 14  | A     | 807  | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 835  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 806  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 821  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 837  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 816  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 811  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 819  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 813  | CLA  | C5-C6-C7-C8     |
| 14  | Z     | 802  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 818  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 811  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 810  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 813  | CLA  | C2C-C3C-CAC-CBC |
| 14  | Y     | 804  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 801  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 827  | CLA  | C16-C17-C18-C20 |
| 18  | B     | 850  | LHG  | C14-C15-C16-C17 |
| 19  | B     | 849  | LMG  | C36-C37-C38-C39 |
| 14  | G     | 839  | CLA  | C3-C5-C6-C7     |
| 14  | Y     | 840  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 836  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Y     | 811  | CLA  | CAD-CBD-CGD-O1D |
| 14  | S     | 1102 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 816  | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 827  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 810  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Z     | 834  | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 801  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 827  | CLA  | CAD-CBD-CGD-O1D |
| 14  | H     | 812  | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 825  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Y     | 816  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Y     | 813  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 830  | CLA  | CAD-CBD-CGD-O1D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | H     | 834  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 815  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 806  | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 831  | CLA  | CAD-CBD-CGD-O1D |
| 14  | Y     | 819  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 813  | CLA  | CAD-CBD-CGD-O1D |
| 14  | S     | 1103 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 837  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 815  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 814  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 838  | CLA  | C6-C7-C8-C9     |
| 14  | L     | 207  | CLA  | C14-C13-C15-C16 |
| 14  | Z     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | H     | 827  | CLA  | C6-C7-C8-C9     |
| 14  | Z     | 806  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 841  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 824  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 808  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 806  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 822  | CLA  | C6-C7-C8-C9     |
| 14  | H     | 835  | CLA  | C5-C6-C7-C8     |
| 14  | Y     | 855  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 826  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 822  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 821  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 806  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 804  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 805  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Z     | 839  | CLA  | CAA-CBA-CGA-O2A |
| 14  | L     | 206  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 829  | CLA  | C5-C6-C7-C8     |
| 19  | H     | 846  | LMG  | C28-C29-C30-C31 |
| 14  | G     | 813  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 836  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 809  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 808  | CLA  | C4-C3-C5-C6     |
| 14  | Y     | 854  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 802  | CLA  | C8-C10-C11-C12  |
| 14  | Y     | 827  | CLA  | C12-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | U     | 1002 | CLA  | C12-C13-C15-C16 |
| 14  | H     | 815  | CLA  | C2-C3-C5-C6     |
| 14  | Y     | 820  | CLA  | C11-C10-C8-C7   |
| 14  | L     | 207  | CLA  | C6-C7-C8-C10    |
| 14  | Y     | 808  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 827  | CLA  | C6-C7-C8-C10    |
| 14  | Z     | 830  | CLA  | C2-C3-C5-C6     |
| 14  | H     | 803  | CLA  | C11-C10-C8-C7   |
| 15  | G     | 844  | PQN  | C16-C17-C18-C20 |
| 14  | Z     | 806  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 806  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 805  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | H     | 812  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 842  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 825  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 824  | CLA  | C6-C7-C8-C10    |
| 14  | L     | 202  | CLA  | C11-C10-C8-C7   |
| 14  | Z     | 825  | CLA  | C11-C12-C13-C15 |
| 14  | Z     | 823  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 828  | CLA  | C12-C13-C15-C16 |
| 14  | Z     | 802  | CLA  | C6-C7-C8-C10    |
| 14  | Z     | 821  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 830  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 821  | CLA  | C3A-C2A-CAA-CBA |
| 14  | Z     | 836  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 838  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 805  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 820  | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 843  | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 19  | Z     | 847  | LMG  | O7-C10-C11-C12  |
| 14  | H     | 808  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 830  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 822  | CLA  | CAA-CBA-CGA-O2A |
| 14  | Y     | 828  | CLA  | CAA-CBA-CGA-O2A |
| 15  | H     | 839  | PQN  | C13-C15-C16-C17 |
| 17  | U     | 1005 | BCR  | C21-C22-C23-C24 |
| 17  | e     | 101  | BCR  | C11-C12-C13-C14 |
| 17  | R     | 101  | BCR  | C7-C8-C9-C10    |
| 17  | L     | 208  | BCR  | C21-C22-C23-C24 |
| 17  | H     | 843  | BCR  | C17-C18-C19-C20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | R     | 102 | BCR  | C21-C22-C23-C24 |
| 14  | G     | 824 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Z     | 817 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Z     | 839 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 809 | CLA  | C2C-C3C-CAC-CBC |
| 19  | B     | 849 | LMG  | C13-C14-C15-C16 |
| 14  | G     | 824 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 840 | CLA  | C10-C11-C12-C13 |
| 14  | Z     | 804 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 822 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 826 | CLA  | CAA-CBA-CGA-O1A |
| 14  | Y     | 828 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 809 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 824 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 831 | CLA  | CAA-CBA-CGA-O2A |
| 14  | d     | 202 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 835 | CLA  | C2A-CAA-CBA-CGA |
| 14  | H     | 826 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 811 | CLA  | CAA-CBA-CGA-O1A |
| 14  | H     | 821 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 811 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Z     | 823 | CLA  | C2A-CAA-CBA-CGA |
| 14  | Y     | 838 | CLA  | C15-C16-C17-C18 |
| 14  | Z     | 816 | CLA  | C5-C6-C7-C8     |
| 19  | B     | 849 | LMG  | C42-C43-C44-C45 |
| 14  | H     | 807 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 821 | CLA  | CAA-CBA-CGA-O1A |

There are no ring outliers.

349 monomers are involved in 1963 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | B     | 811 | CLA  | 3       | 0            |
| 14  | B     | 817 | CLA  | 7       | 0            |
| 14  | B     | 833 | CLA  | 7       | 0            |
| 14  | H     | 820 | CLA  | 4       | 0            |
| 14  | Y     | 810 | CLA  | 5       | 0            |
| 14  | Y     | 827 | CLA  | 8       | 0            |
| 14  | A     | 852 | CLA  | 14      | 0            |
| 14  | A     | 826 | CLA  | 12      | 0            |
| 14  | Y     | 835 | CLA  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18  | Y     | 852  | LHG  | 4       | 0            |
| 14  | Z     | 808  | CLA  | 11      | 0            |
| 14  | B     | 841  | CLA  | 5       | 0            |
| 17  | M     | 101  | BCR  | 6       | 0            |
| 14  | H     | 817  | CLA  | 8       | 0            |
| 14  | H     | 818  | CLA  | 7       | 0            |
| 14  | H     | 831  | CLA  | 7       | 0            |
| 17  | U     | 1005 | BCR  | 3       | 0            |
| 14  | A     | 832  | CLA  | 7       | 0            |
| 17  | G     | 846  | BCR  | 6       | 0            |
| 14  | G     | 824  | CLA  | 11      | 0            |
| 14  | B     | 802  | CLA  | 6       | 0            |
| 14  | Z     | 831  | CLA  | 7       | 0            |
| 14  | B     | 838  | CLA  | 6       | 0            |
| 14  | H     | 804  | CLA  | 4       | 0            |
| 14  | Y     | 855  | CLA  | 18      | 0            |
| 14  | G     | 839  | CLA  | 10      | 0            |
| 14  | H     | 813  | CLA  | 5       | 0            |
| 14  | A     | 822  | CLA  | 7       | 0            |
| 14  | H     | 837  | CLA  | 4       | 0            |
| 14  | L     | 205  | CLA  | 8       | 0            |
| 14  | F     | 202  | CLA  | 1       | 0            |
| 14  | Y     | 830  | CLA  | 15      | 0            |
| 14  | Y     | 825  | CLA  | 9       | 0            |
| 14  | Y     | 809  | CLA  | 4       | 0            |
| 14  | A     | 840  | CLA  | 16      | 0            |
| 14  | G     | 813  | CLA  | 11      | 0            |
| 14  | Y     | 840  | CLA  | 6       | 0            |
| 14  | B     | 837  | CLA  | 9       | 0            |
| 14  | U     | 1003 | CLA  | 6       | 0            |
| 17  | H     | 845  | BCR  | 9       | 0            |
| 14  | B     | 834  | CLA  | 7       | 0            |
| 18  | G     | 852  | LHG  | 5       | 0            |
| 14  | A     | 836  | CLA  | 8       | 0            |
| 17  | J     | 103  | BCR  | 11      | 0            |
| 14  | U     | 1002 | CLA  | 8       | 0            |
| 14  | A     | 812  | CLA  | 9       | 0            |
| 17  | A     | 847  | BCR  | 3       | 0            |
| 17  | G     | 854  | BCR  | 11      | 0            |
| 14  | H     | 805  | CLA  | 9       | 0            |
| 17  | Y     | 846  | BCR  | 8       | 0            |
| 18  | A     | 850  | LHG  | 4       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | G     | 816  | CLA  | 1       | 0            |
| 14  | G     | 836  | CLA  | 4       | 0            |
| 14  | A     | 820  | CLA  | 3       | 0            |
| 14  | G     | 817  | CLA  | 6       | 0            |
| 14  | H     | 807  | CLA  | 14      | 0            |
| 14  | Y     | 811  | CLA  | 8       | 0            |
| 14  | Y     | 838  | CLA  | 6       | 0            |
| 14  | H     | 815  | CLA  | 1       | 0            |
| 14  | B     | 825  | CLA  | 13      | 0            |
| 14  | Y     | 812  | CLA  | 3       | 0            |
| 14  | Z     | 821  | CLA  | 4       | 0            |
| 14  | J     | 102  | CLA  | 4       | 0            |
| 17  | B     | 844  | BCR  | 3       | 0            |
| 14  | S     | 1102 | CLA  | 2       | 0            |
| 17  | H     | 841  | BCR  | 5       | 0            |
| 17  | A     | 845  | BCR  | 3       | 0            |
| 14  | A     | 807  | CLA  | 6       | 0            |
| 14  | Z     | 815  | CLA  | 7       | 0            |
| 14  | H     | 810  | CLA  | 6       | 0            |
| 18  | A     | 851  | LHG  | 1       | 0            |
| 14  | H     | 802  | CLA  | 16      | 0            |
| 14  | Y     | 820  | CLA  | 4       | 0            |
| 17  | G     | 849  | BCR  | 16      | 0            |
| 17  | H     | 842  | BCR  | 6       | 0            |
| 17  | Y     | 851  | BCR  | 14      | 0            |
| 14  | T     | 101  | CLA  | 4       | 0            |
| 14  | U     | 1006 | CLA  | 10      | 0            |
| 14  | Y     | 834  | CLA  | 15      | 0            |
| 14  | Z     | 832  | CLA  | 12      | 0            |
| 14  | Z     | 833  | CLA  | 9       | 0            |
| 17  | A     | 849  | BCR  | 11      | 0            |
| 17  | Y     | 856  | BCR  | 5       | 0            |
| 17  | B     | 851  | BCR  | 12      | 0            |
| 14  | H     | 821  | CLA  | 9       | 0            |
| 14  | L     | 207  | CLA  | 4       | 0            |
| 14  | B     | 819  | CLA  | 7       | 0            |
| 14  | G     | 809  | CLA  | 7       | 0            |
| 18  | H     | 847  | LHG  | 2       | 0            |
| 17  | B     | 848  | BCR  | 10      | 0            |
| 14  | A     | 841  | CLA  | 11      | 0            |
| 14  | G     | 834  | CLA  | 7       | 0            |
| 14  | A     | 816  | CLA  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | Z     | 837  | CLA  | 8       | 0            |
| 14  | A     | 815  | CLA  | 2       | 0            |
| 14  | H     | 823  | CLA  | 8       | 0            |
| 14  | B     | 801  | CLA  | 11      | 0            |
| 14  | H     | 824  | CLA  | 14      | 0            |
| 14  | Y     | 833  | CLA  | 9       | 0            |
| 14  | H     | 835  | CLA  | 10      | 0            |
| 14  | G     | 806  | CLA  | 8       | 0            |
| 14  | Z     | 814  | CLA  | 1       | 0            |
| 14  | A     | 804  | CLA  | 7       | 0            |
| 14  | A     | 829  | CLA  | 10      | 0            |
| 14  | G     | 812  | CLA  | 1       | 0            |
| 14  | Y     | 808  | CLA  | 11      | 0            |
| 14  | H     | 832  | CLA  | 6       | 0            |
| 14  | Z     | 801  | CLA  | 13      | 0            |
| 14  | Z     | 807  | CLA  | 12      | 0            |
| 14  | U     | 1004 | CLA  | 7       | 0            |
| 17  | J     | 104  | BCR  | 10      | 0            |
| 14  | H     | 827  | CLA  | 10      | 0            |
| 17  | Y     | 848  | BCR  | 5       | 0            |
| 19  | Z     | 847  | LMG  | 3       | 0            |
| 14  | G     | 804  | CLA  | 10      | 0            |
| 14  | Y     | 802  | CLA  | 9       | 0            |
| 14  | G     | 811  | CLA  | 11      | 0            |
| 14  | H     | 808  | CLA  | 16      | 0            |
| 14  | H     | 838  | CLA  | 3       | 0            |
| 14  | A     | 825  | CLA  | 9       | 0            |
| 17  | L     | 203  | BCR  | 7       | 0            |
| 13  | G     | 801  | CL0  | 16      | 0            |
| 14  | B     | 804  | CLA  | 12      | 0            |
| 14  | Z     | 812  | CLA  | 4       | 0            |
| 14  | L     | 206  | CLA  | 12      | 0            |
| 18  | Y     | 853  | LHG  | 5       | 0            |
| 14  | A     | 838  | CLA  | 7       | 0            |
| 14  | Z     | 830  | CLA  | 2       | 0            |
| 16  | N     | 102  | SF4  | 2       | 0            |
| 14  | B     | 832  | CLA  | 11      | 0            |
| 14  | B     | 810  | CLA  | 9       | 0            |
| 14  | S     | 1103 | CLA  | 2       | 0            |
| 14  | T     | 103  | CLA  | 2       | 0            |
| 14  | H     | 833  | CLA  | 5       | 0            |
| 17  | Y     | 850  | BCR  | 10      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | R     | 101 | BCR  | 3       | 0            |
| 14  | H     | 809 | CLA  | 11      | 0            |
| 14  | Y     | 822 | CLA  | 2       | 0            |
| 14  | H     | 803 | CLA  | 12      | 0            |
| 14  | G     | 837 | CLA  | 5       | 0            |
| 15  | G     | 844 | PQN  | 3       | 0            |
| 14  | Y     | 832 | CLA  | 9       | 0            |
| 14  | A     | 827 | CLA  | 9       | 0            |
| 14  | H     | 830 | CLA  | 9       | 0            |
| 14  | Y     | 818 | CLA  | 7       | 0            |
| 14  | A     | 809 | CLA  | 1       | 0            |
| 14  | B     | 813 | CLA  | 15      | 0            |
| 14  | G     | 840 | CLA  | 4       | 0            |
| 14  | Z     | 806 | CLA  | 14      | 0            |
| 14  | Z     | 834 | CLA  | 5       | 0            |
| 14  | B     | 806 | CLA  | 6       | 0            |
| 14  | Z     | 809 | CLA  | 6       | 0            |
| 14  | G     | 808 | CLA  | 13      | 0            |
| 14  | G     | 832 | CLA  | 2       | 0            |
| 14  | H     | 801 | CLA  | 24      | 0            |
| 14  | Y     | 821 | CLA  | 14      | 0            |
| 14  | Z     | 828 | CLA  | 6       | 0            |
| 14  | B     | 812 | CLA  | 1       | 0            |
| 14  | H     | 806 | CLA  | 8       | 0            |
| 14  | G     | 810 | CLA  | 4       | 0            |
| 17  | A     | 848 | BCR  | 8       | 0            |
| 14  | G     | 841 | CLA  | 6       | 0            |
| 14  | A     | 805 | CLA  | 11      | 0            |
| 14  | Z     | 817 | CLA  | 5       | 0            |
| 14  | Z     | 803 | CLA  | 2       | 0            |
| 14  | Y     | 814 | CLA  | 1       | 0            |
| 14  | Z     | 819 | CLA  | 4       | 0            |
| 14  | B     | 827 | CLA  | 8       | 0            |
| 17  | B     | 847 | BCR  | 17      | 0            |
| 17  | G     | 847 | BCR  | 11      | 0            |
| 14  | Y     | 815 | CLA  | 1       | 0            |
| 14  | B     | 803 | CLA  | 16      | 0            |
| 14  | B     | 824 | CLA  | 7       | 0            |
| 14  | B     | 821 | CLA  | 5       | 0            |
| 17  | Z     | 841 | BCR  | 3       | 0            |
| 14  | Z     | 804 | CLA  | 6       | 0            |
| 14  | H     | 812 | CLA  | 8       | 0            |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | A     | 821  | CLA  | 7       | 0            |
| 14  | G     | 830  | CLA  | 13      | 0            |
| 15  | H     | 839  | PQN  | 7       | 0            |
| 14  | A     | 842  | CLA  | 2       | 0            |
| 14  | A     | 802  | CLA  | 10      | 0            |
| 17  | L     | 208  | BCR  | 7       | 0            |
| 14  | A     | 831  | CLA  | 5       | 0            |
| 14  | Y     | 823  | CLA  | 2       | 0            |
| 17  | Z     | 846  | BCR  | 6       | 0            |
| 17  | Y     | 847  | BCR  | 9       | 0            |
| 14  | A     | 839  | CLA  | 9       | 0            |
| 19  | B     | 849  | LMG  | 6       | 0            |
| 17  | Z     | 845  | BCR  | 6       | 0            |
| 14  | Y     | 839  | CLA  | 6       | 0            |
| 17  | B     | 845  | BCR  | 7       | 0            |
| 14  | G     | 825  | CLA  | 15      | 0            |
| 14  | Y     | 816  | CLA  | 3       | 0            |
| 14  | Q     | 201  | CLA  | 9       | 0            |
| 17  | G     | 850  | BCR  | 13      | 0            |
| 14  | K     | 101  | CLA  | 3       | 0            |
| 14  | L     | 201  | CLA  | 7       | 0            |
| 14  | A     | 833  | CLA  | 5       | 0            |
| 14  | H     | 829  | CLA  | 6       | 0            |
| 14  | A     | 824  | CLA  | 4       | 0            |
| 14  | L     | 202  | CLA  | 7       | 0            |
| 14  | G     | 820  | CLA  | 5       | 0            |
| 14  | G     | 835  | CLA  | 4       | 0            |
| 14  | Y     | 826  | CLA  | 7       | 0            |
| 14  | Y     | 804  | CLA  | 4       | 0            |
| 17  | Q     | 204  | BCR  | 4       | 0            |
| 17  | V     | 1202 | BCR  | 6       | 0            |
| 14  | Z     | 825  | CLA  | 12      | 0            |
| 14  | Y     | 837  | CLA  | 6       | 0            |
| 14  | Z     | 818  | CLA  | 3       | 0            |
| 14  | A     | 814  | CLA  | 2       | 0            |
| 17  | U     | 1008 | BCR  | 6       | 0            |
| 14  | G     | 803  | CLA  | 15      | 0            |
| 14  | Y     | 813  | CLA  | 6       | 0            |
| 14  | S     | 1101 | CLA  | 7       | 0            |
| 14  | B     | 820  | CLA  | 2       | 0            |
| 17  | U     | 1007 | BCR  | 10      | 0            |
| 14  | G     | 833  | CLA  | 4       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | Z     | 838  | CLA  | 6       | 0            |
| 14  | Z     | 811  | CLA  | 8       | 0            |
| 14  | H     | 822  | CLA  | 4       | 0            |
| 17  | G     | 848  | BCR  | 5       | 0            |
| 14  | G     | 829  | CLA  | 11      | 0            |
| 16  | C     | 101  | SF4  | 2       | 0            |
| 17  | H     | 843  | BCR  | 5       | 0            |
| 14  | Y     | 806  | CLA  | 12      | 0            |
| 14  | Y     | 829  | CLA  | 11      | 0            |
| 14  | G     | 853  | CLA  | 4       | 0            |
| 16  | C     | 102  | SF4  | 3       | 0            |
| 14  | A     | 828  | CLA  | 16      | 0            |
| 17  | A     | 846  | BCR  | 9       | 0            |
| 14  | A     | 803  | CLA  | 6       | 0            |
| 17  | Z     | 843  | BCR  | 6       | 0            |
| 14  | B     | 830  | CLA  | 5       | 0            |
| 14  | Z     | 820  | CLA  | 4       | 0            |
| 14  | G     | 838  | CLA  | 4       | 0            |
| 14  | Y     | 841  | CLA  | 10      | 0            |
| 17  | B     | 843  | BCR  | 2       | 0            |
| 14  | Z     | 822  | CLA  | 8       | 0            |
| 15  | B     | 842  | PQN  | 11      | 0            |
| 14  | Y     | 842  | CLA  | 9       | 0            |
| 14  | A     | 819  | CLA  | 11      | 0            |
| 14  | V     | 1201 | CLA  | 6       | 0            |
| 14  | W     | 1701 | CLA  | 4       | 0            |
| 14  | Z     | 802  | CLA  | 11      | 0            |
| 14  | H     | 834  | CLA  | 7       | 0            |
| 16  | A     | 844  | SF4  | 1       | 0            |
| 14  | B     | 814  | CLA  | 3       | 0            |
| 14  | Y     | 805  | CLA  | 15      | 0            |
| 14  | Y     | 854  | CLA  | 12      | 0            |
| 14  | G     | 802  | CLA  | 19      | 0            |
| 16  | N     | 101  | SF4  | 1       | 0            |
| 14  | A     | 830  | CLA  | 8       | 0            |
| 14  | G     | 828  | CLA  | 15      | 0            |
| 14  | H     | 836  | CLA  | 11      | 0            |
| 17  | Z     | 842  | BCR  | 4       | 0            |
| 14  | B     | 808  | CLA  | 10      | 0            |
| 14  | B     | 816  | CLA  | 1       | 0            |
| 14  | Z     | 839  | CLA  | 4       | 0            |
| 14  | G     | 826  | CLA  | 6       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | A     | 823  | CLA  | 1       | 0            |
| 14  | G     | 821  | CLA  | 14      | 0            |
| 14  | B     | 822  | CLA  | 7       | 0            |
| 14  | Y     | 843  | CLA  | 5       | 0            |
| 14  | B     | 839  | CLA  | 8       | 0            |
| 14  | A     | 808  | CLA  | 9       | 0            |
| 14  | H     | 811  | CLA  | 3       | 0            |
| 14  | B     | 823  | CLA  | 2       | 0            |
| 14  | A     | 811  | CLA  | 7       | 0            |
| 14  | Z     | 810  | CLA  | 3       | 0            |
| 14  | Y     | 803  | CLA  | 7       | 0            |
| 14  | H     | 826  | CLA  | 10      | 0            |
| 14  | B     | 807  | CLA  | 10      | 0            |
| 19  | H     | 846  | LMG  | 4       | 0            |
| 14  | Z     | 816  | CLA  | 10      | 0            |
| 14  | B     | 836  | CLA  | 7       | 0            |
| 14  | G     | 805  | CLA  | 14      | 0            |
| 14  | H     | 828  | CLA  | 11      | 0            |
| 14  | B     | 831  | CLA  | 3       | 0            |
| 14  | Z     | 824  | CLA  | 7       | 0            |
| 14  | Z     | 835  | CLA  | 9       | 0            |
| 14  | B     | 826  | CLA  | 8       | 0            |
| 15  | A     | 843  | PQN  | 6       | 0            |
| 14  | A     | 835  | CLA  | 9       | 0            |
| 17  | L     | 209  | BCR  | 8       | 0            |
| 14  | B     | 815  | CLA  | 7       | 0            |
| 14  | Z     | 813  | CLA  | 5       | 0            |
| 17  | F     | 201  | BCR  | 8       | 0            |
| 14  | A     | 806  | CLA  | 14      | 0            |
| 14  | B     | 829  | CLA  | 6       | 0            |
| 14  | Y     | 828  | CLA  | 20      | 0            |
| 17  | H     | 844  | BCR  | 10      | 0            |
| 14  | Z     | 826  | CLA  | 7       | 0            |
| 14  | B     | 805  | CLA  | 10      | 0            |
| 14  | G     | 815  | CLA  | 7       | 0            |
| 14  | G     | 831  | CLA  | 5       | 0            |
| 14  | B     | 809  | CLA  | 12      | 0            |
| 17  | H     | 840  | BCR  | 8       | 0            |
| 14  | G     | 823  | CLA  | 3       | 0            |
| 14  | Y     | 807  | CLA  | 3       | 0            |
| 17  | S     | 1104 | BCR  | 10      | 0            |
| 14  | K     | 103  | CLA  | 4       | 0            |

*Continued on next page...*

*Continued from previous page...*

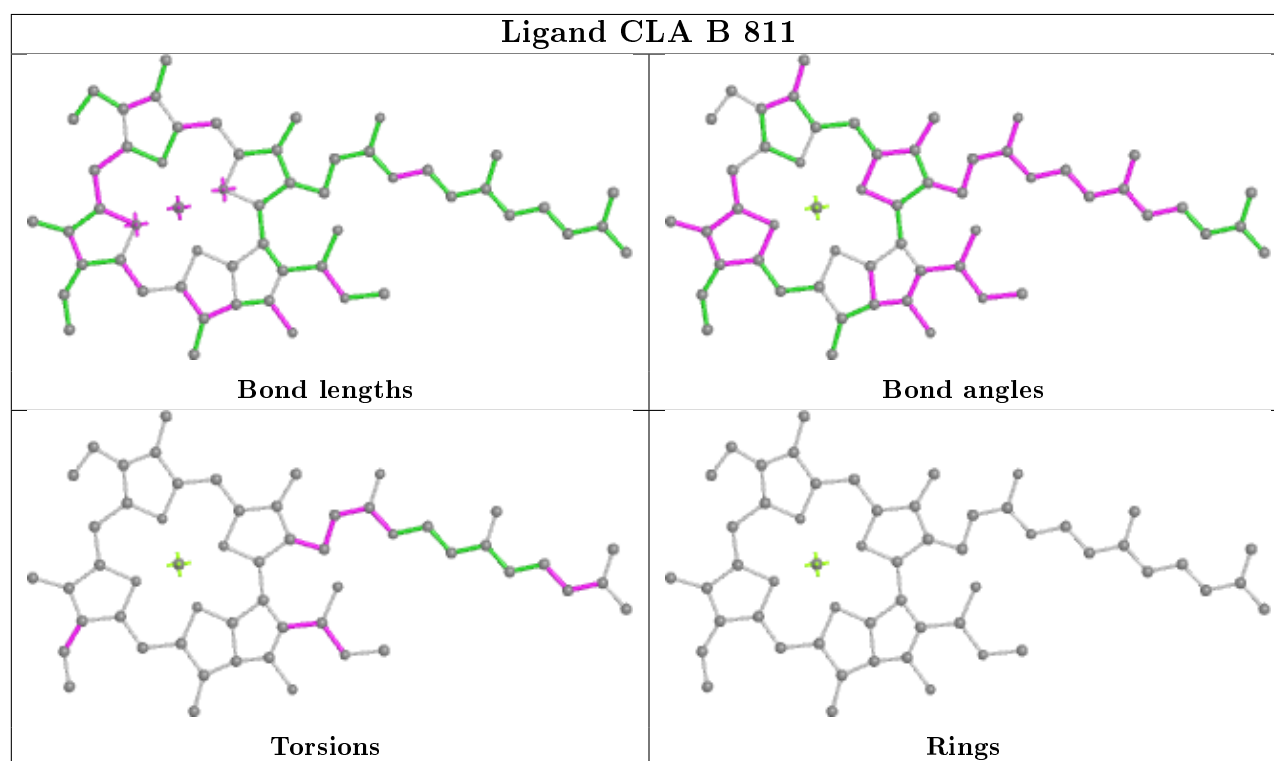
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | Z     | 829 | CLA  | 2       | 0            |
| 14  | B     | 840 | CLA  | 7       | 0            |
| 14  | G     | 822 | CLA  | 2       | 0            |
| 14  | H     | 814 | CLA  | 5       | 0            |
| 14  | Y     | 824 | CLA  | 3       | 0            |
| 14  | A     | 837 | CLA  | 11      | 0            |
| 17  | Q     | 202 | BCR  | 5       | 0            |
| 14  | H     | 819 | CLA  | 3       | 0            |
| 15  | Y     | 844 | PQN  | 2       | 0            |
| 14  | Z     | 823 | CLA  | 7       | 0            |
| 14  | B     | 818 | CLA  | 8       | 0            |
| 14  | H     | 816 | CLA  | 10      | 0            |
| 17  | T     | 102 | BCR  | 6       | 0            |
| 17  | B     | 846 | BCR  | 2       | 0            |
| 14  | G     | 818 | CLA  | 15      | 0            |
| 14  | A     | 818 | CLA  | 10      | 0            |
| 14  | Z     | 827 | CLA  | 10      | 0            |
| 13  | A     | 801 | CL0  | 13      | 0            |
| 17  | I     | 101 | BCR  | 11      | 0            |
| 14  | Y     | 817 | CLA  | 5       | 0            |
| 13  | Y     | 801 | CL0  | 11      | 0            |
| 14  | A     | 817 | CLA  | 5       | 0            |
| 14  | Z     | 836 | CLA  | 2       | 0            |
| 18  | G     | 851 | LHG  | 7       | 0            |
| 14  | G     | 814 | CLA  | 7       | 0            |
| 14  | A     | 810 | CLA  | 7       | 0            |
| 14  | Y     | 836 | CLA  | 3       | 0            |
| 14  | H     | 825 | CLA  | 4       | 0            |
| 14  | A     | 834 | CLA  | 10      | 0            |
| 14  | Y     | 831 | CLA  | 4       | 0            |
| 14  | Z     | 805 | CLA  | 7       | 0            |
| 15  | Z     | 840 | PQN  | 4       | 0            |
| 17  | R     | 102 | BCR  | 9       | 0            |
| 14  | G     | 807 | CLA  | 4       | 0            |
| 17  | Z     | 844 | BCR  | 8       | 0            |
| 14  | B     | 828 | CLA  | 8       | 0            |
| 14  | G     | 819 | CLA  | 15      | 0            |
| 14  | B     | 835 | CLA  | 8       | 0            |
| 17  | H     | 848 | BCR  | 5       | 0            |
| 14  | G     | 842 | CLA  | 6       | 0            |
| 17  | K     | 102 | BCR  | 3       | 0            |
| 14  | Y     | 819 | CLA  | 12      | 0            |

*Continued on next page...*

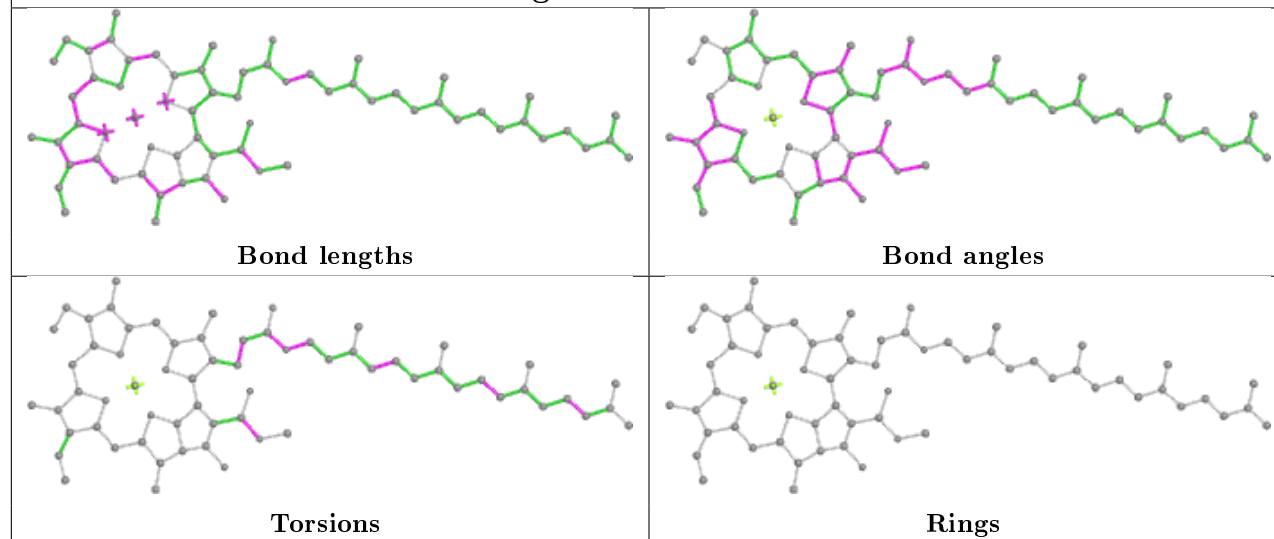
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | G     | 827 | CLA  | 8       | 0            |
| 14  | A     | 813 | CLA  | 10      | 0            |
| 17  | Y     | 849 | BCR  | 7       | 0            |
| 14  | G     | 843 | CLA  | 4       | 0            |

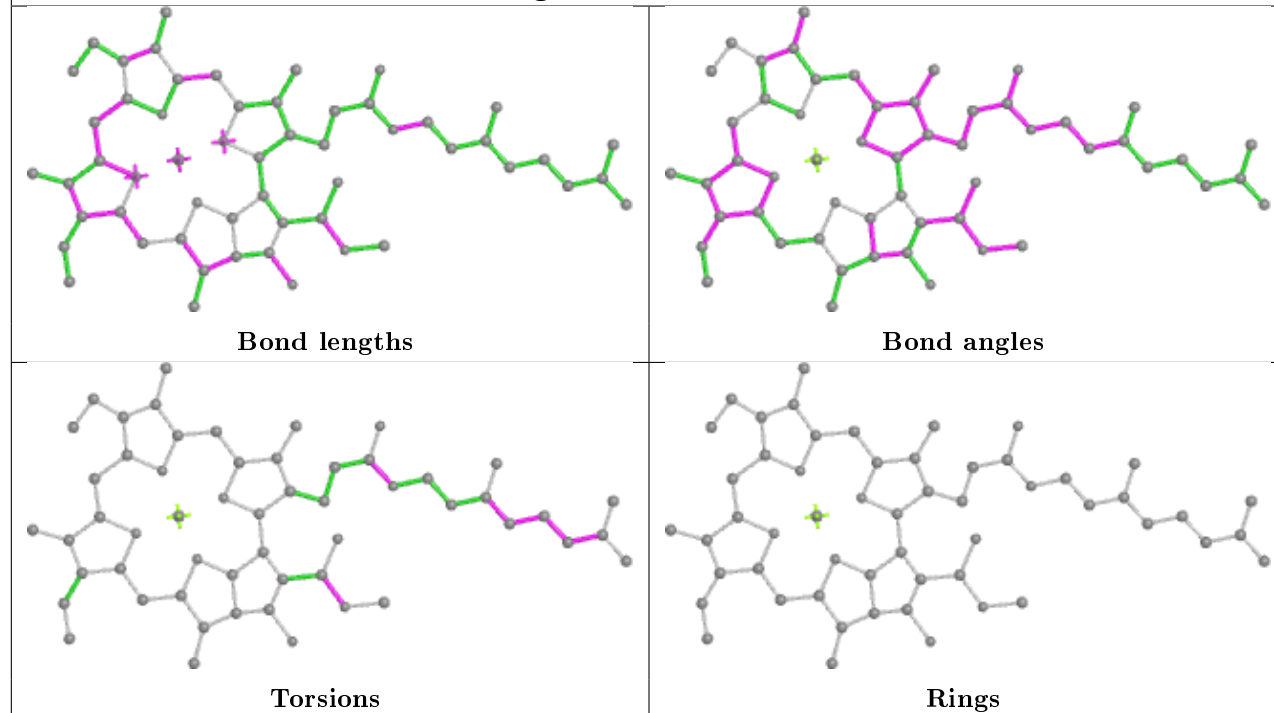
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



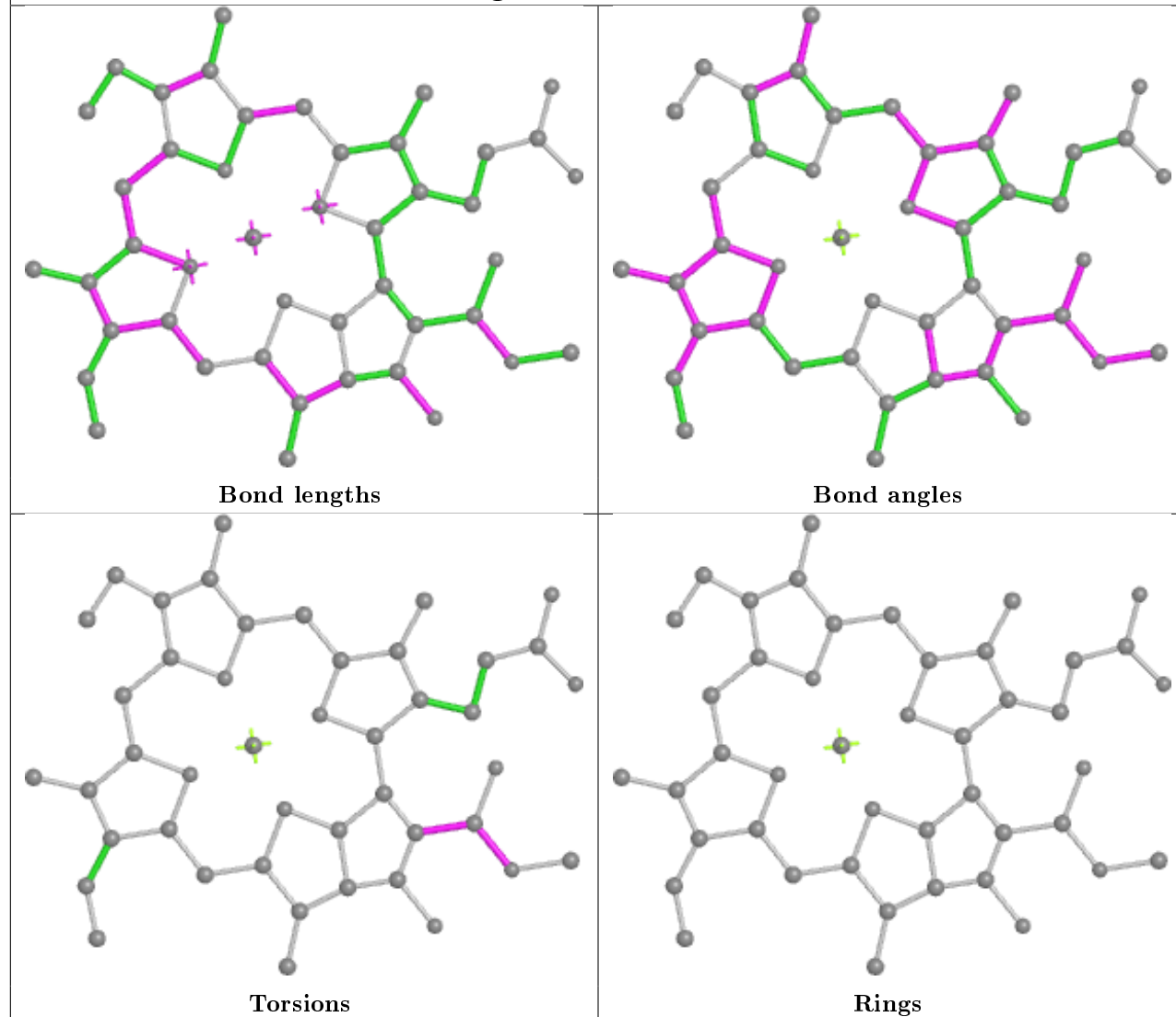
## Ligand CLA B 817



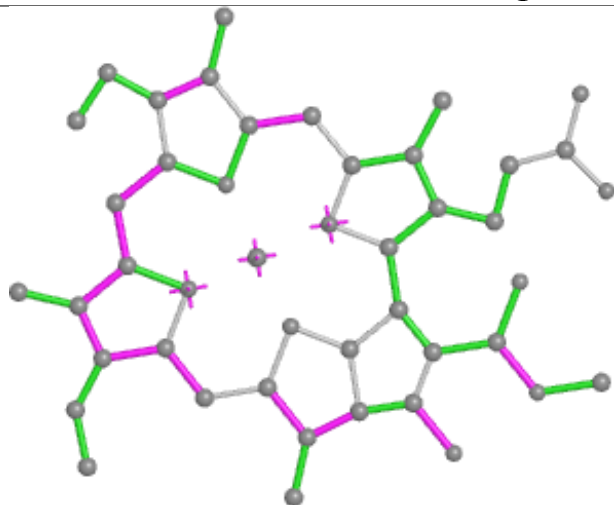
## Ligand CLA B 833



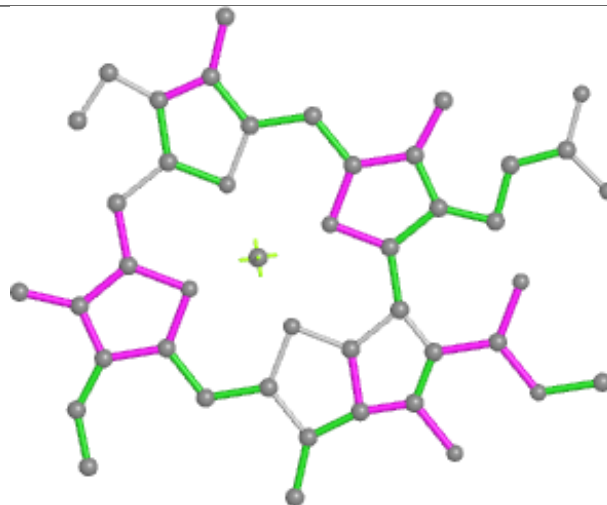
## Ligand CLA H 820



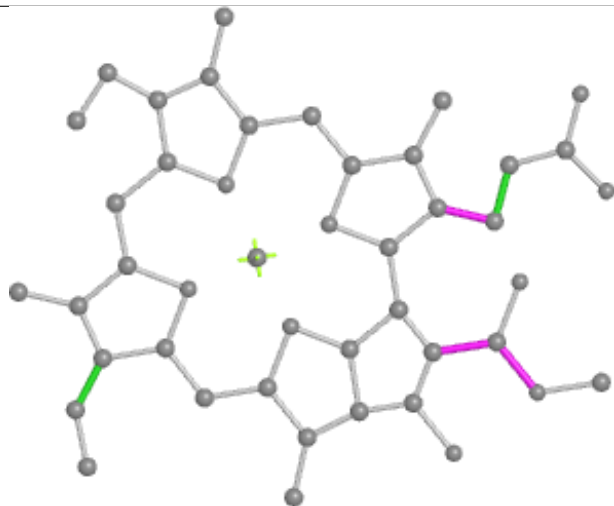
## Ligand CLA Y 810



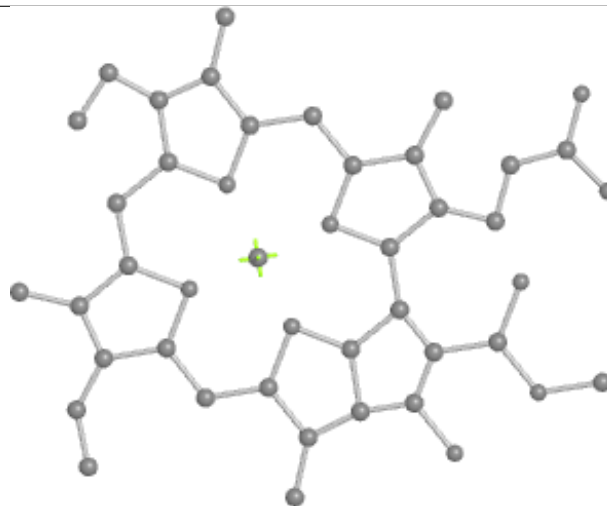
Bond lengths



Bond angles

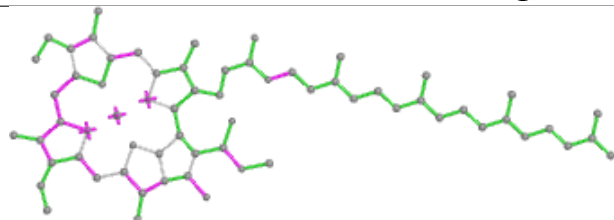


Torsions

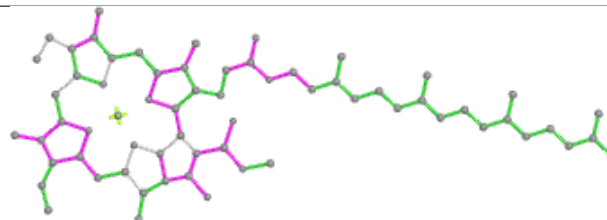


Rings

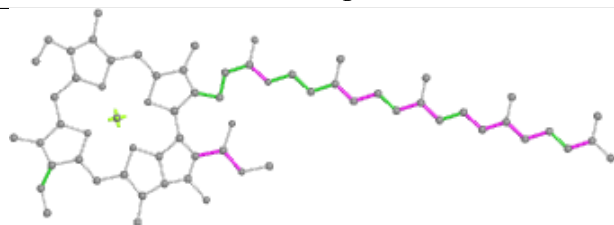
## Ligand CLA Y 827



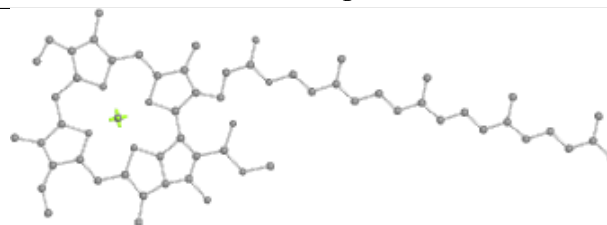
Bond lengths



Bond angles



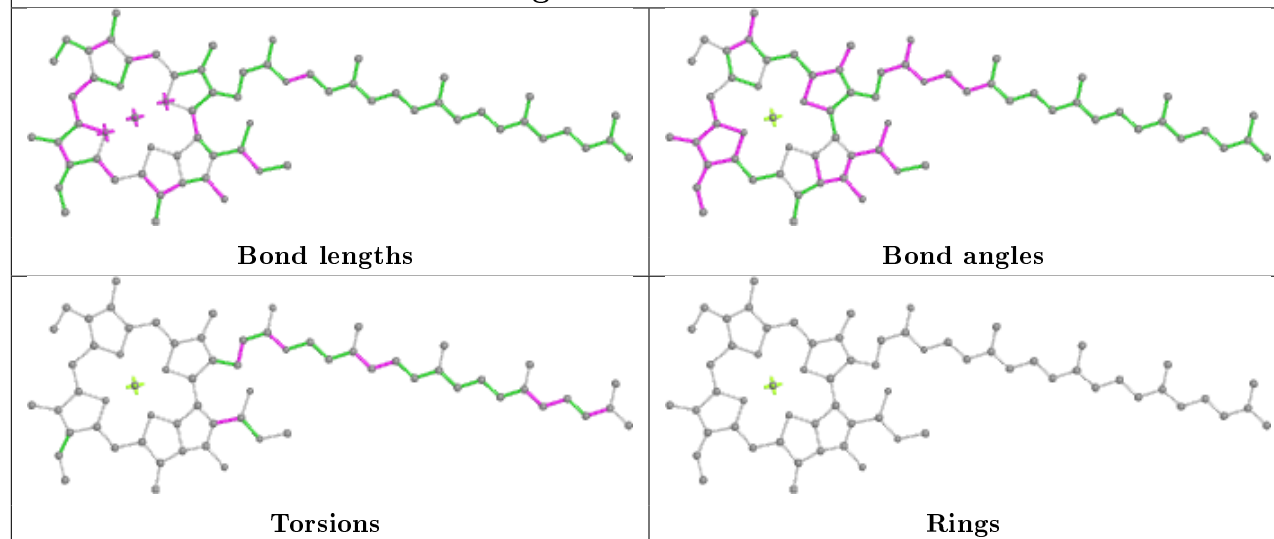
Torsions



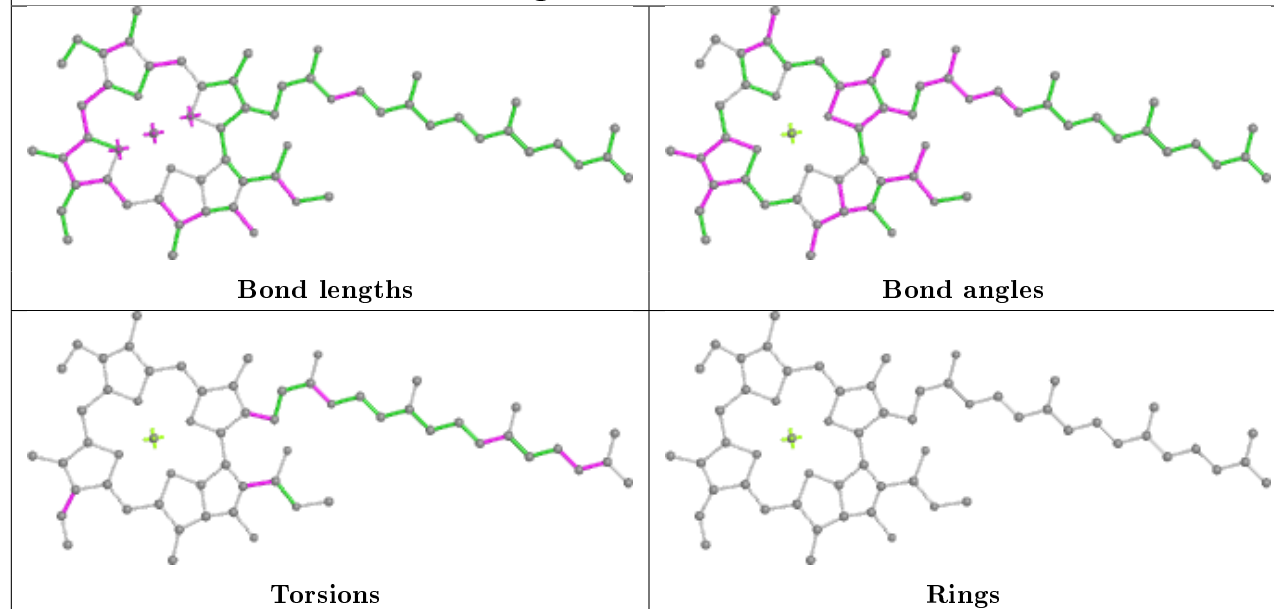
Rings

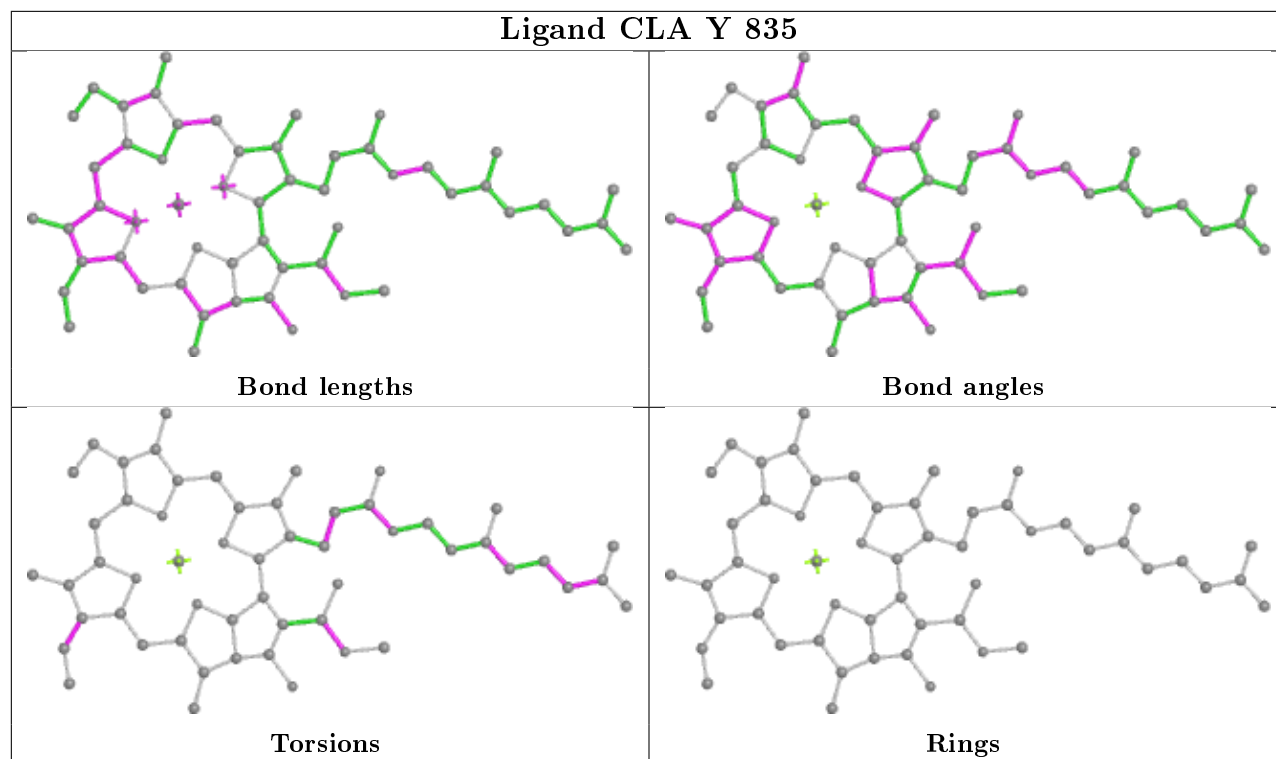


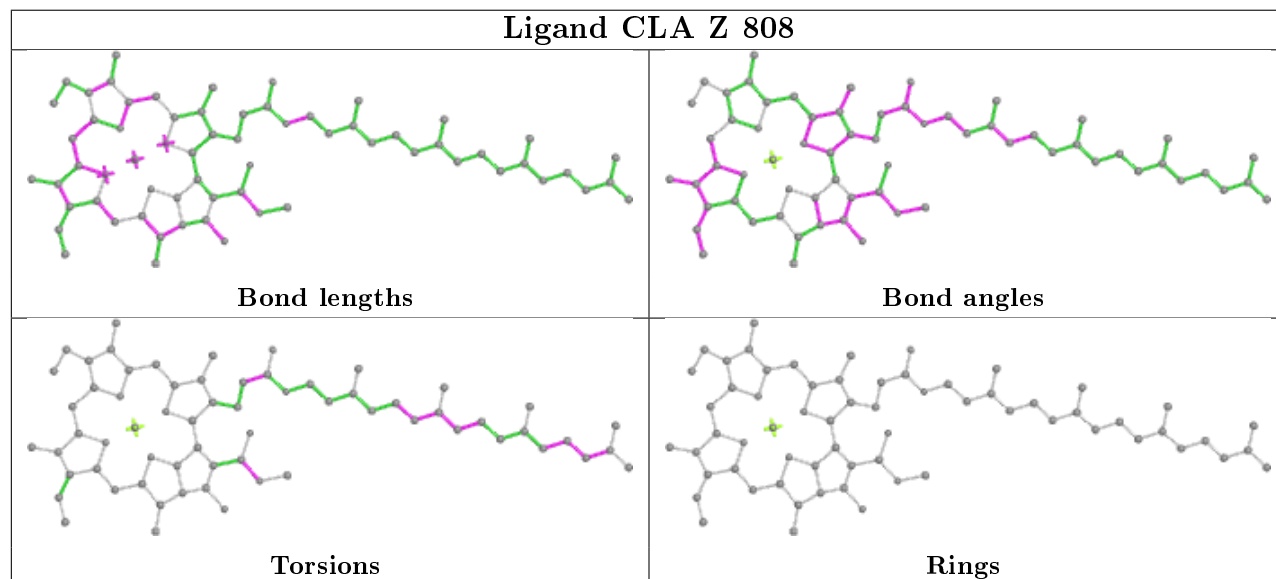
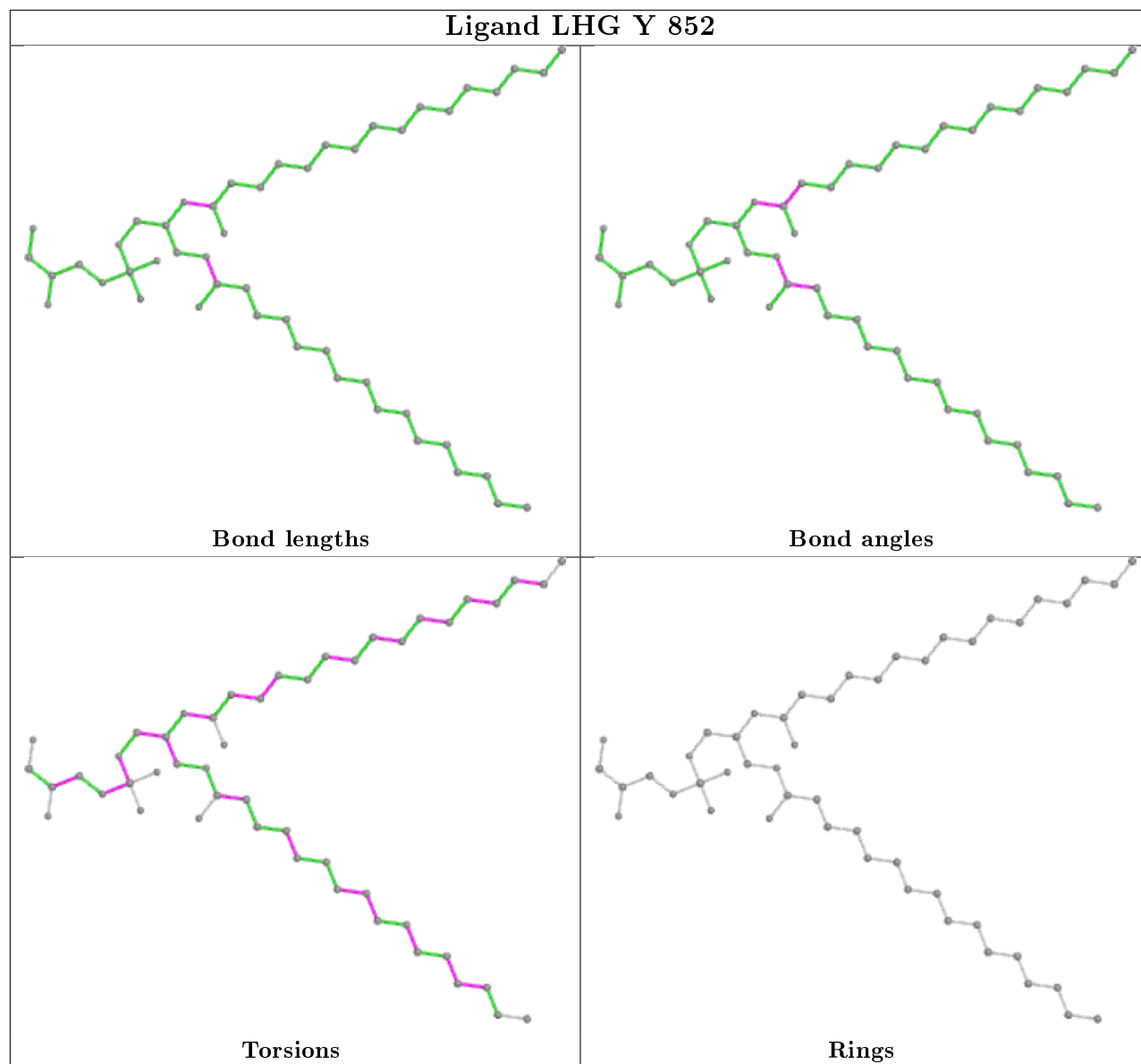
## Ligand CLA A 852



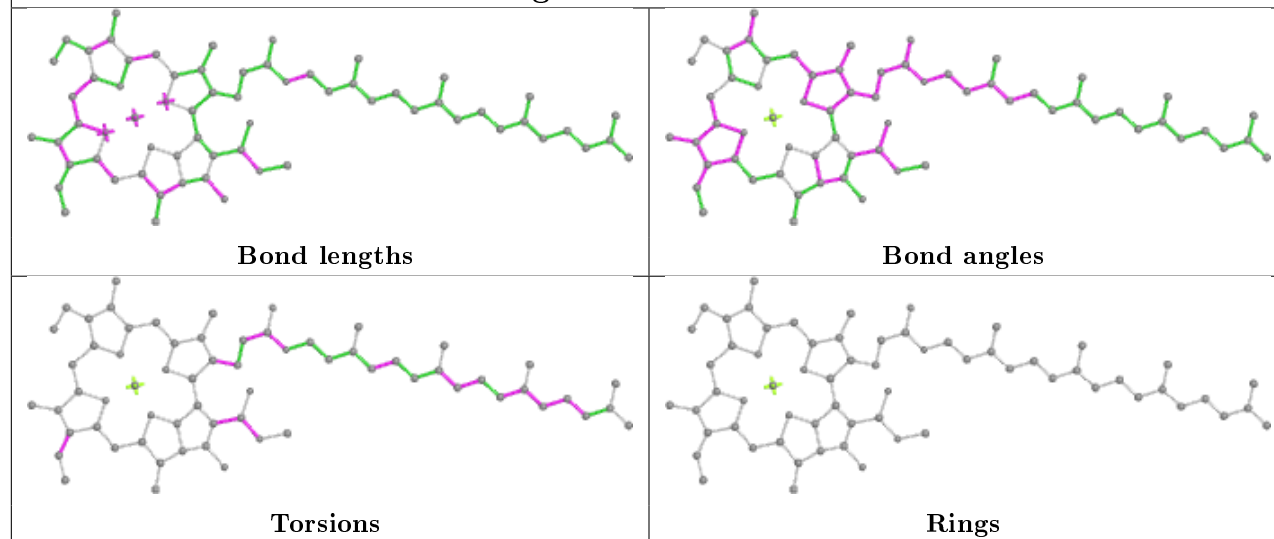
## Ligand CLA A 826



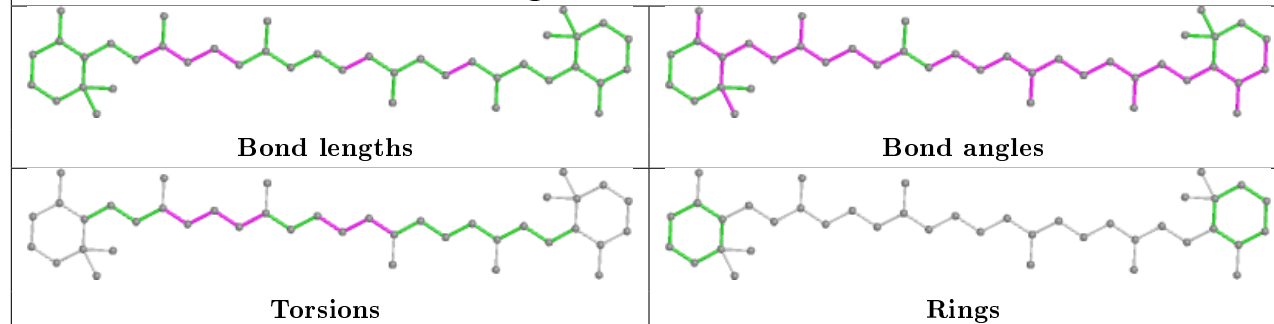




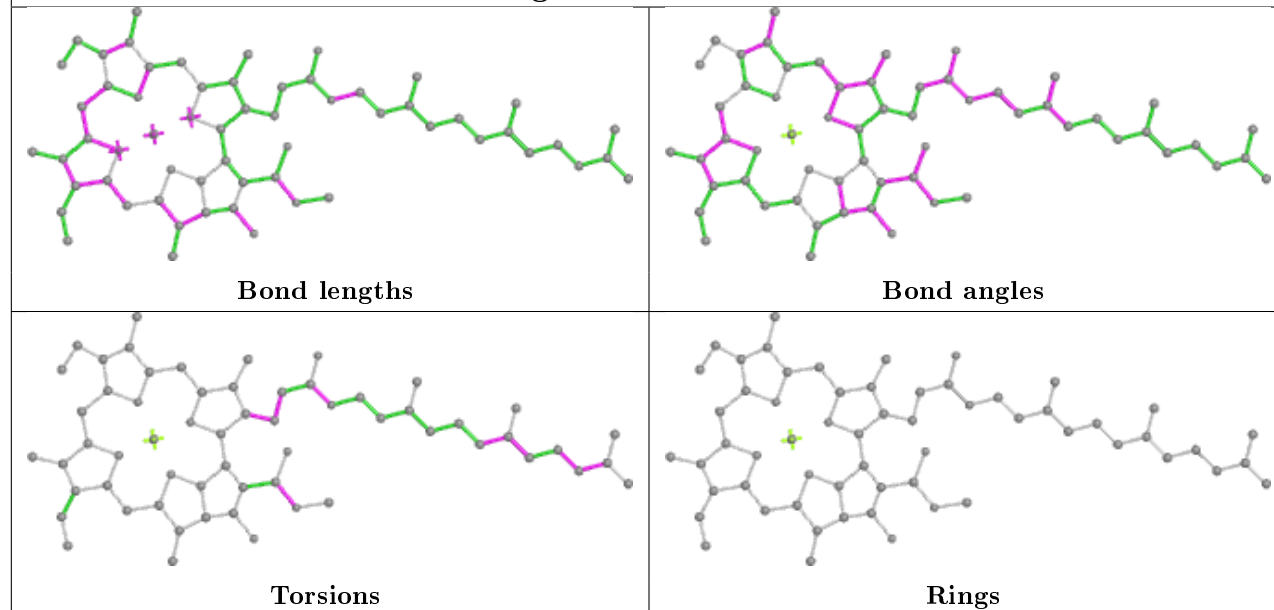
## Ligand CLA B 841



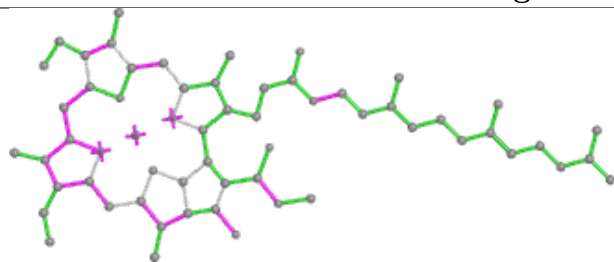
## Ligand BCR M 101



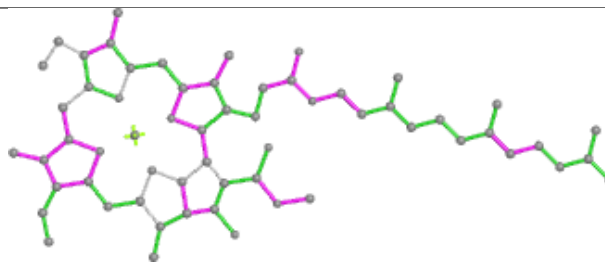
## Ligand CLA H 817



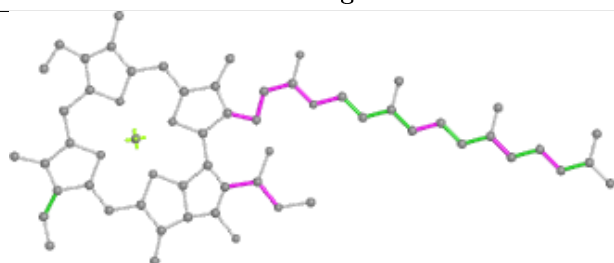
## Ligand CLA H 818



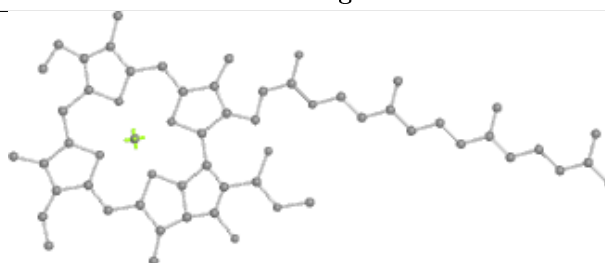
Bond lengths



Bond angles

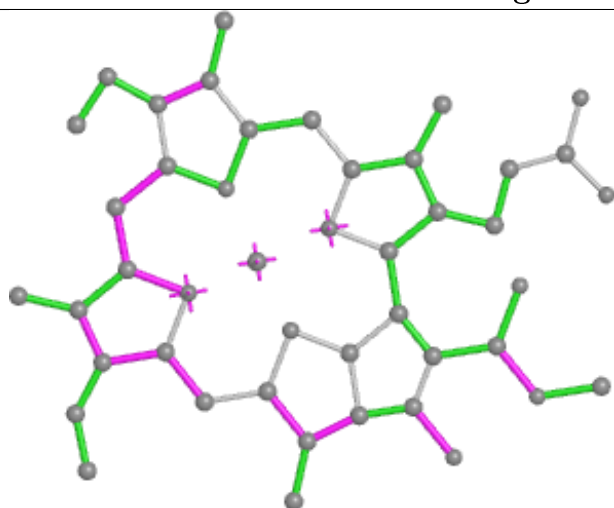


Torsions

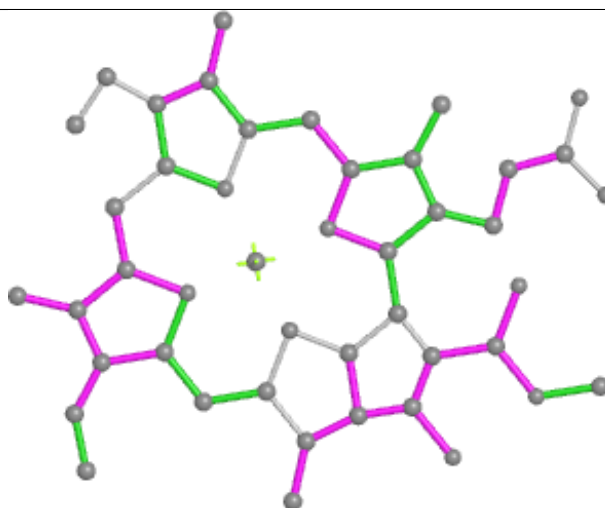


Rings

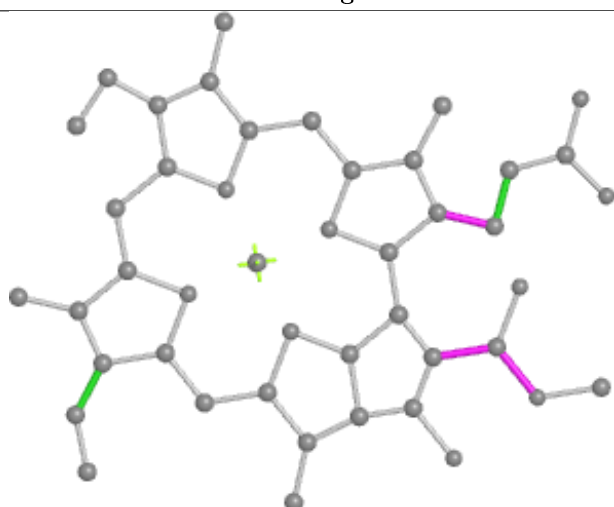
## Ligand CLA H 831



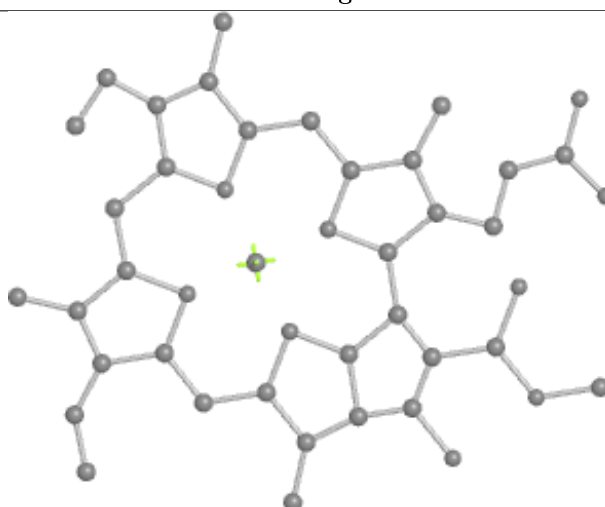
Bond lengths



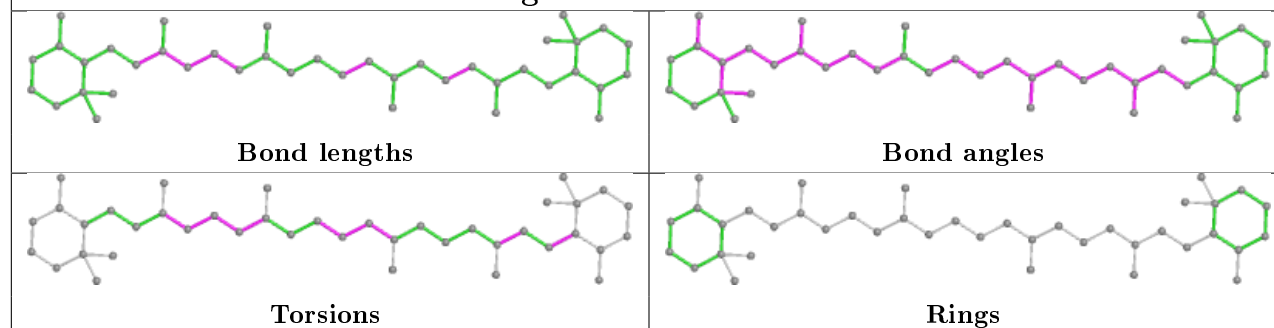
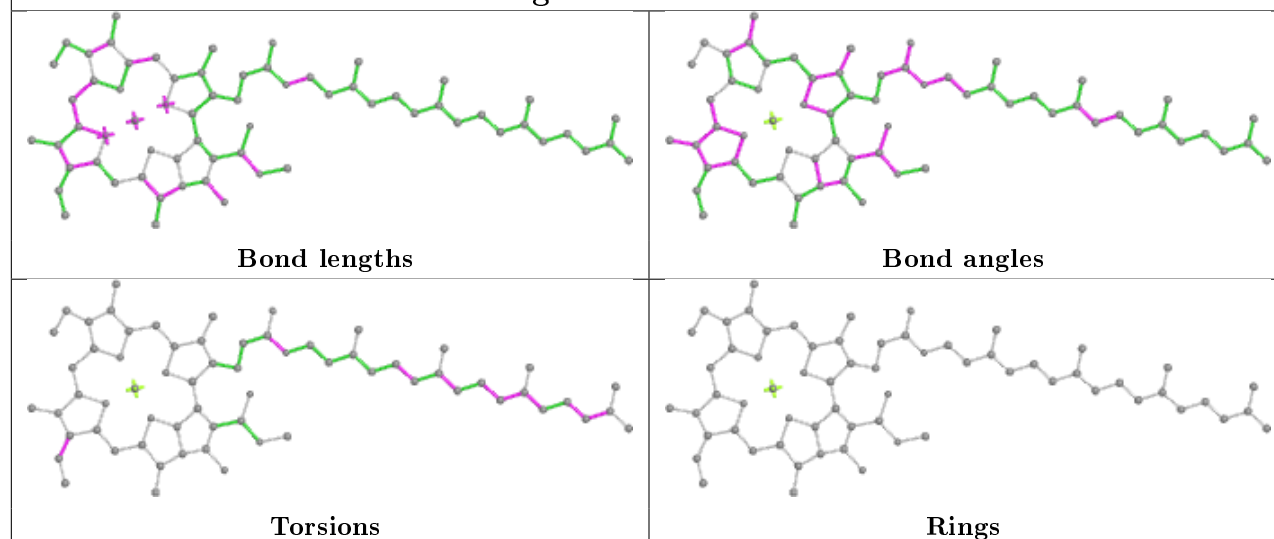
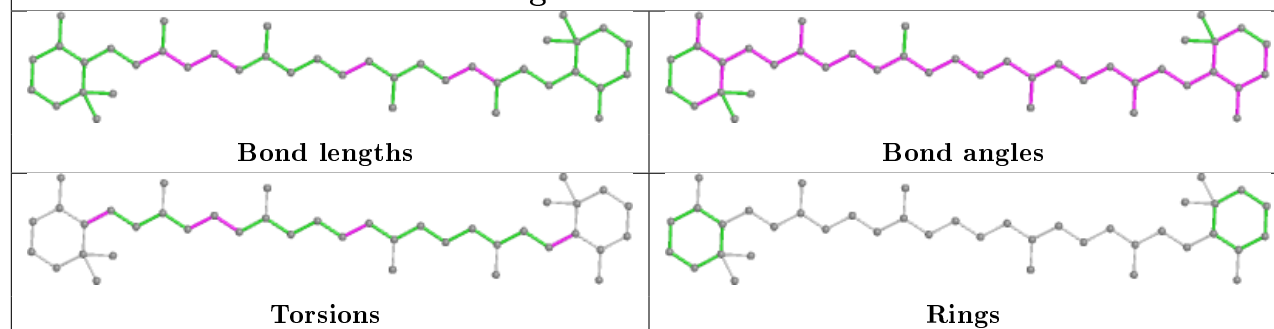
Bond angles



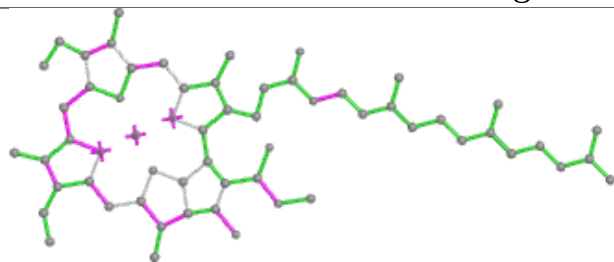
Torsions



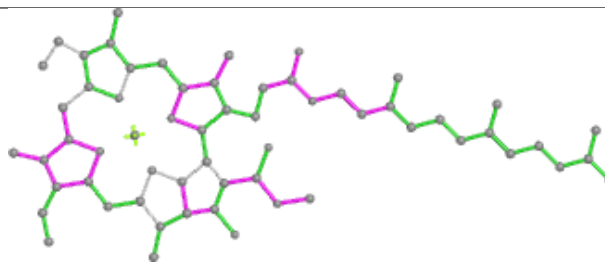
Rings

**Ligand BCR U 1005****Ligand CLA A 832****Ligand BCR G 846**

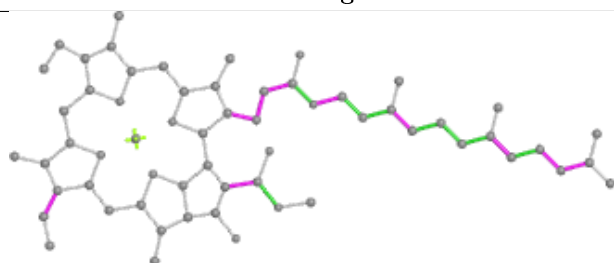
## Ligand CLA G 824



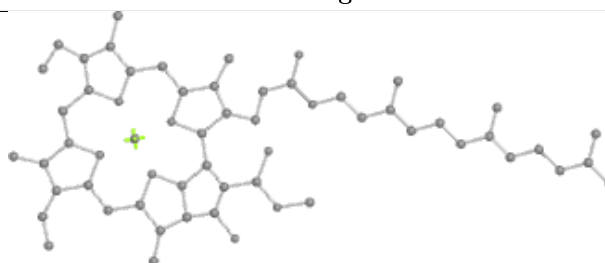
Bond lengths



Bond angles

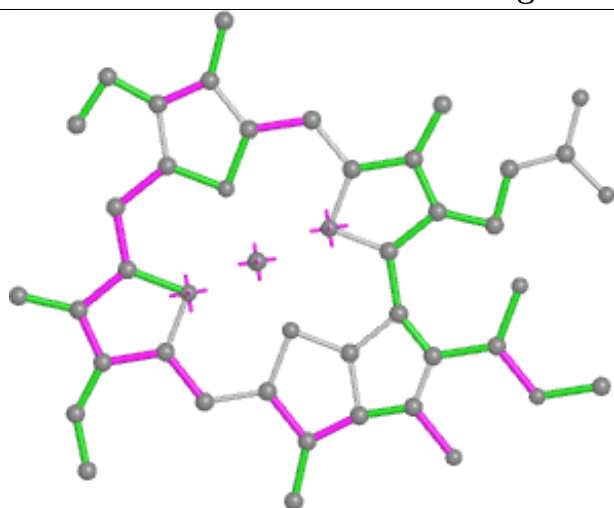


Torsions

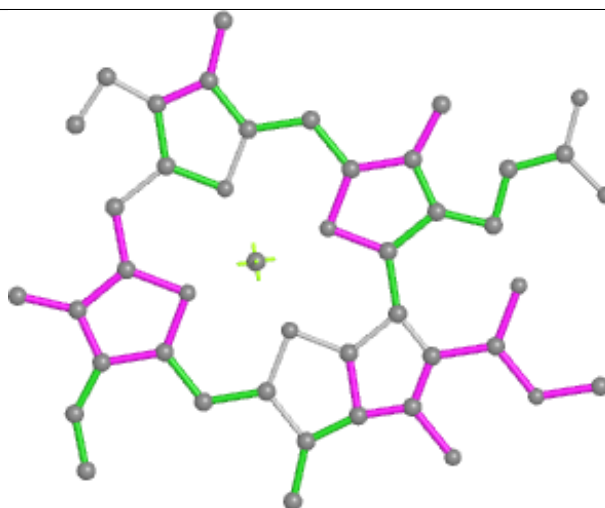


Rings

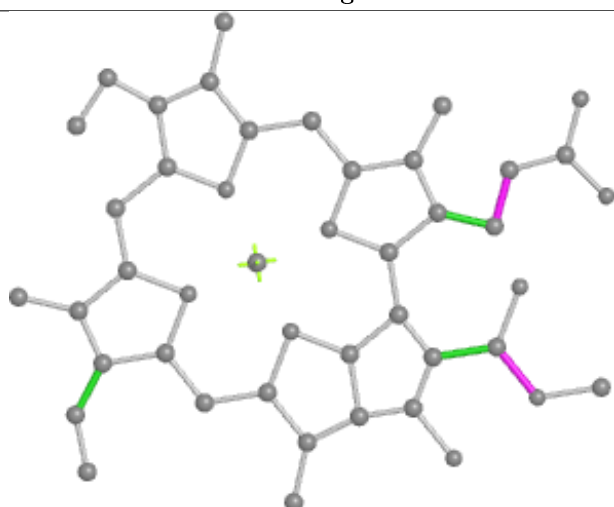
## Ligand CLA d 202



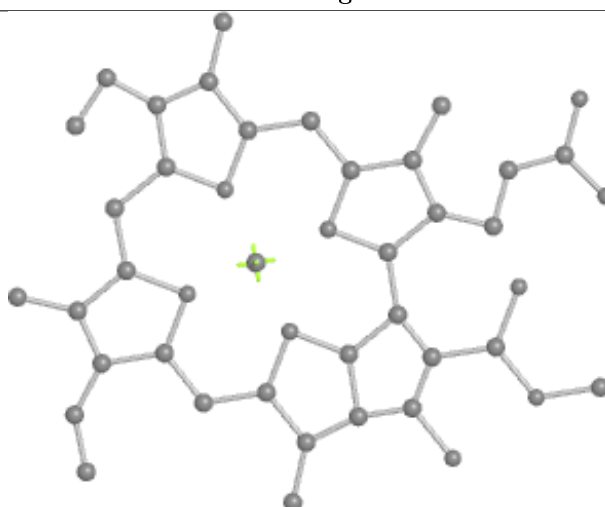
Bond lengths



Bond angles

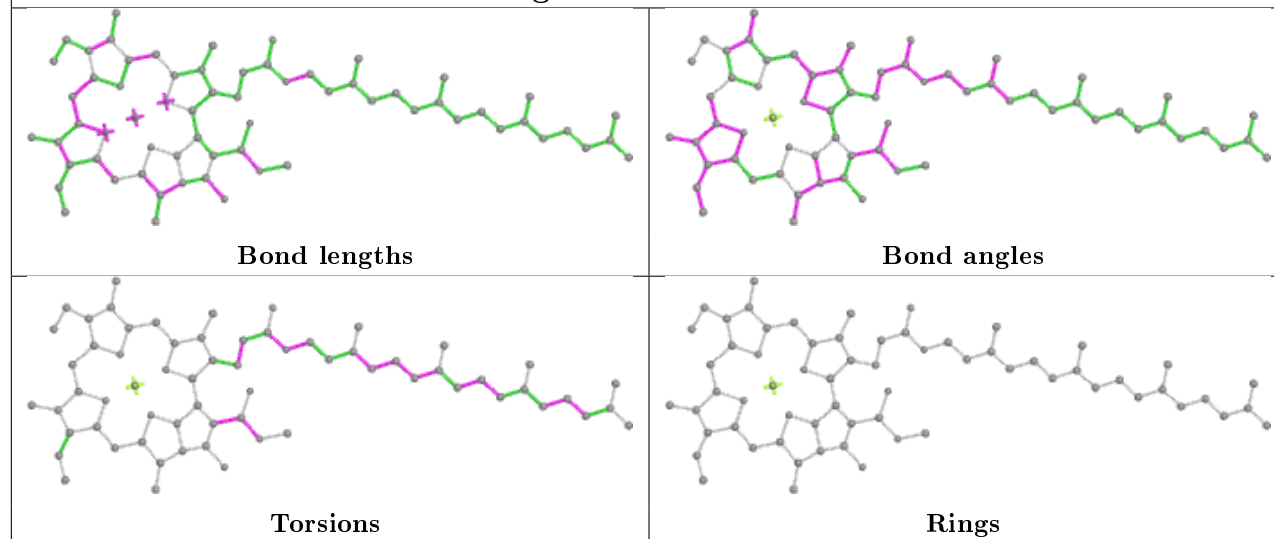


Torsions

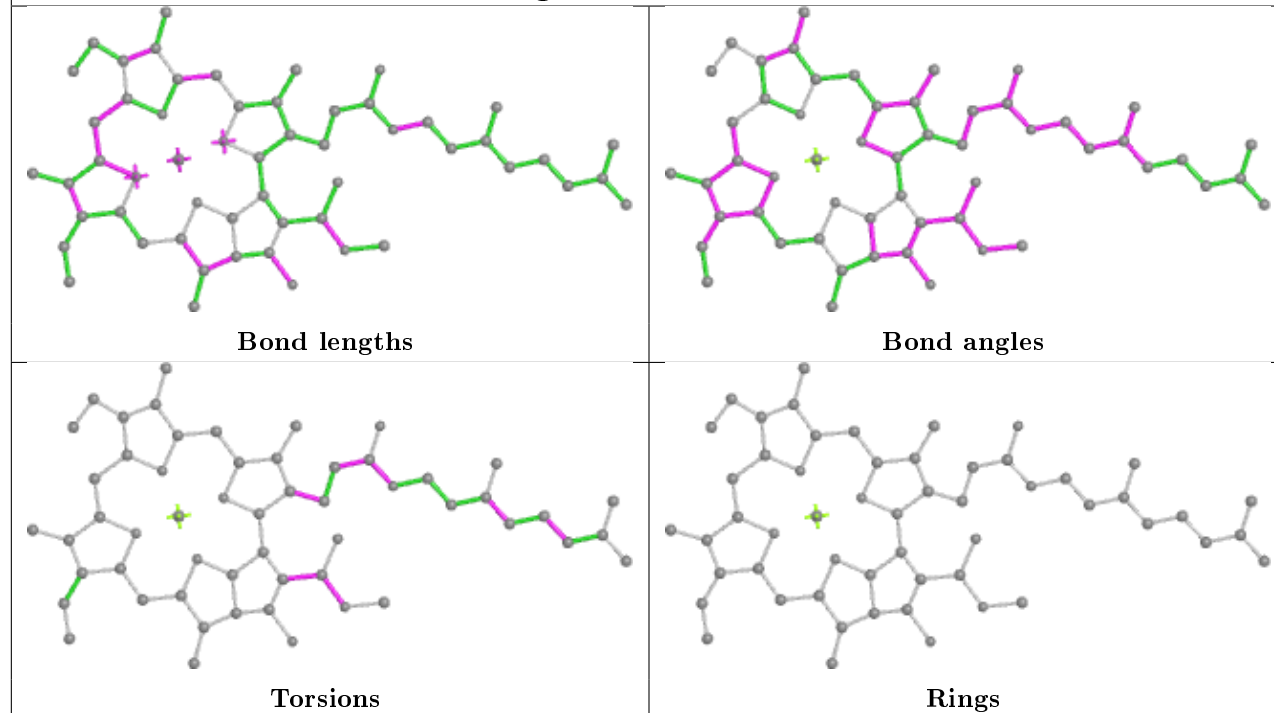


Rings

## Ligand CLA B 802

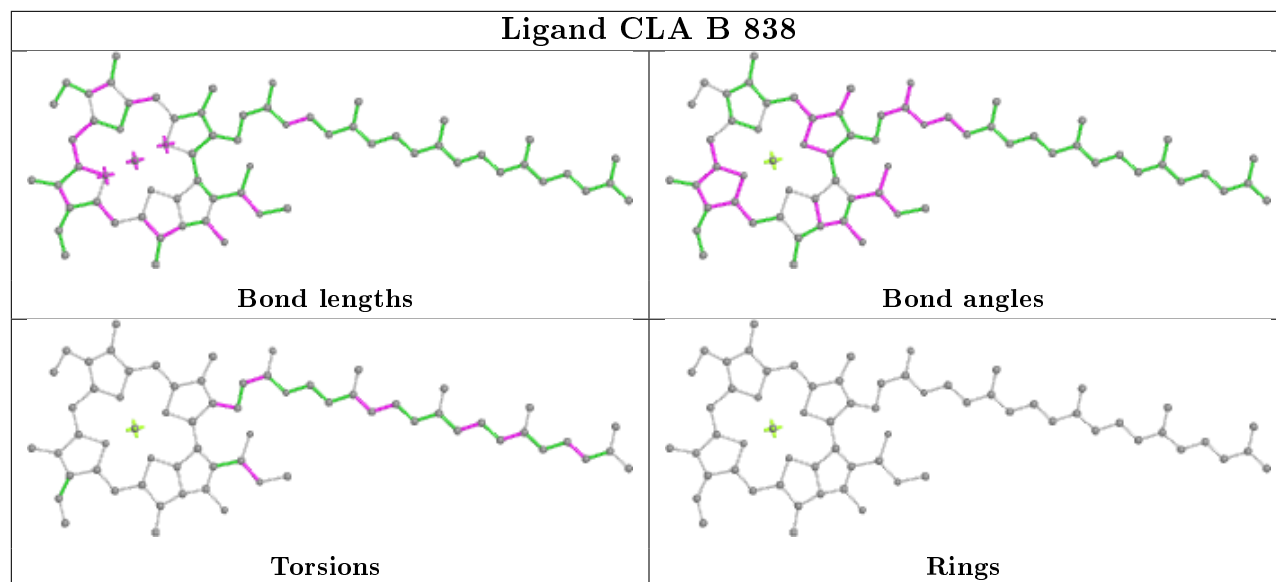


## Ligand CLA Z 831

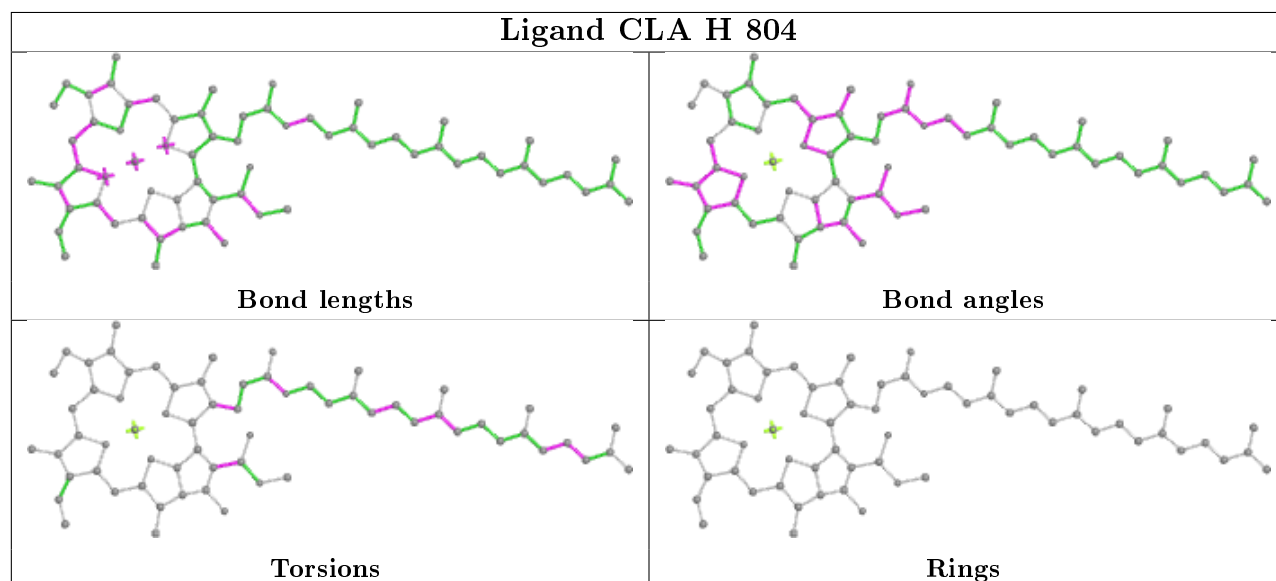




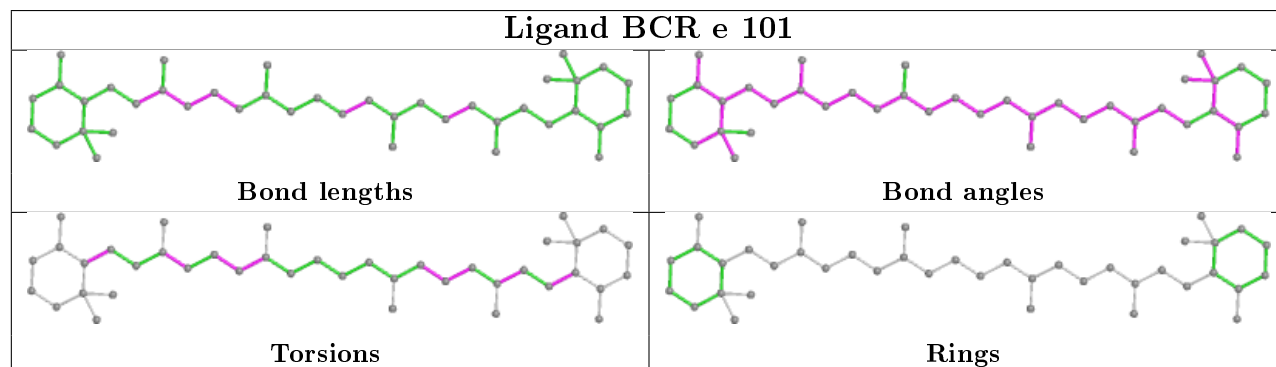
## Ligand CLA B 838



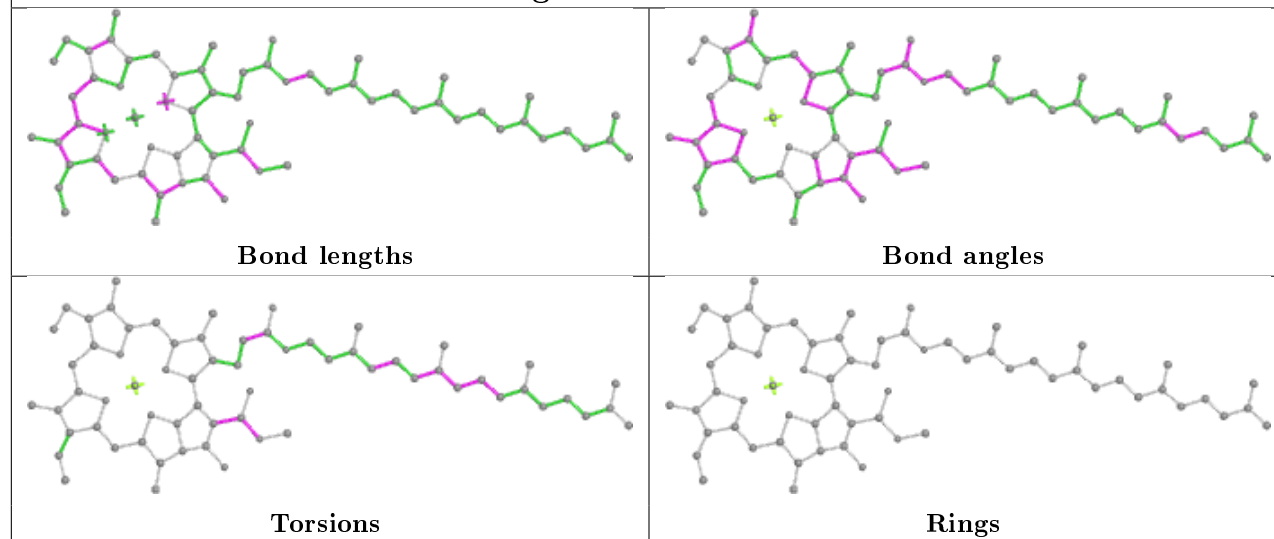
## Ligand CLA H 804



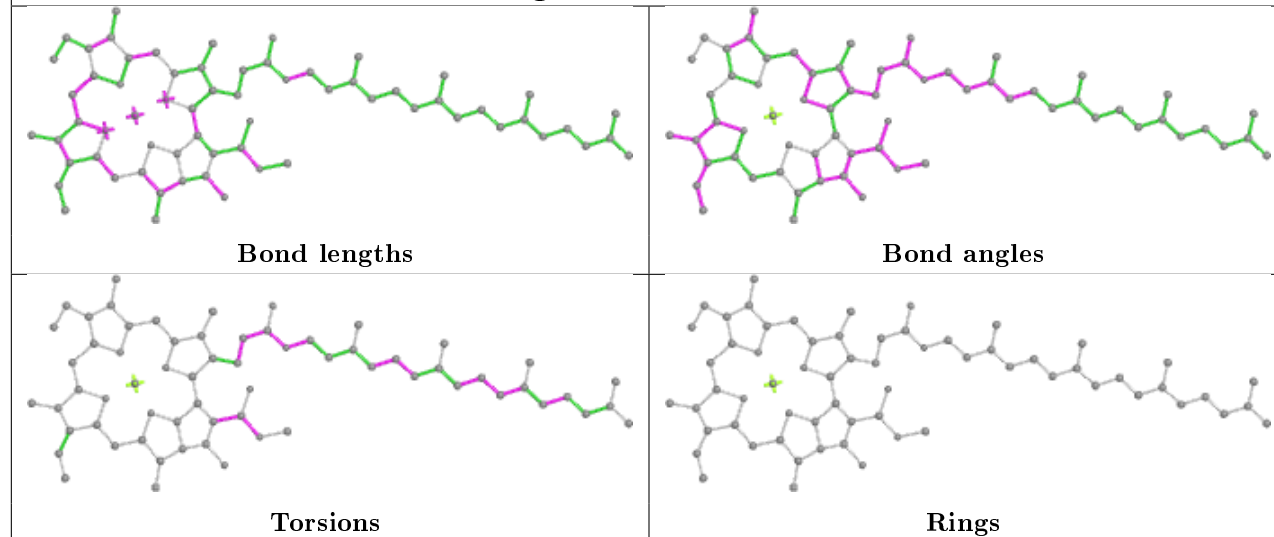
## Ligand BCR e 101



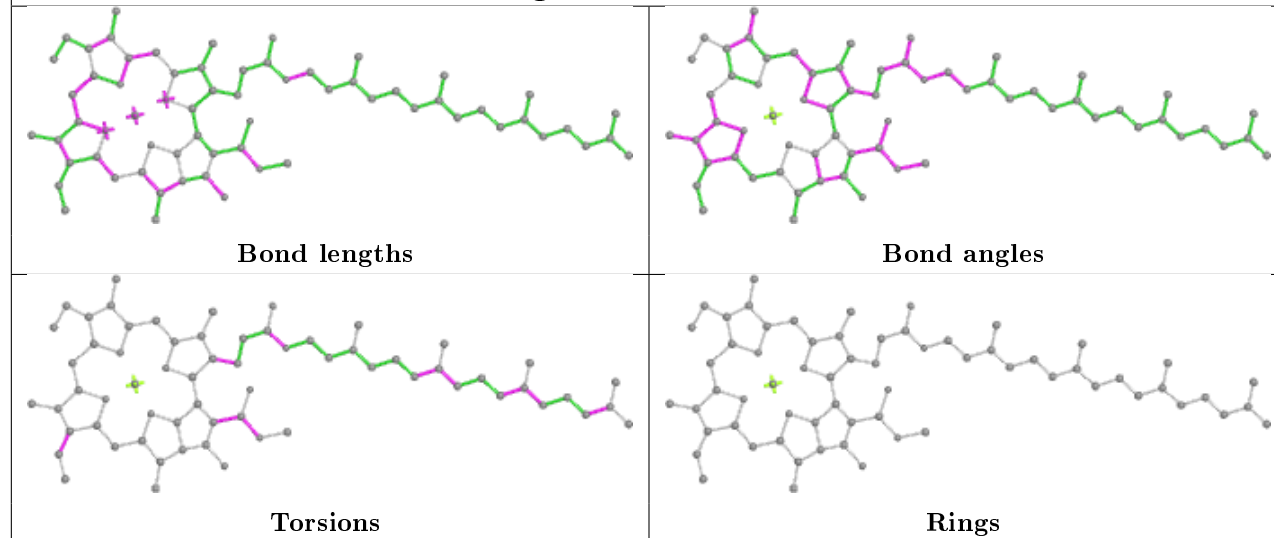
## Ligand CLA Y 855



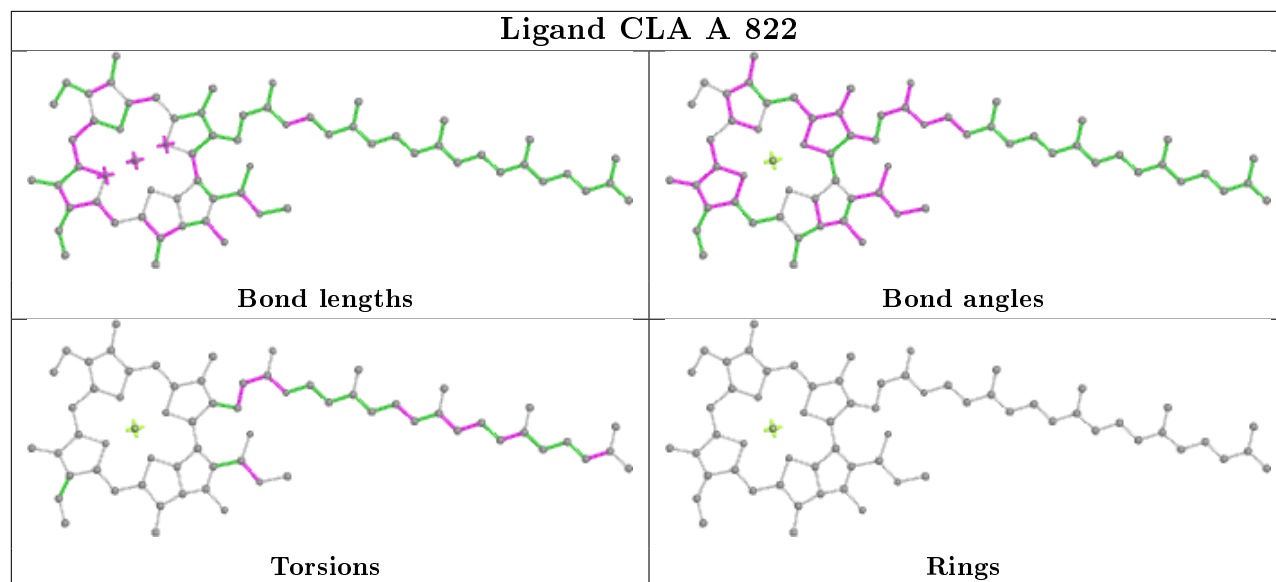
## Ligand CLA G 839



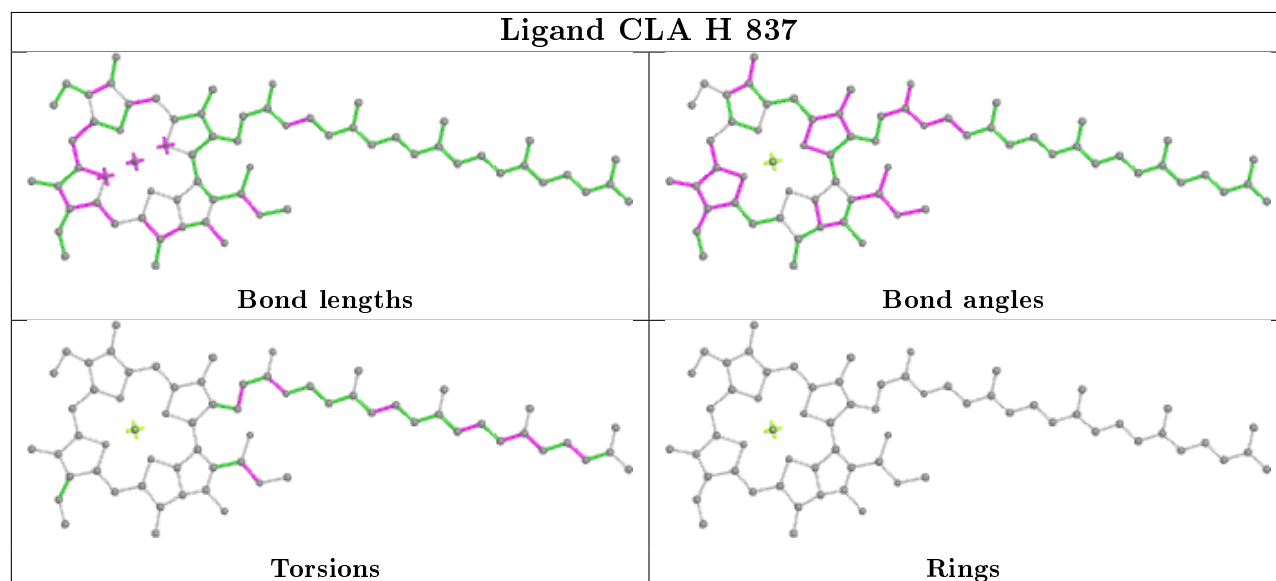
## Ligand CLA H 813



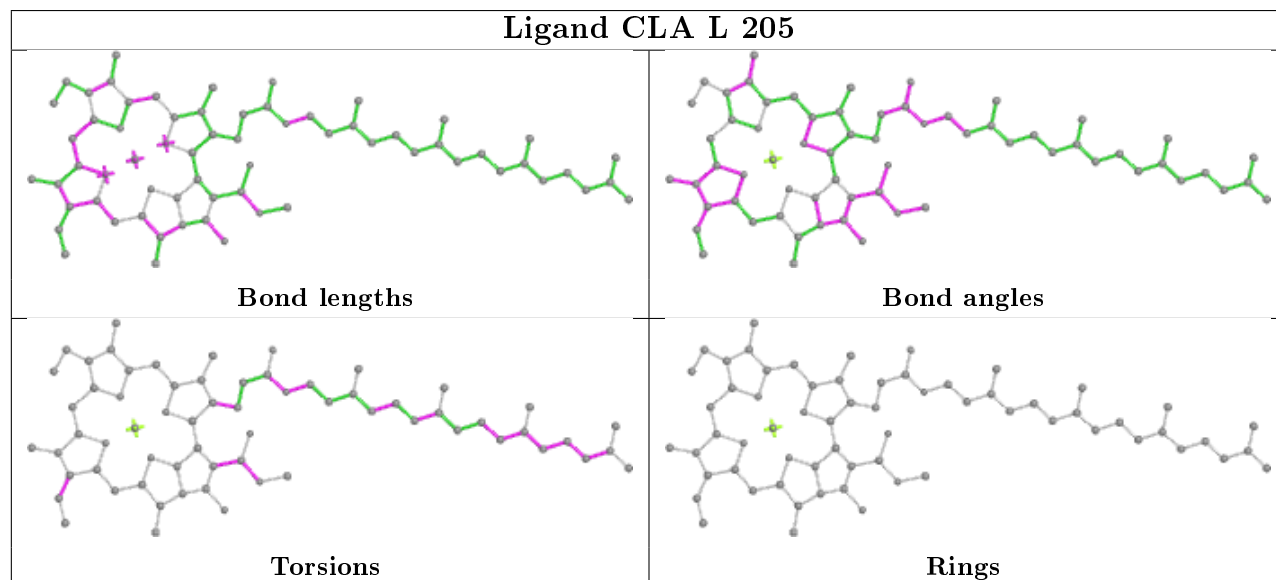
## Ligand CLA A 822



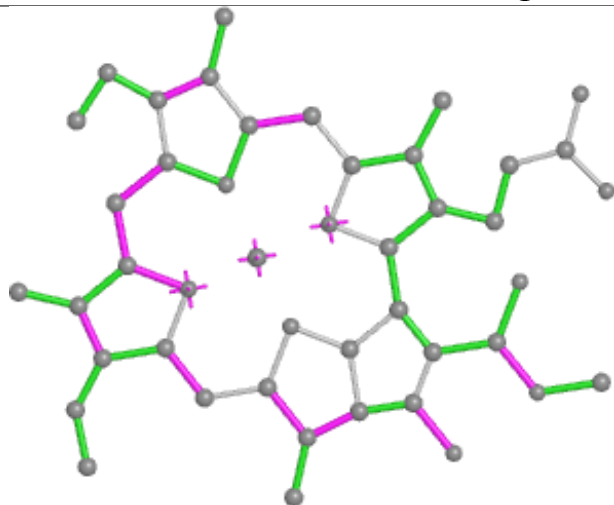
## Ligand CLA H 837



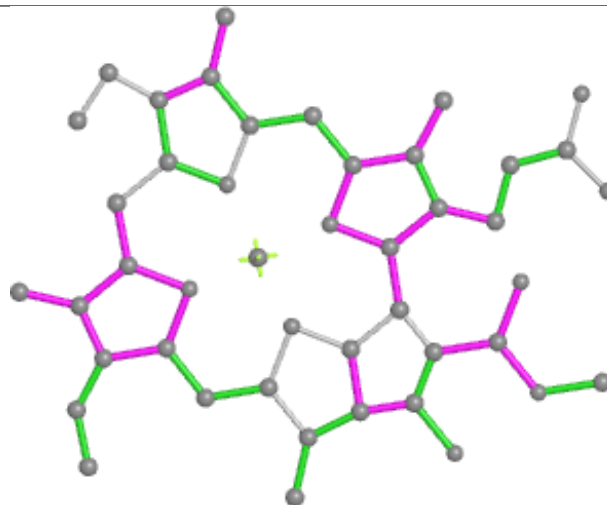
## Ligand CLA L 205



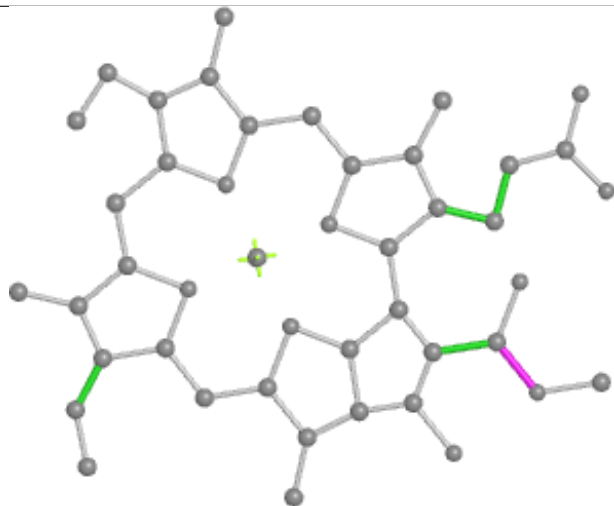
## Ligand CLA F 202



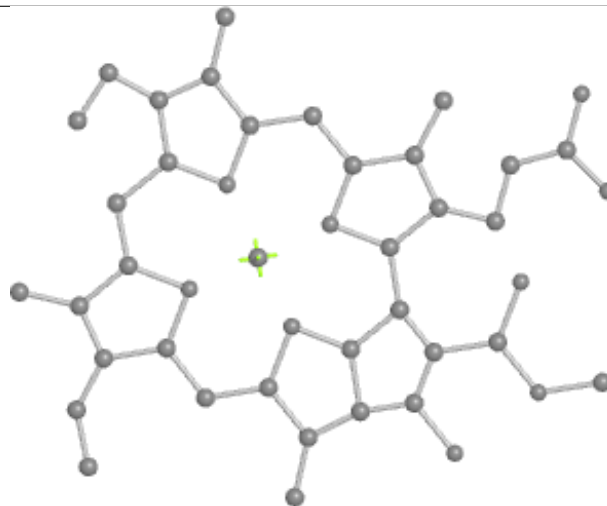
Bond lengths



Bond angles

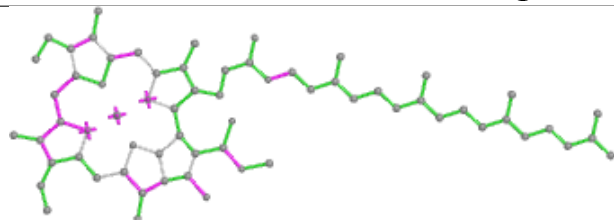


Torsions

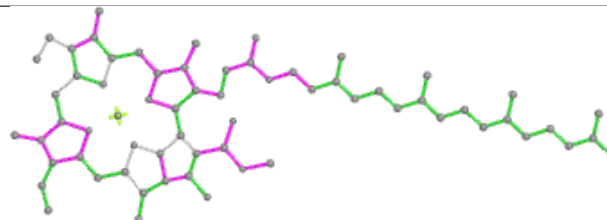


Rings

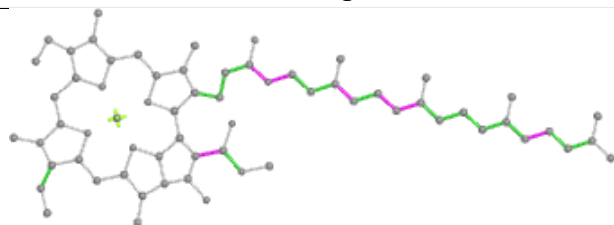
## Ligand CLA Y 830



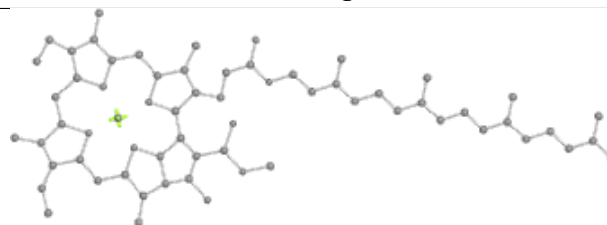
Bond lengths



Bond angles

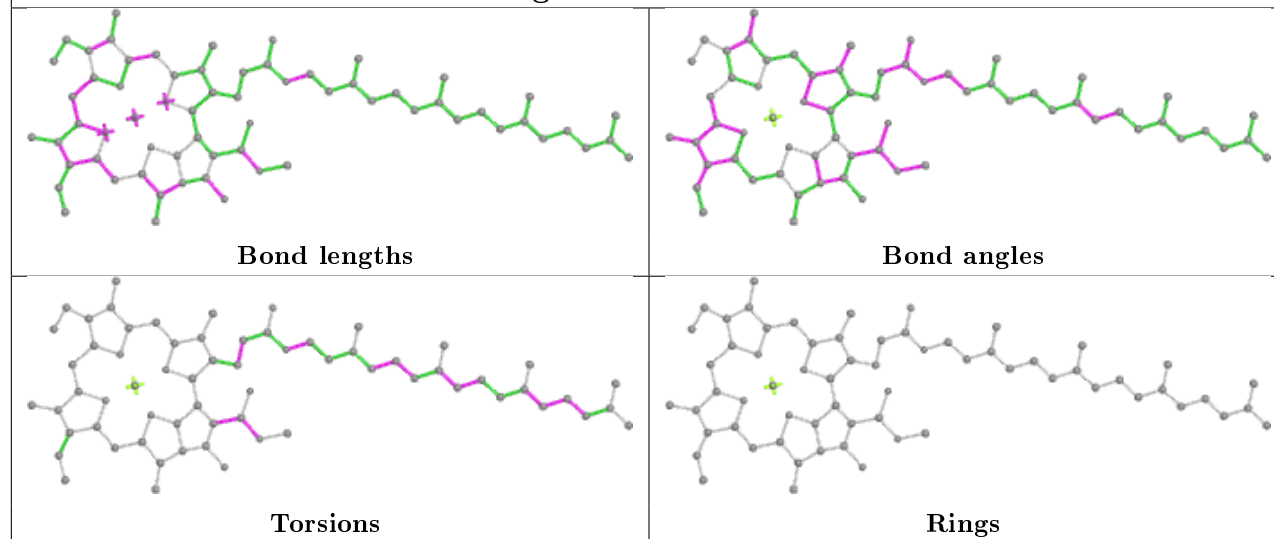


Torsions

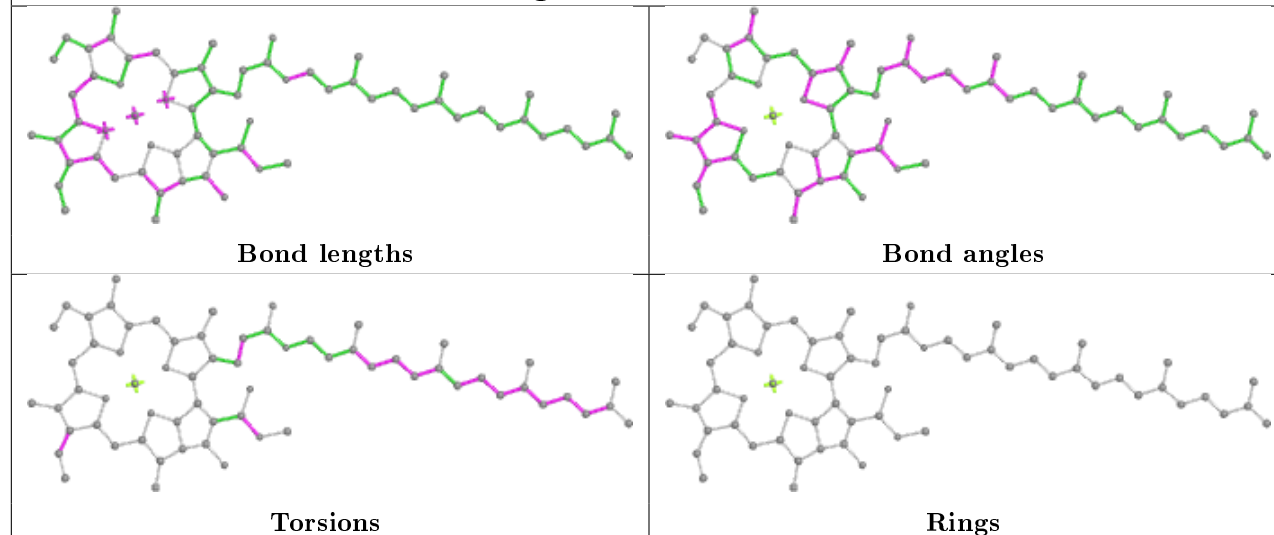


Rings

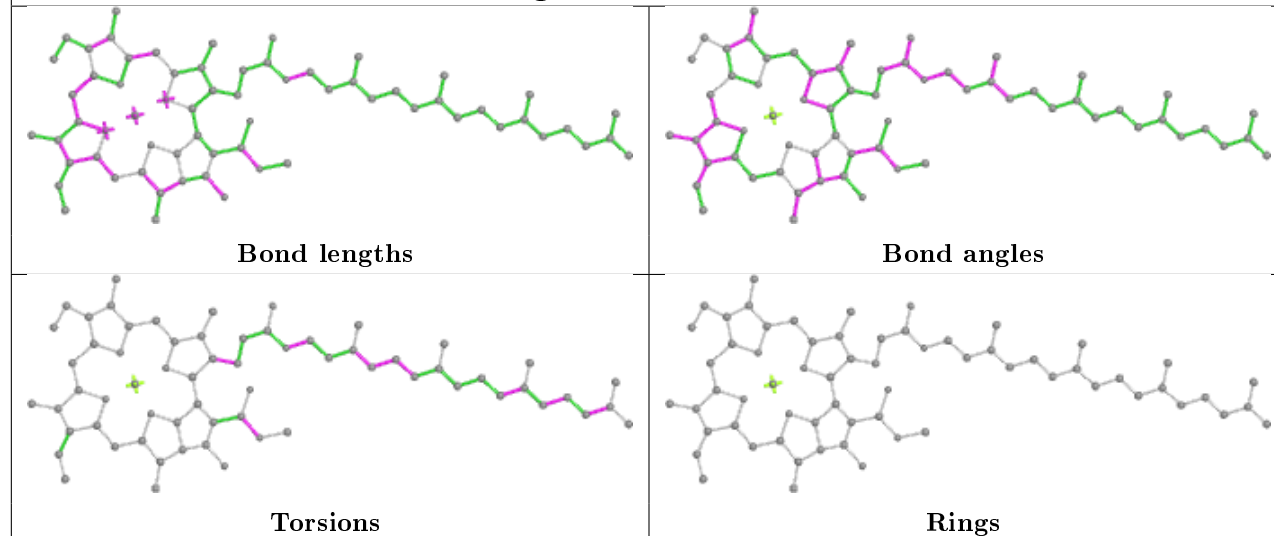
## Ligand CLA Y 825



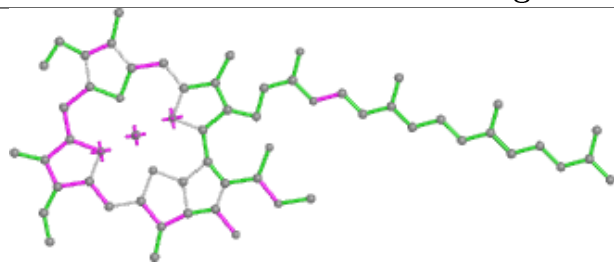
## Ligand CLA Y 809



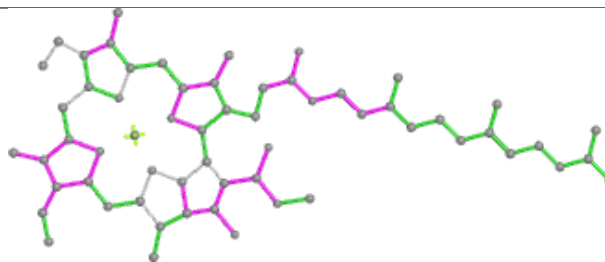
## Ligand CLA A 840



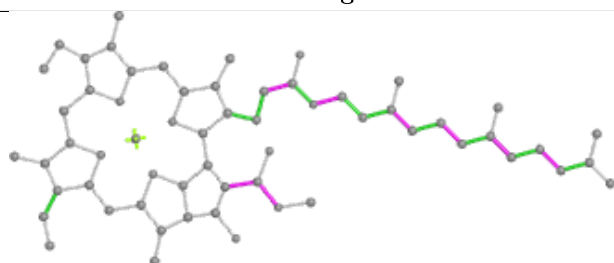
## Ligand CLA G 813



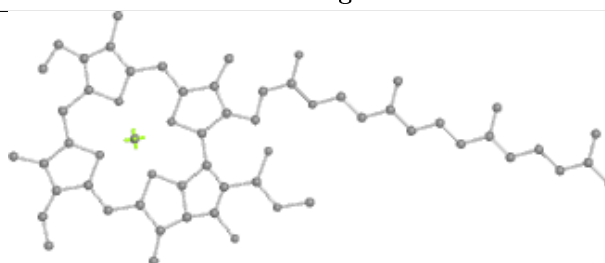
Bond lengths



Bond angles

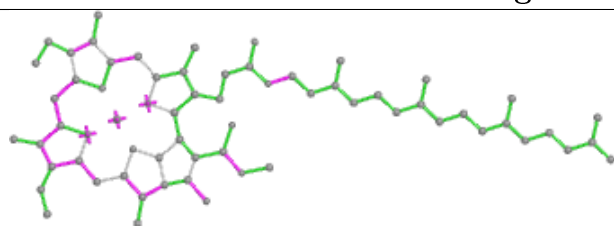


Torsions

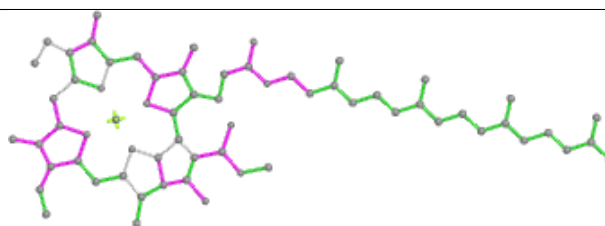


Rings

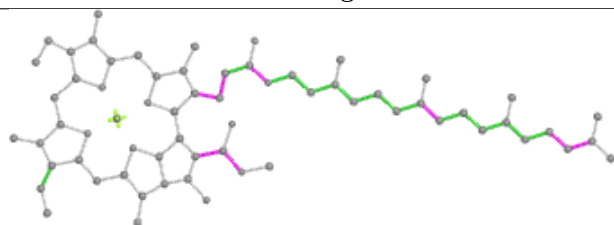
## Ligand CLA Y 840



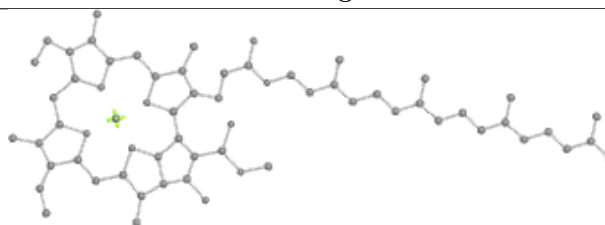
Bond lengths



Bond angles

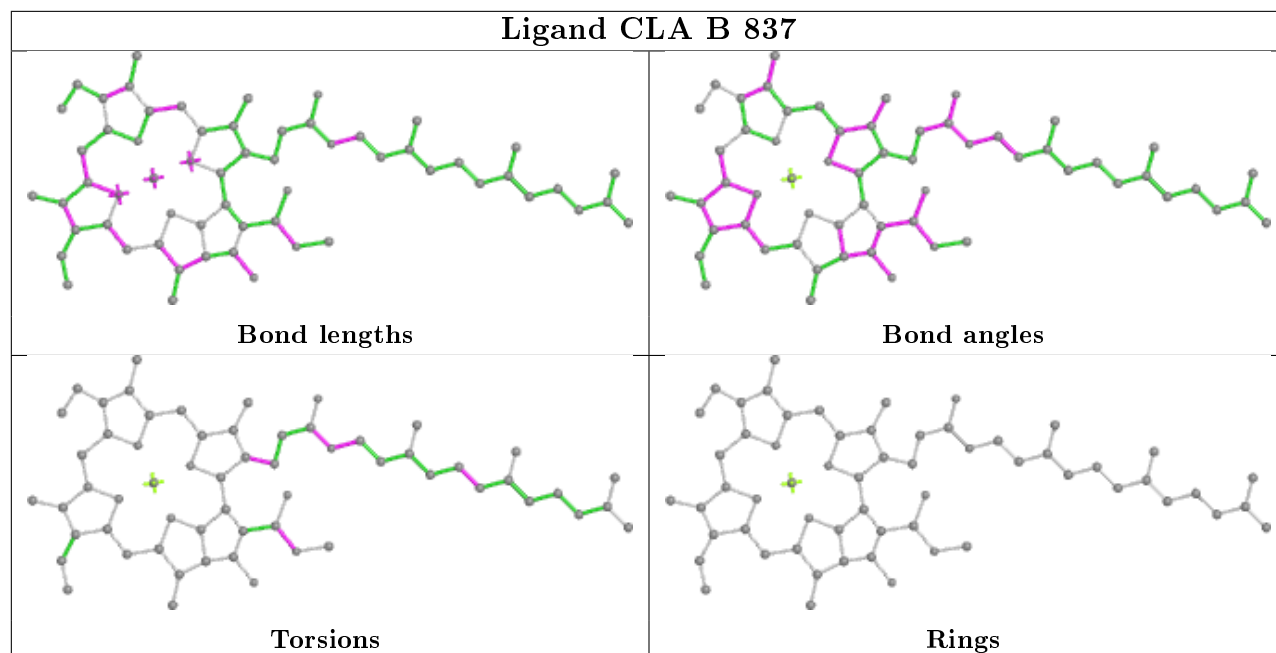


Torsions

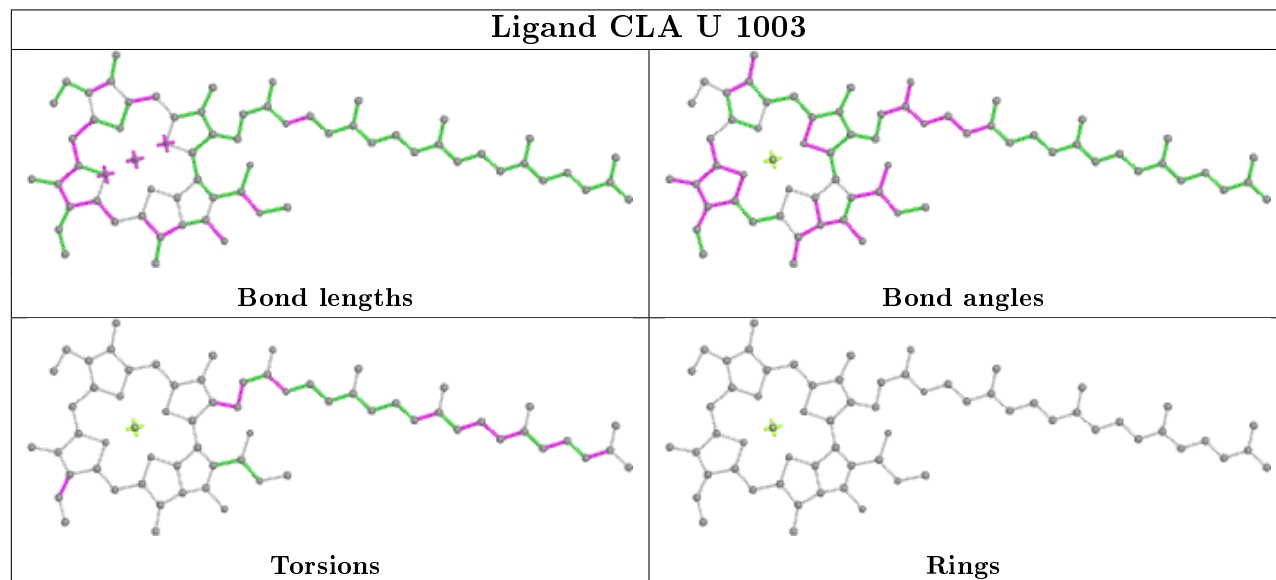


Rings

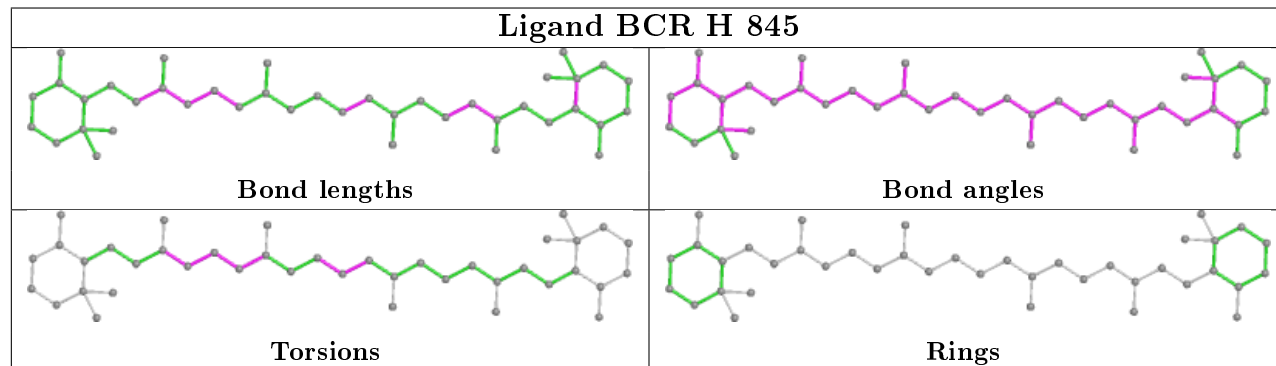
## Ligand CLA B 837



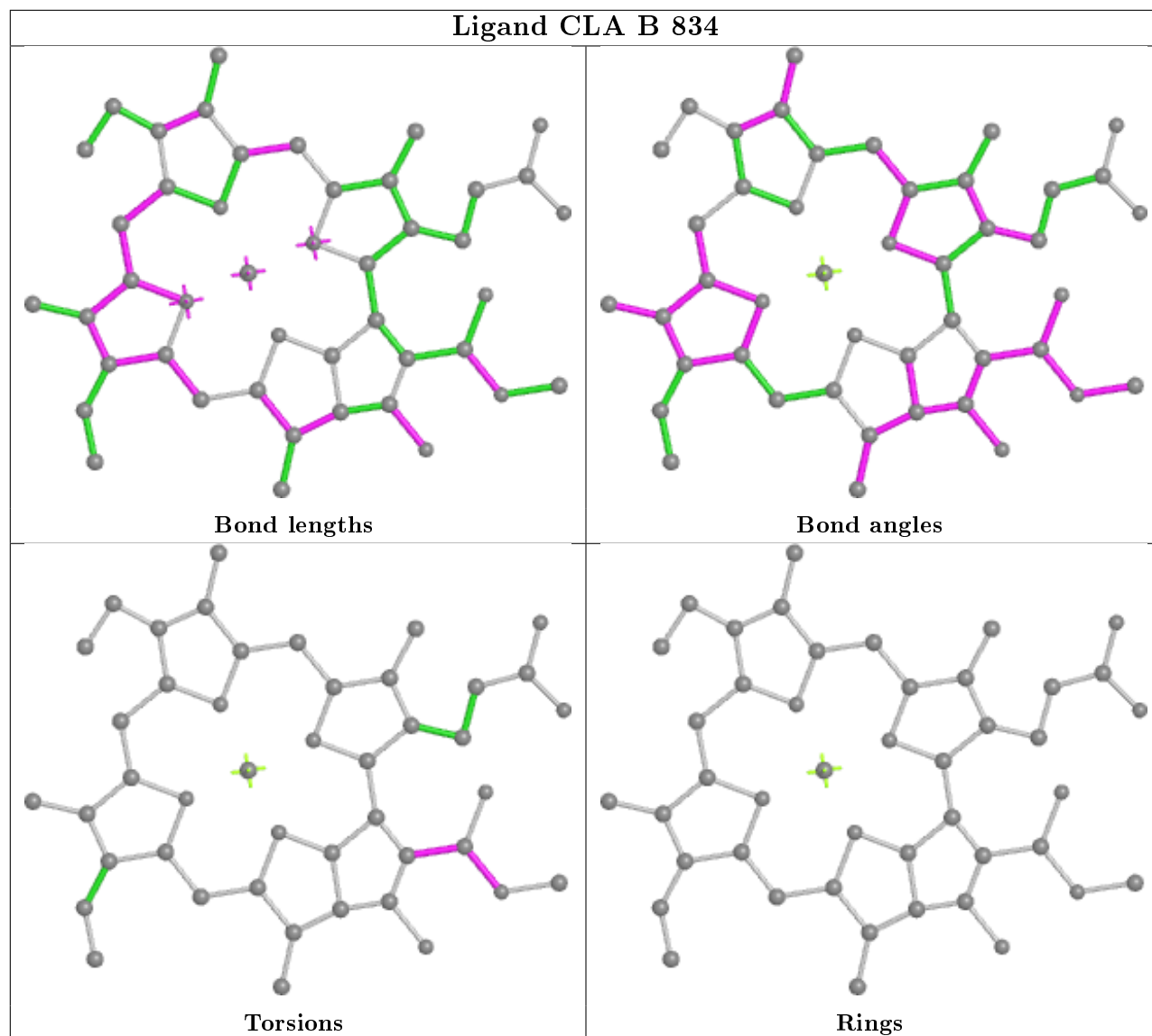
## Ligand CLA U 1003



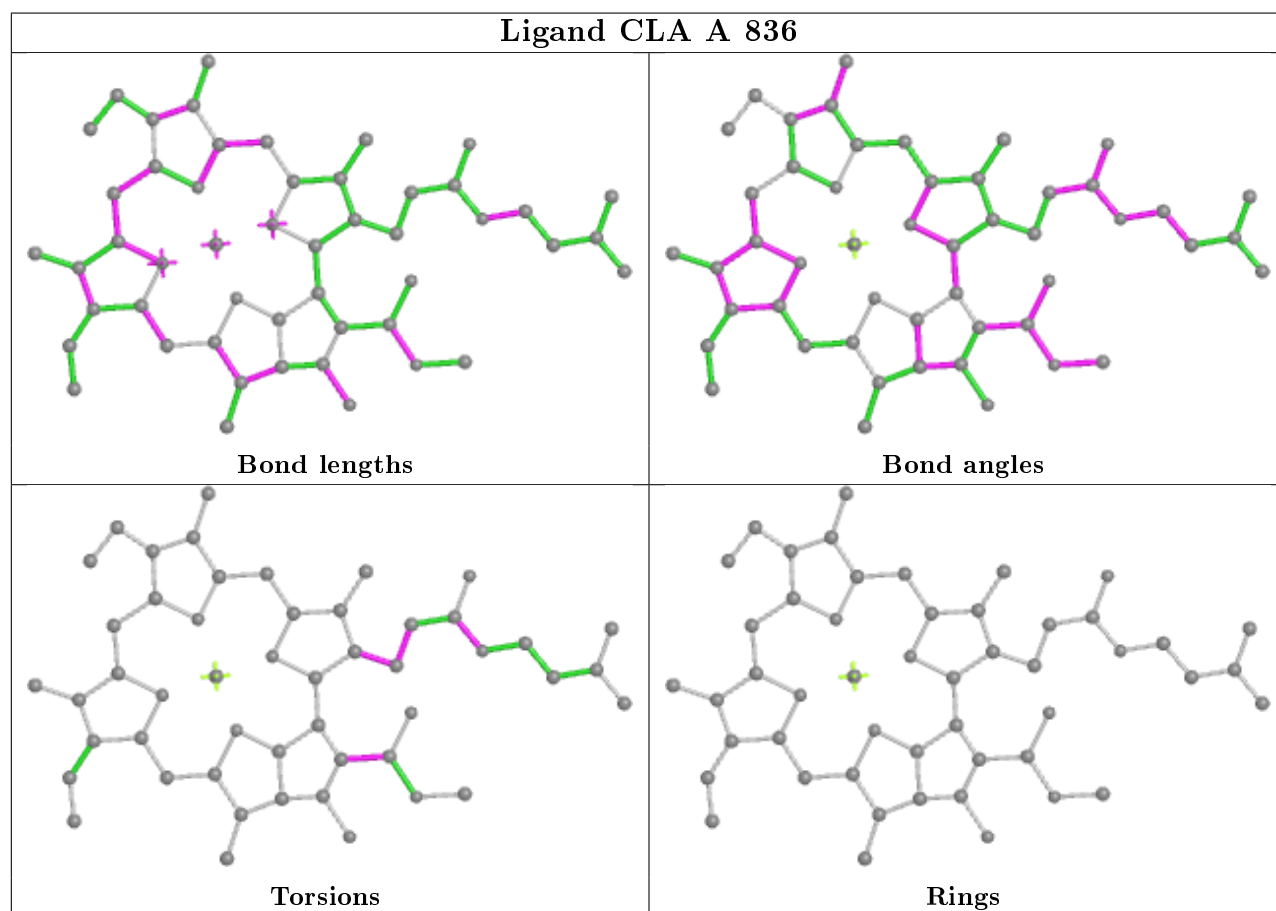
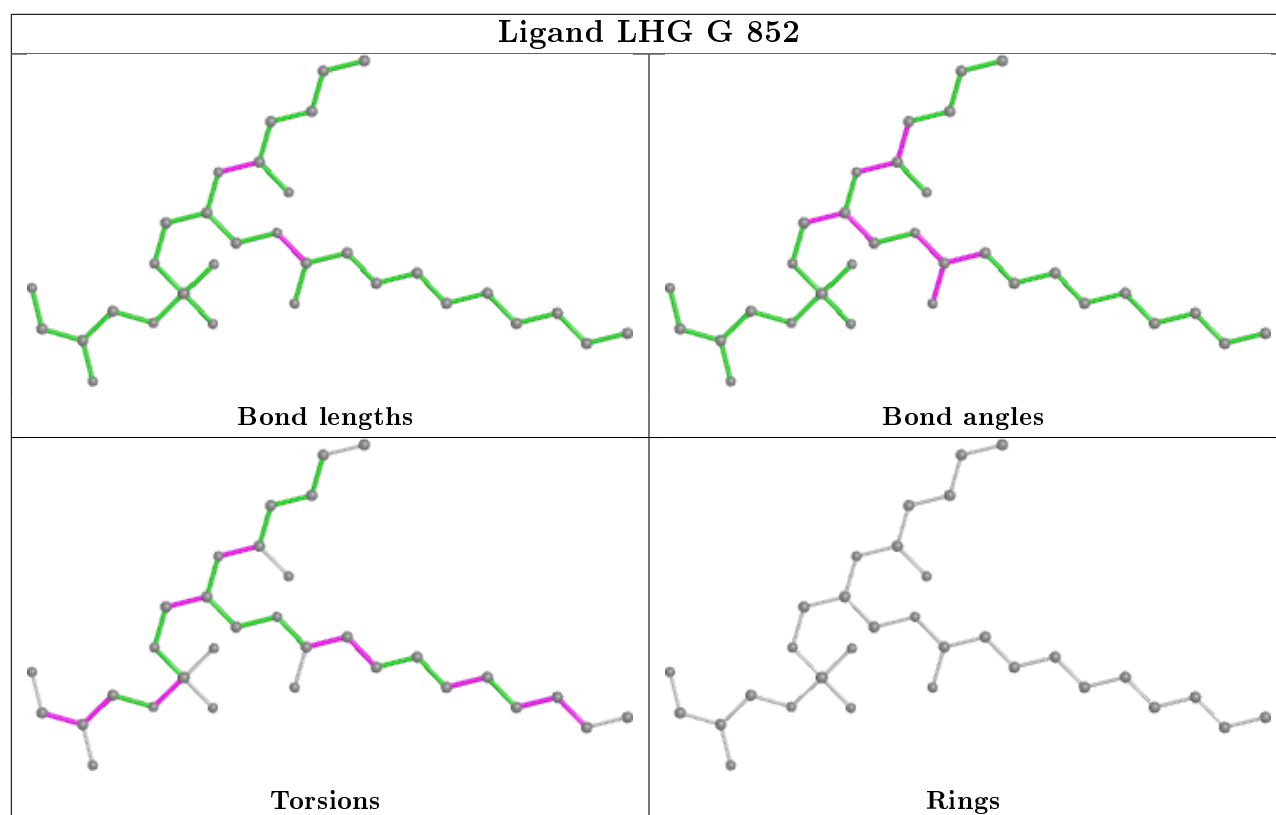
## Ligand BCR H 845



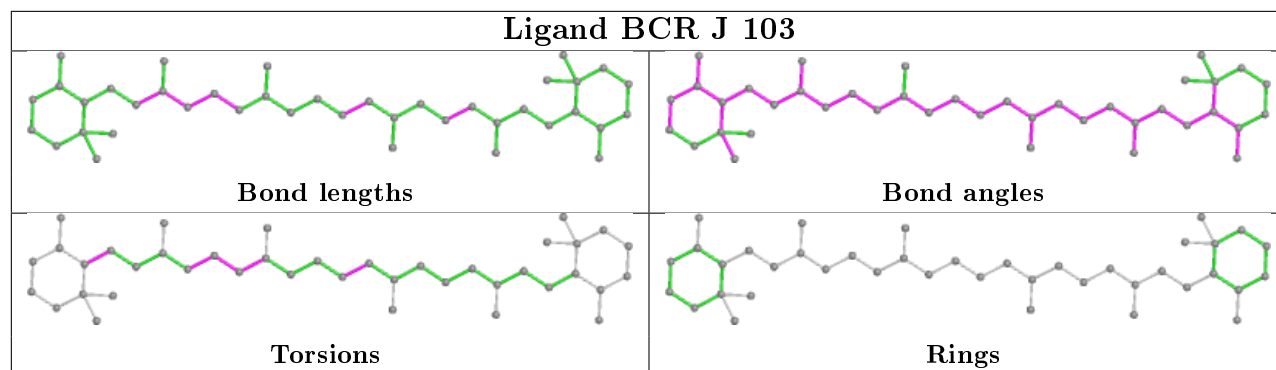
## Ligand CLA B 834



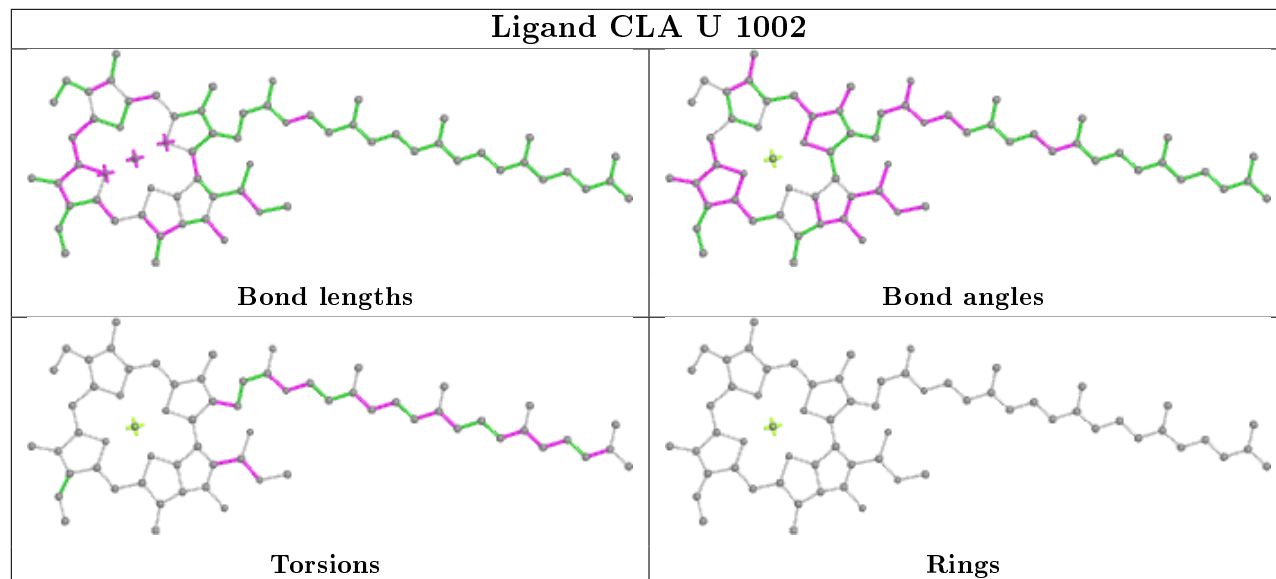




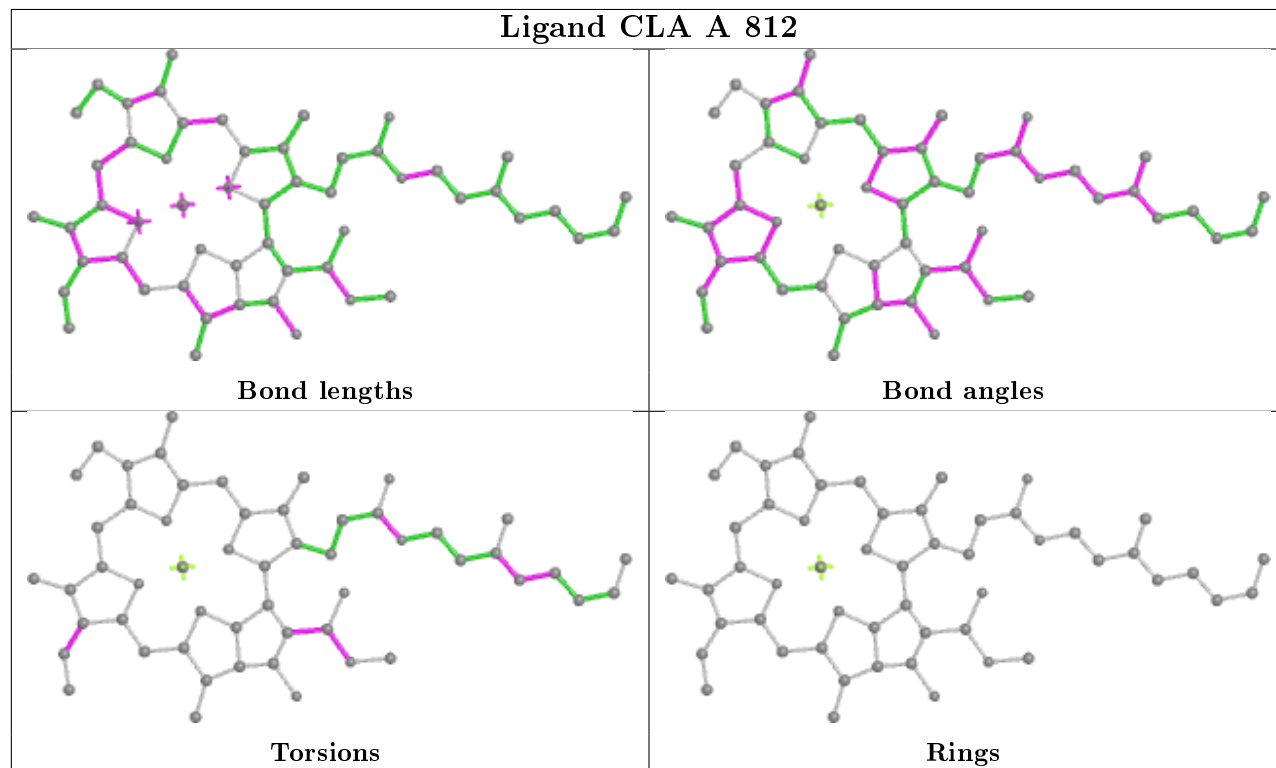
## Ligand BCR J 103

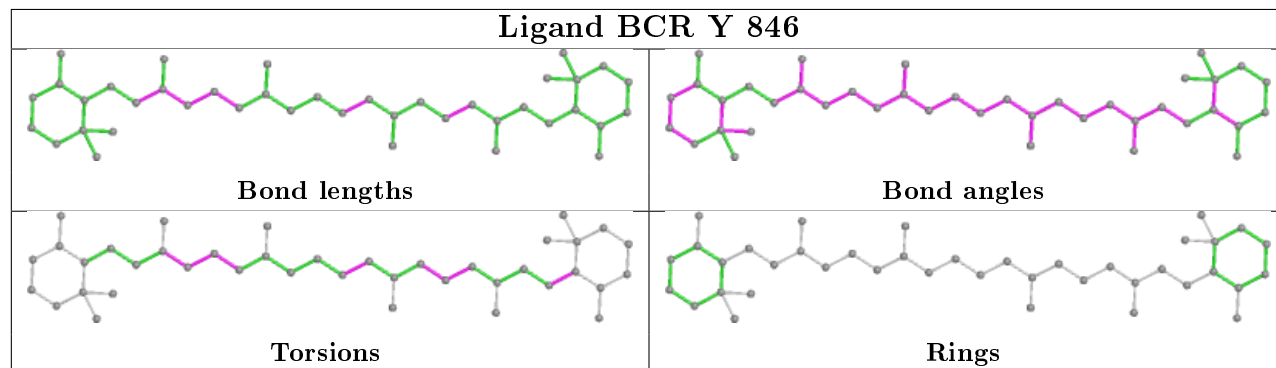
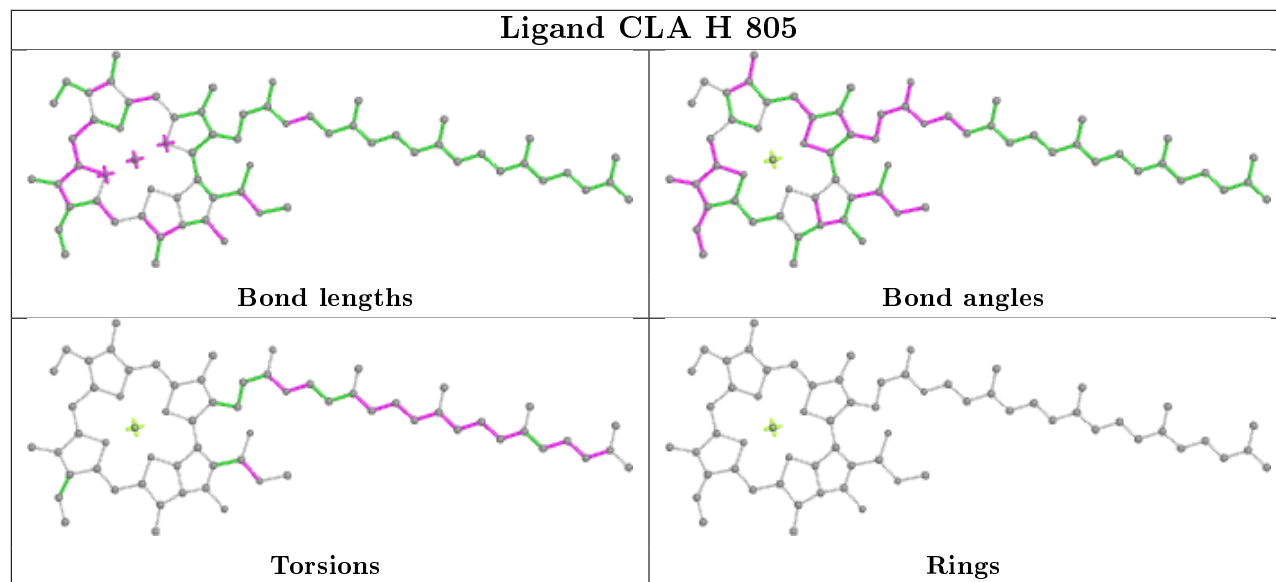
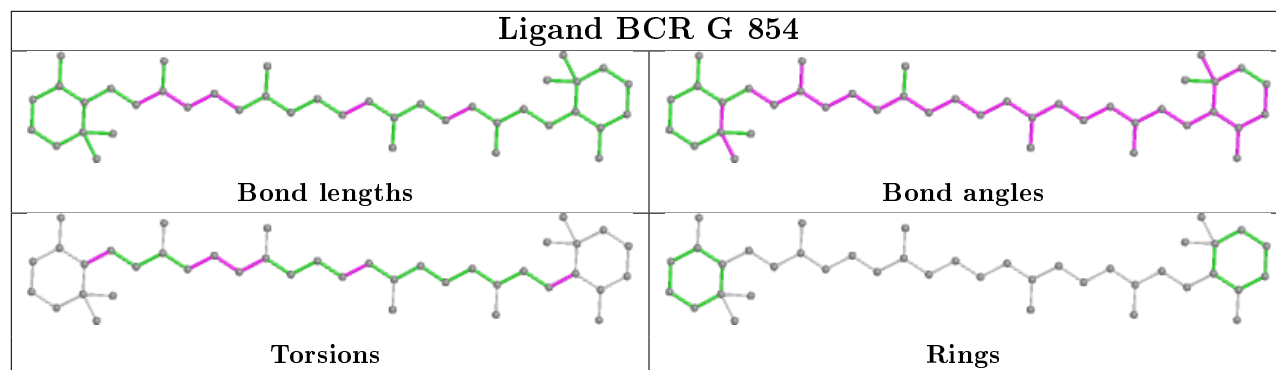
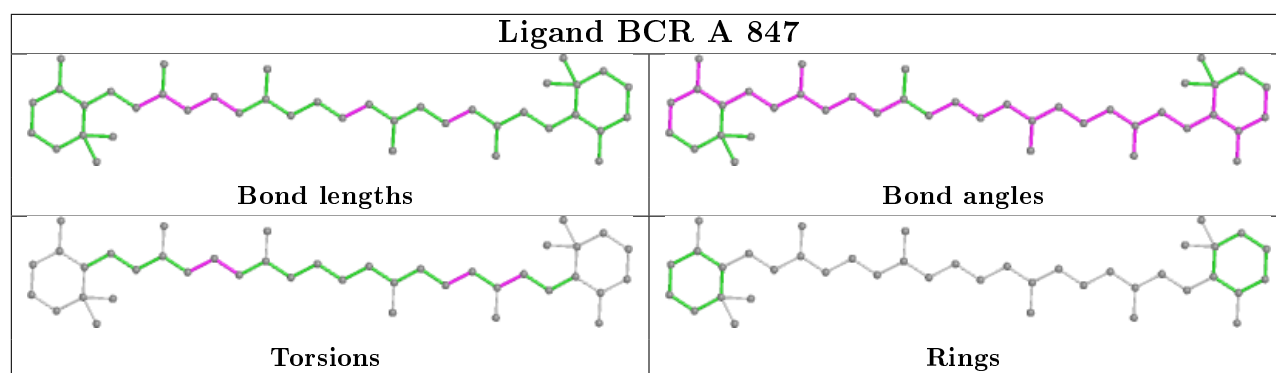


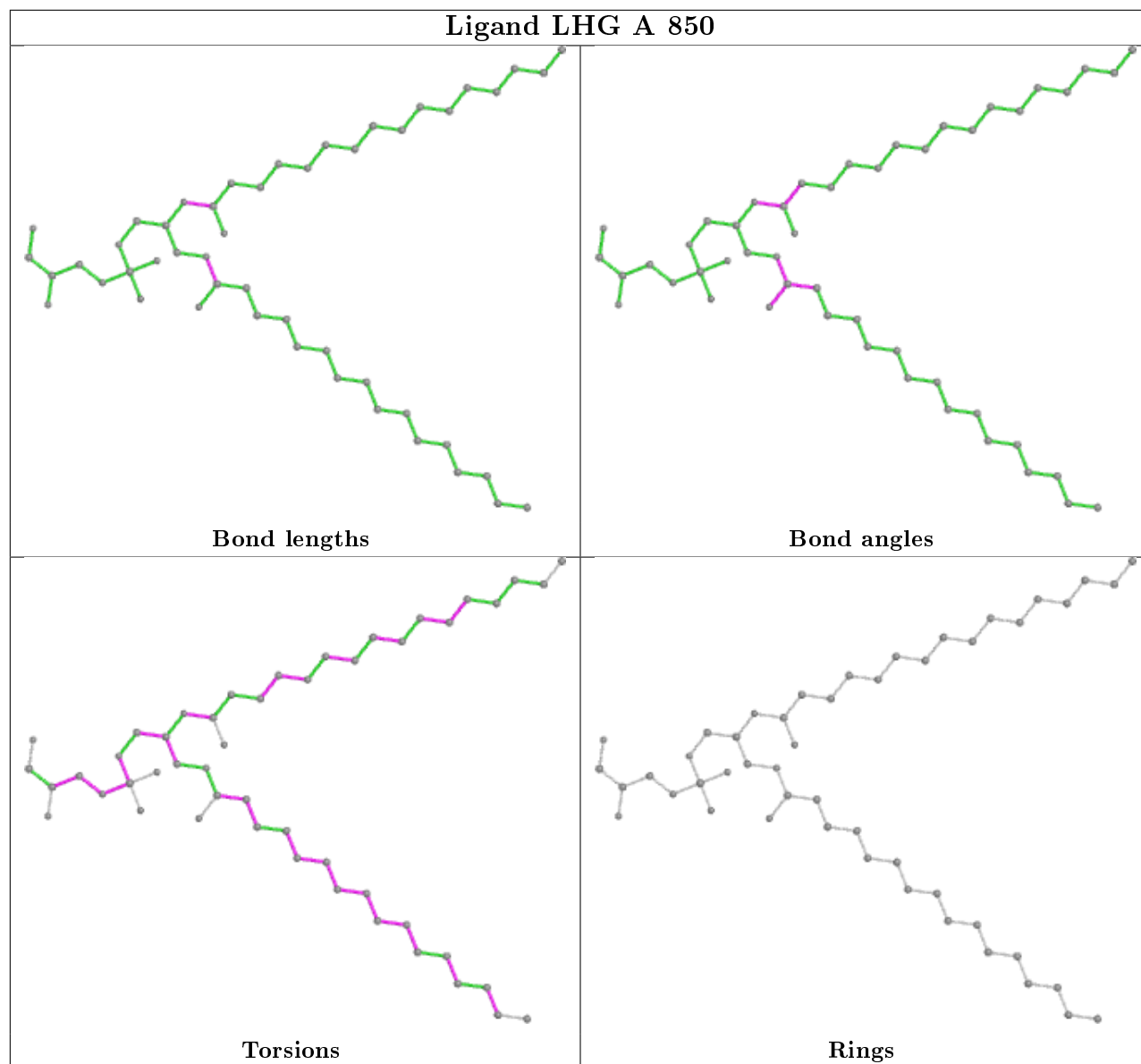
## Ligand CLA U 1002



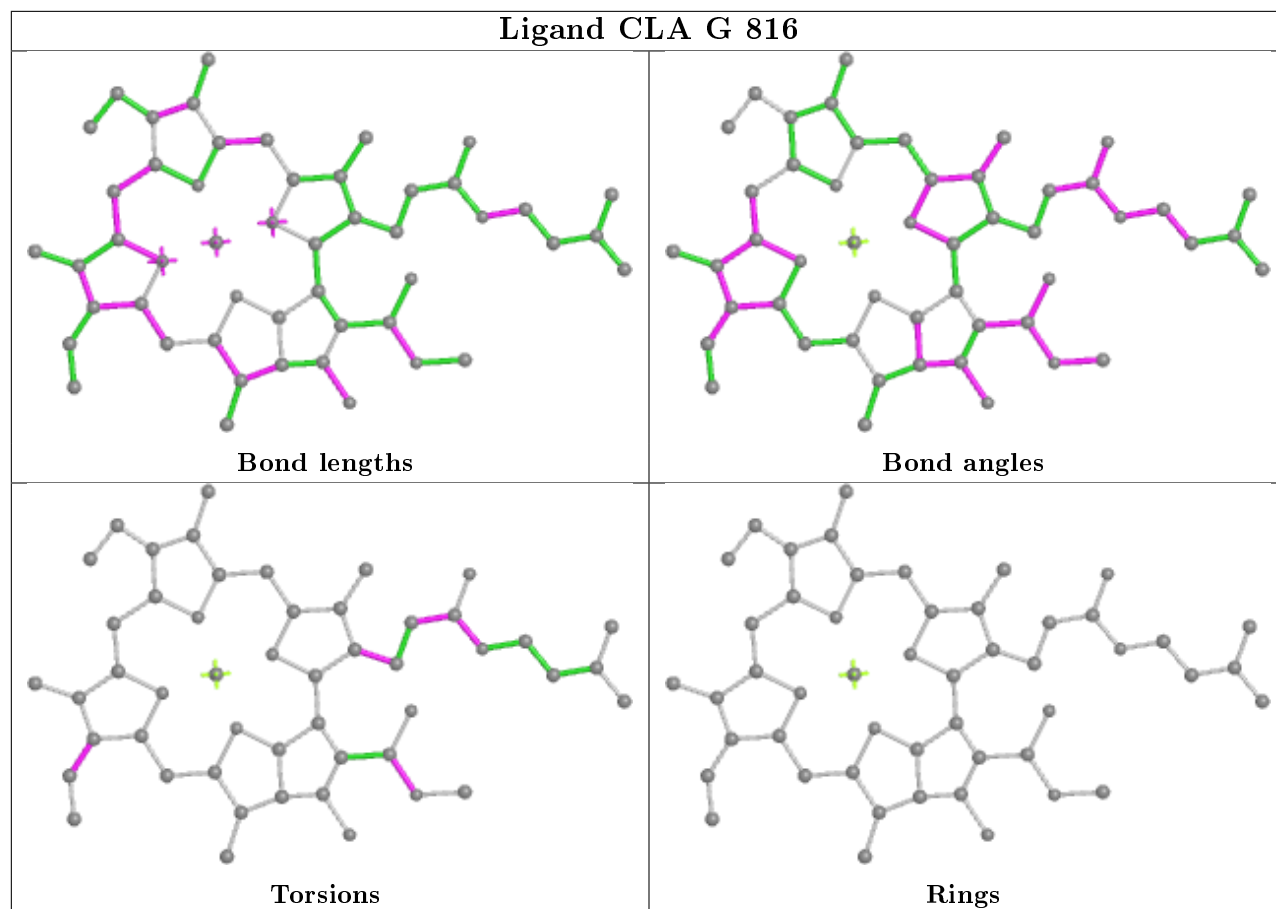
## Ligand CLA A 812



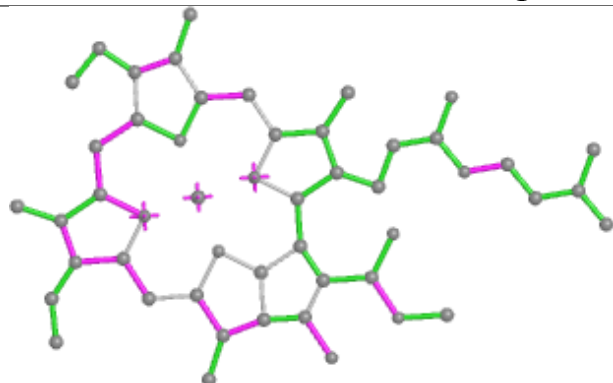




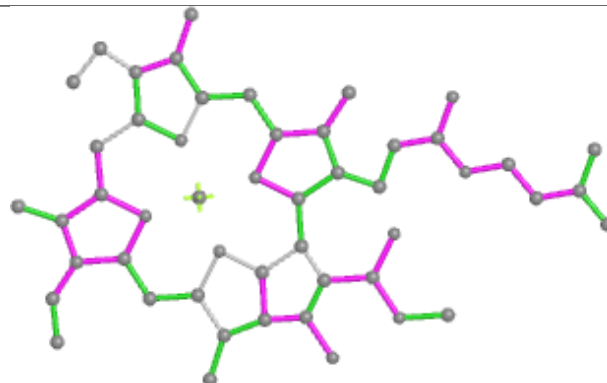
## Ligand CLA G 816



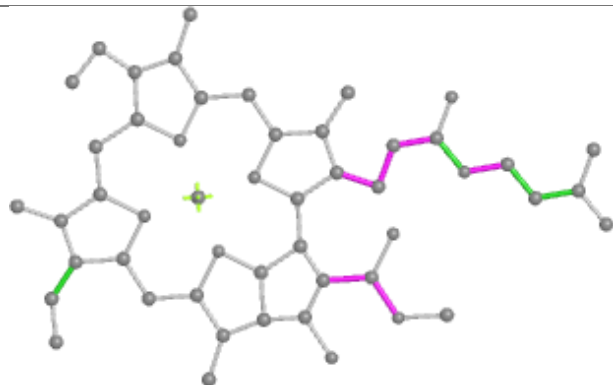
## Ligand CLA G 836



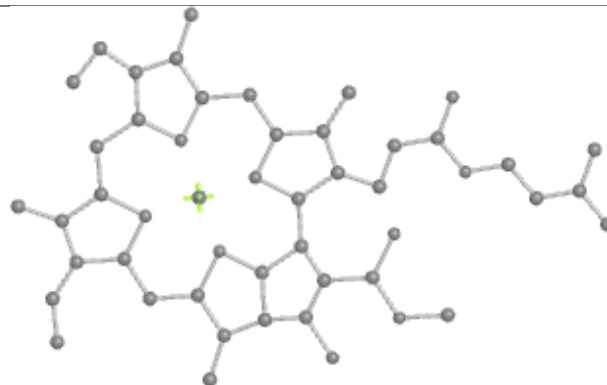
Bond lengths



Bond angles

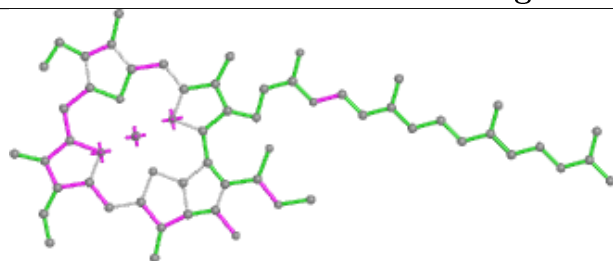


Torsions

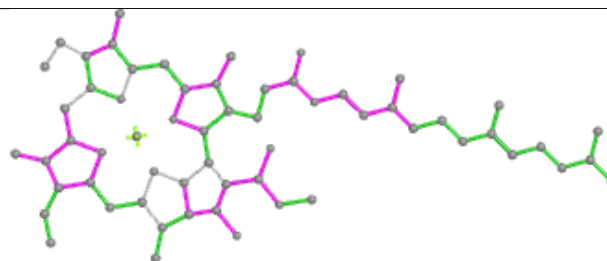


Rings

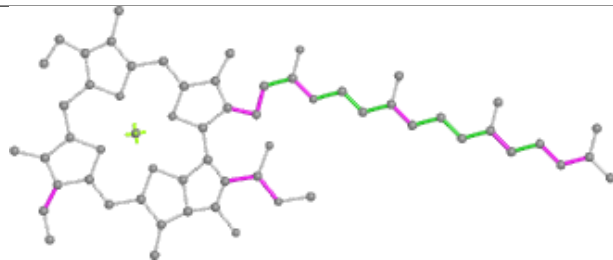
## Ligand CLA A 820



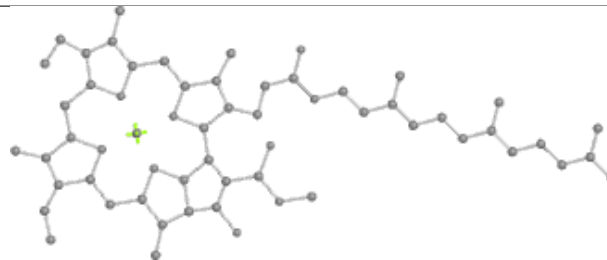
Bond lengths



Bond angles

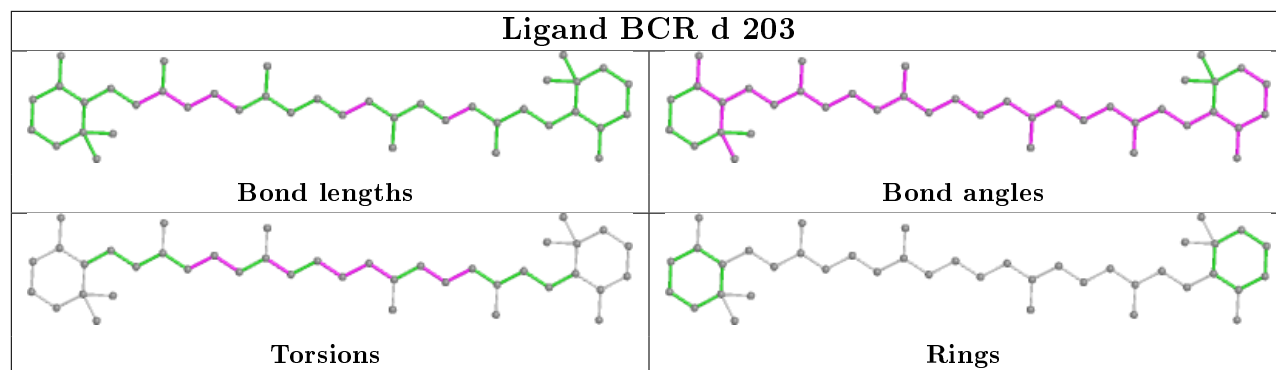


Torsions

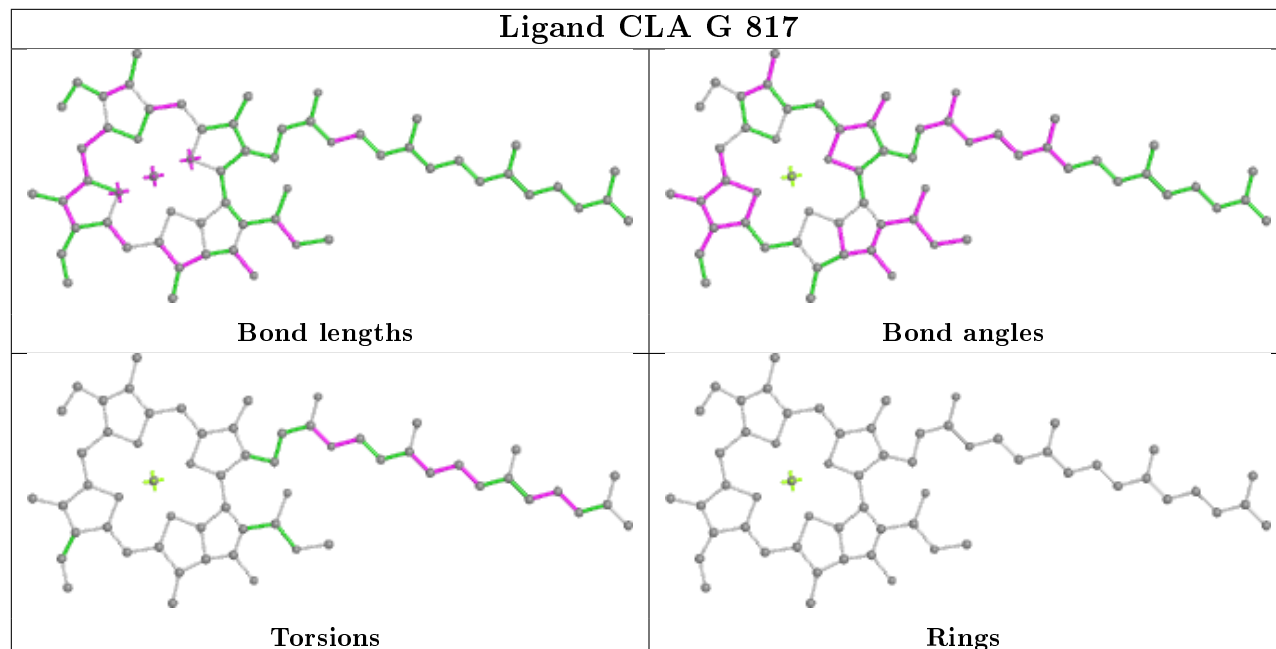


Rings

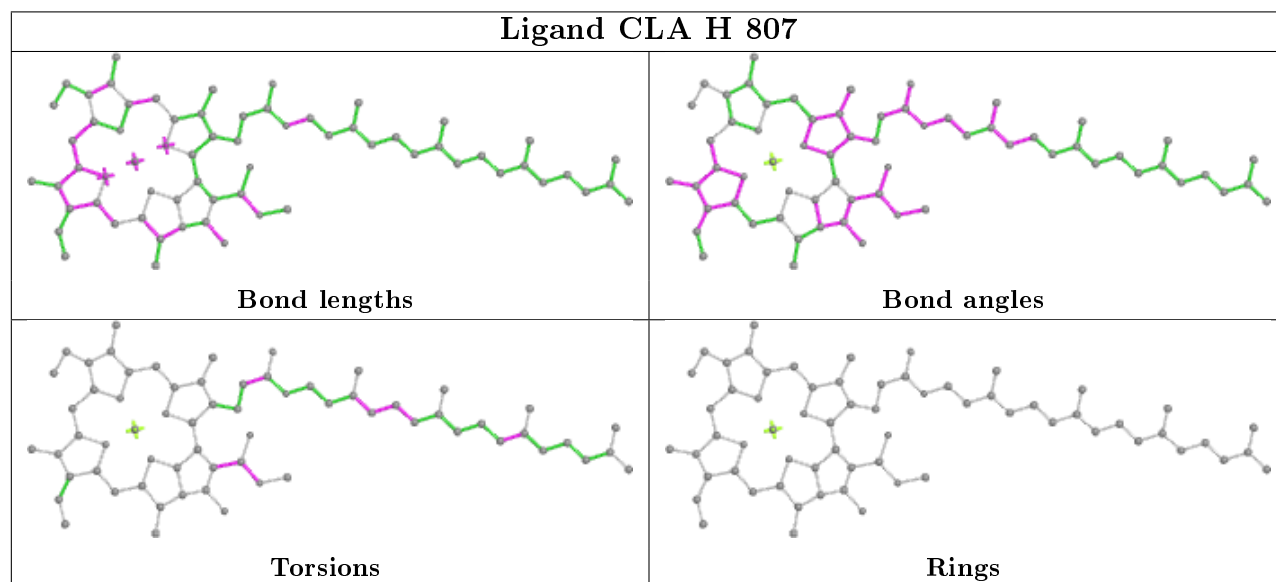
## Ligand BCR d 203



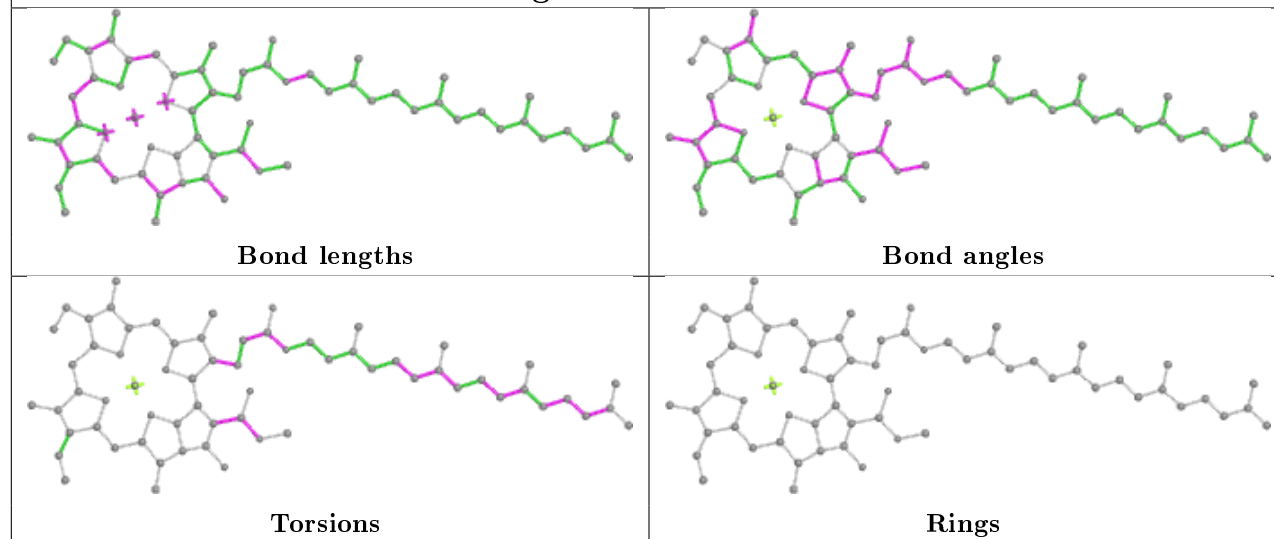
## Ligand CLA G 817



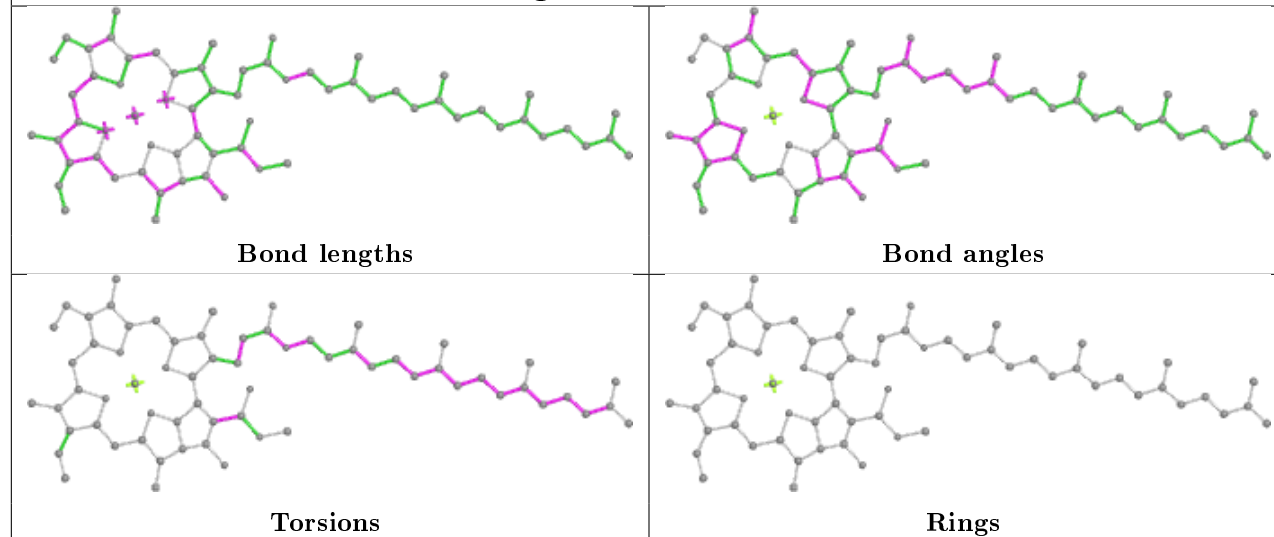
## Ligand CLA H 807



## Ligand CLA Y 811

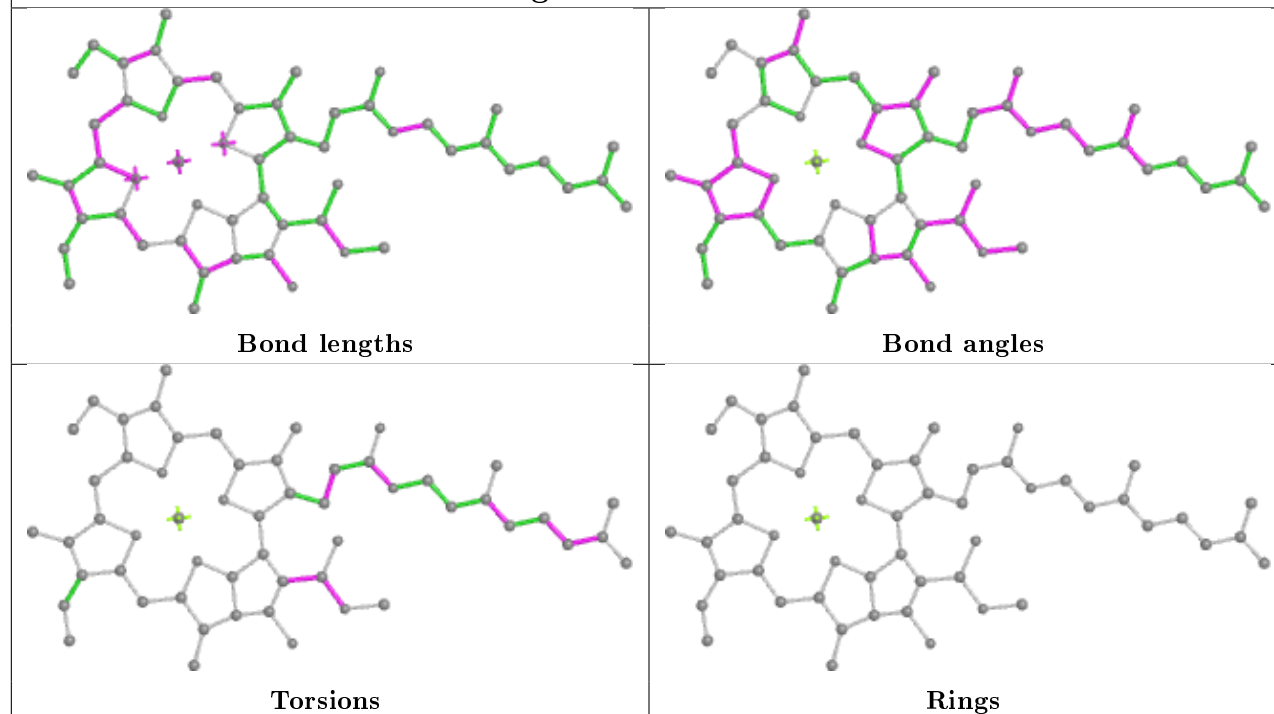


## Ligand CLA Y 838

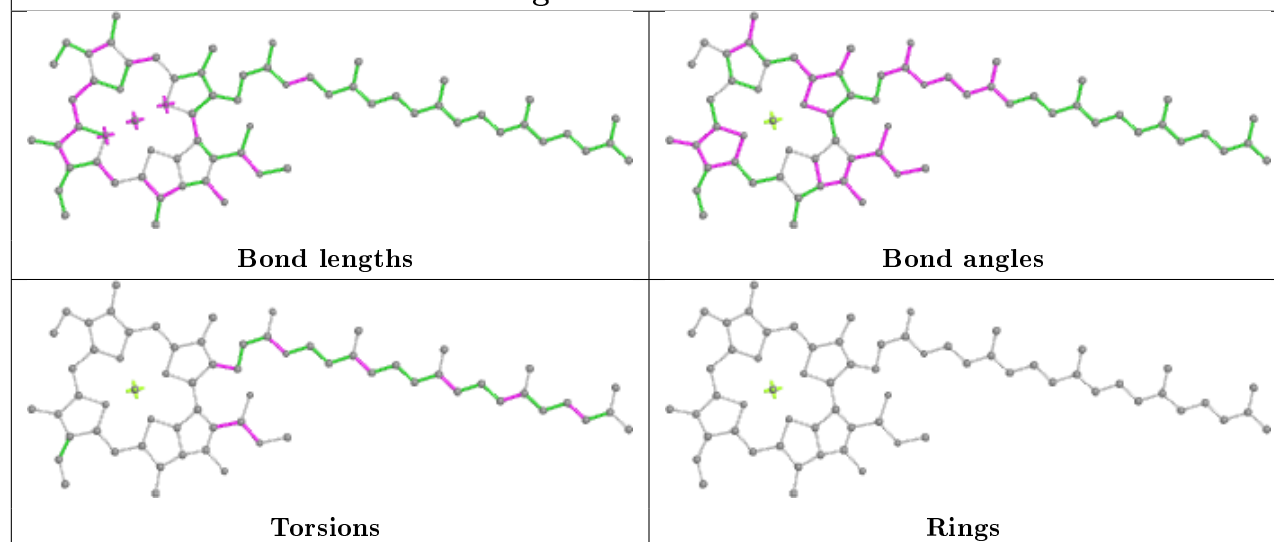




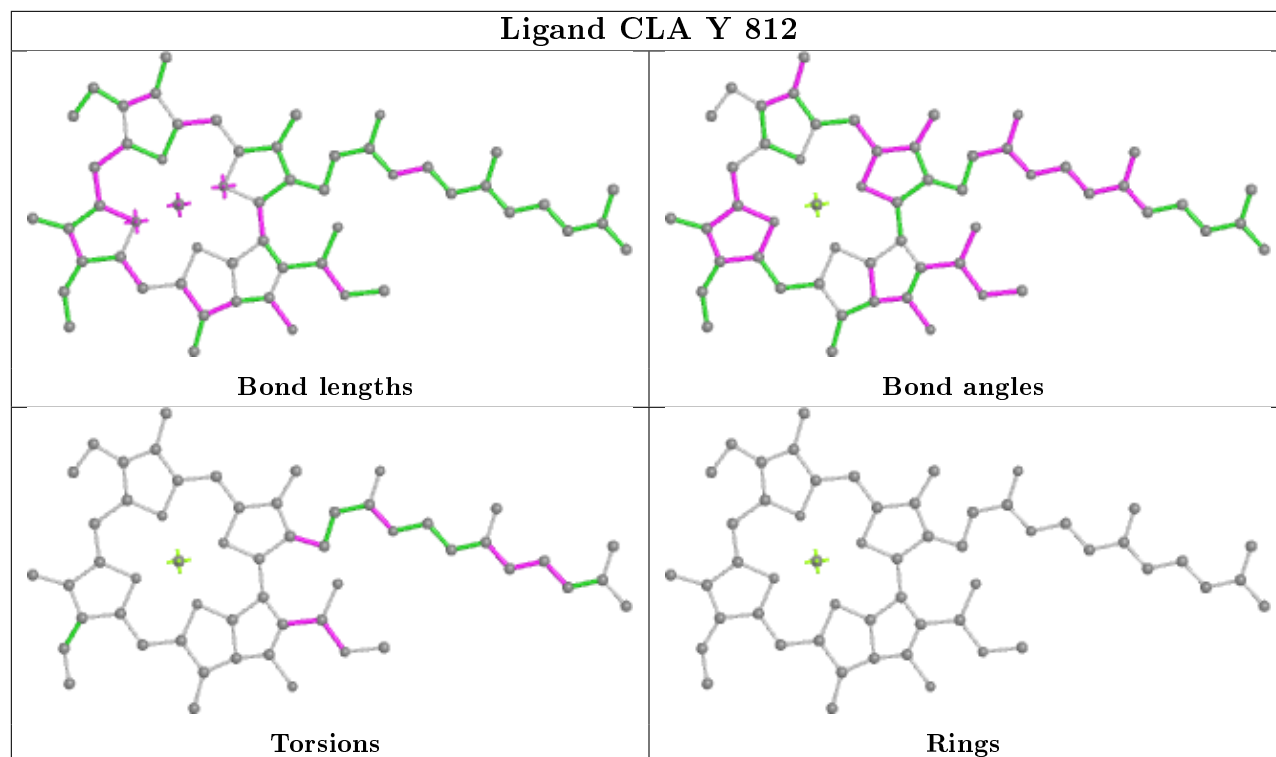
## Ligand CLA H 815



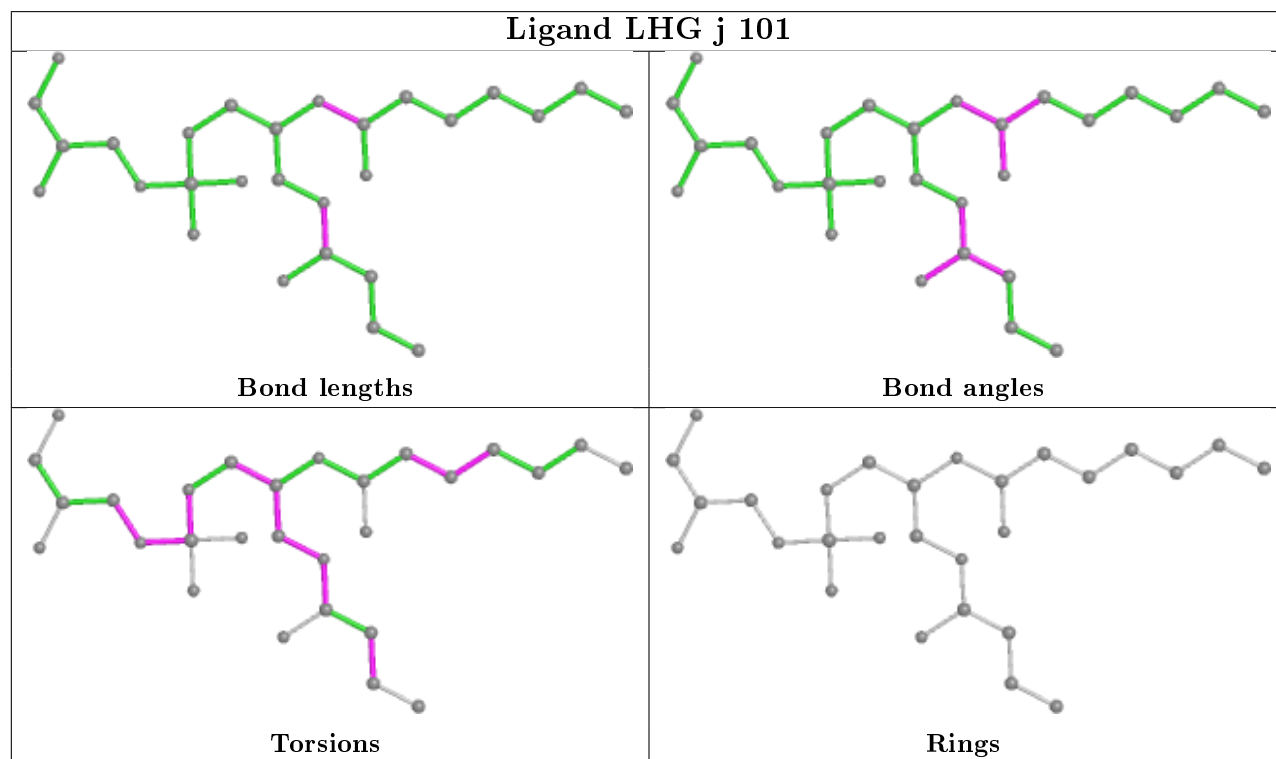
## Ligand CLA B 825



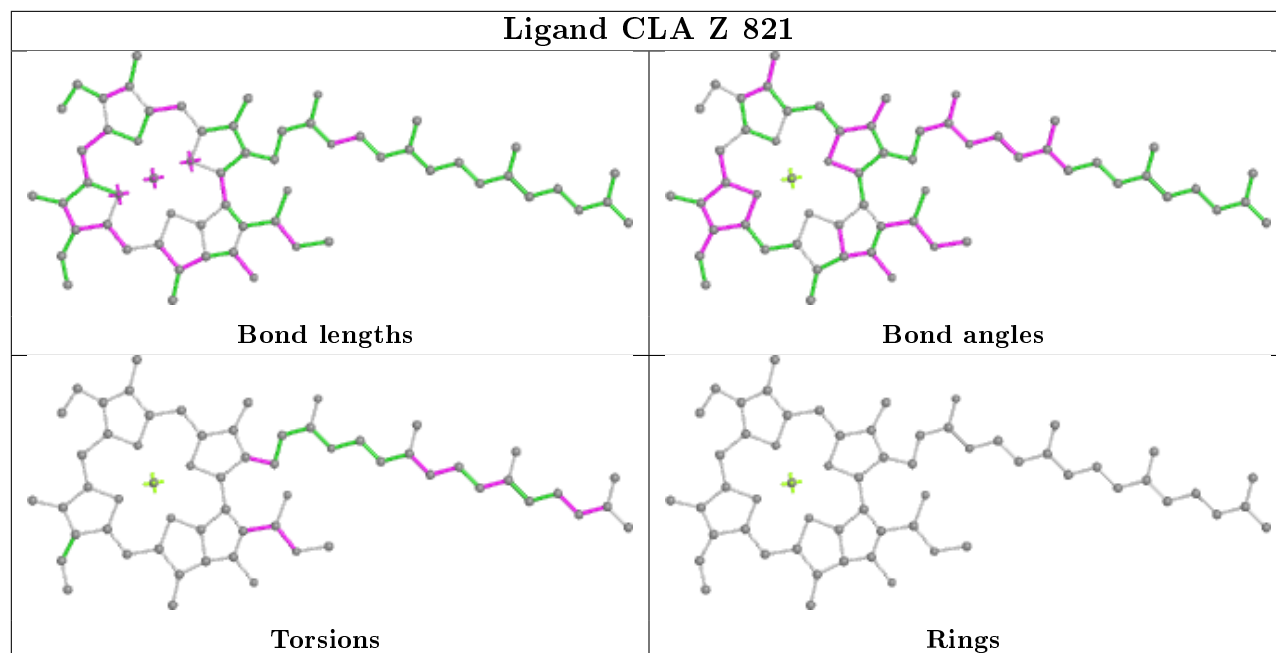
## Ligand CLA Y 812



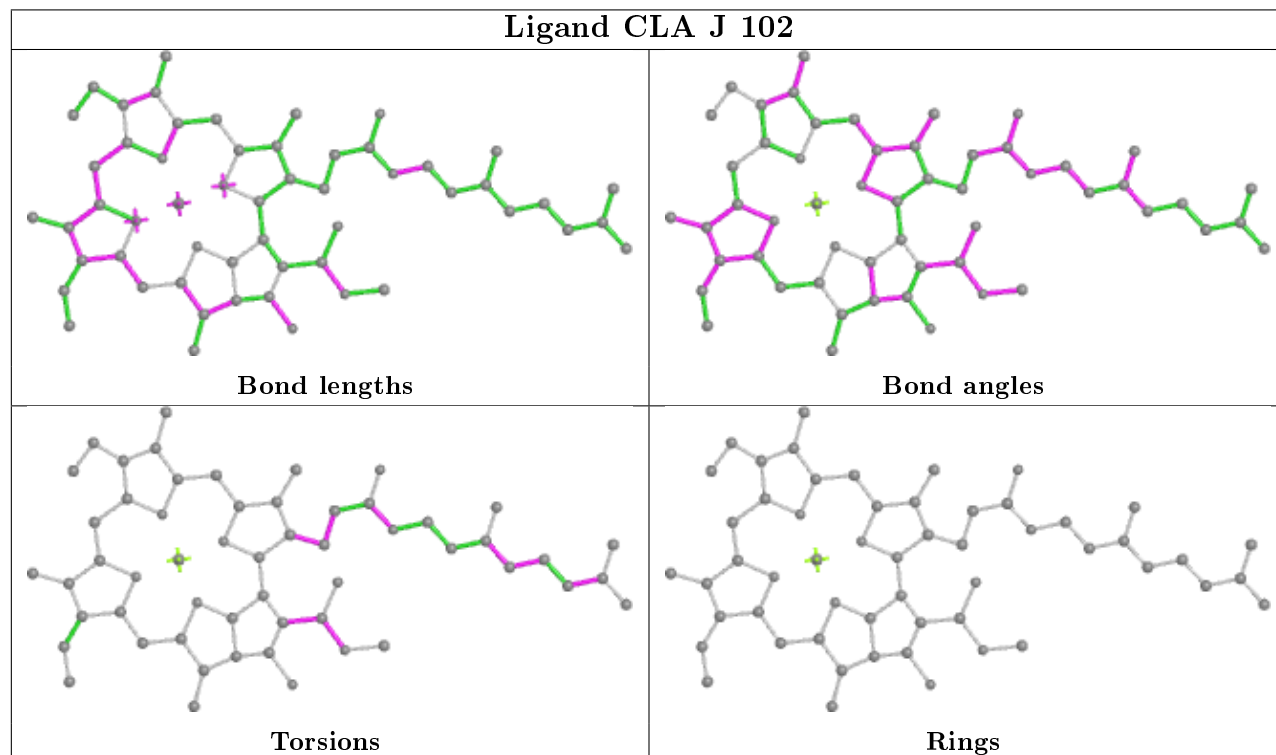
## Ligand LHG j 101



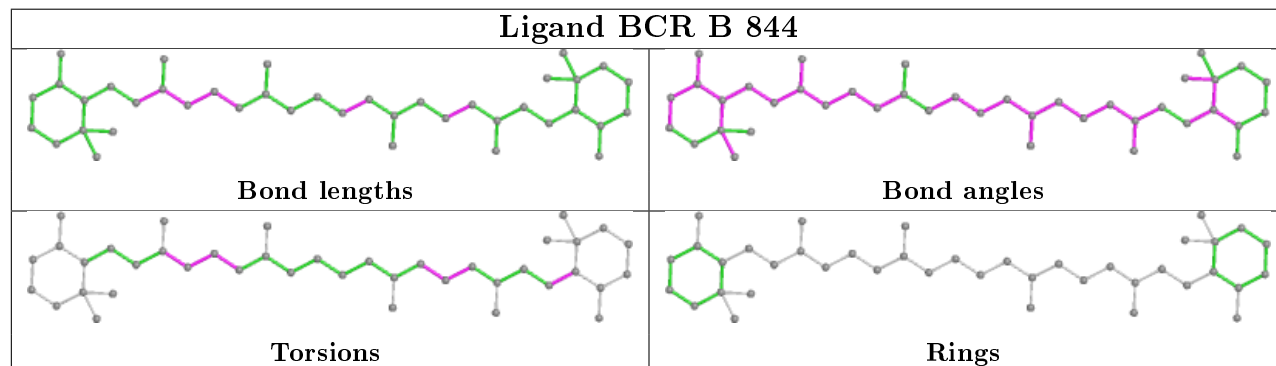
## Ligand CLA Z 821

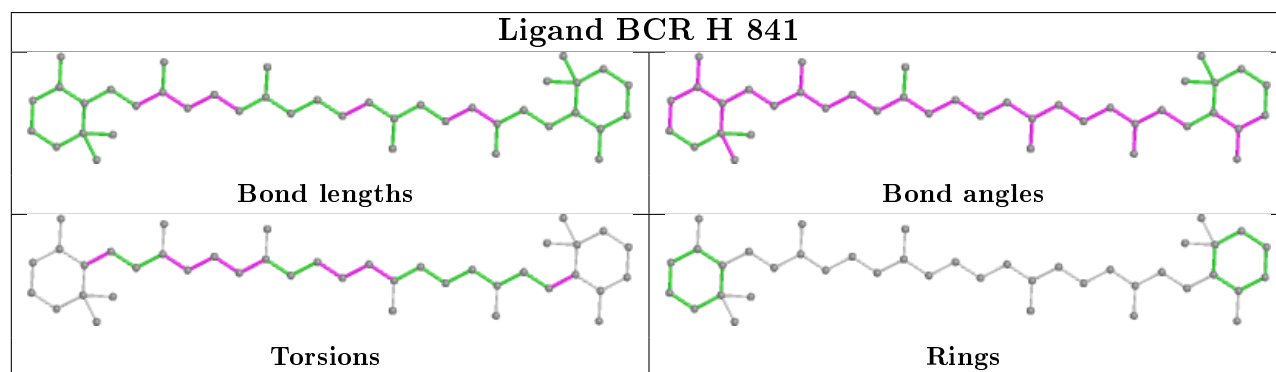
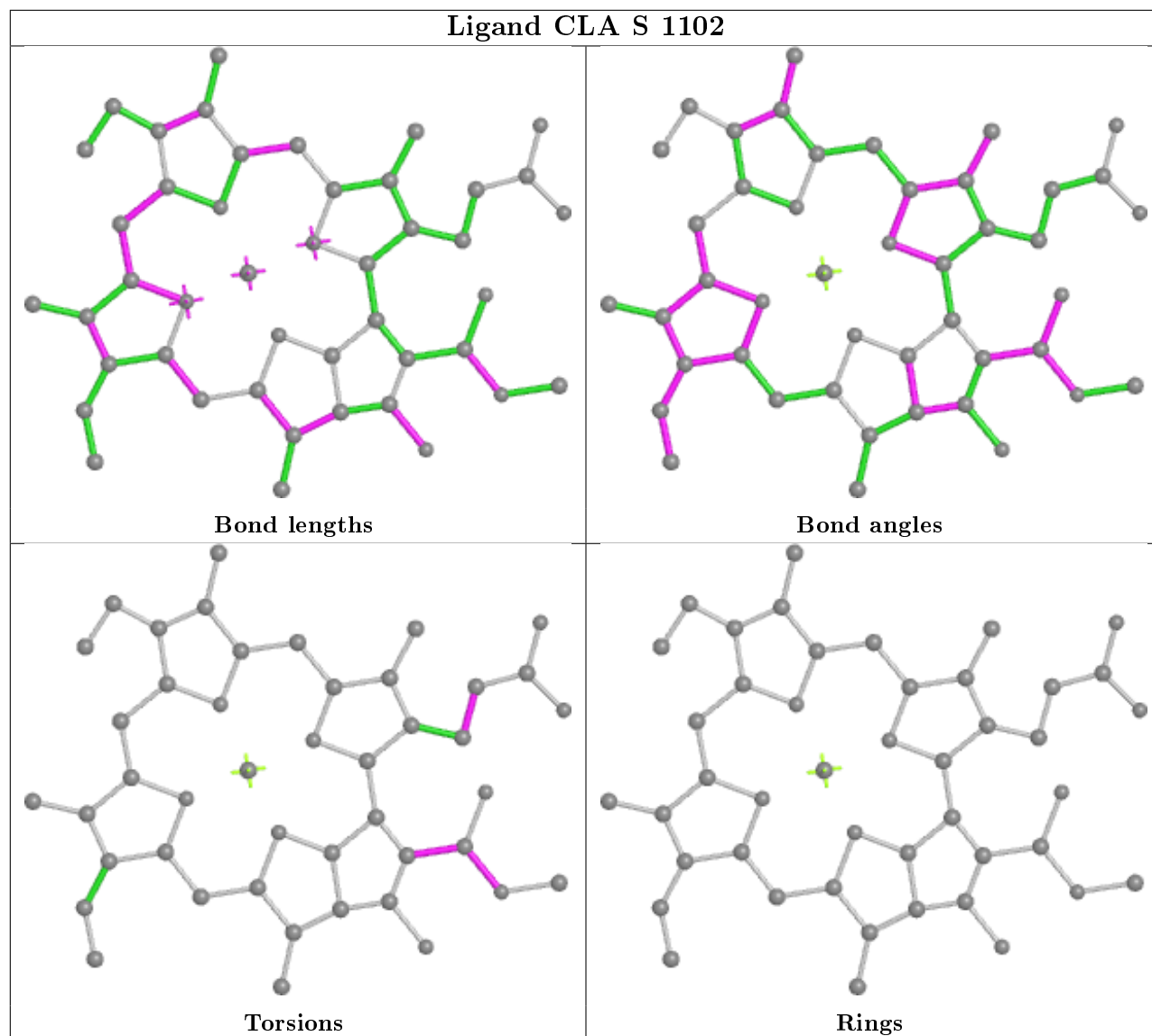


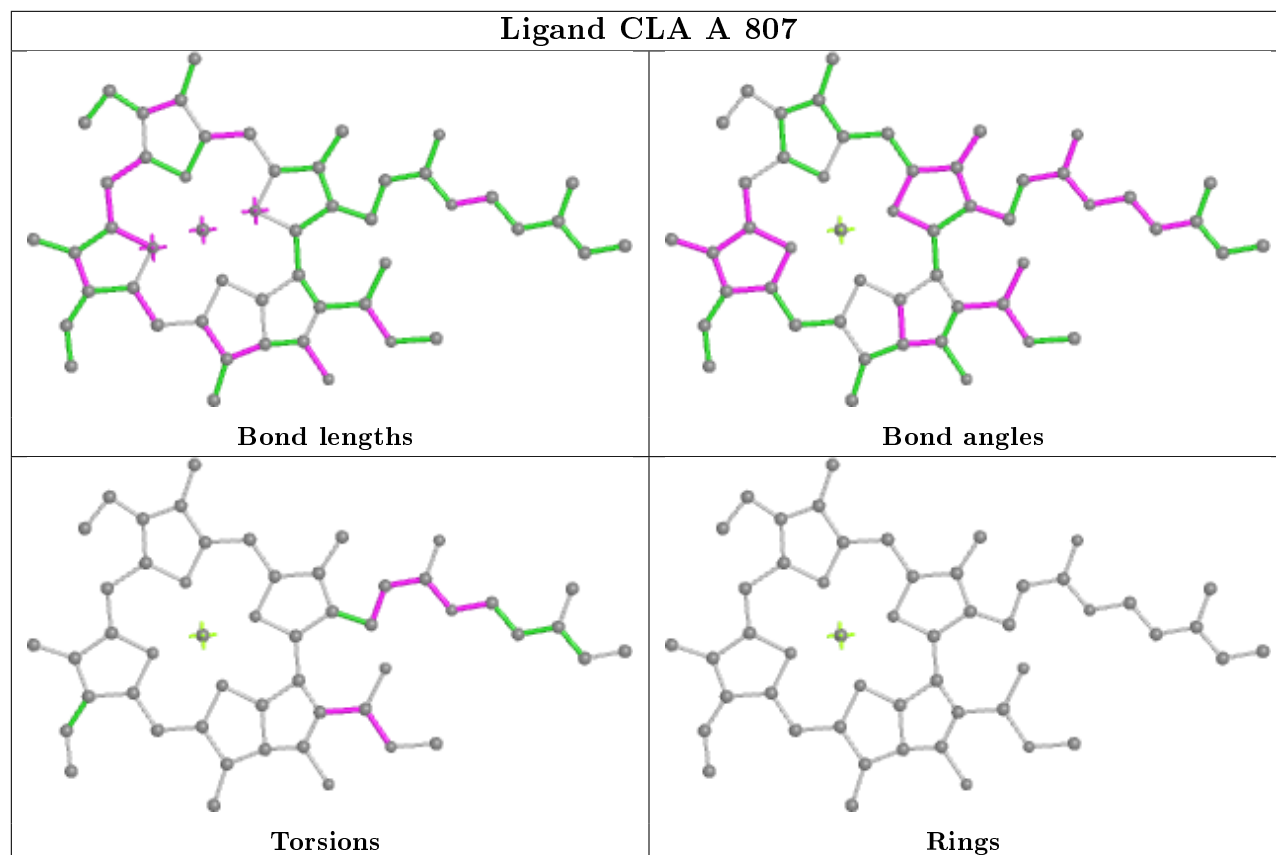
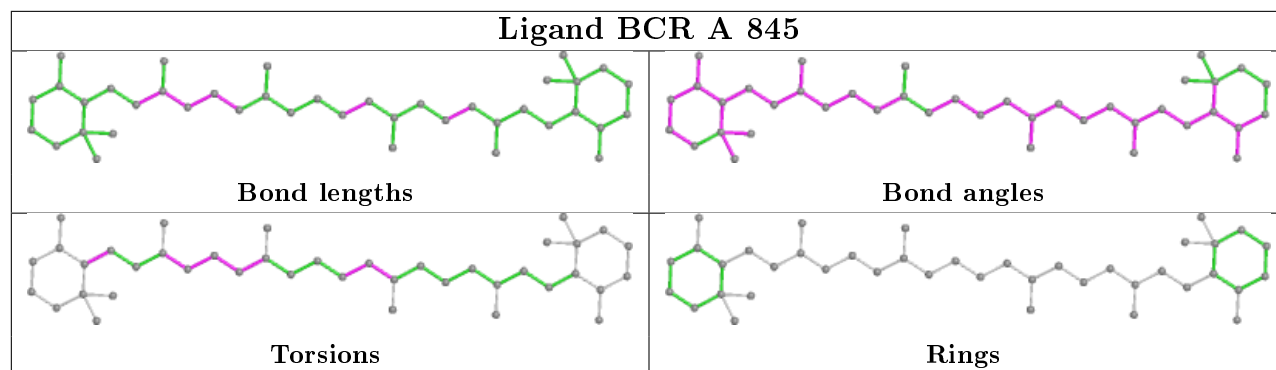
## Ligand CLA J 102



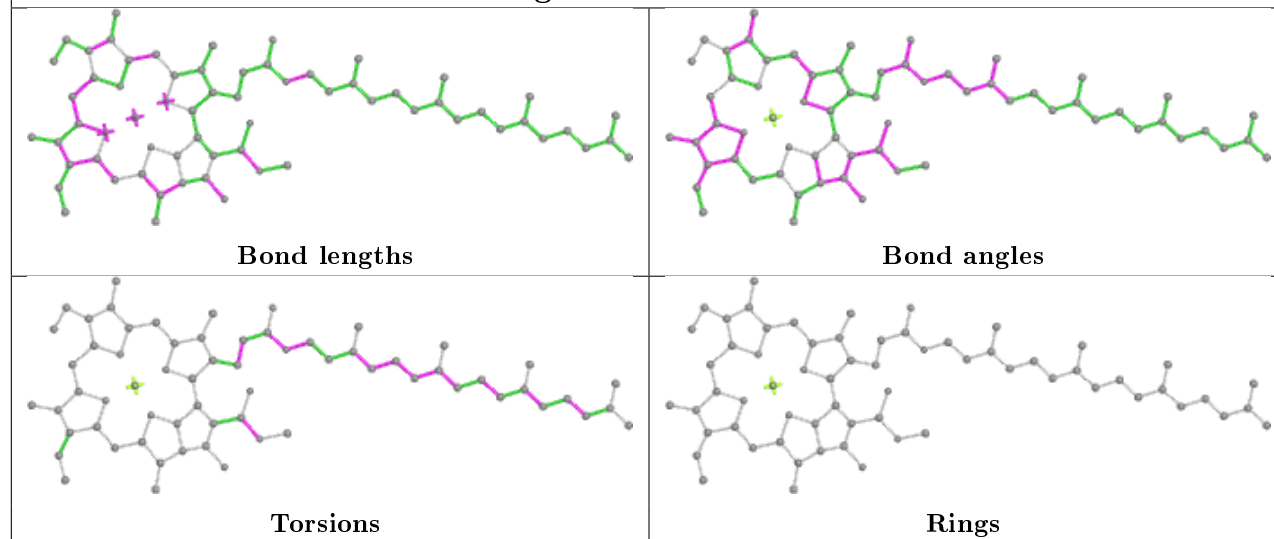
## Ligand BCR B 844



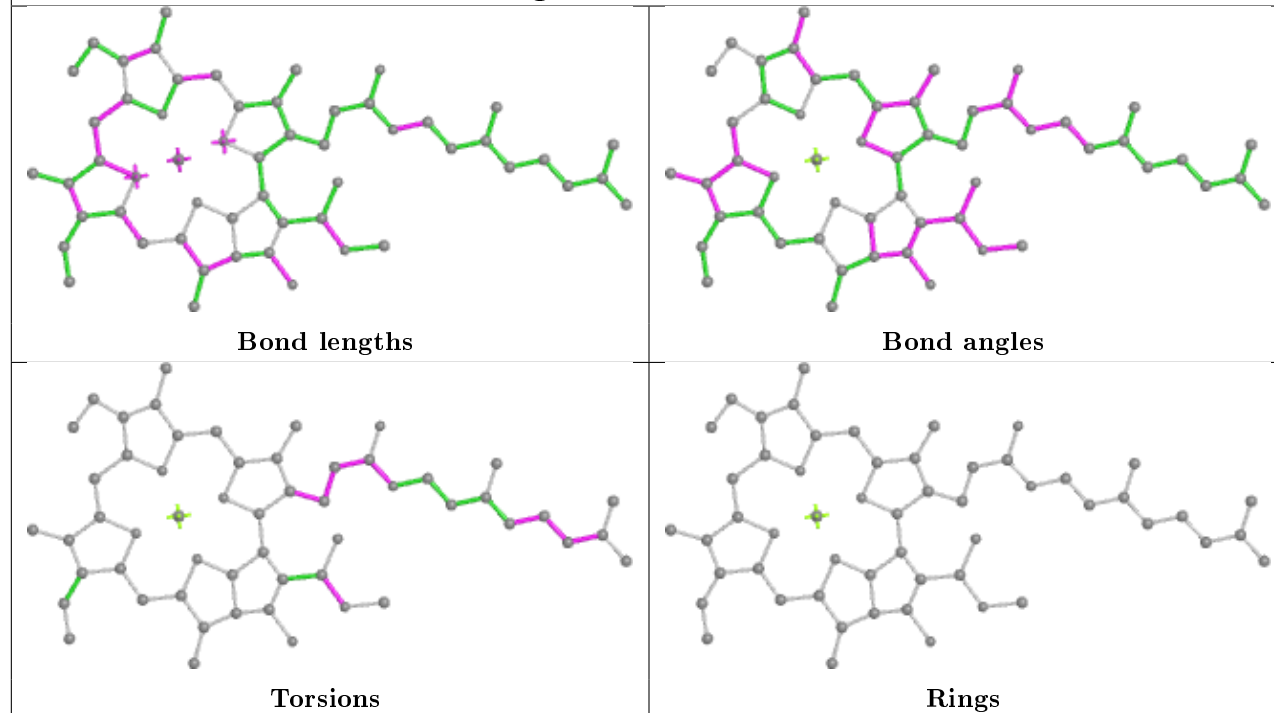


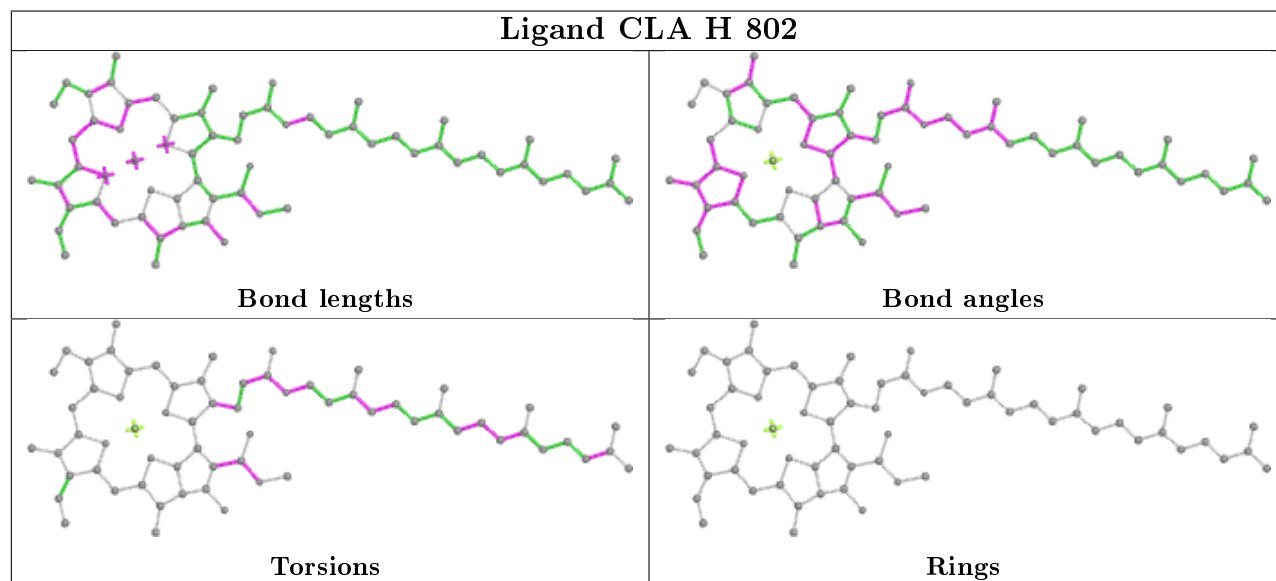
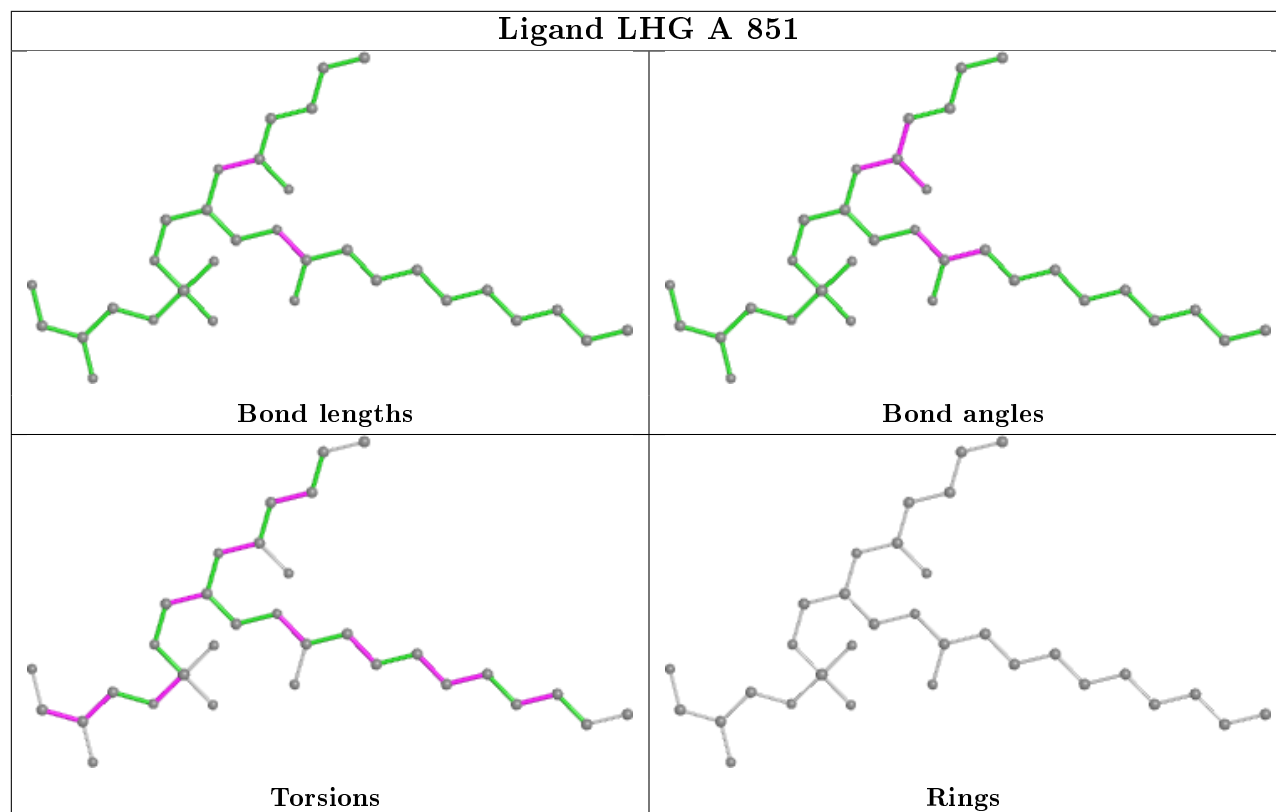


## Ligand CLA Z 815

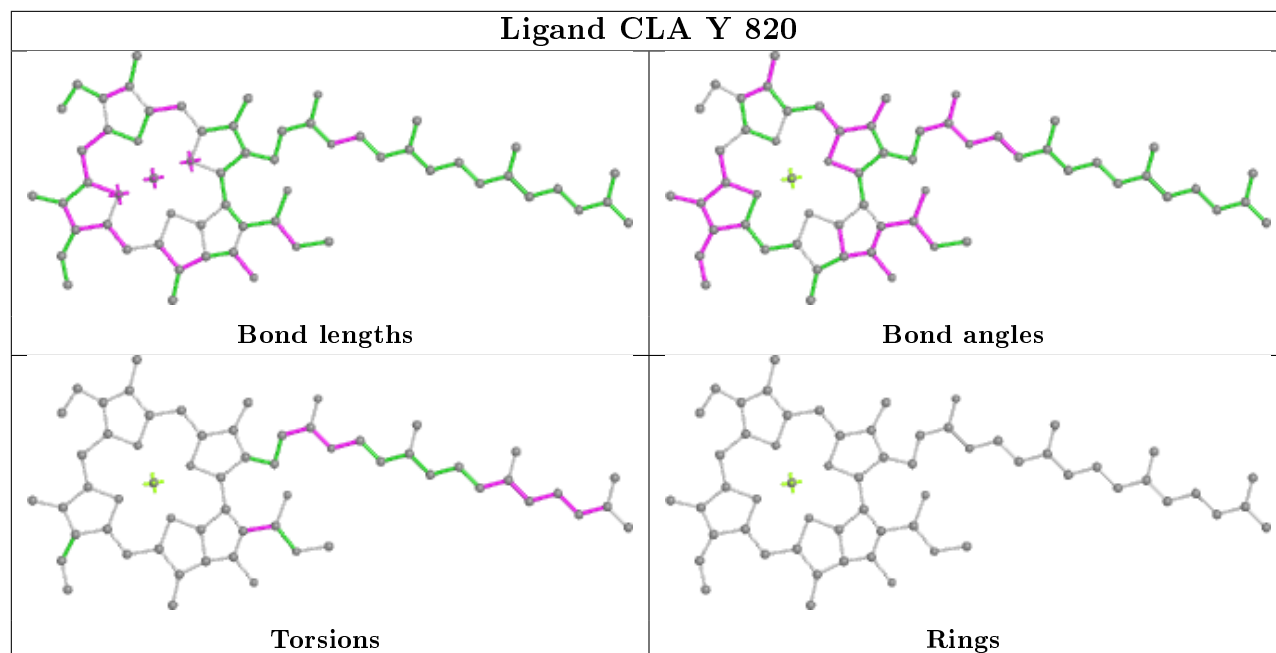


## Ligand CLA H 810

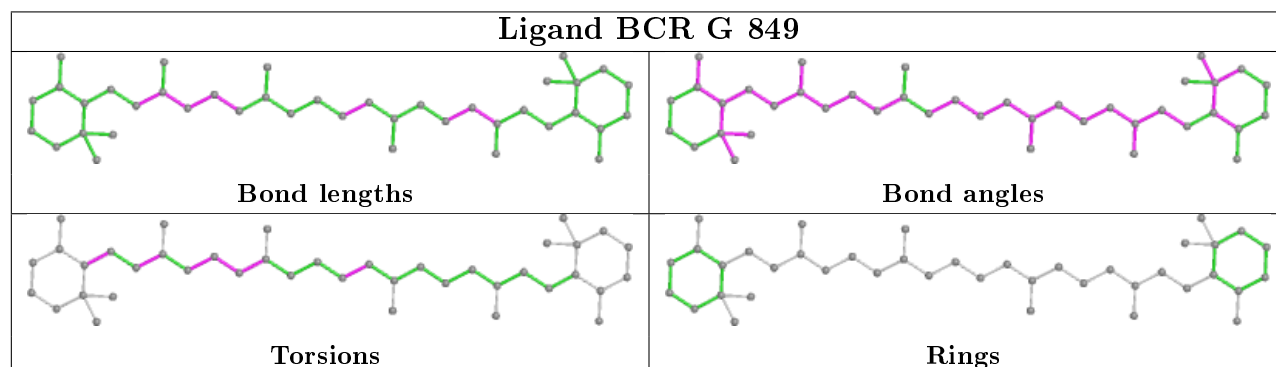




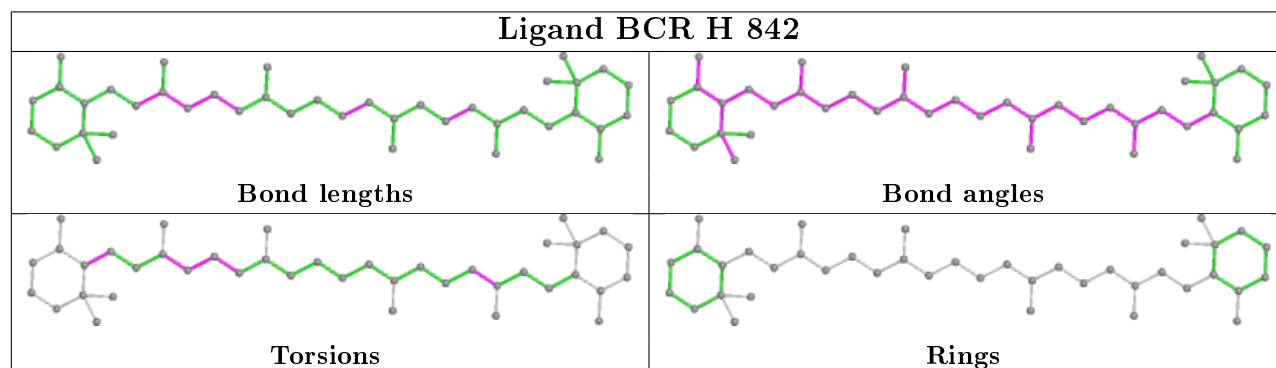
## Ligand CLA Y 820



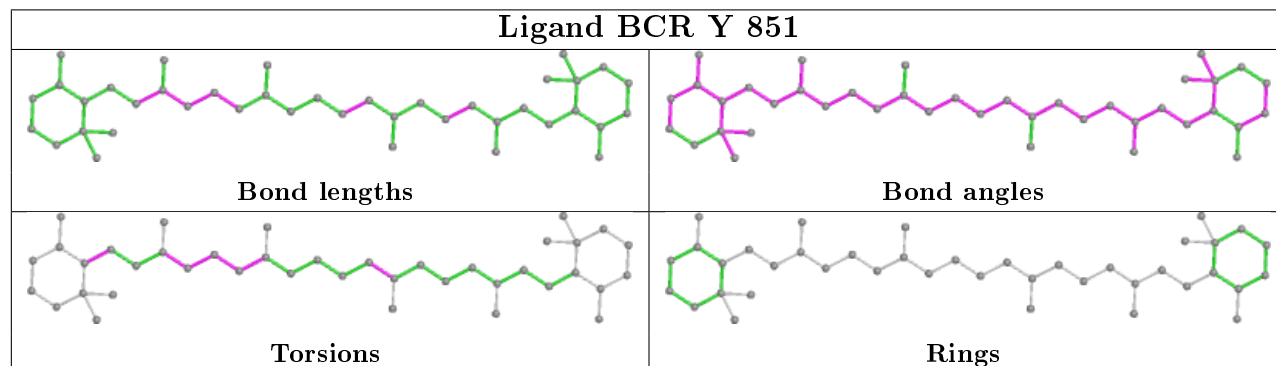
## Ligand BCR G 849



## Ligand BCR H 842

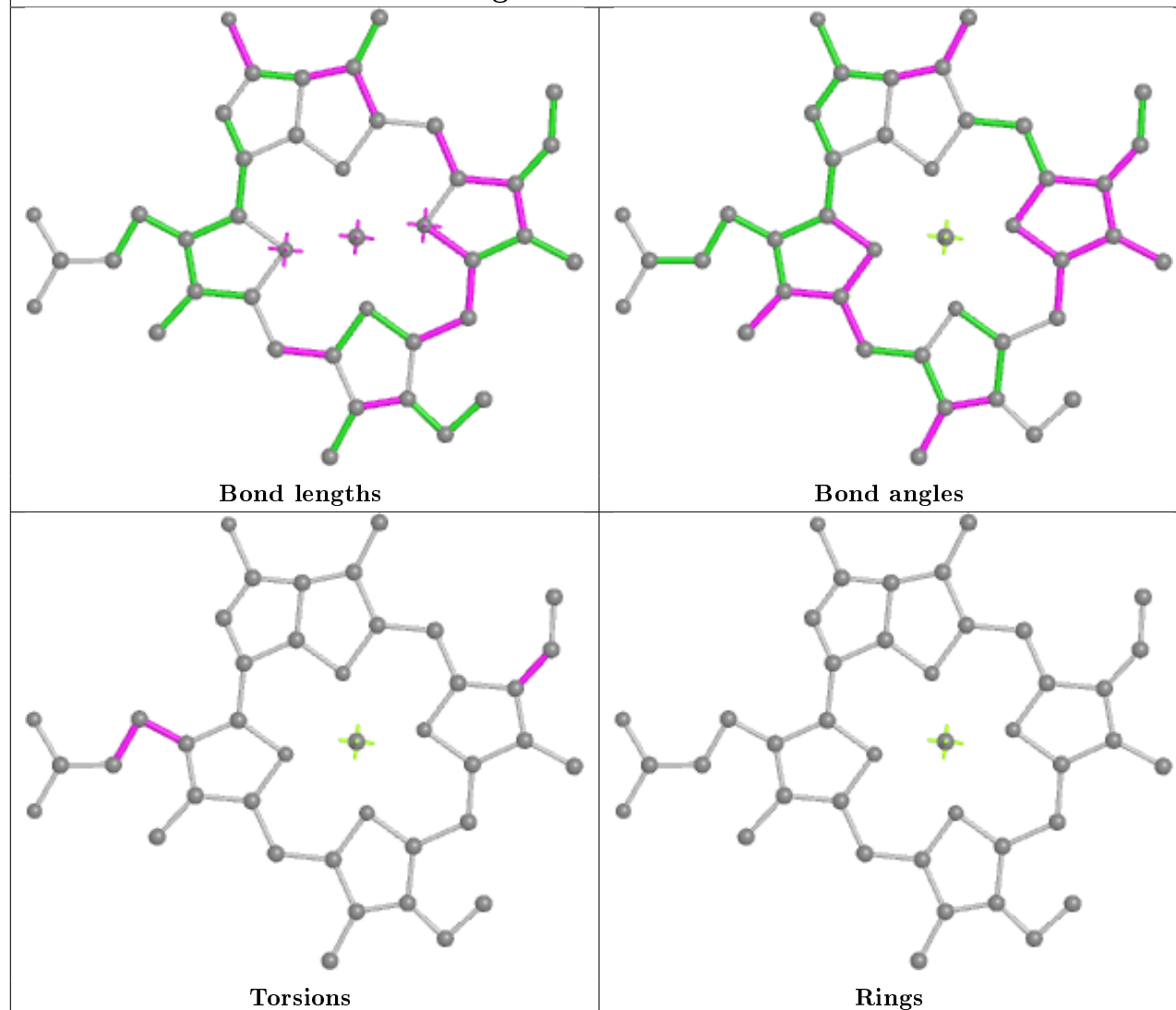


## Ligand BCR Y 851

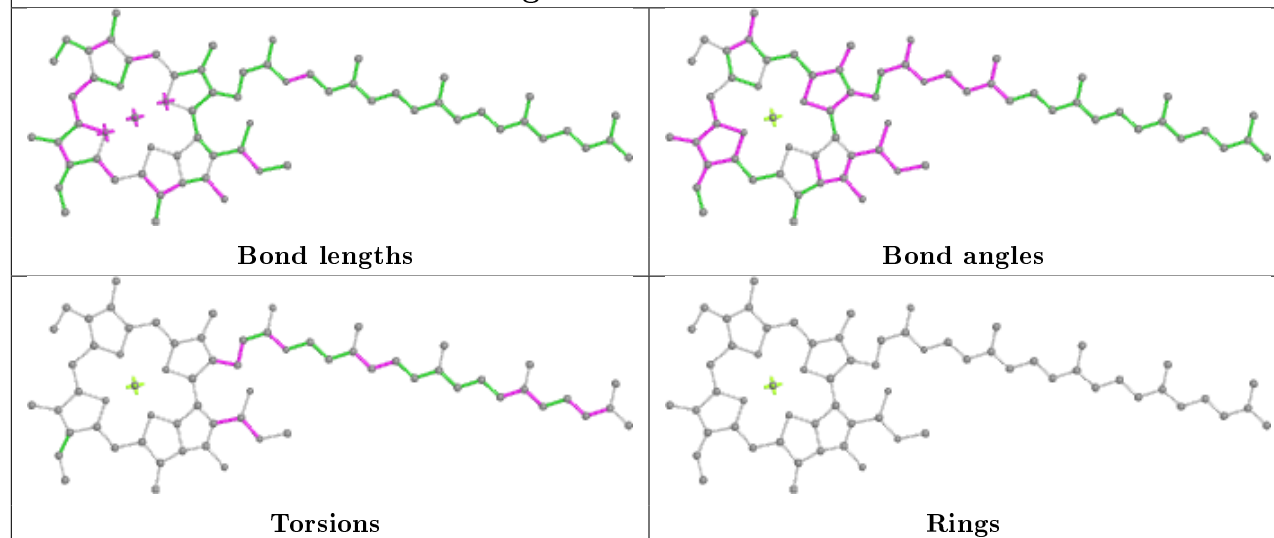




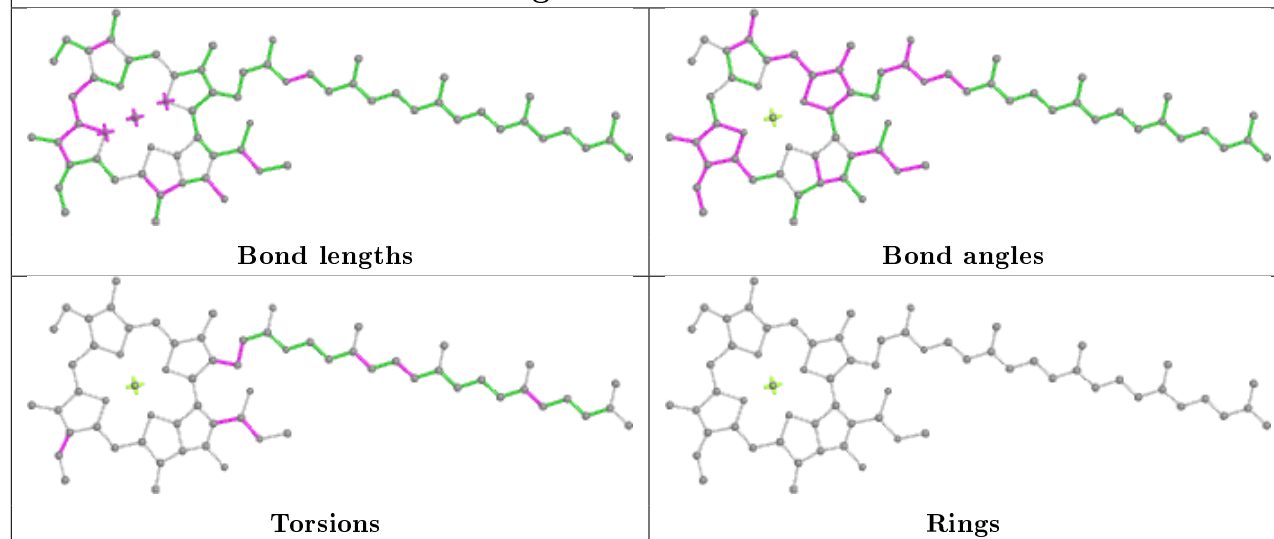
## Ligand CLA T 101



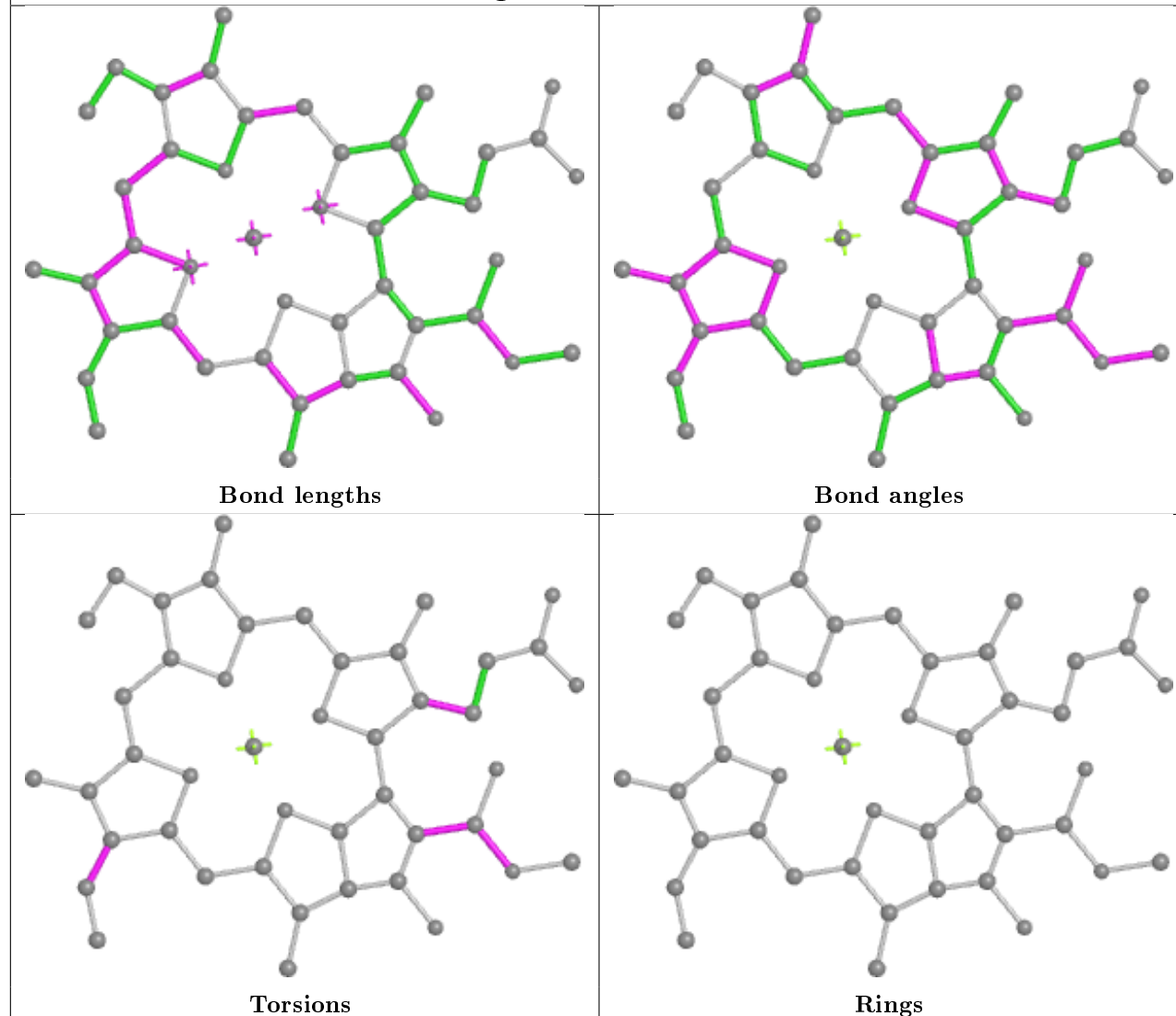
## Ligand CLA U 1006



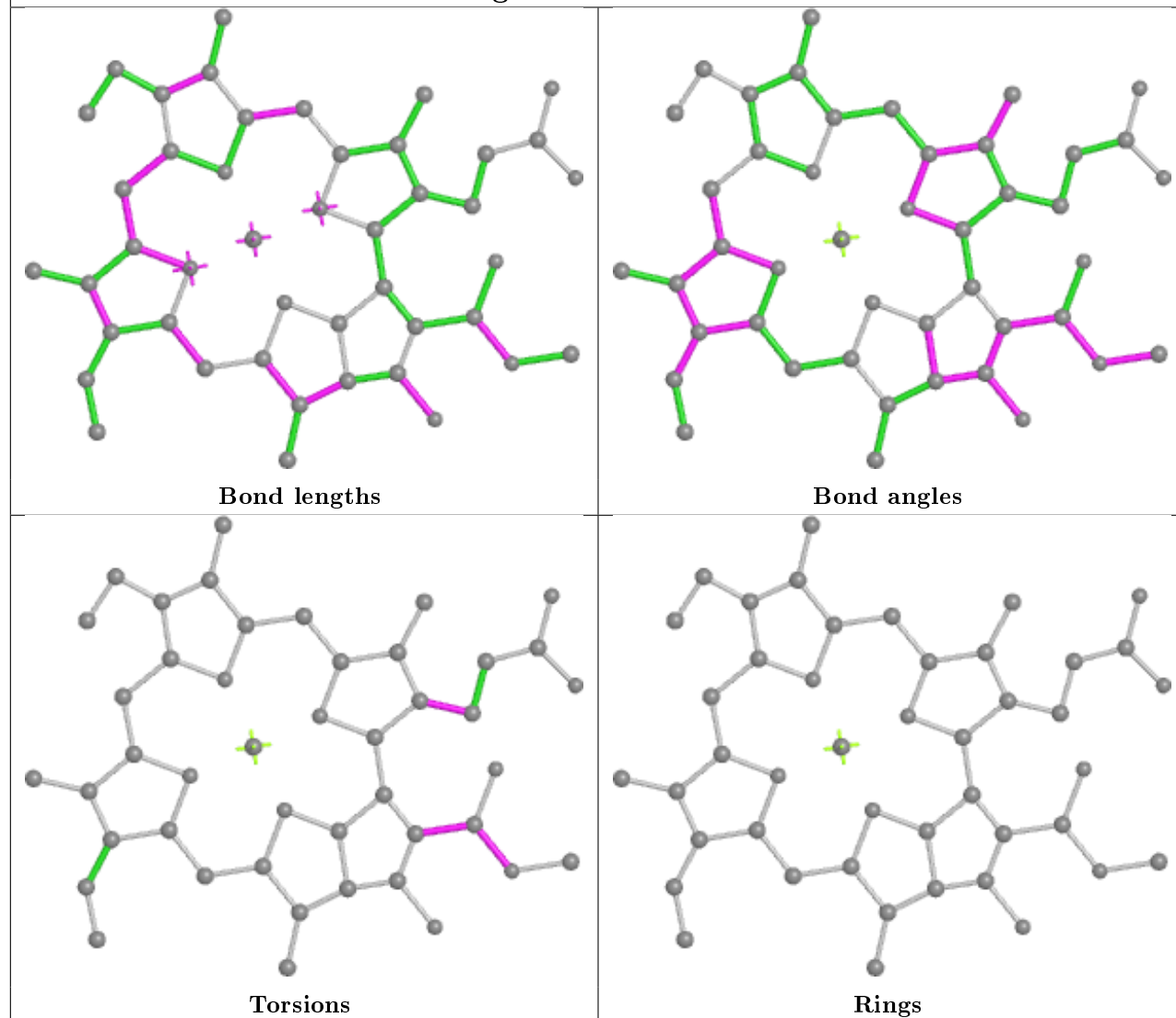
## Ligand CLA Y 834



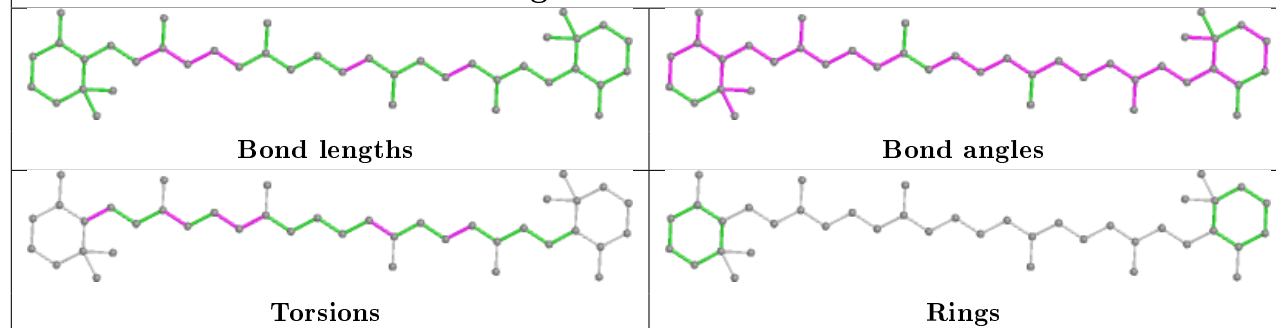
## Ligand CLA Z 832

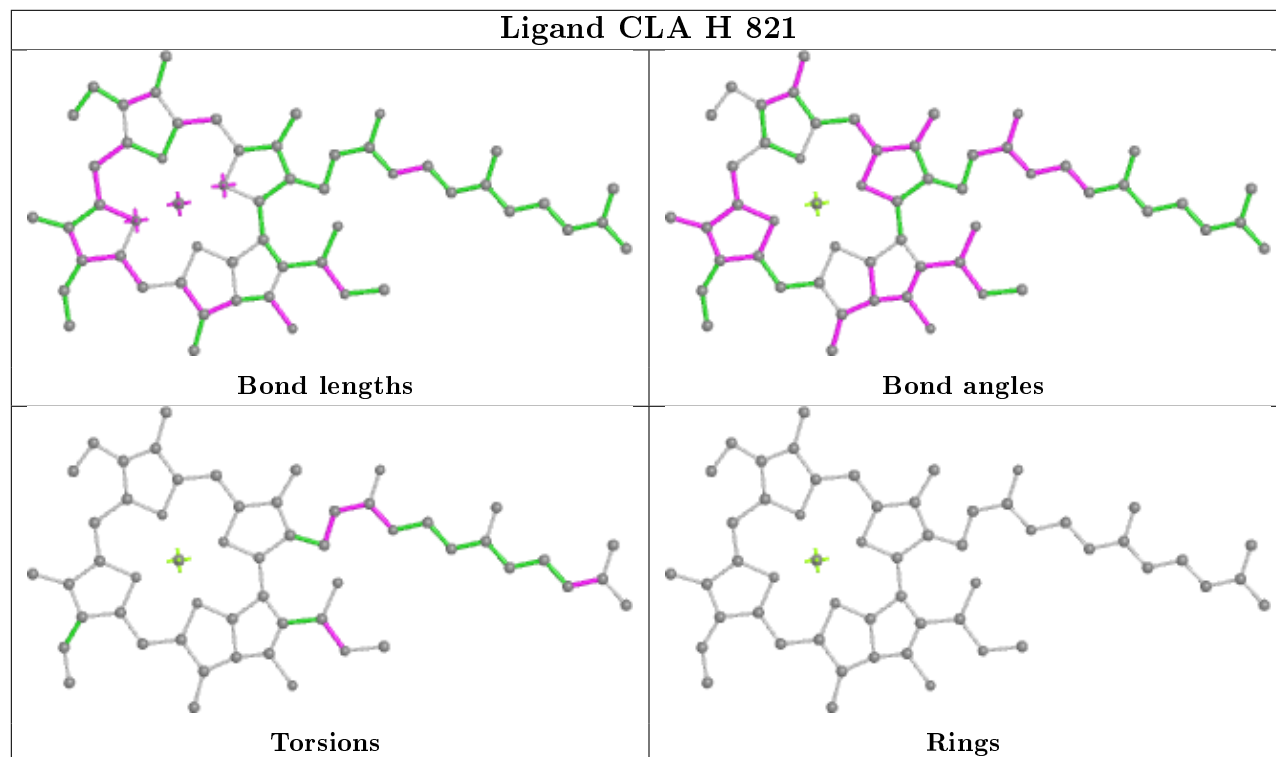
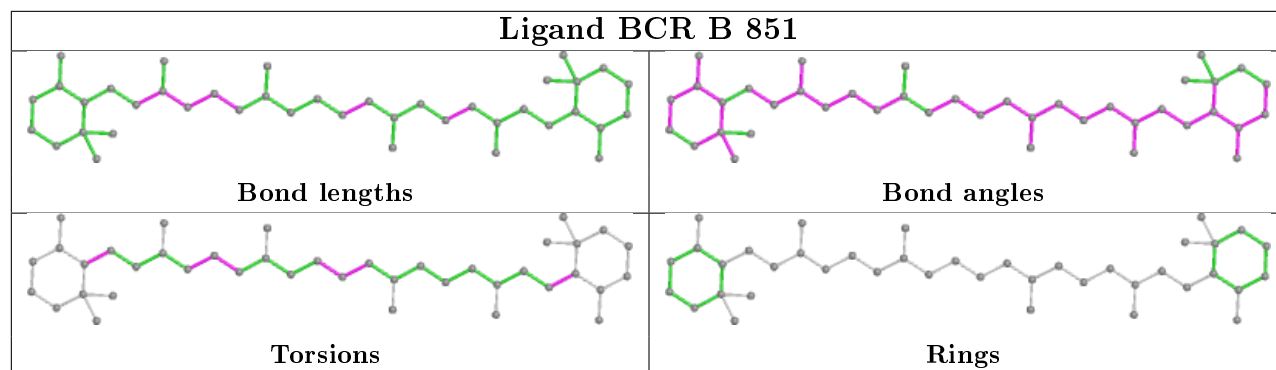
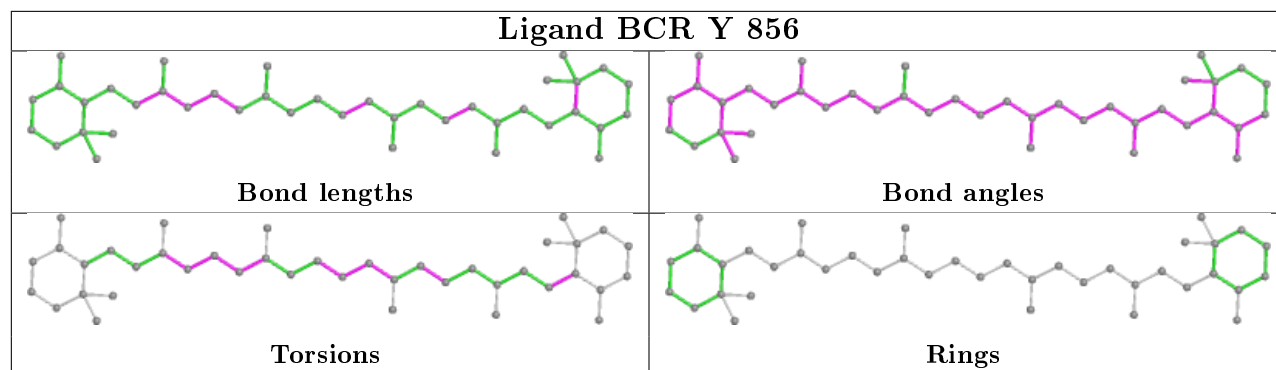


## Ligand CLA Z 833

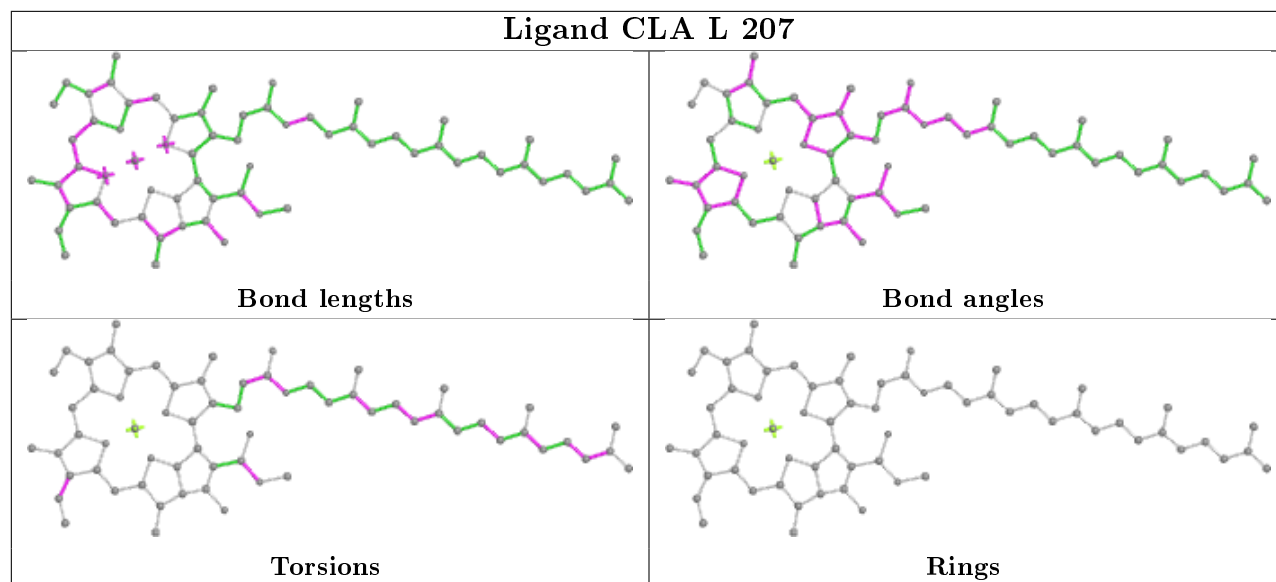


## Ligand BCR A 849

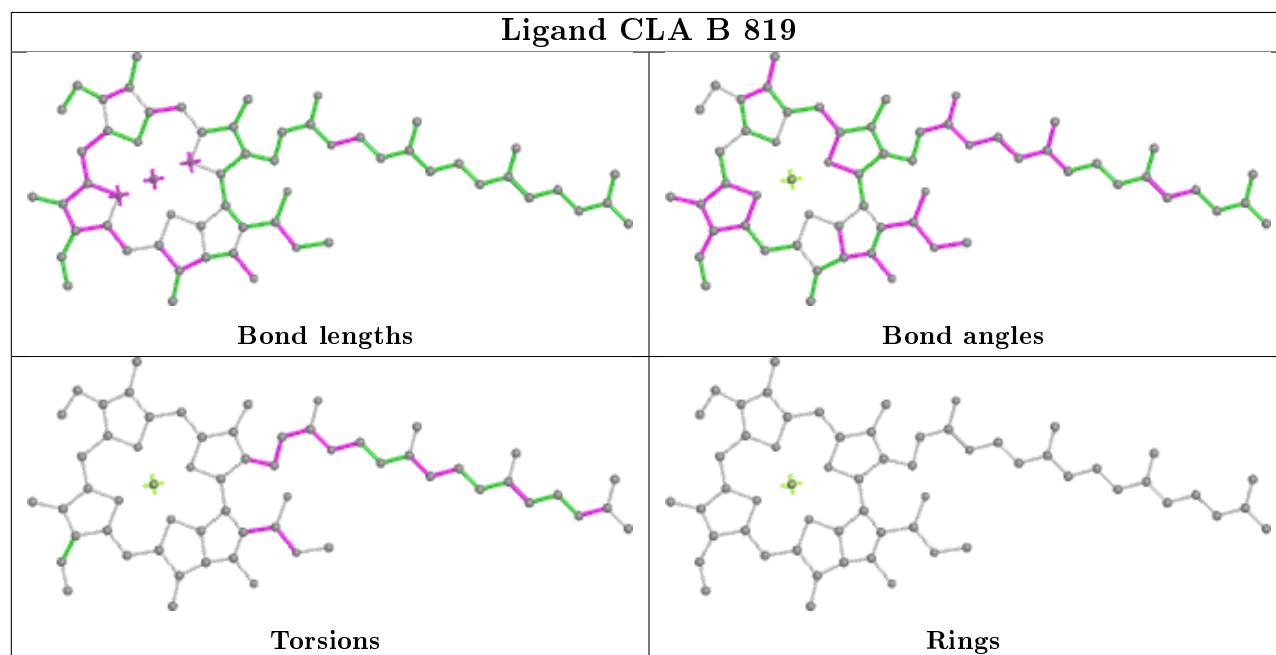




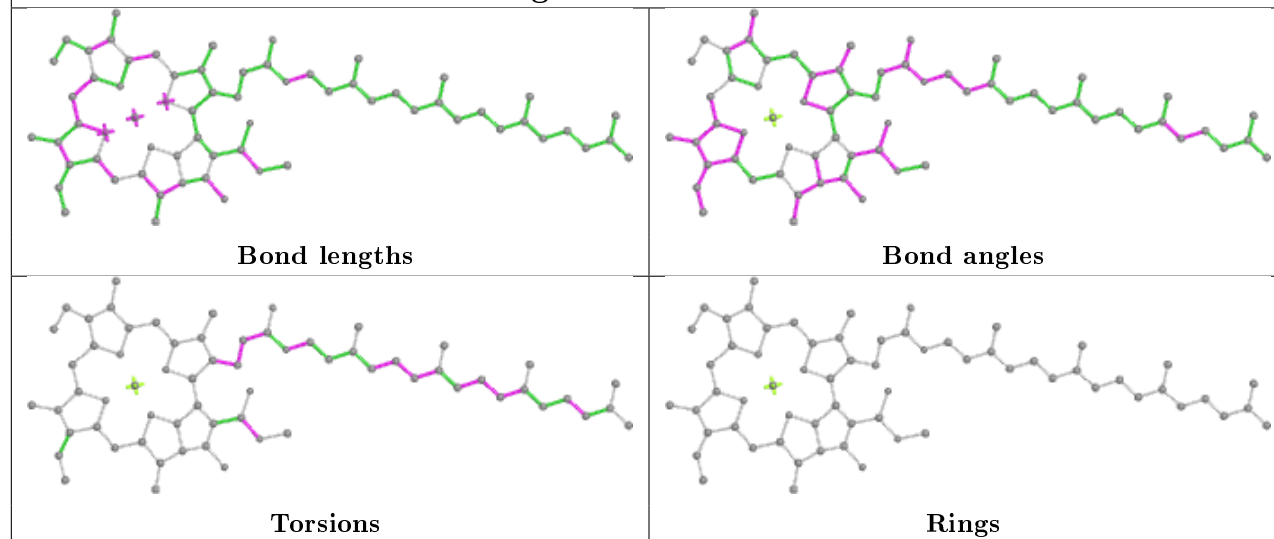
## Ligand CLA L 207



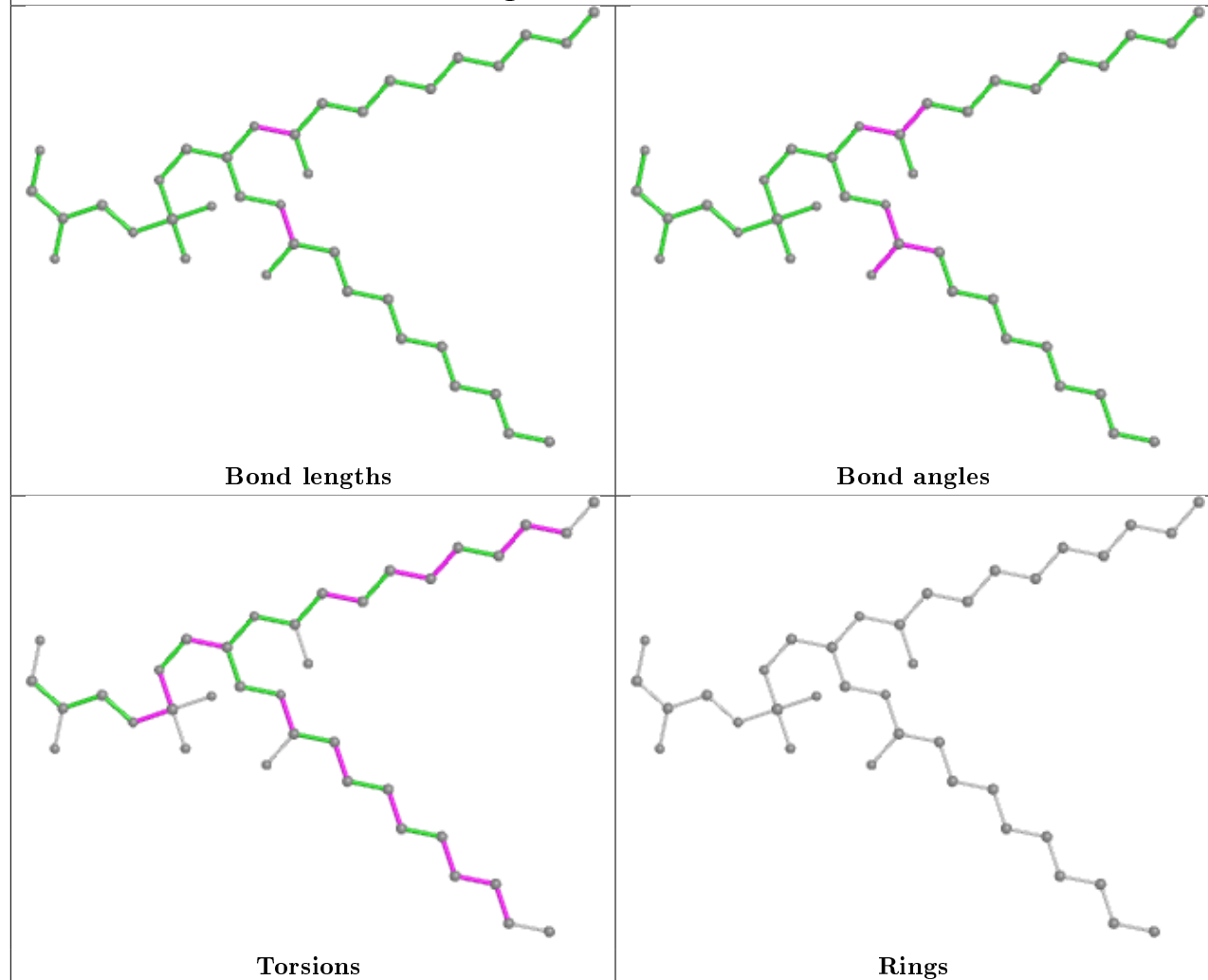
## Ligand CLA B 819

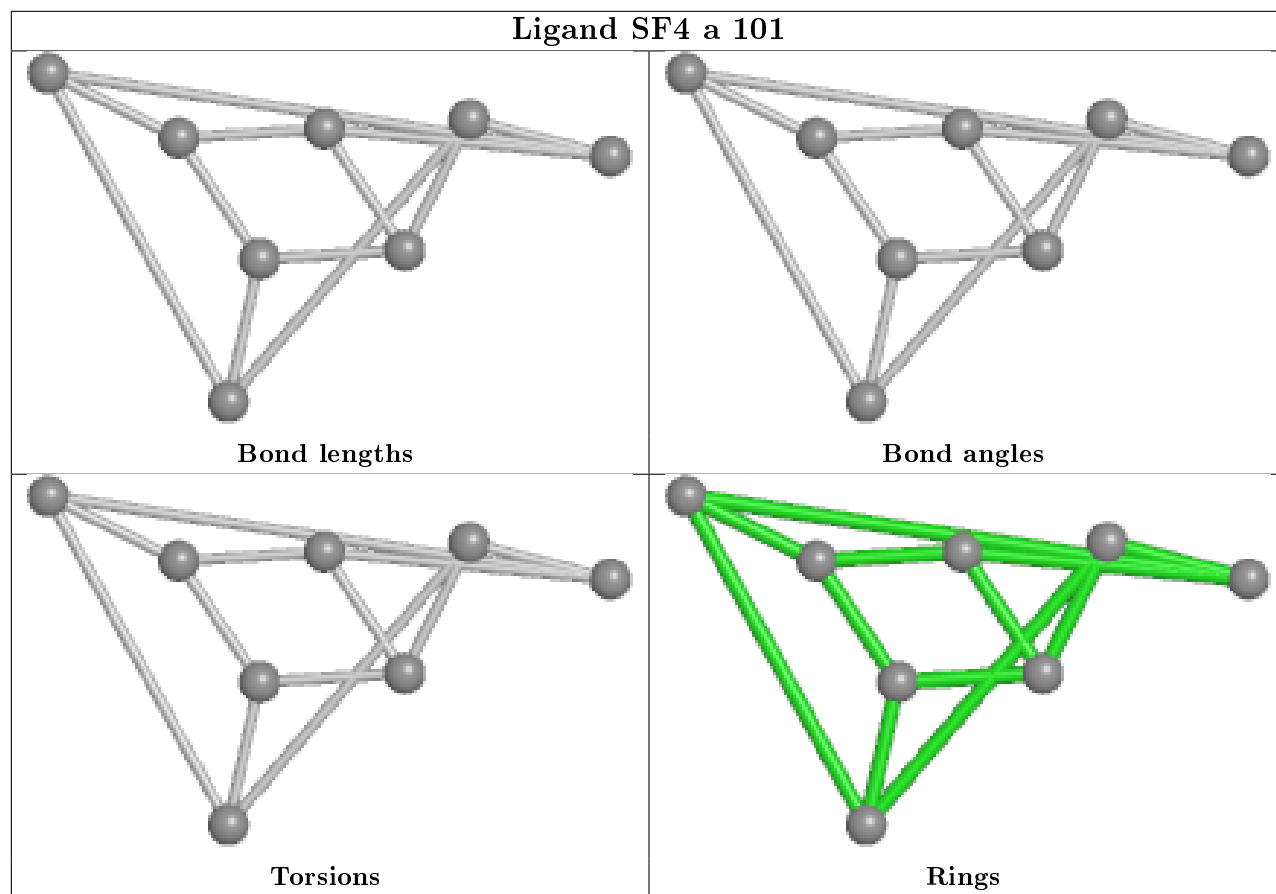
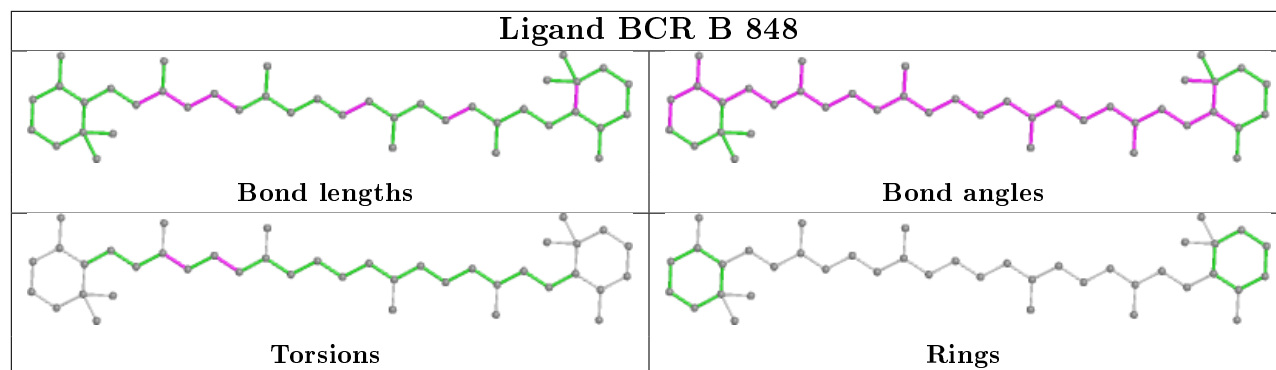


## Ligand CLA G 809

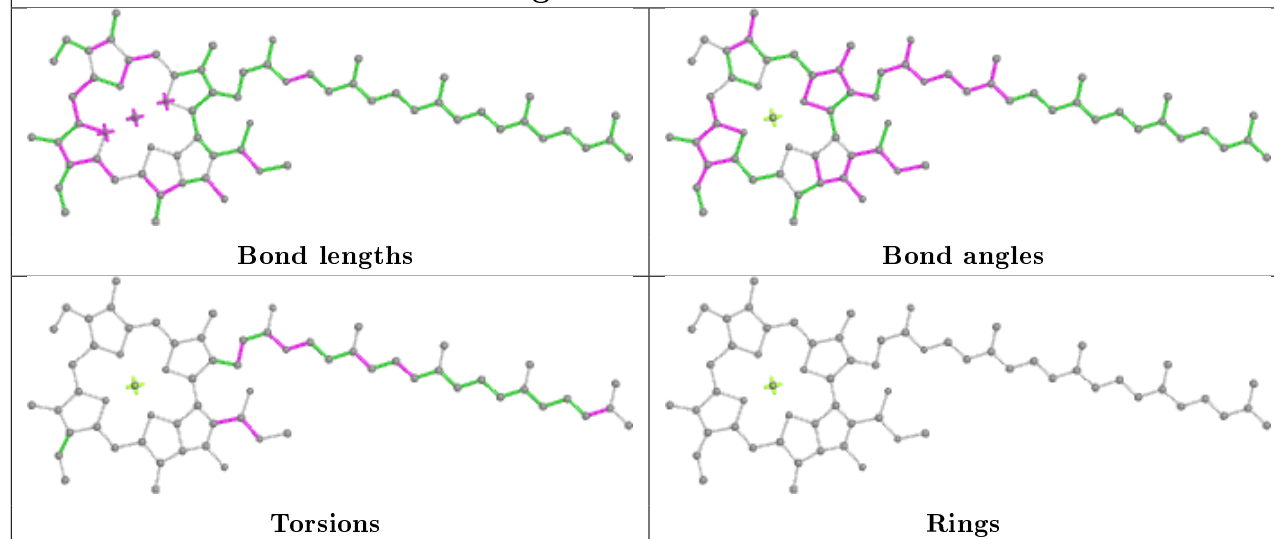


## Ligand LHG H 847

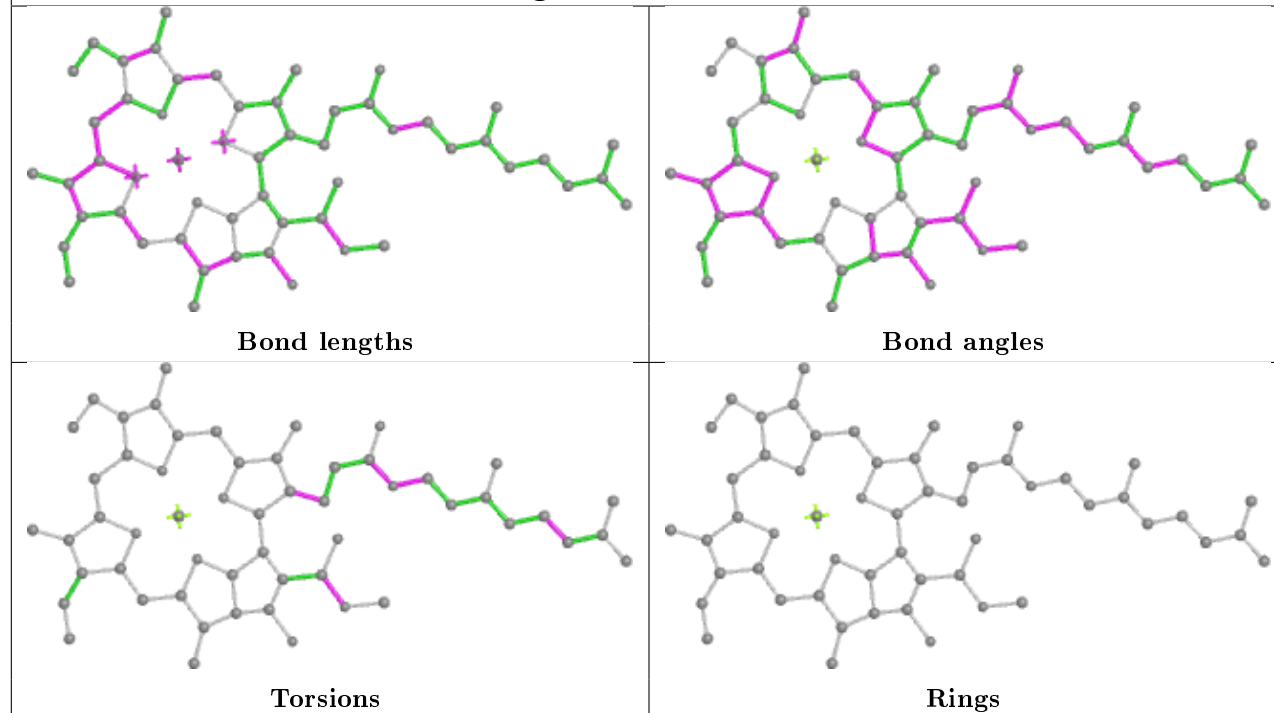




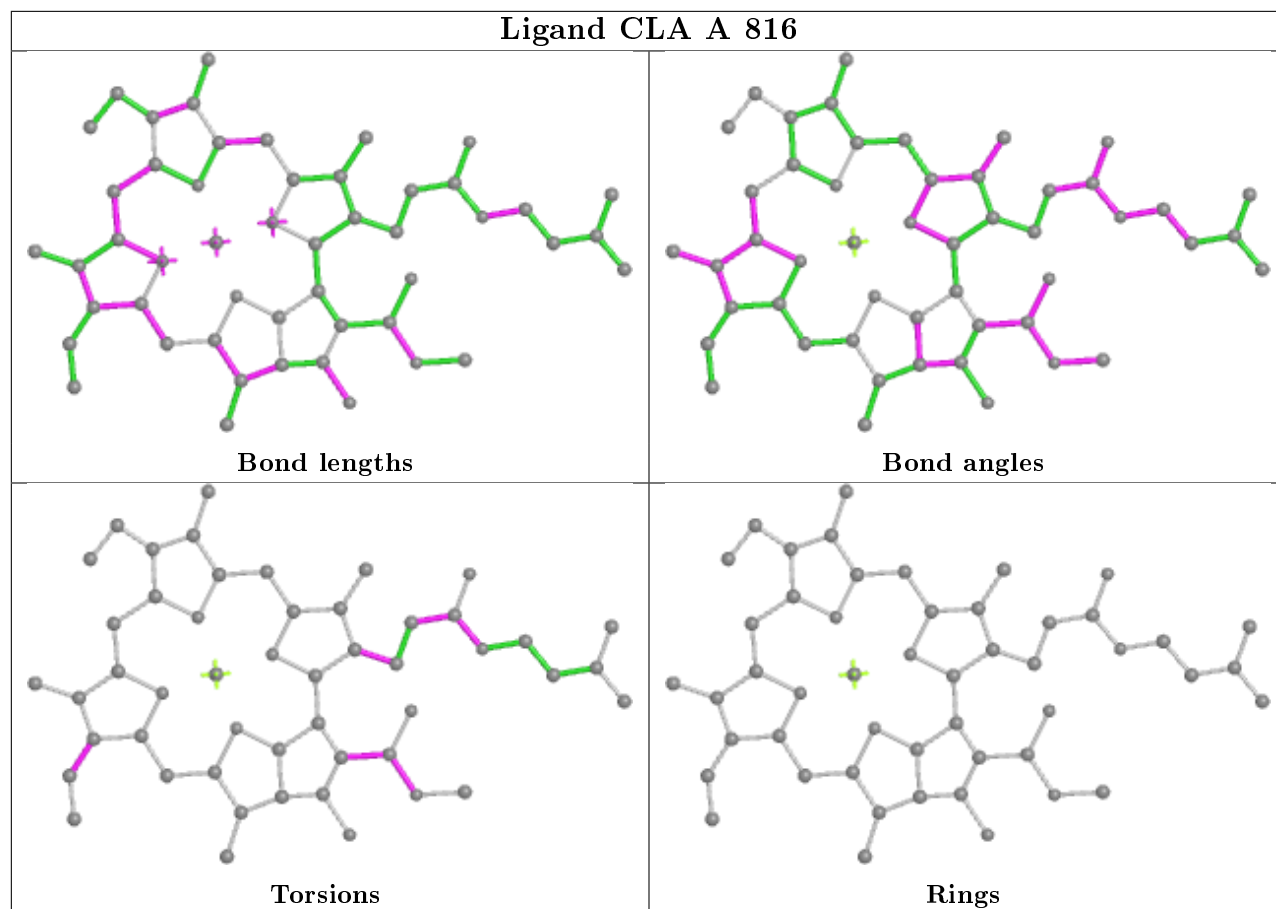
## Ligand CLA A 841



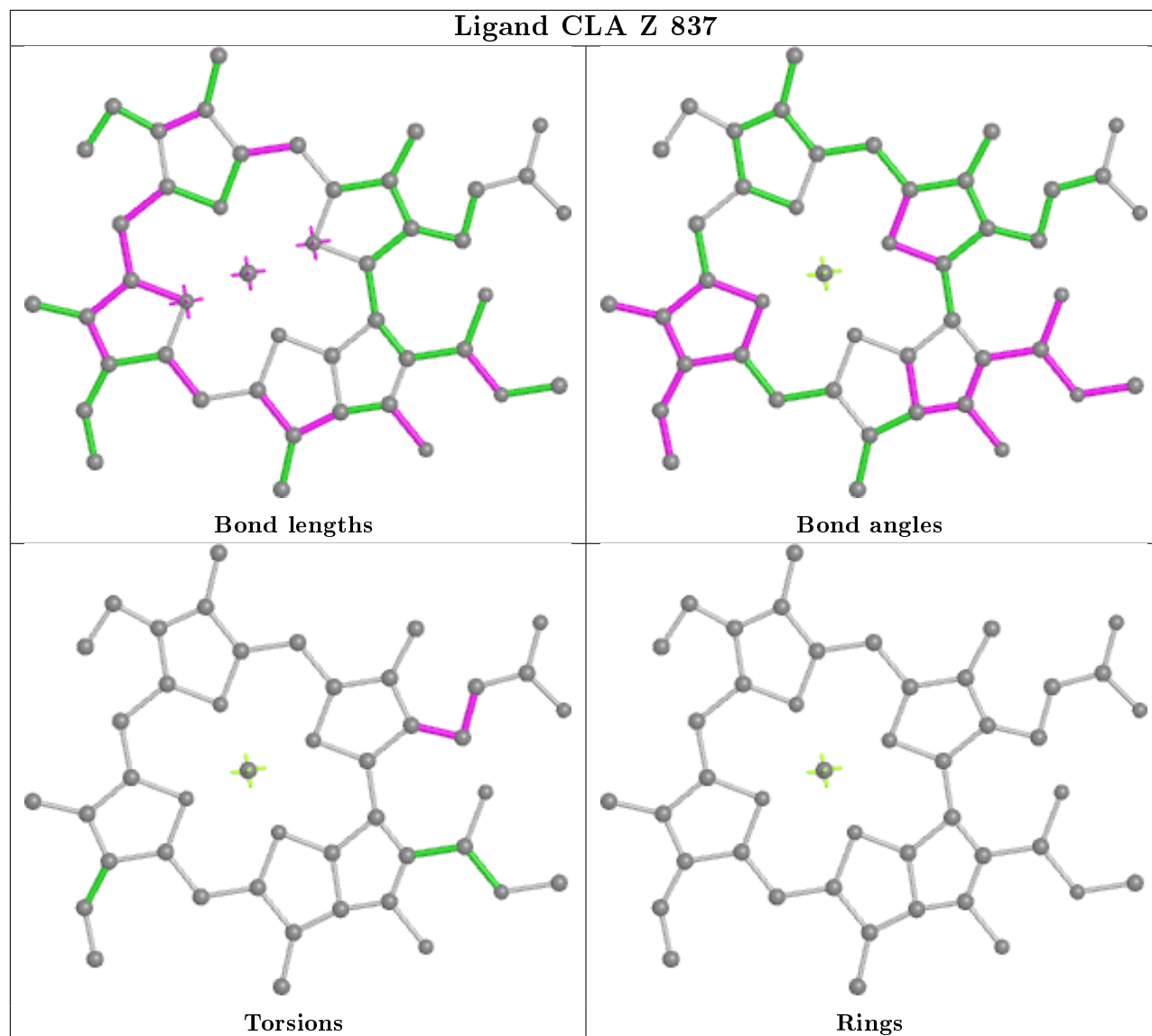
## Ligand CLA G 834



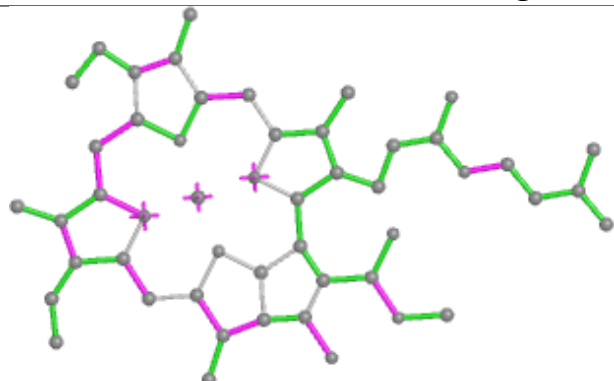




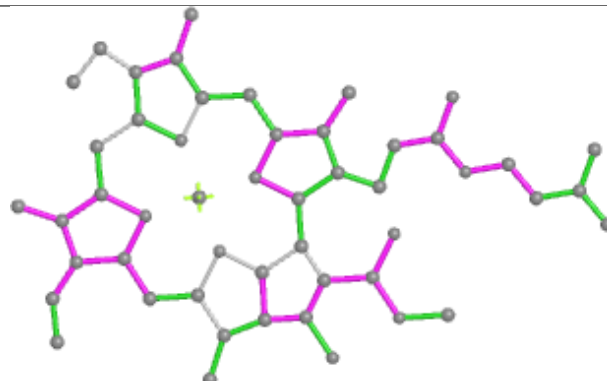
## Ligand CLA Z 837



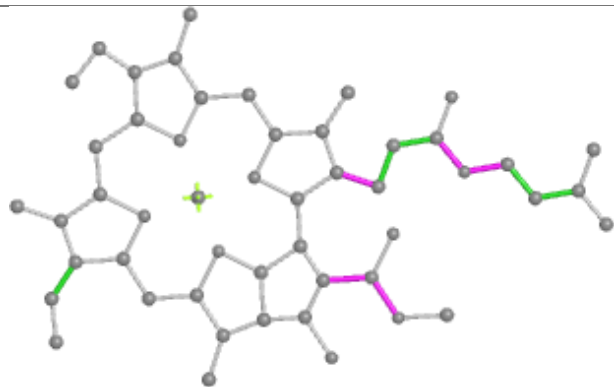
## Ligand CLA A 815



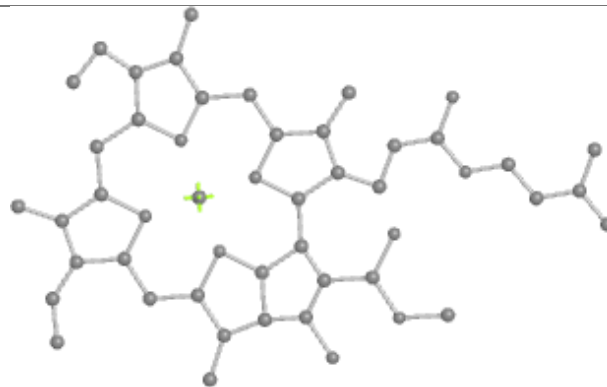
Bond lengths



Bond angles

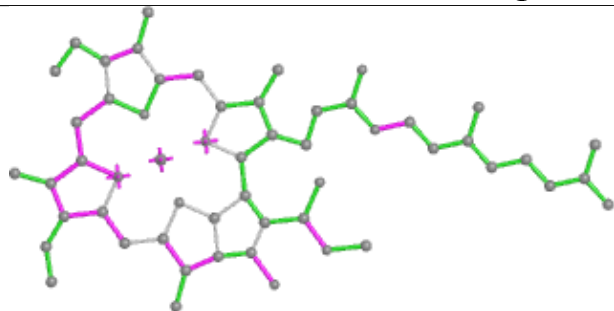


Torsions

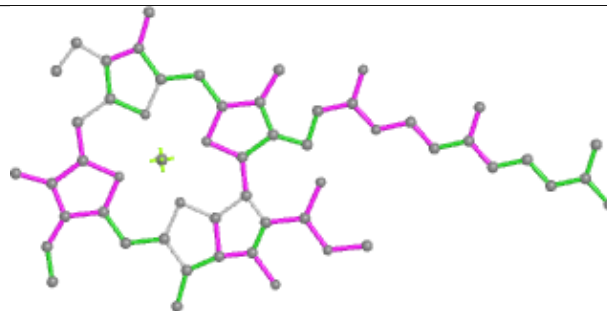


Rings

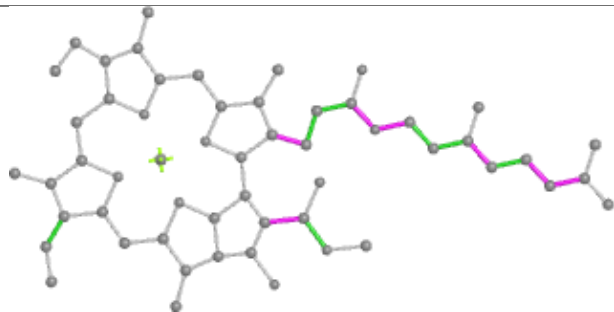
## Ligand CLA H 823



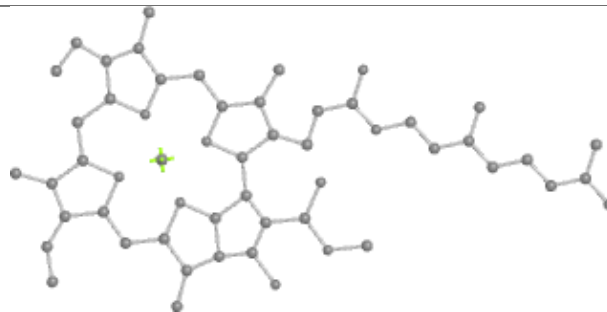
Bond lengths



Bond angles

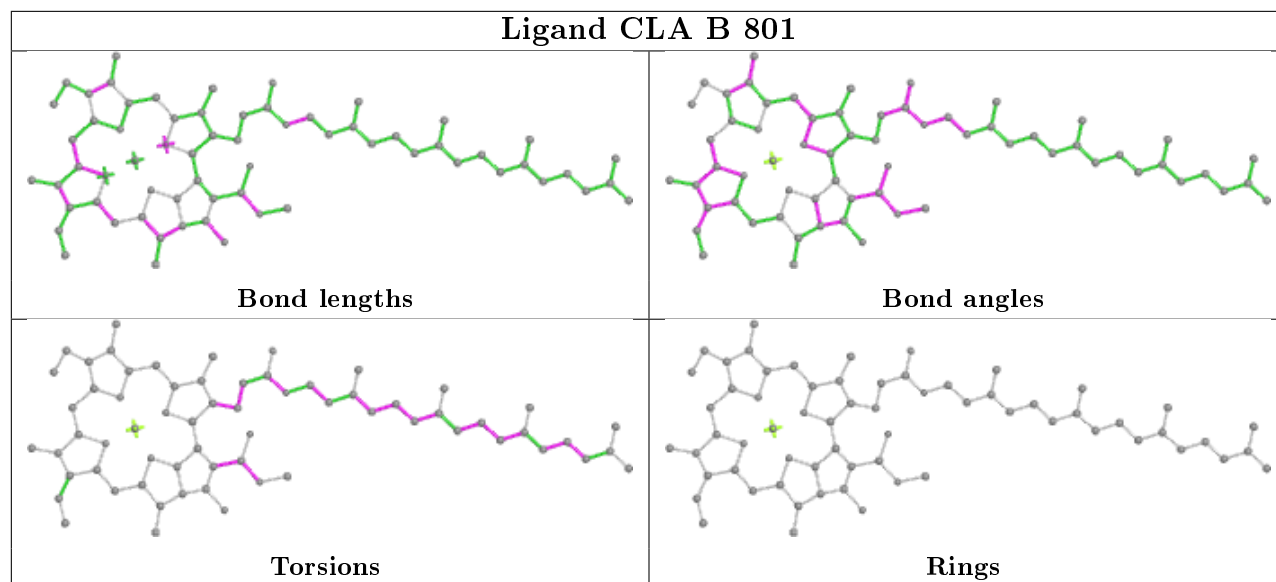


Torsions

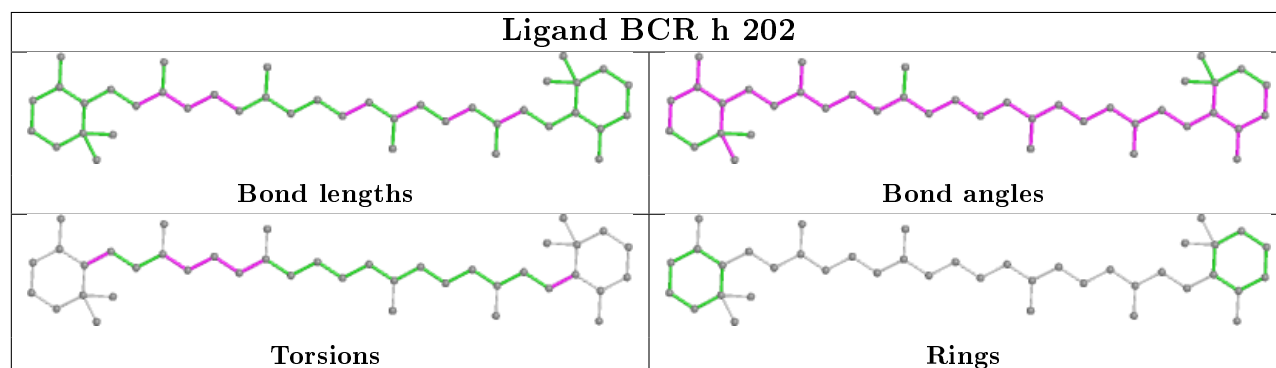


Rings

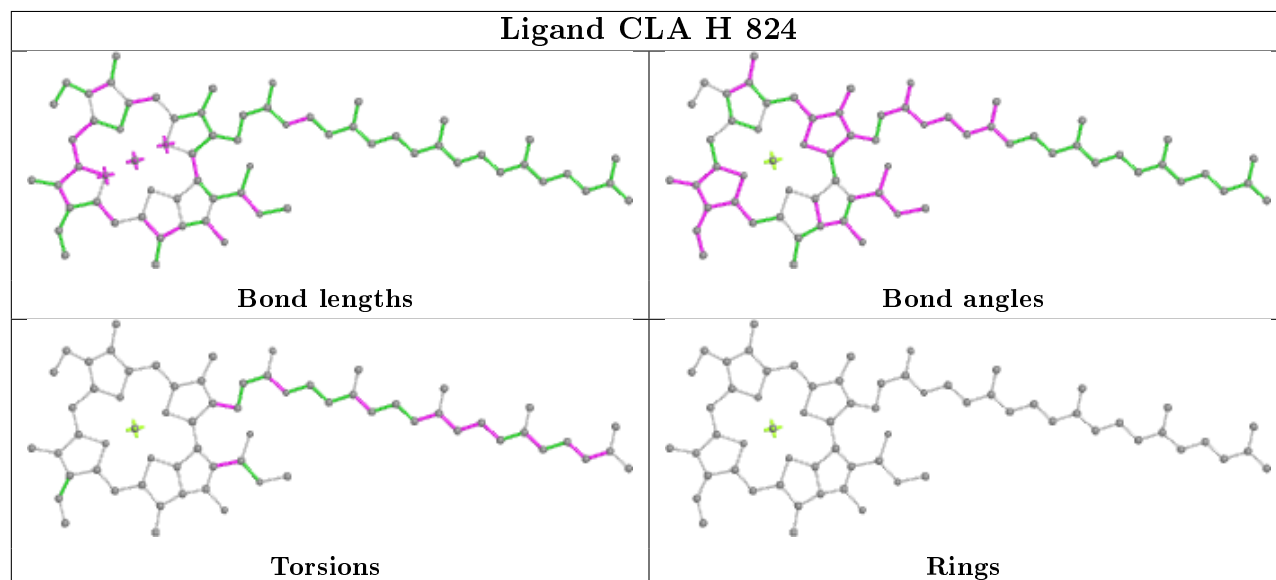
## Ligand CLA B 801



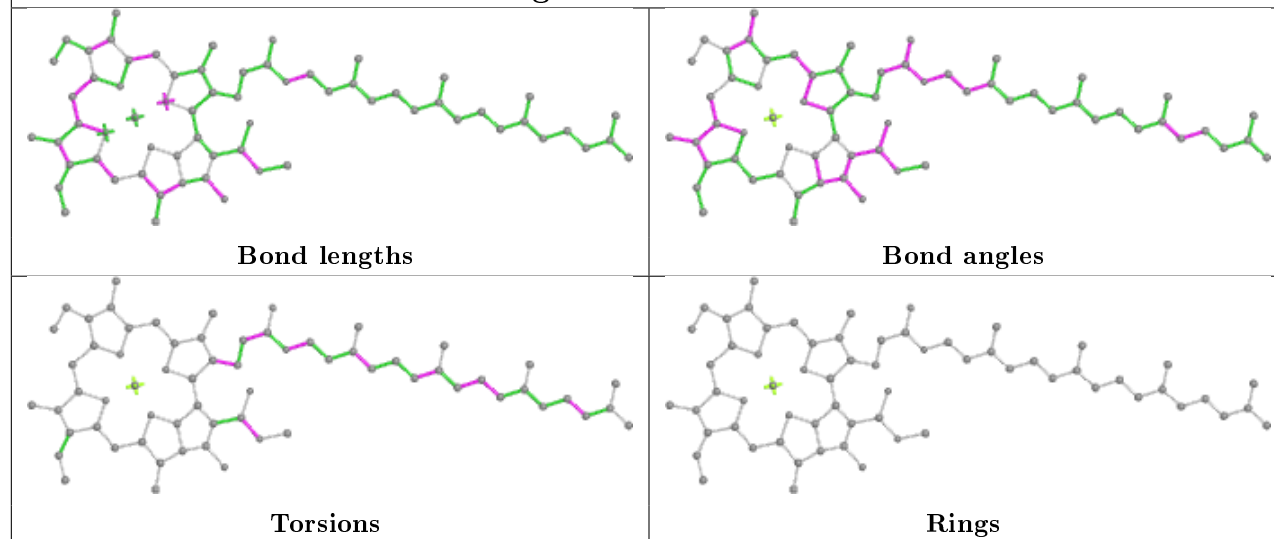
## Ligand BCR h 202



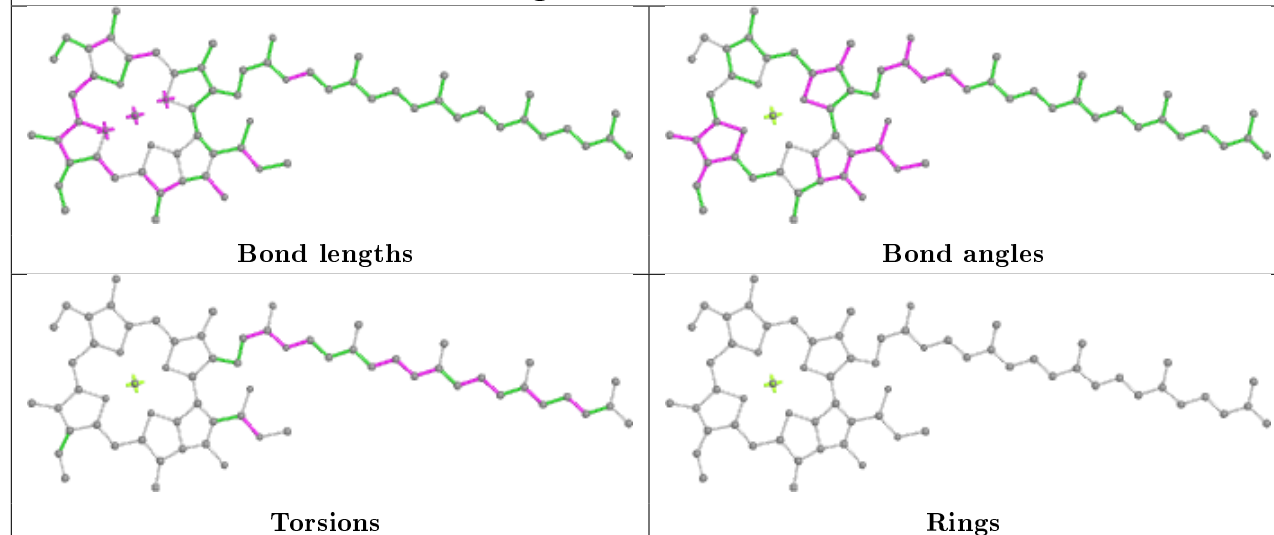
## Ligand CLA H 824



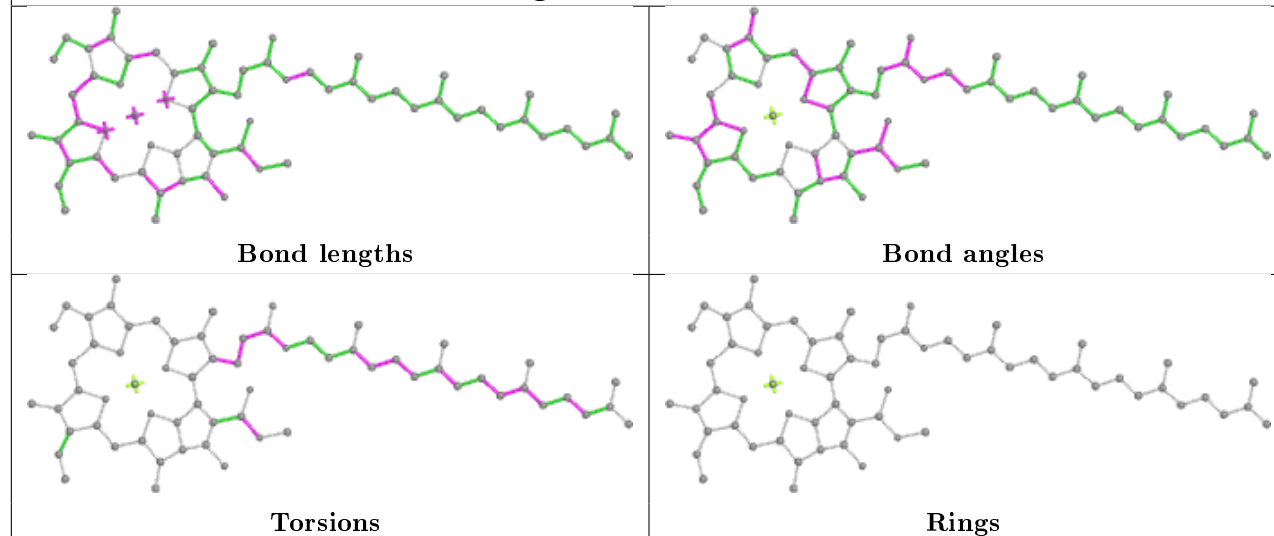
## Ligand CLA Y 833



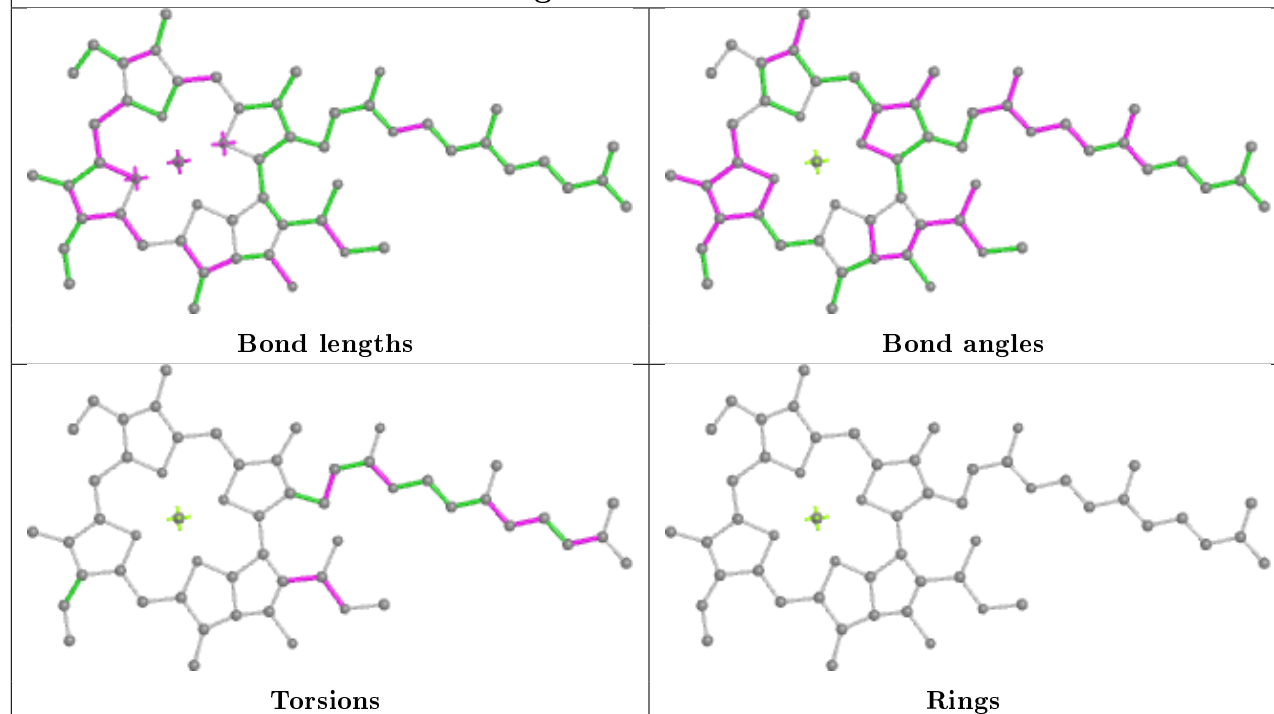
## Ligand CLA H 835



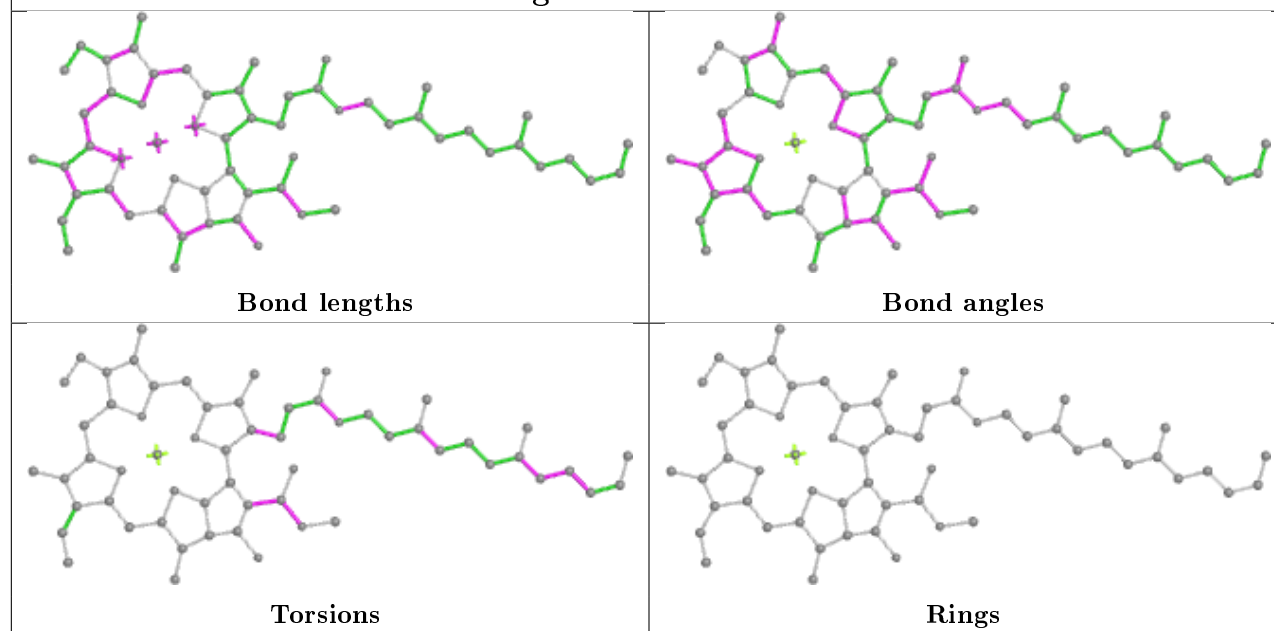
## Ligand CLA G 806



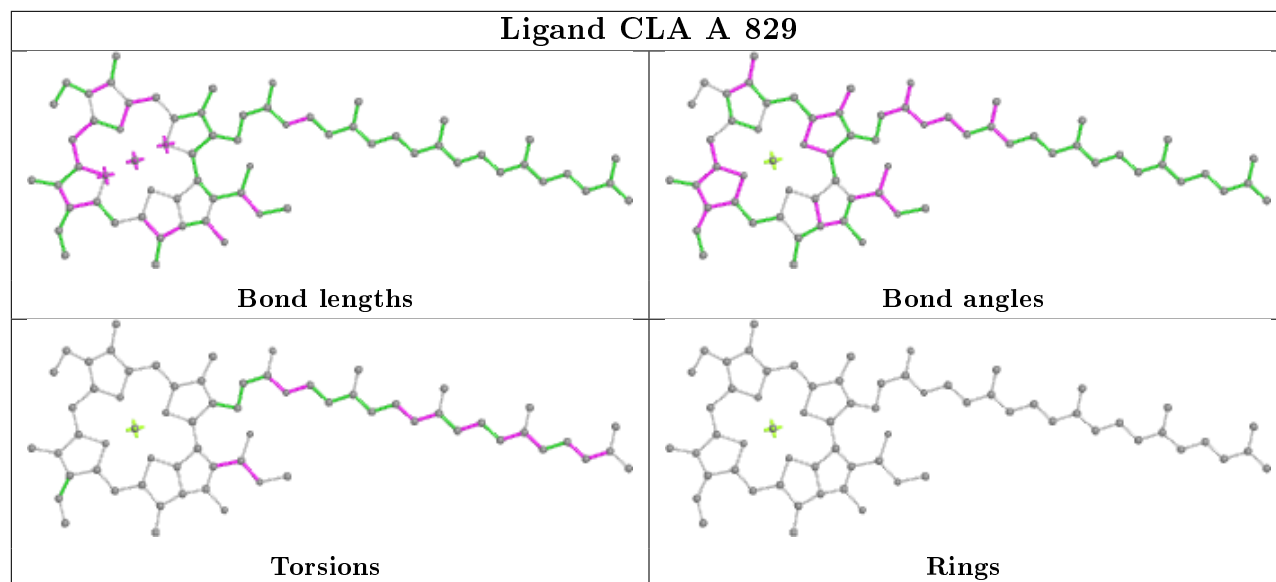
## Ligand CLA Z 814



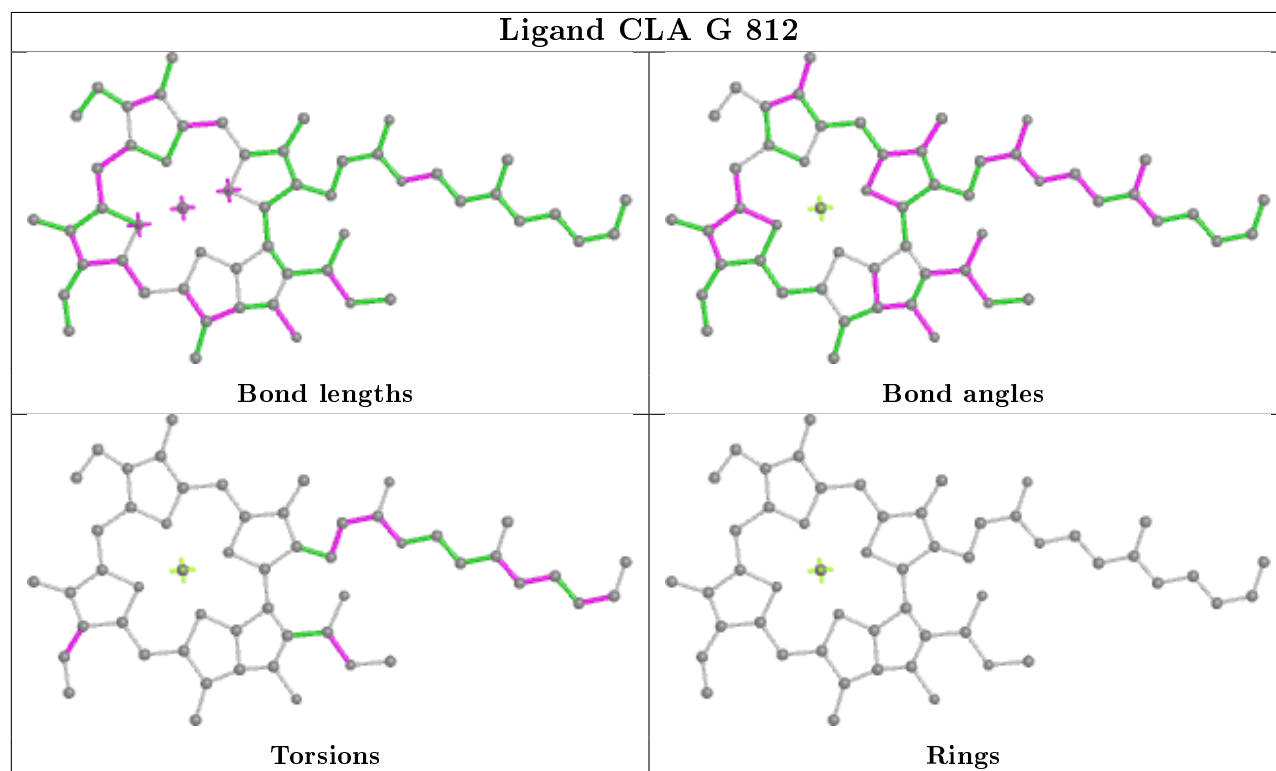
## Ligand CLA A 804



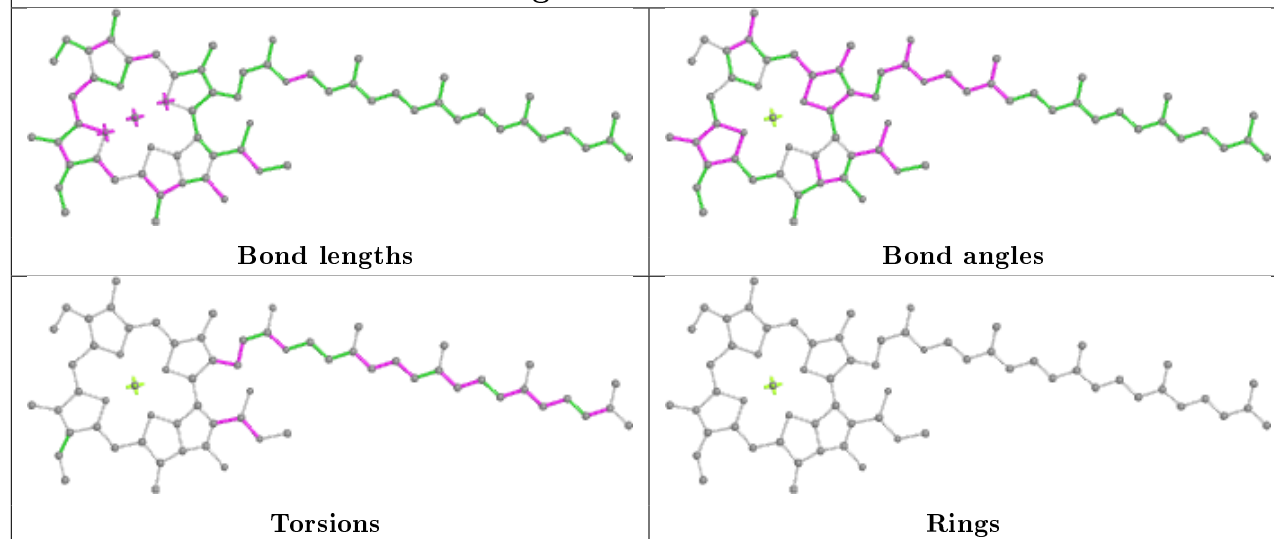
## Ligand CLA A 829



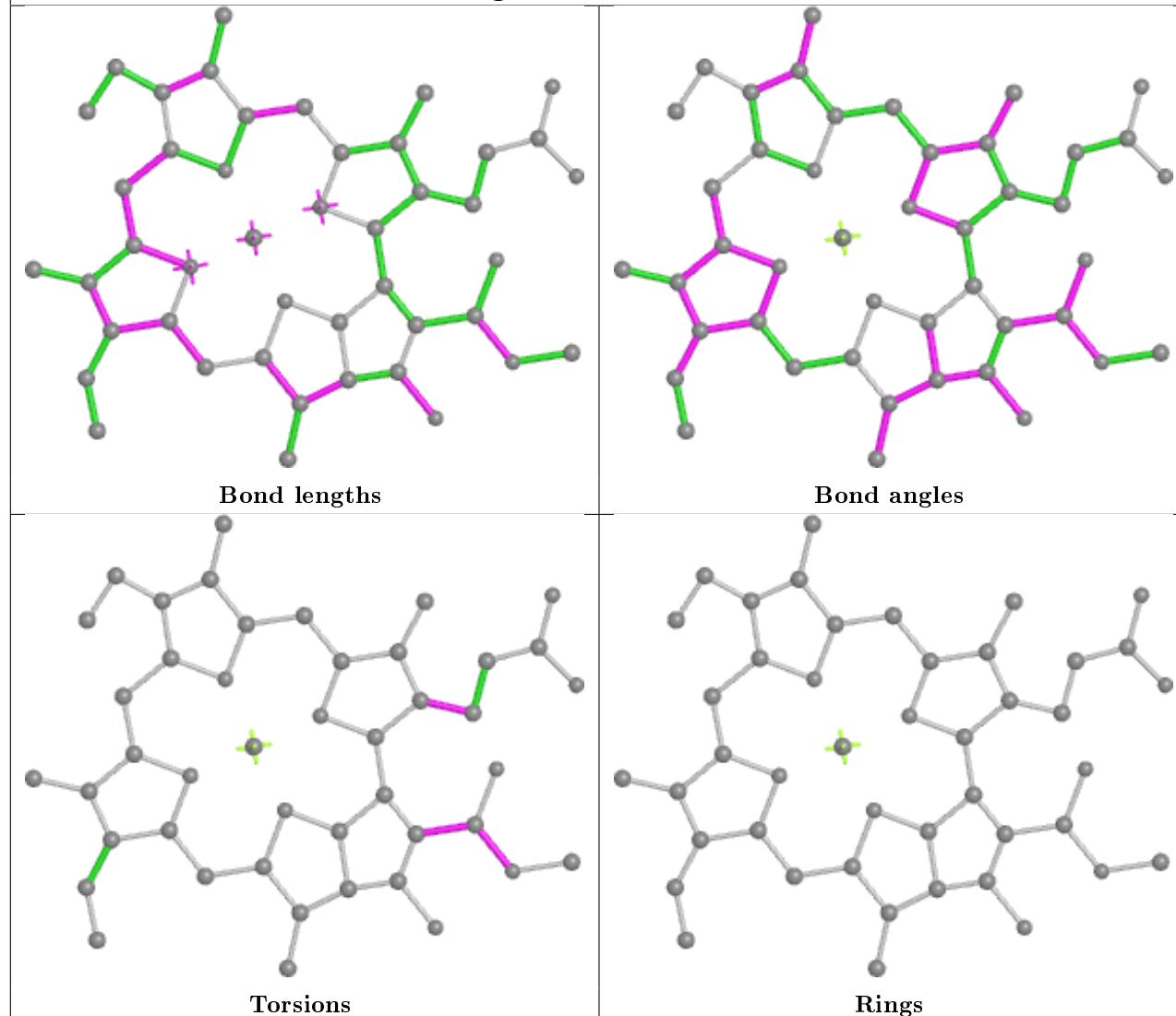
## Ligand CLA G 812



## Ligand CLA Y 808

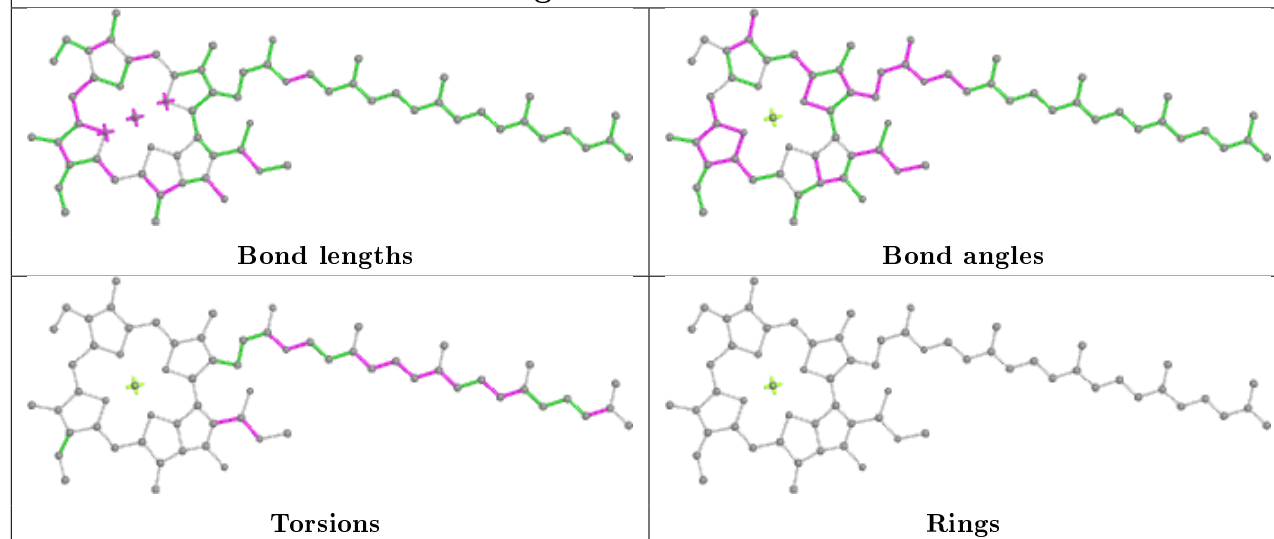


## Ligand CLA H 832

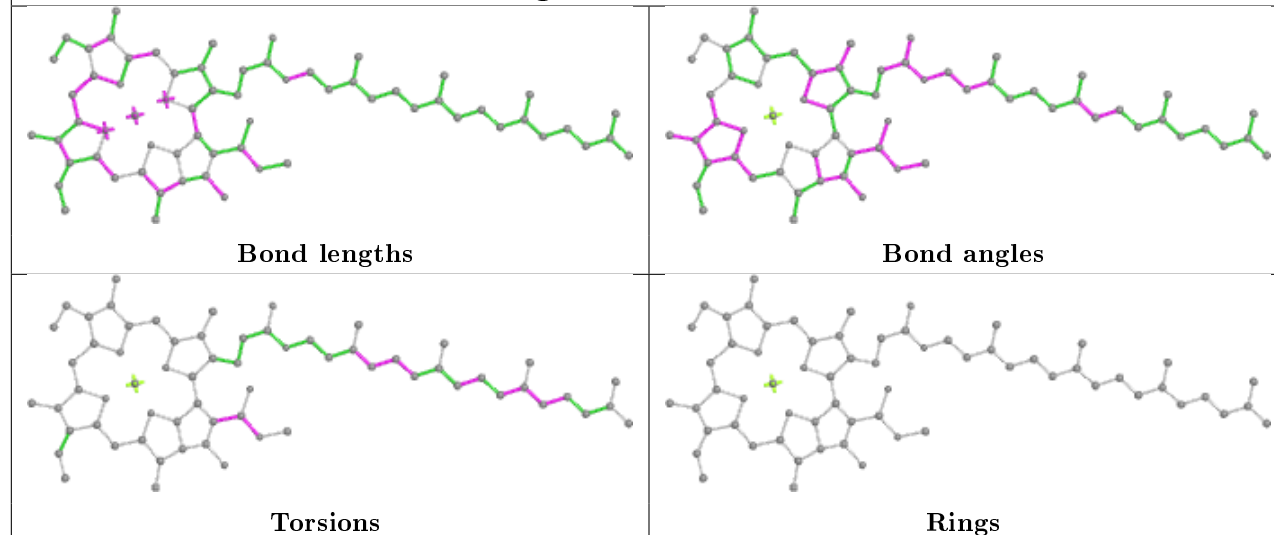




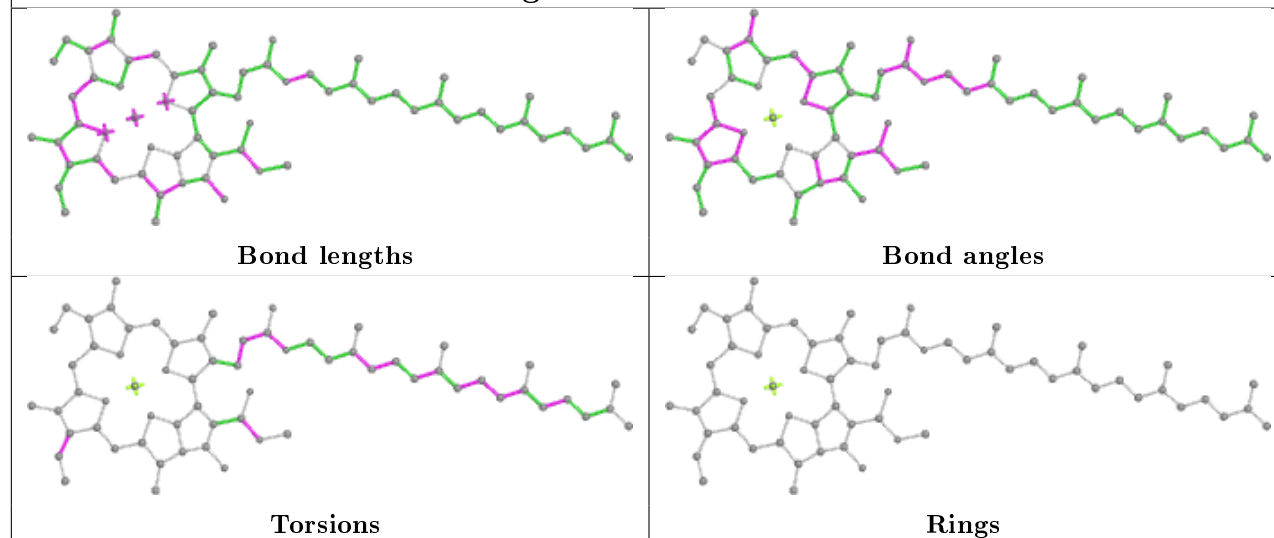
## Ligand CLA Z 801



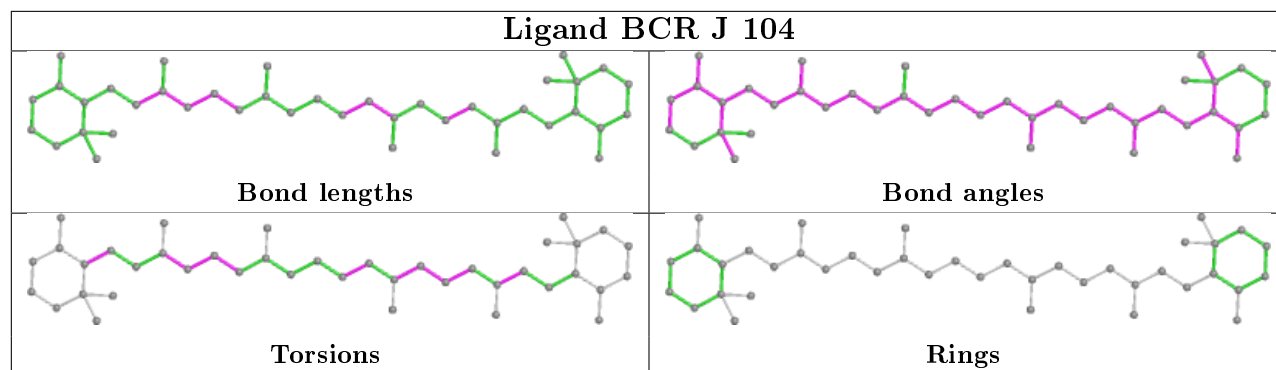
## Ligand CLA Z 807



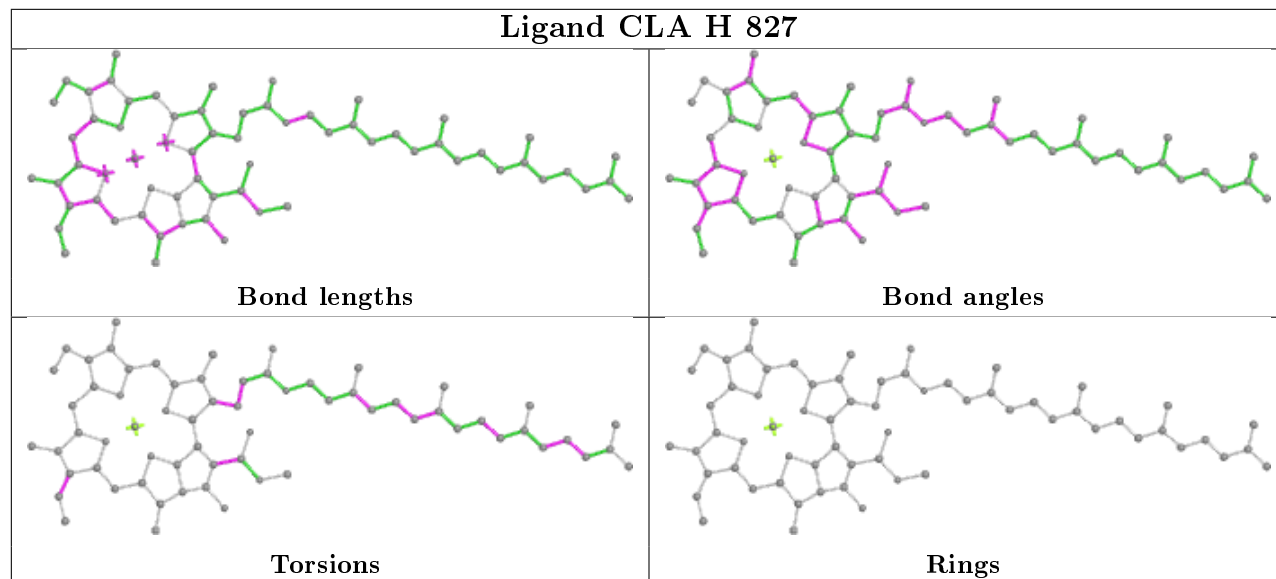
## Ligand CLA U 1004



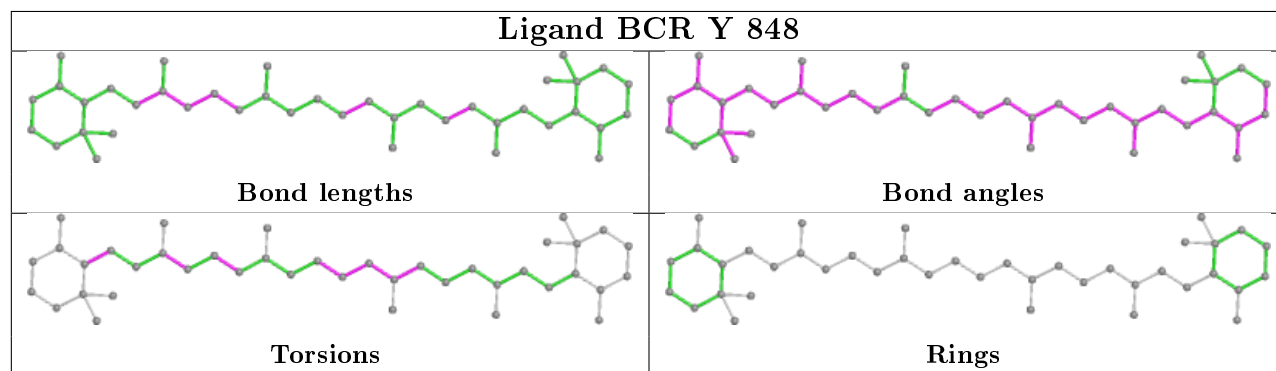
## Ligand BCR J 104

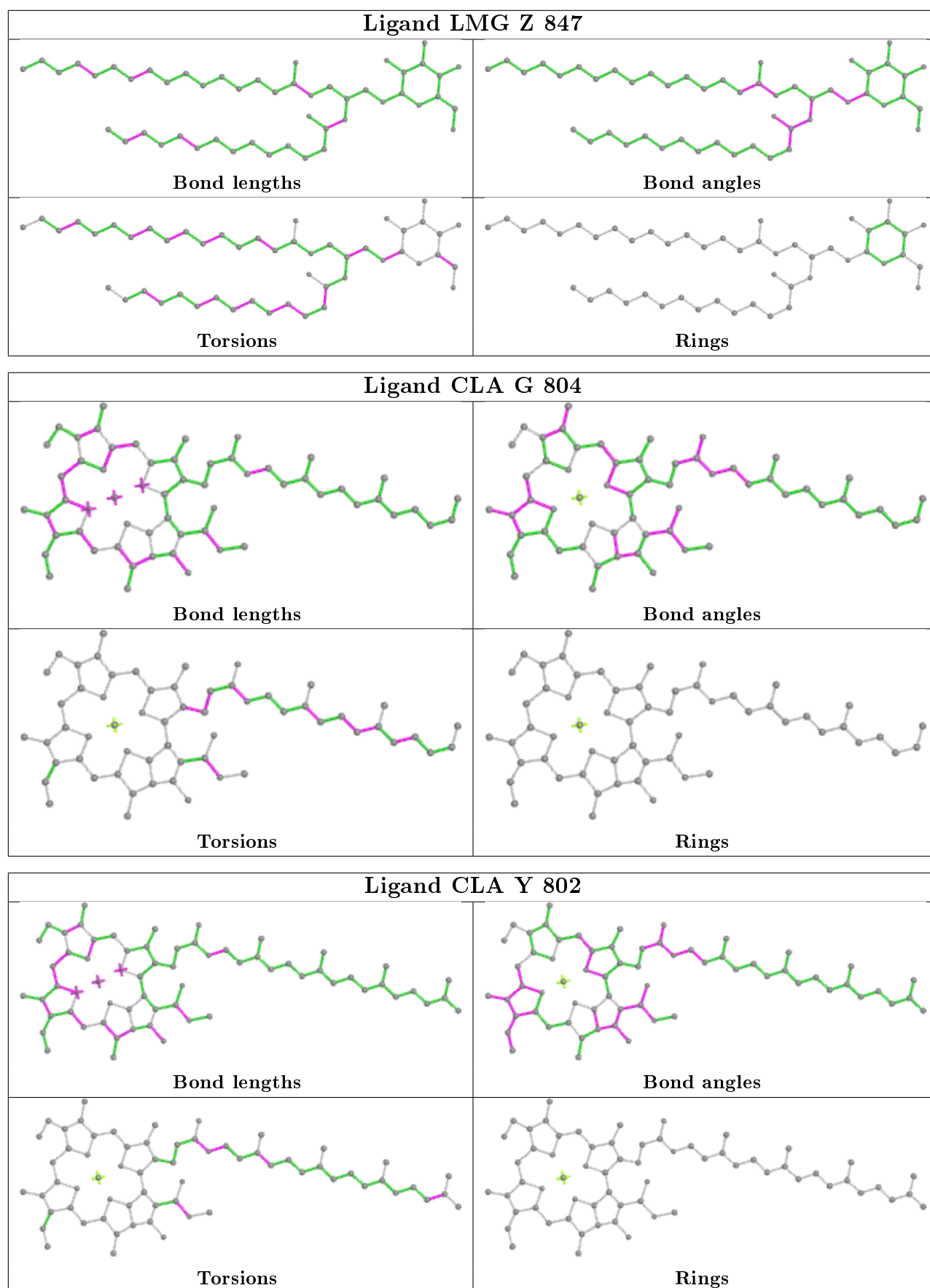


## Ligand CLA H 827

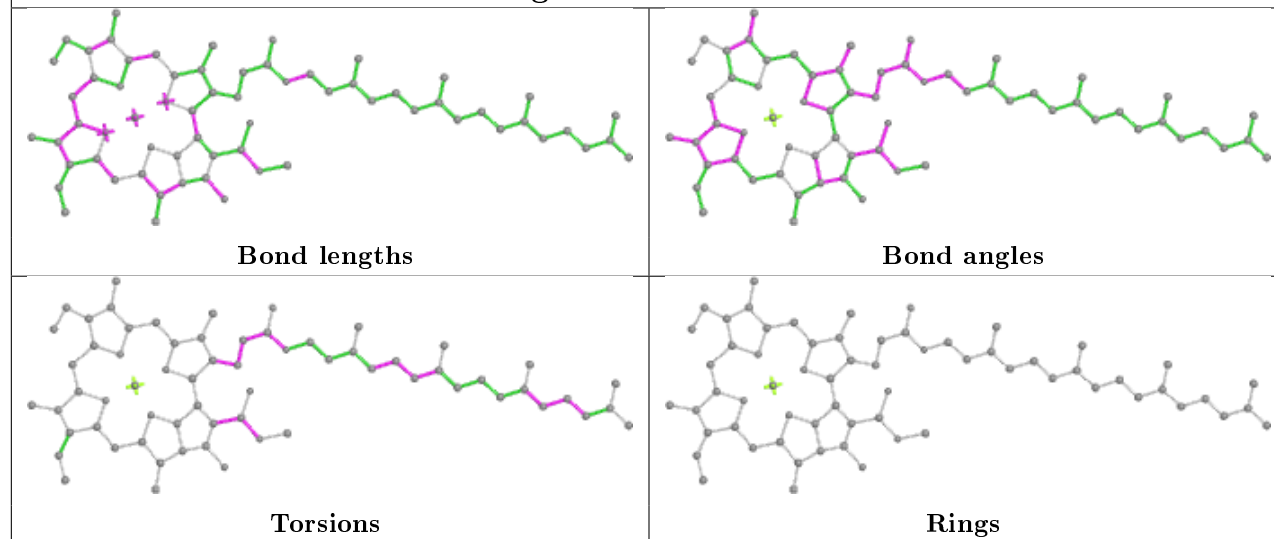


## Ligand BCR Y 848

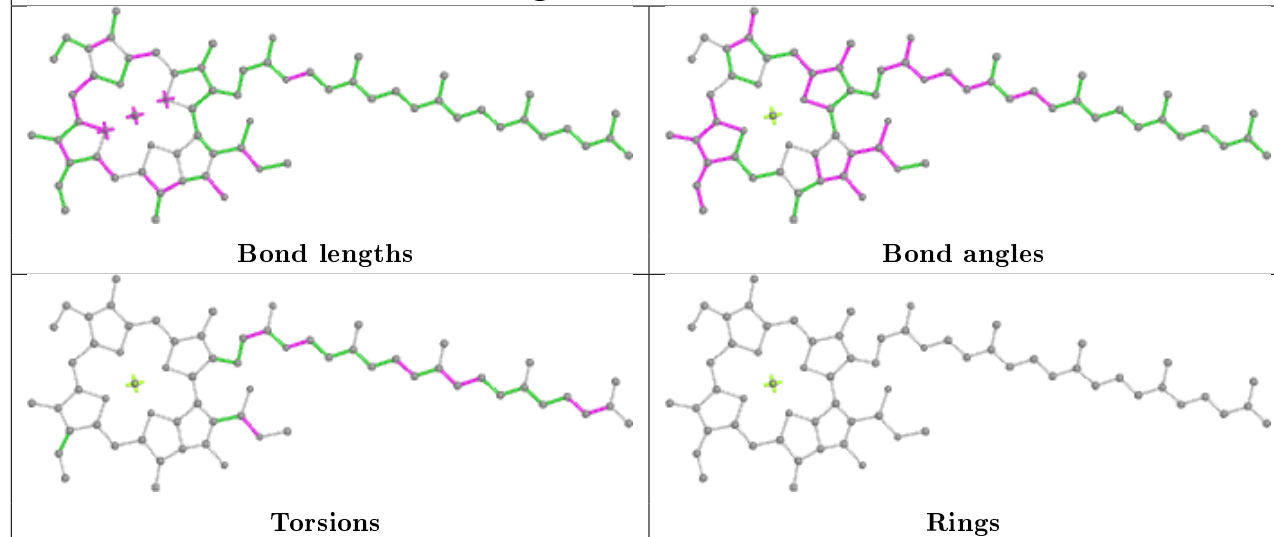




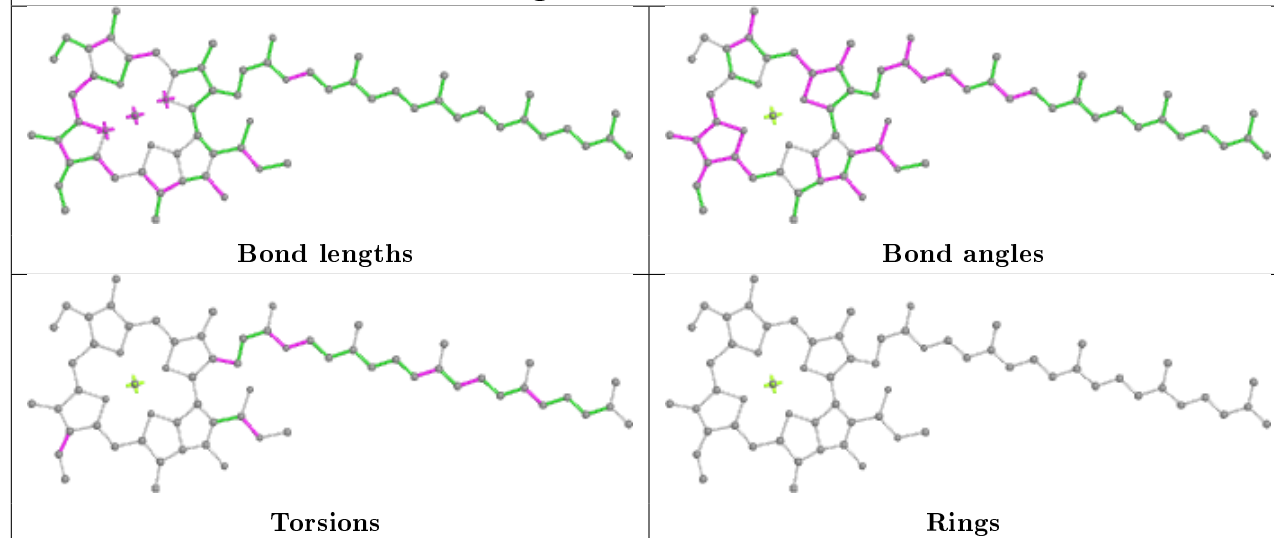
## Ligand CLA G 811



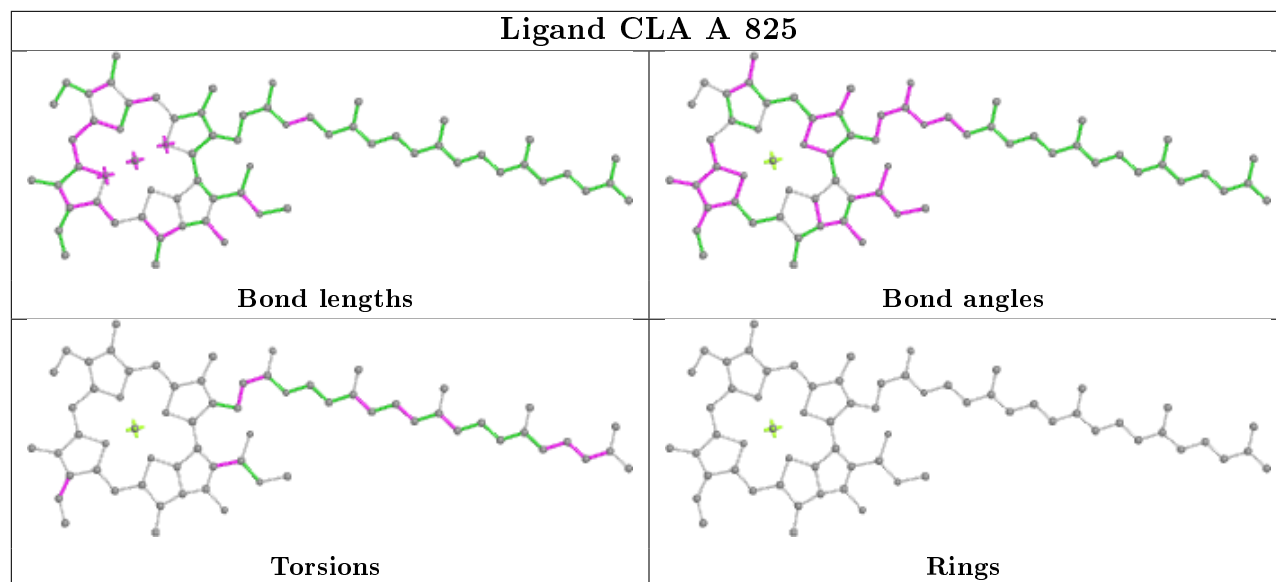
## Ligand CLA H 808



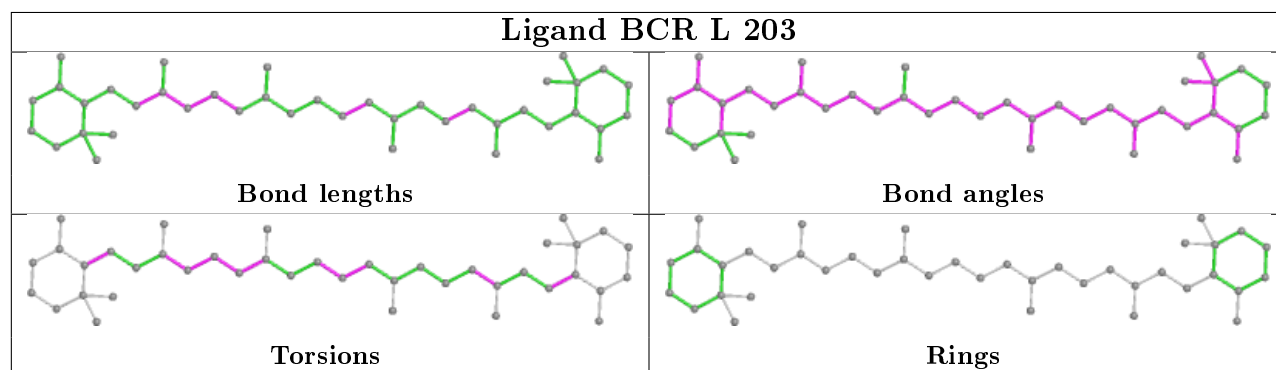
## Ligand CLA H 838



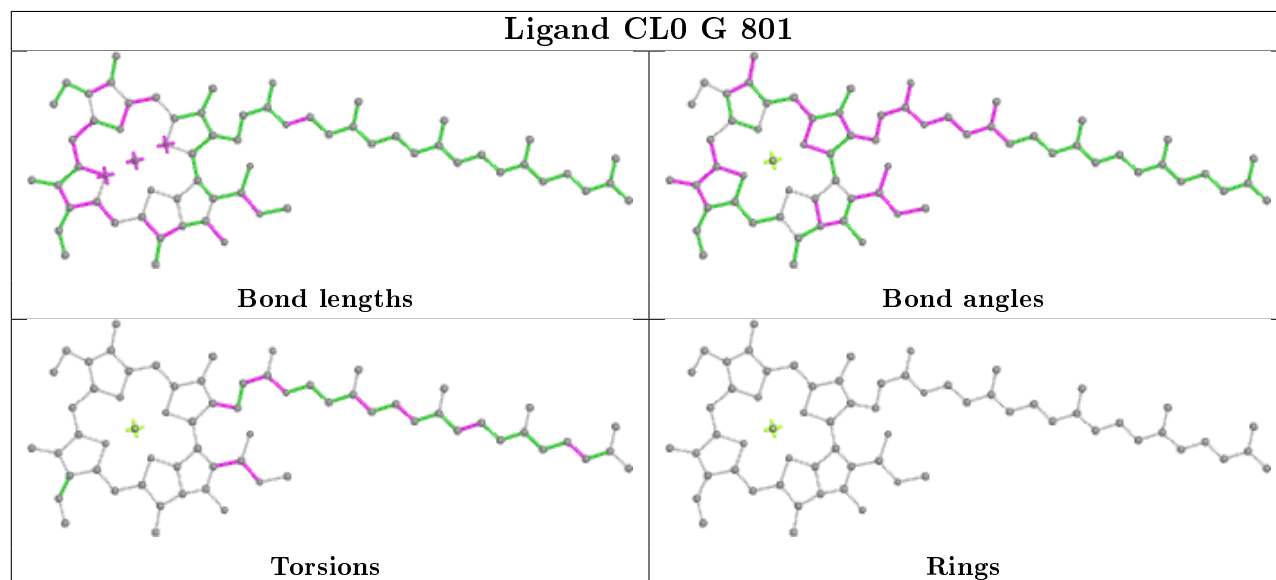
## Ligand CLA A 825

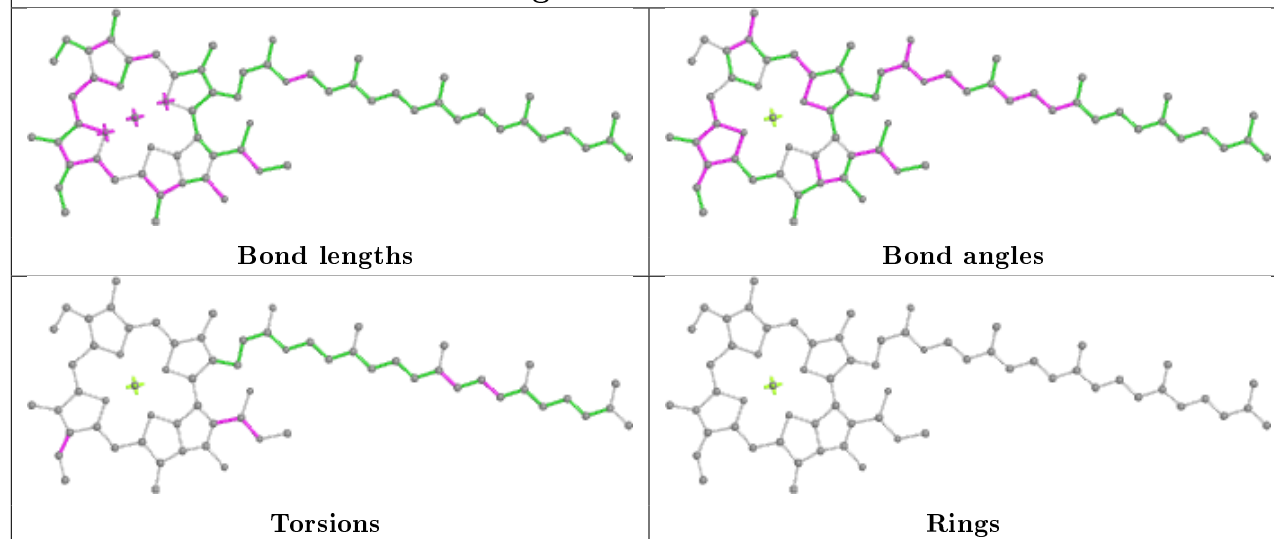
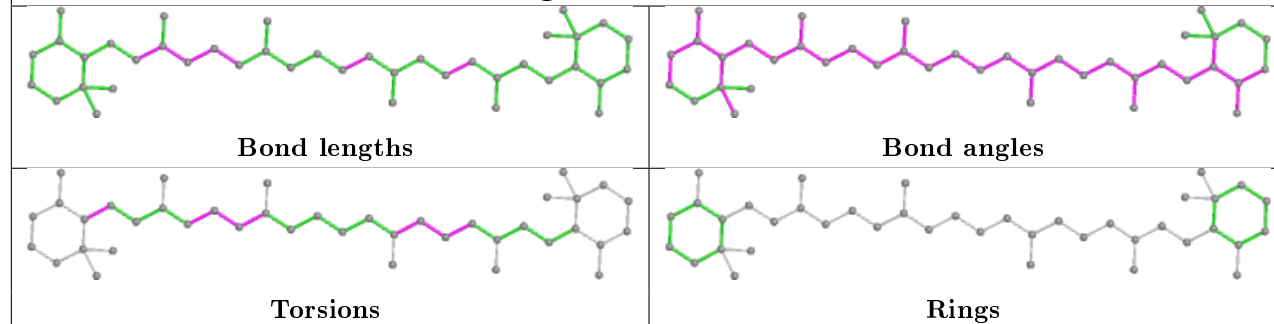
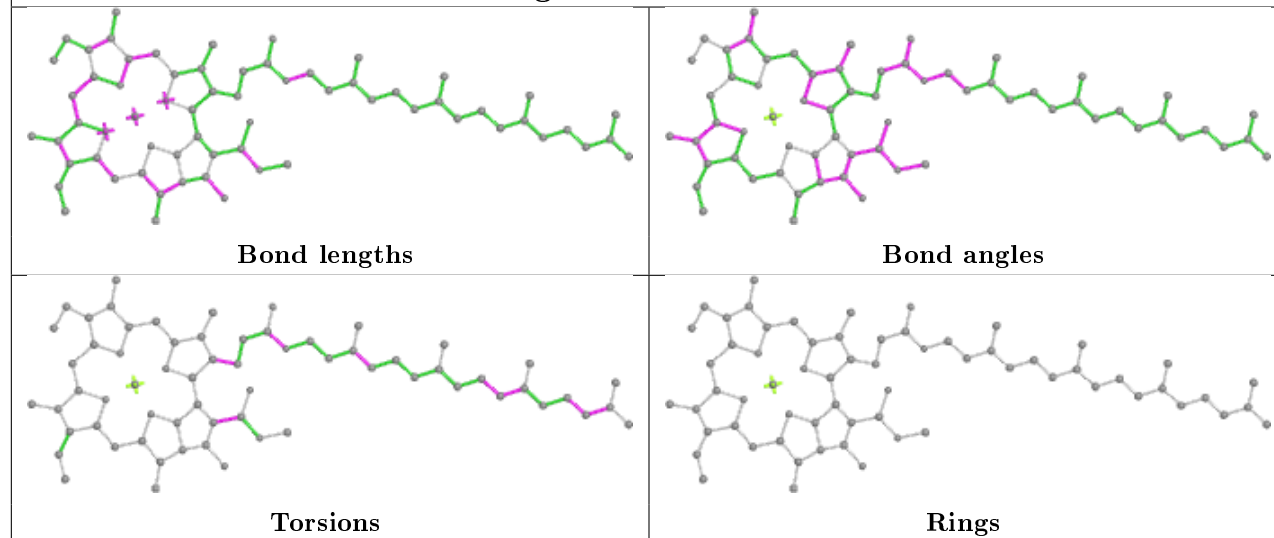


## Ligand BCR L 203

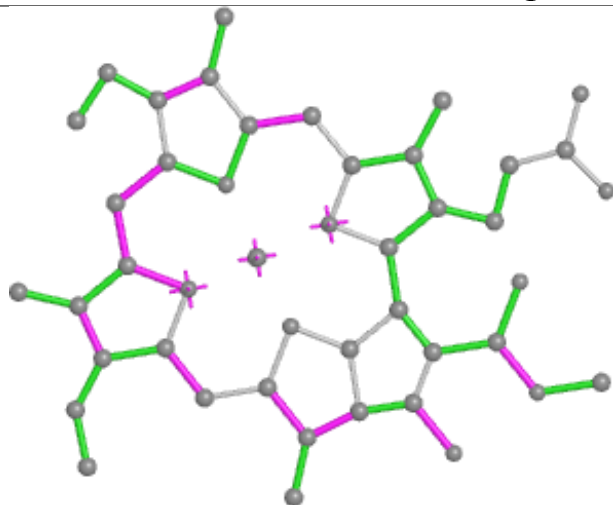


## Ligand CL0 G 801

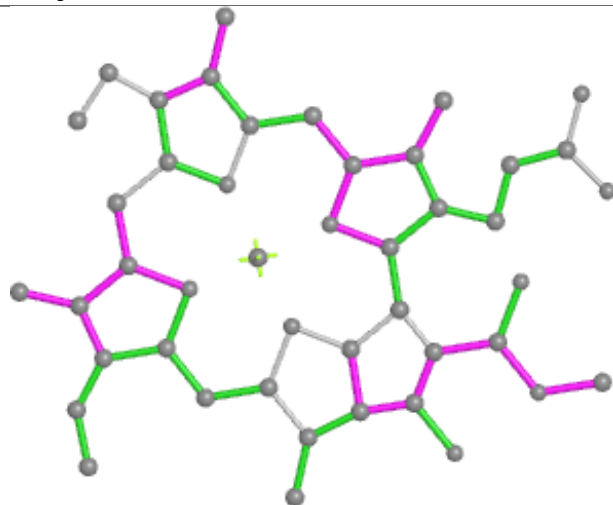


**Ligand CLA B 804****Ligand BCR f 103****Ligand CLA Z 812**

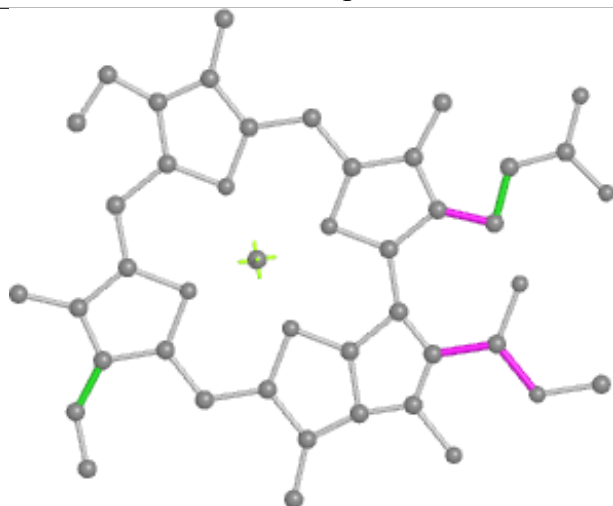
## Ligand CLA j 102



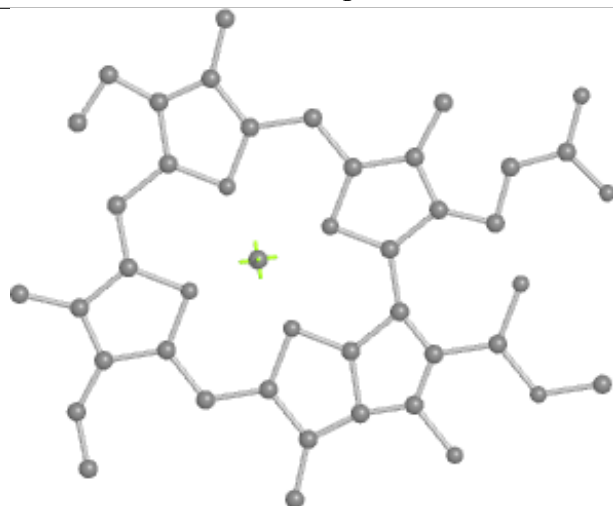
Bond lengths



Bond angles

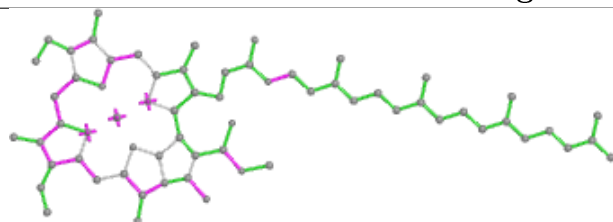


Torsions

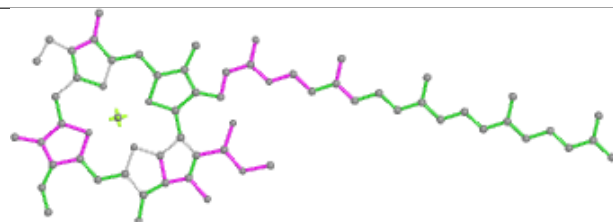


Rings

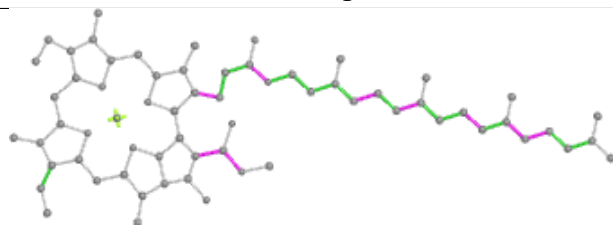
## Ligand CLA L 206



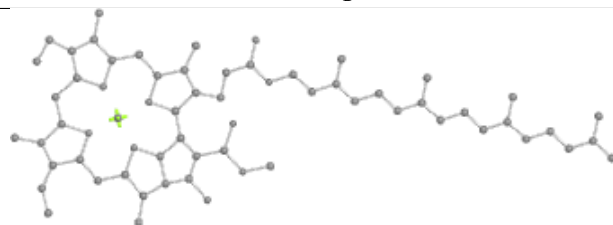
Bond lengths



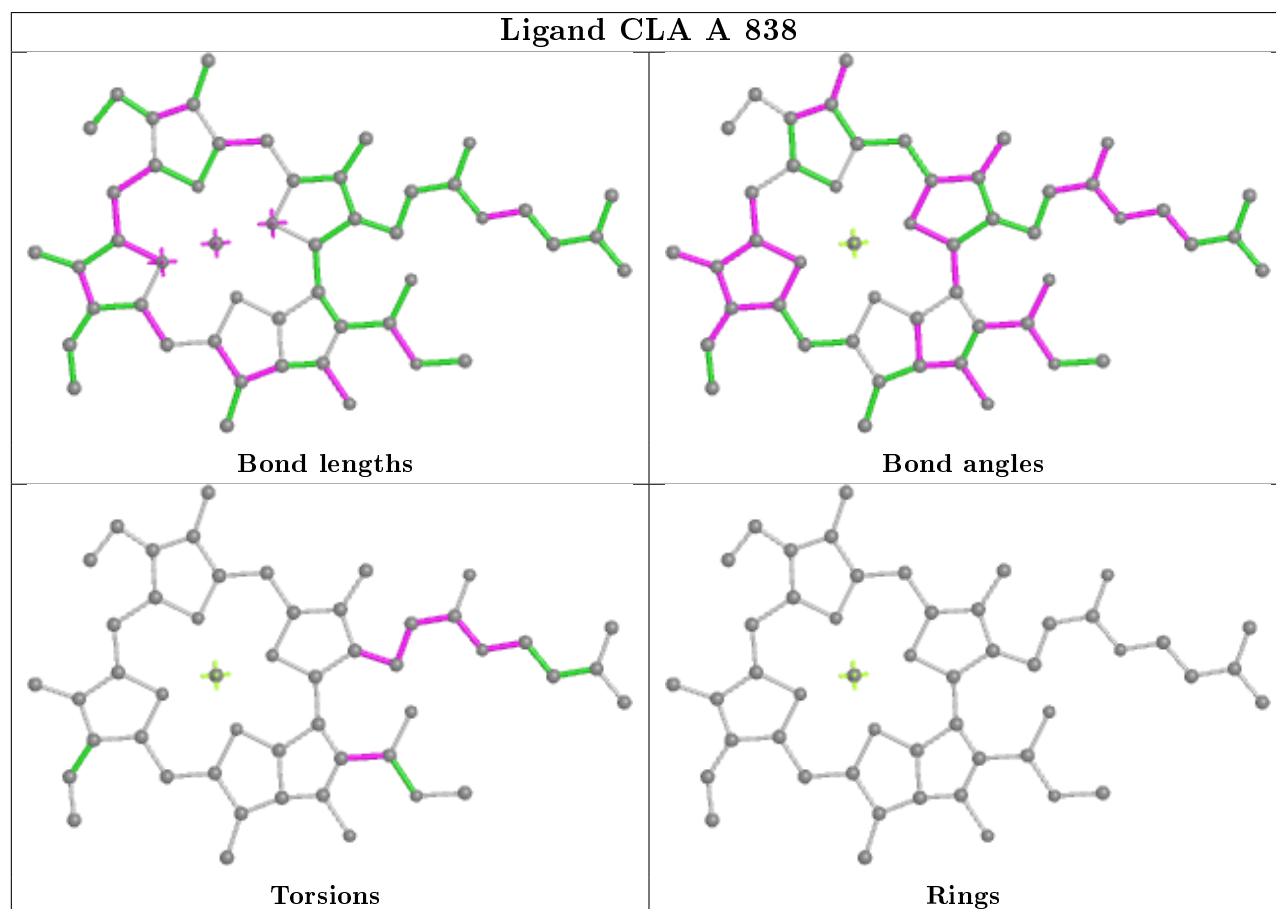
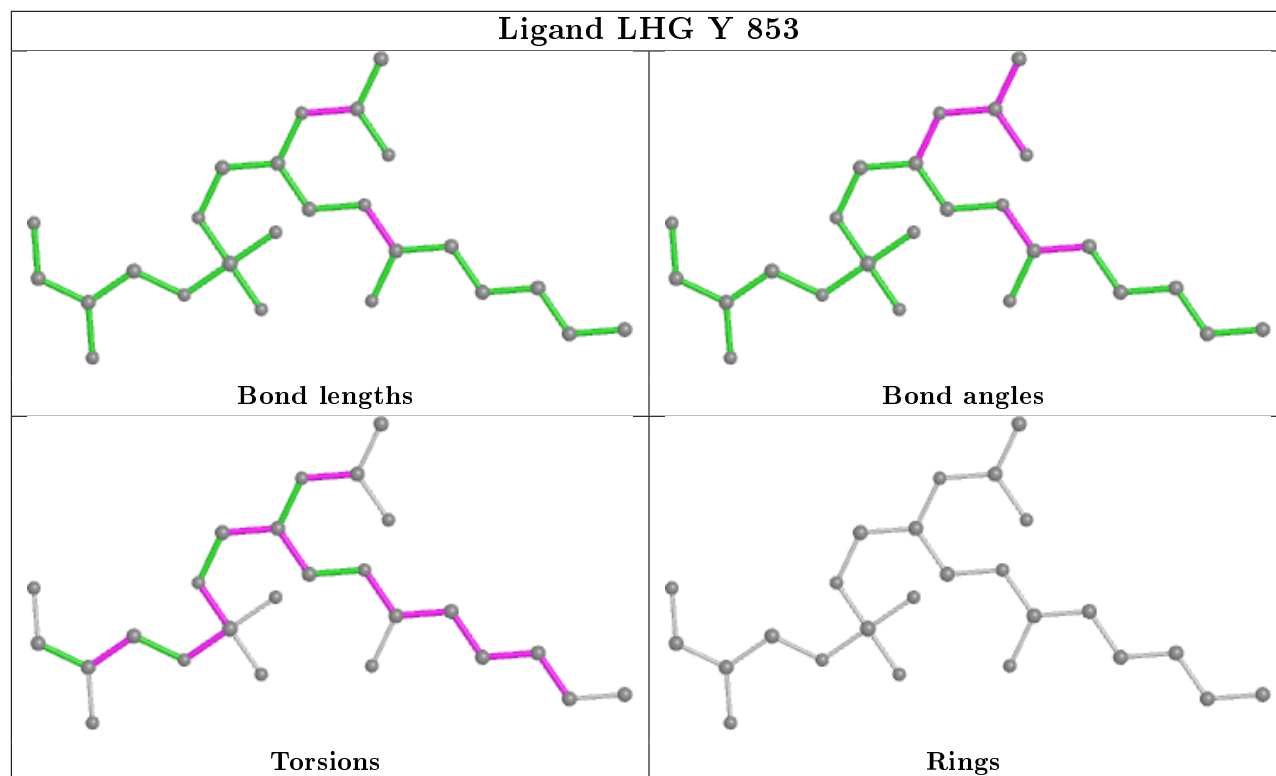
Bond angles



Torsions

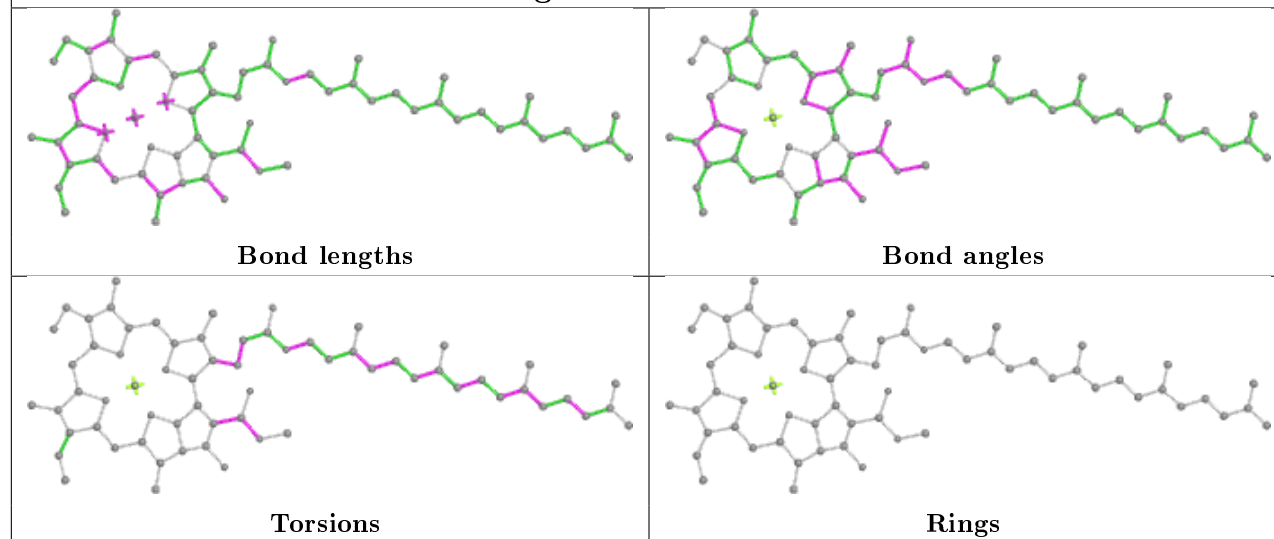


Rings

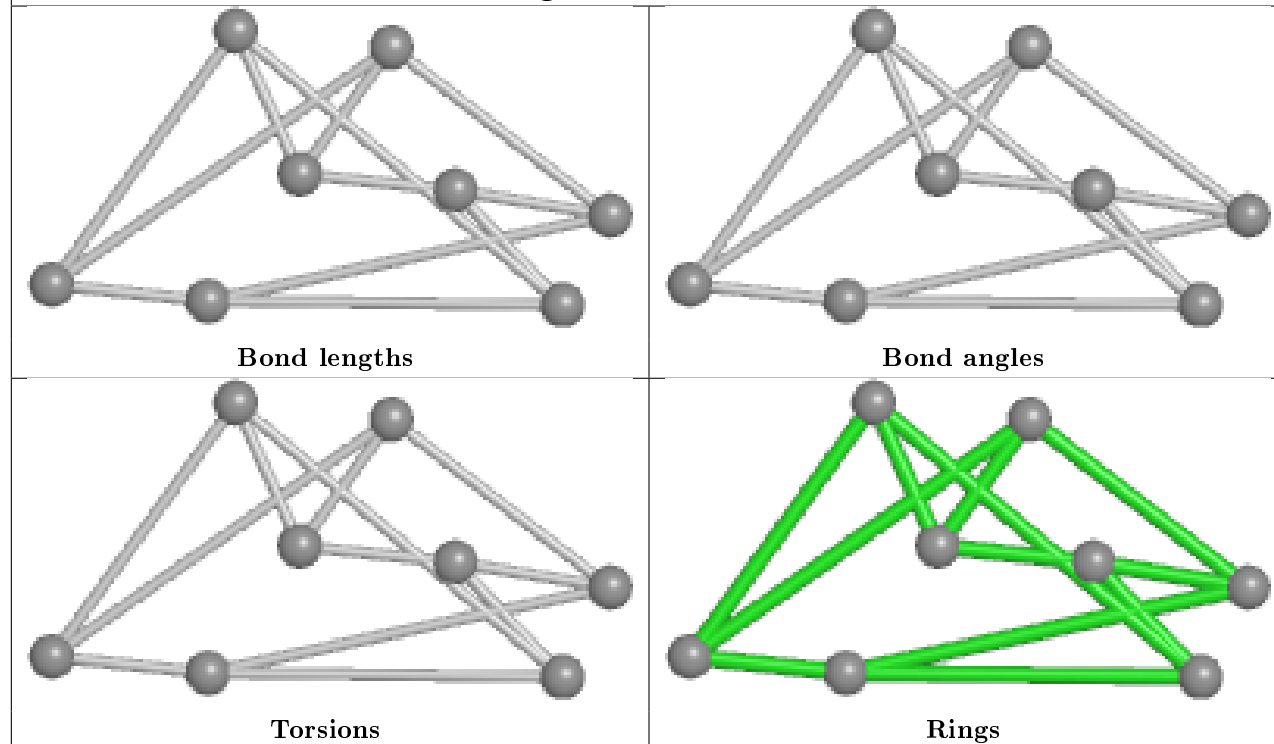


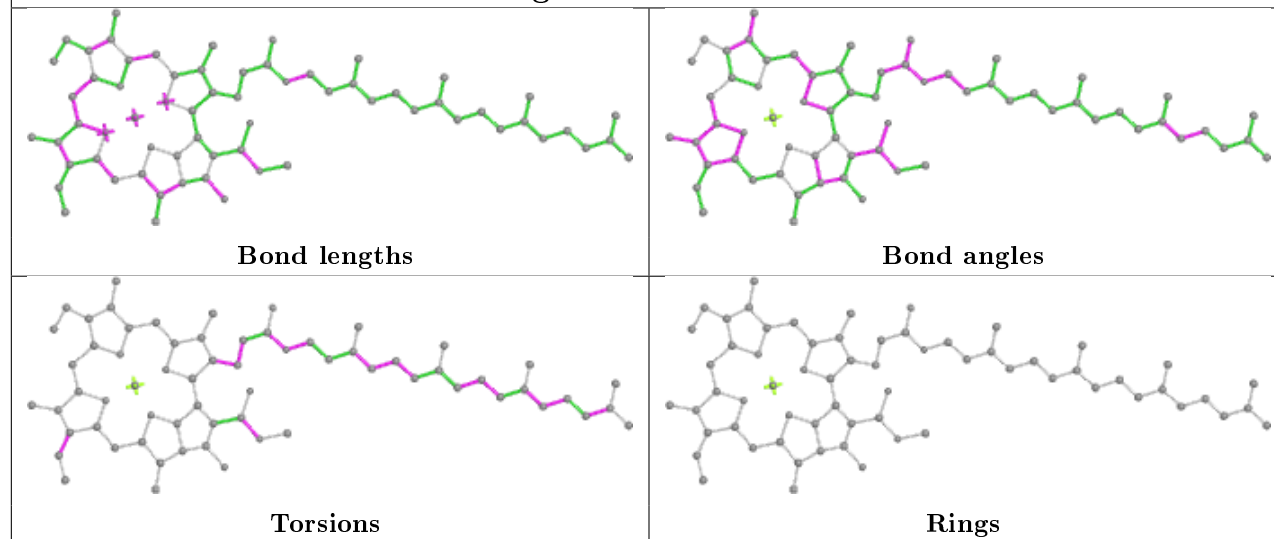
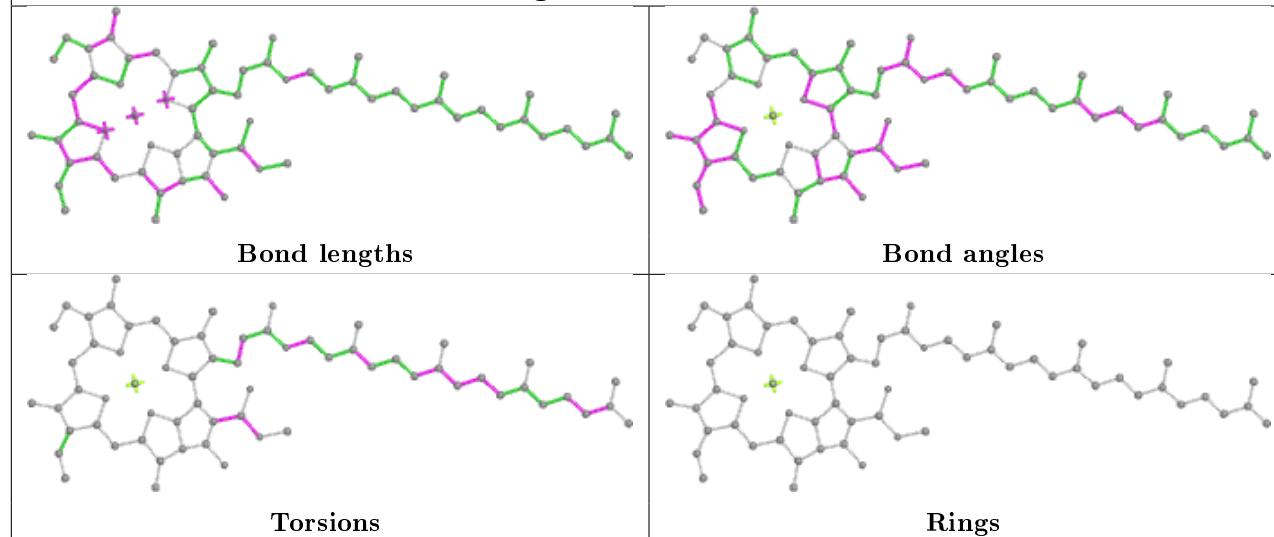


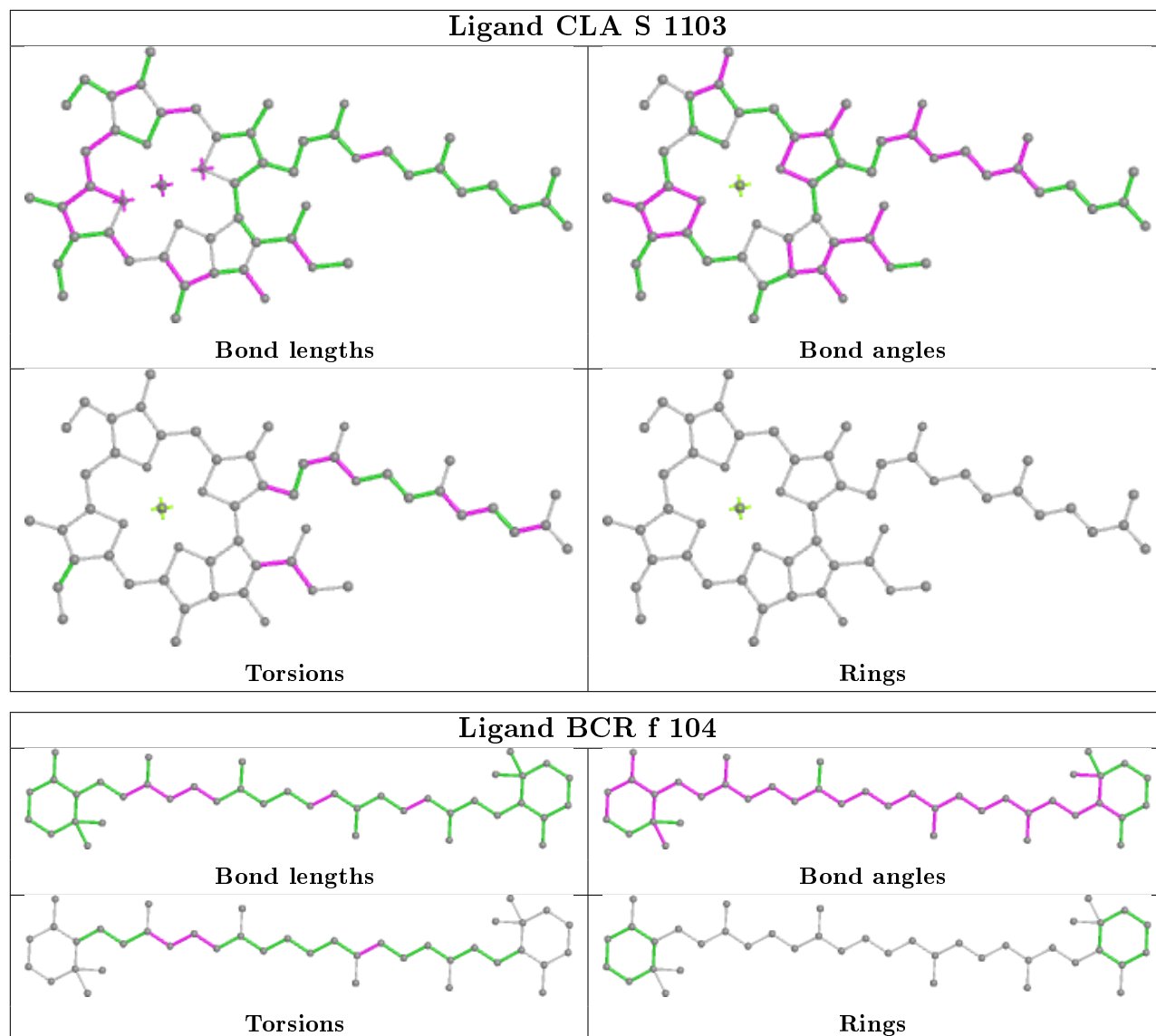
## Ligand CLA Z 830



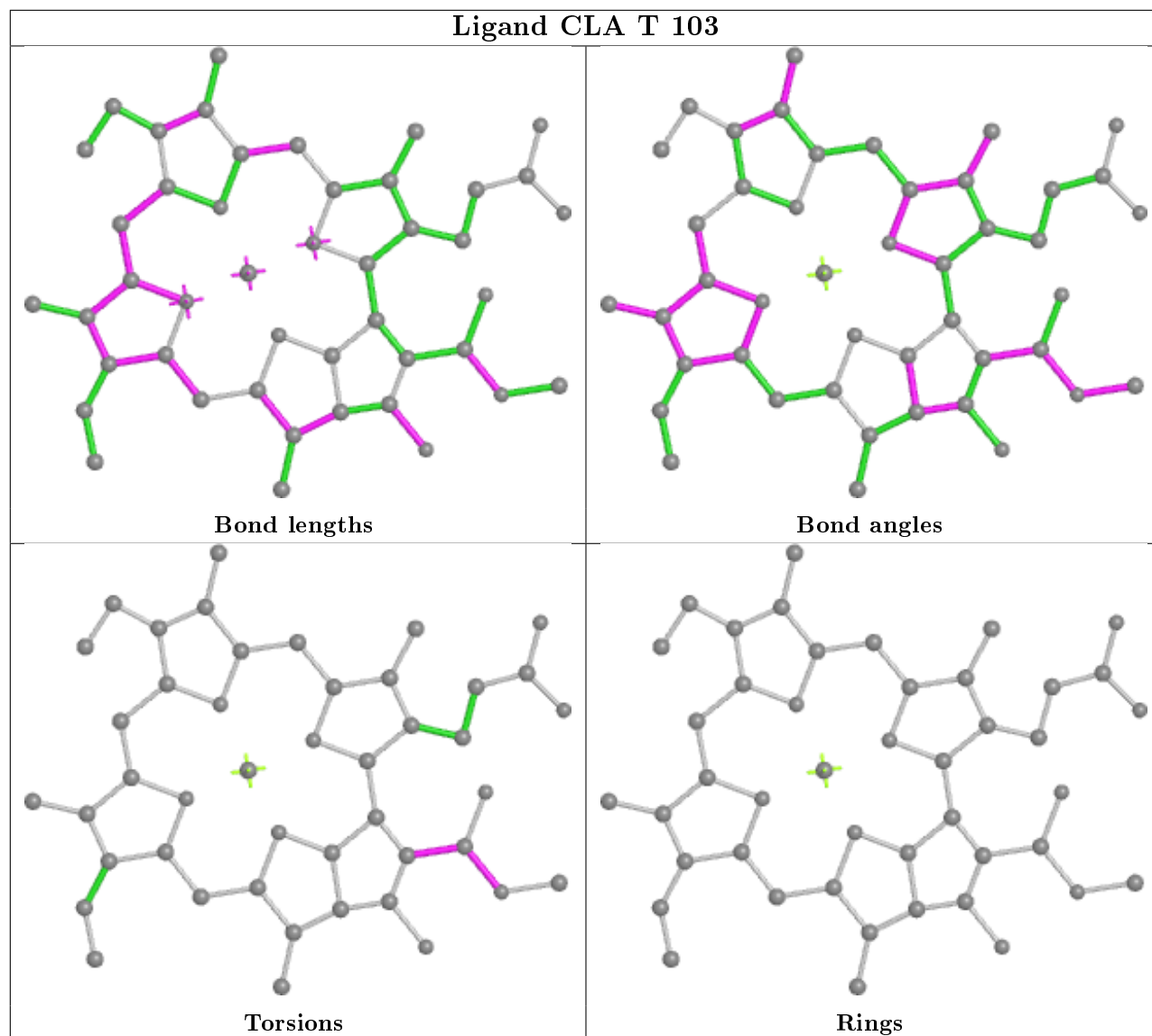
## Ligand SF4 N 102



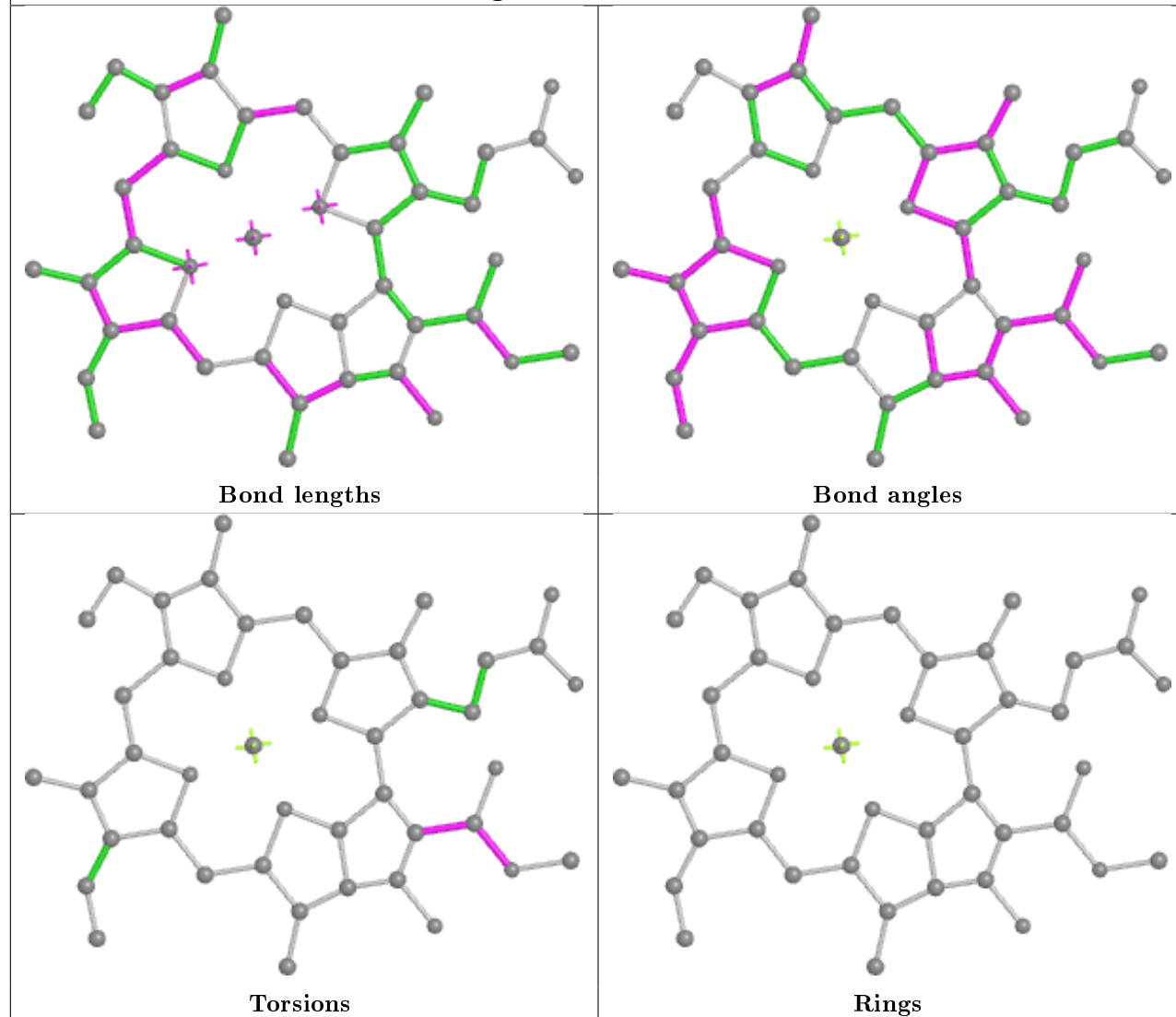
**Ligand CLA B 832****Ligand CLA B 810**



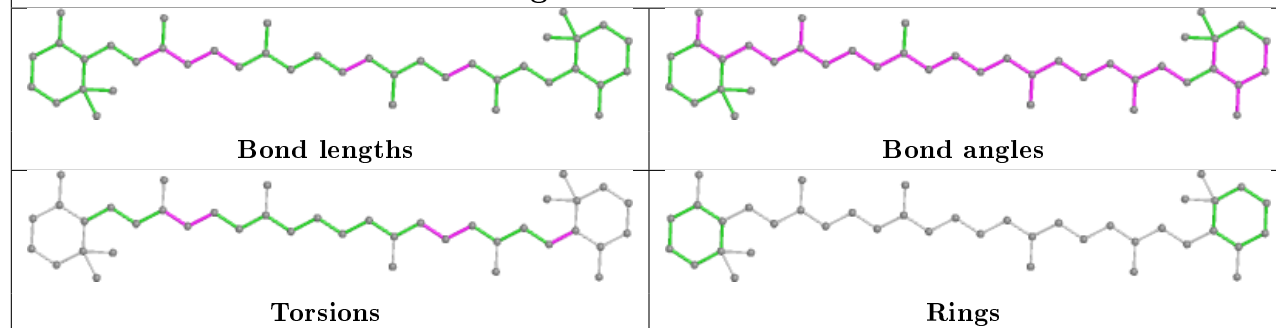
## Ligand CLA T 103

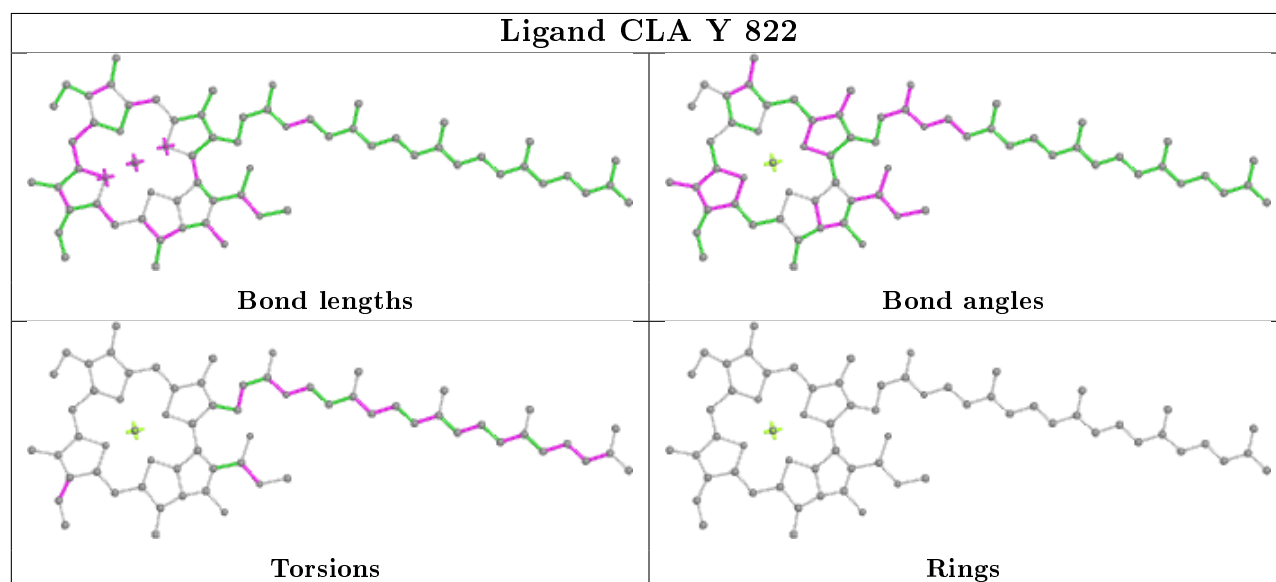
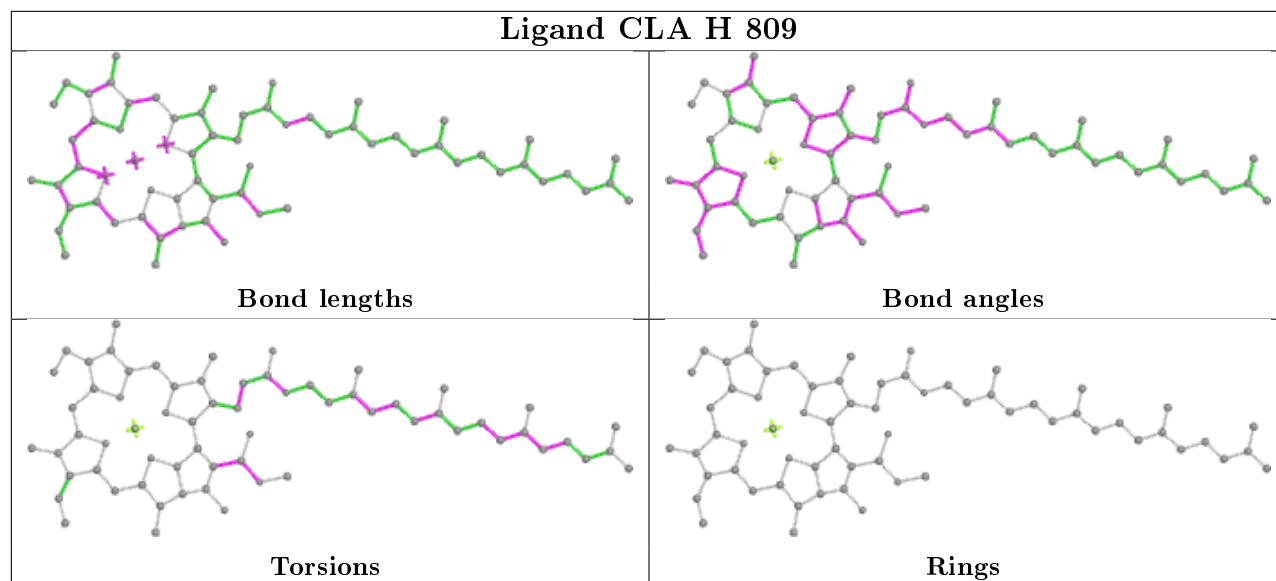
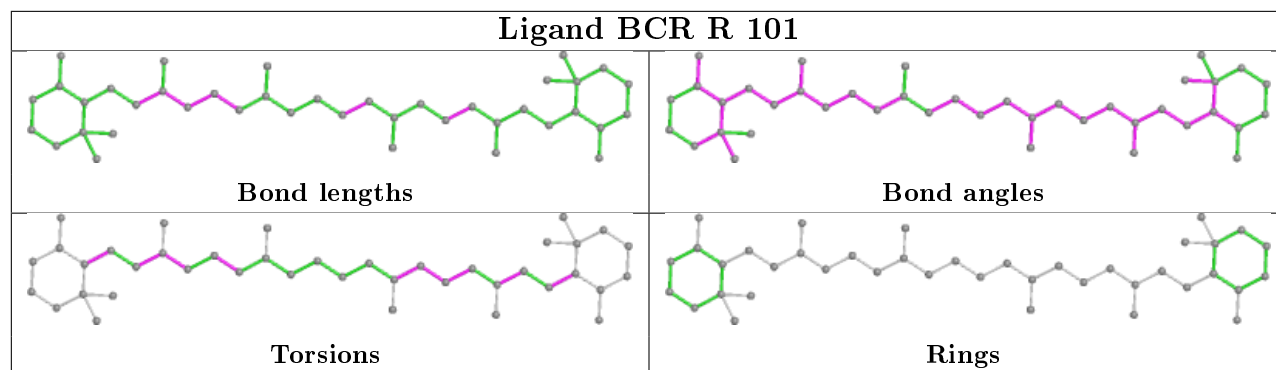


## Ligand CLA H 833

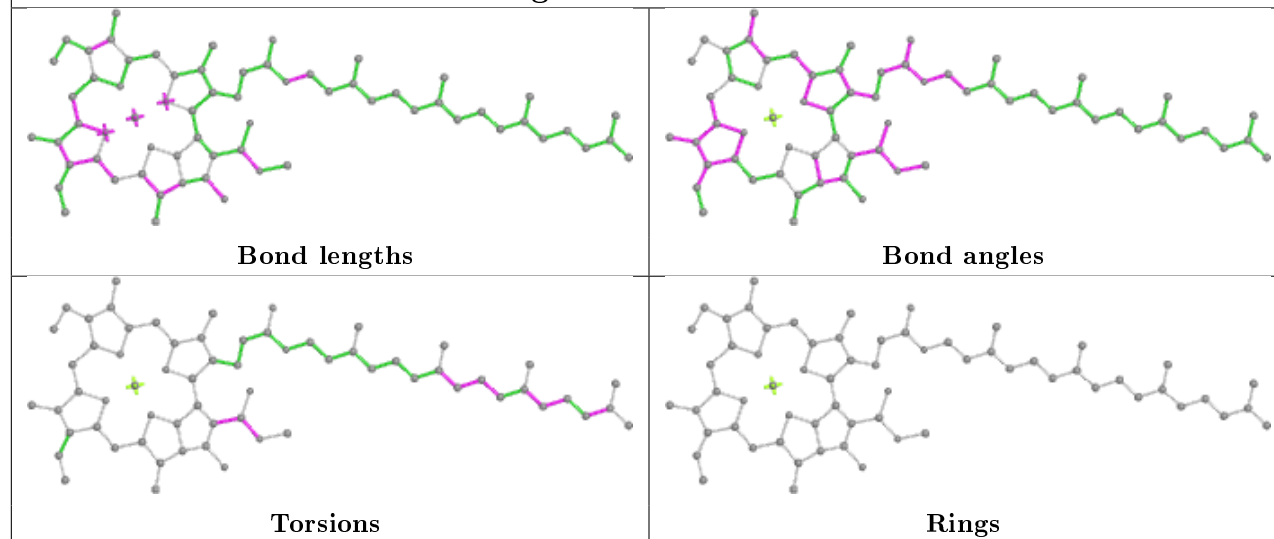


## Ligand BCR Y 850

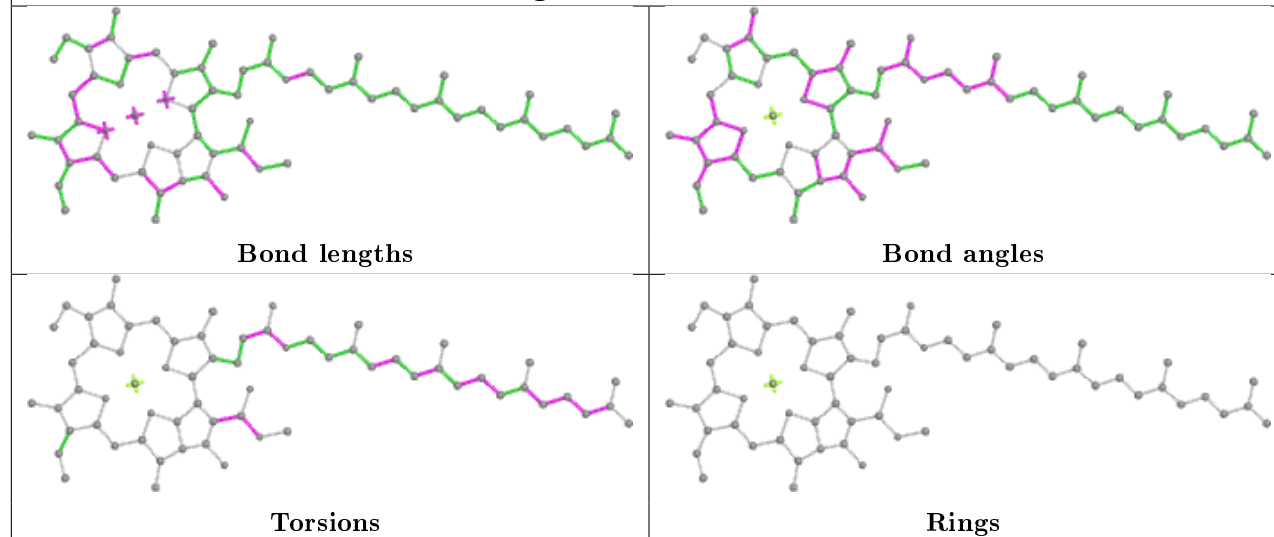




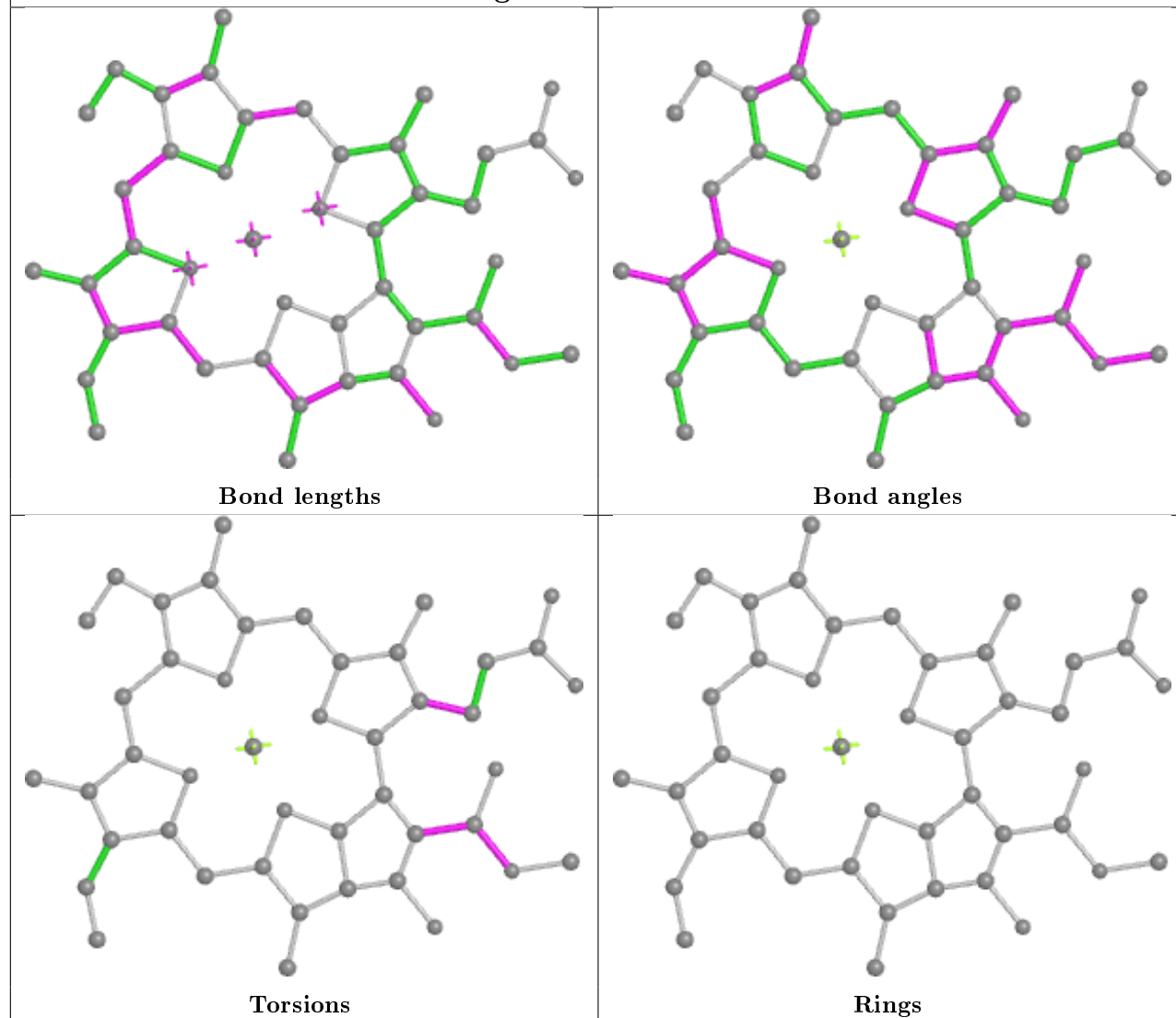
## Ligand CLA H 803



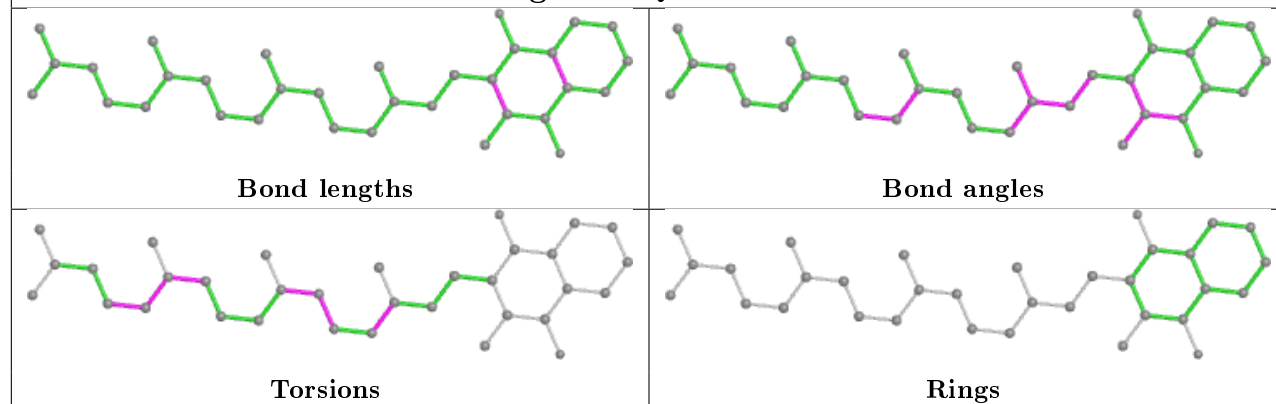
## Ligand CLA G 837



## Ligand CLA J 101

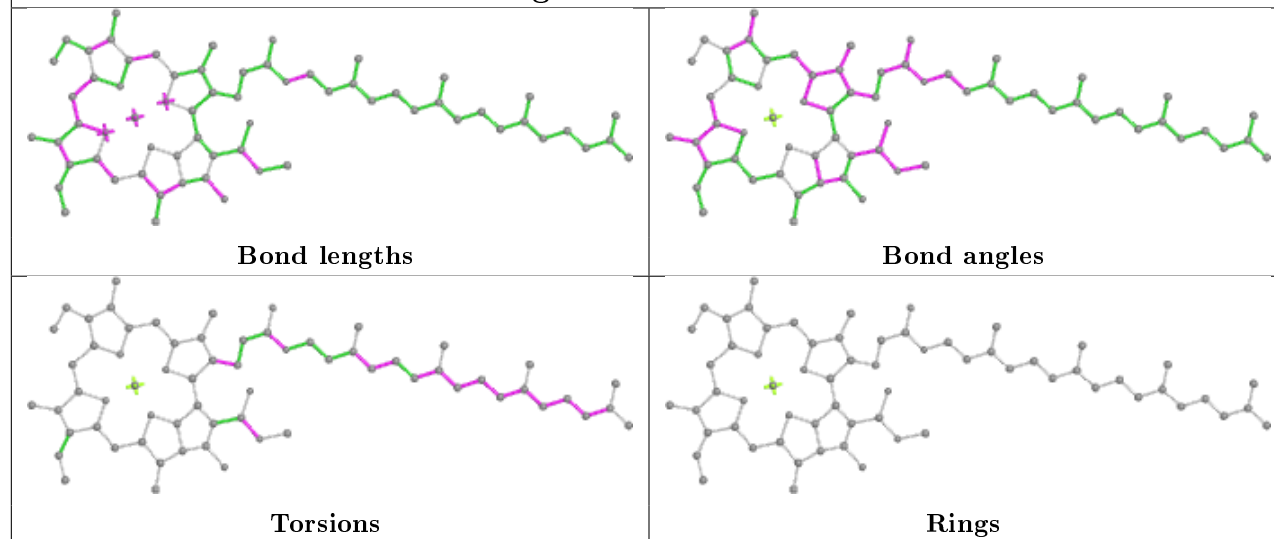


## Ligand PQN G 844

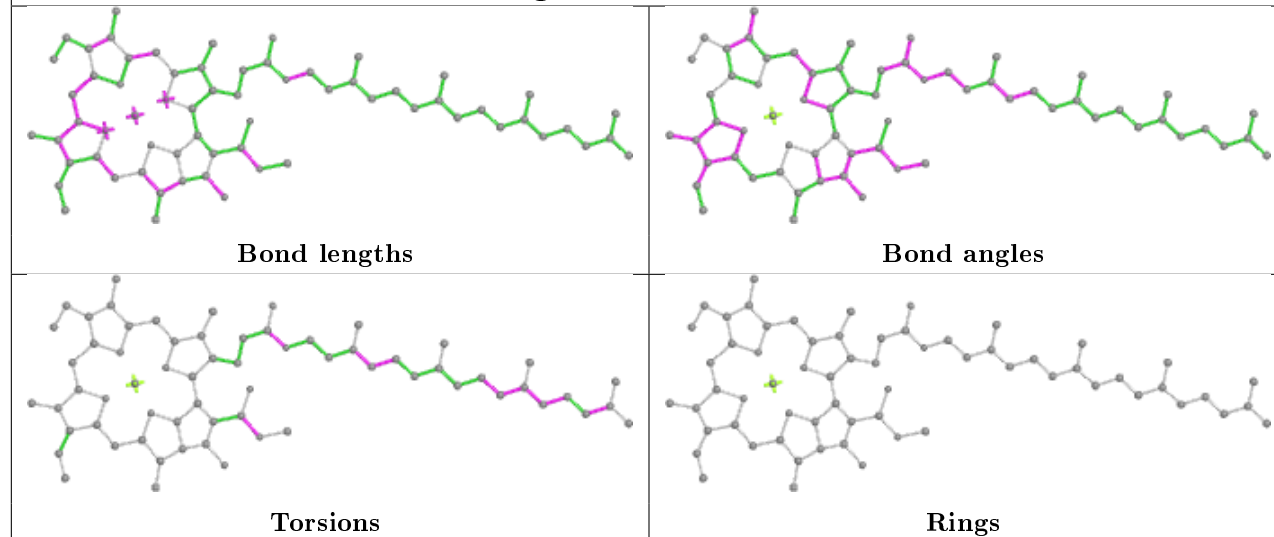




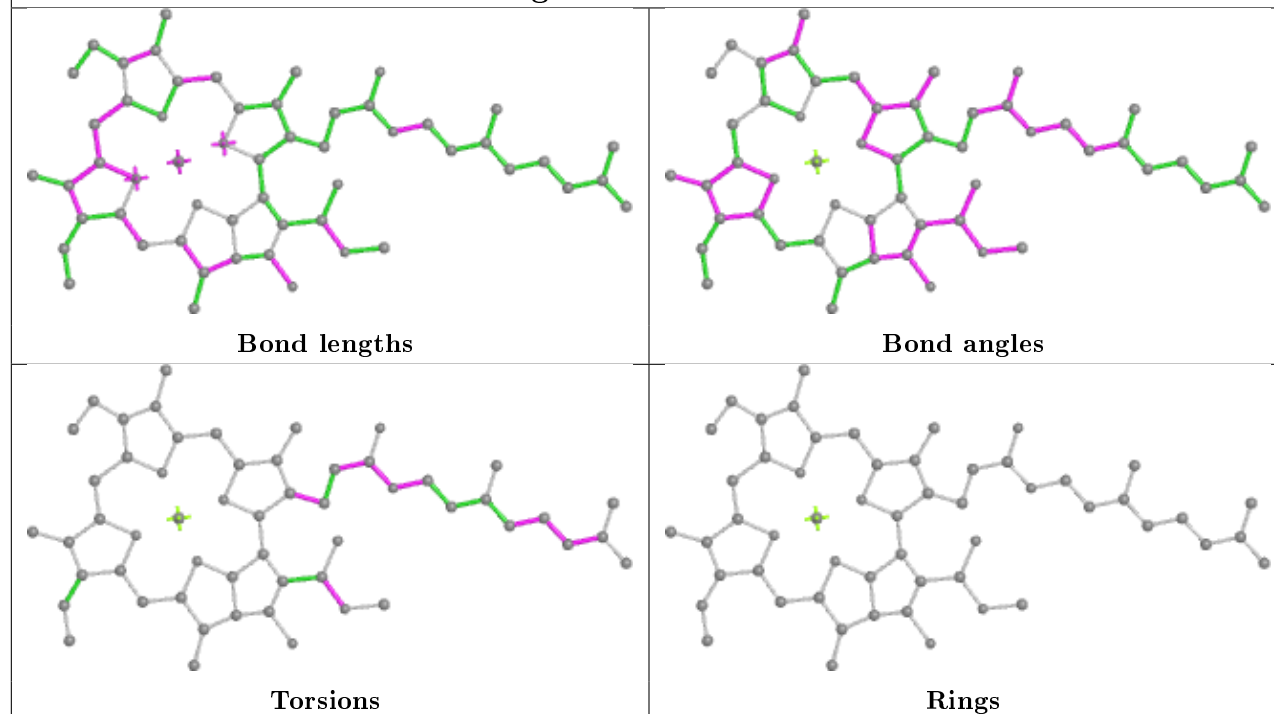
## Ligand CLA Y 832



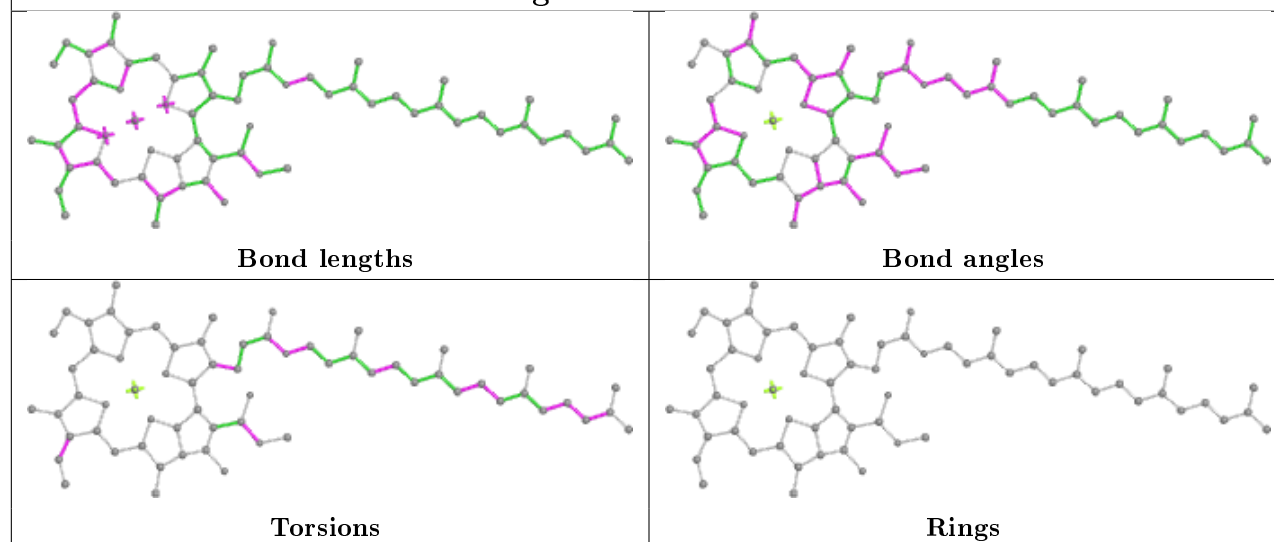
## Ligand CLA A 827



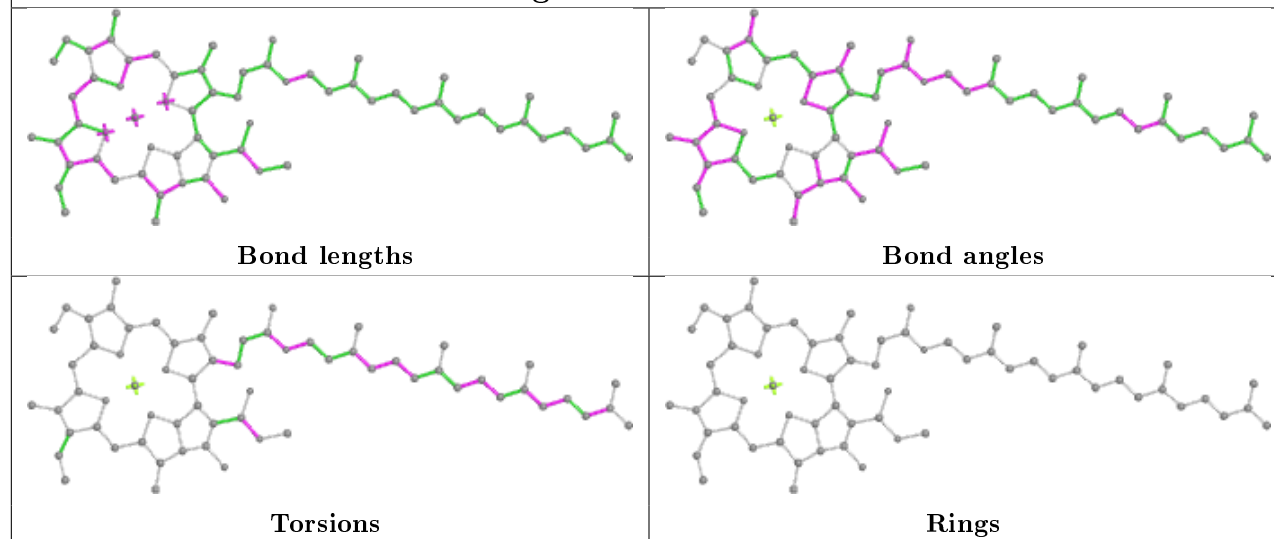
## Ligand CLA H 830



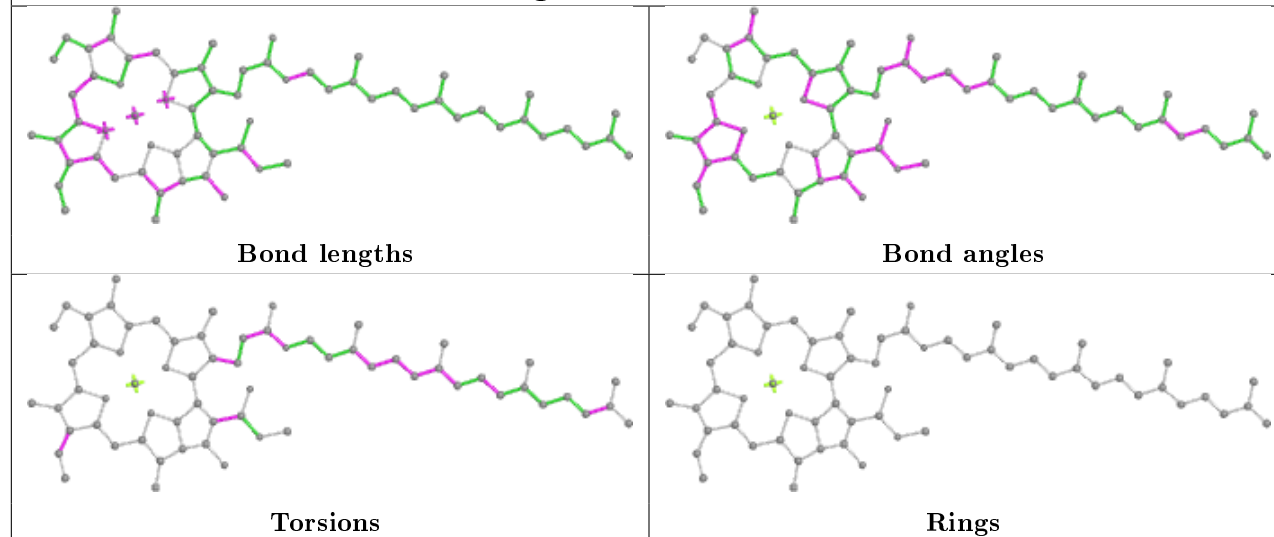
## Ligand CLA Y 818

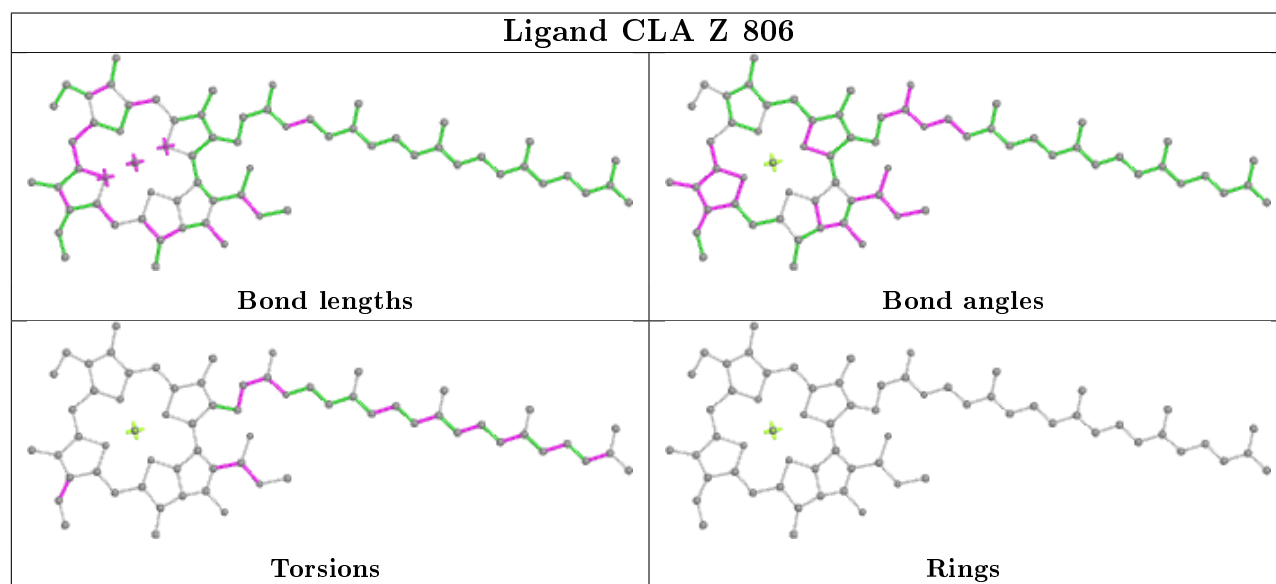
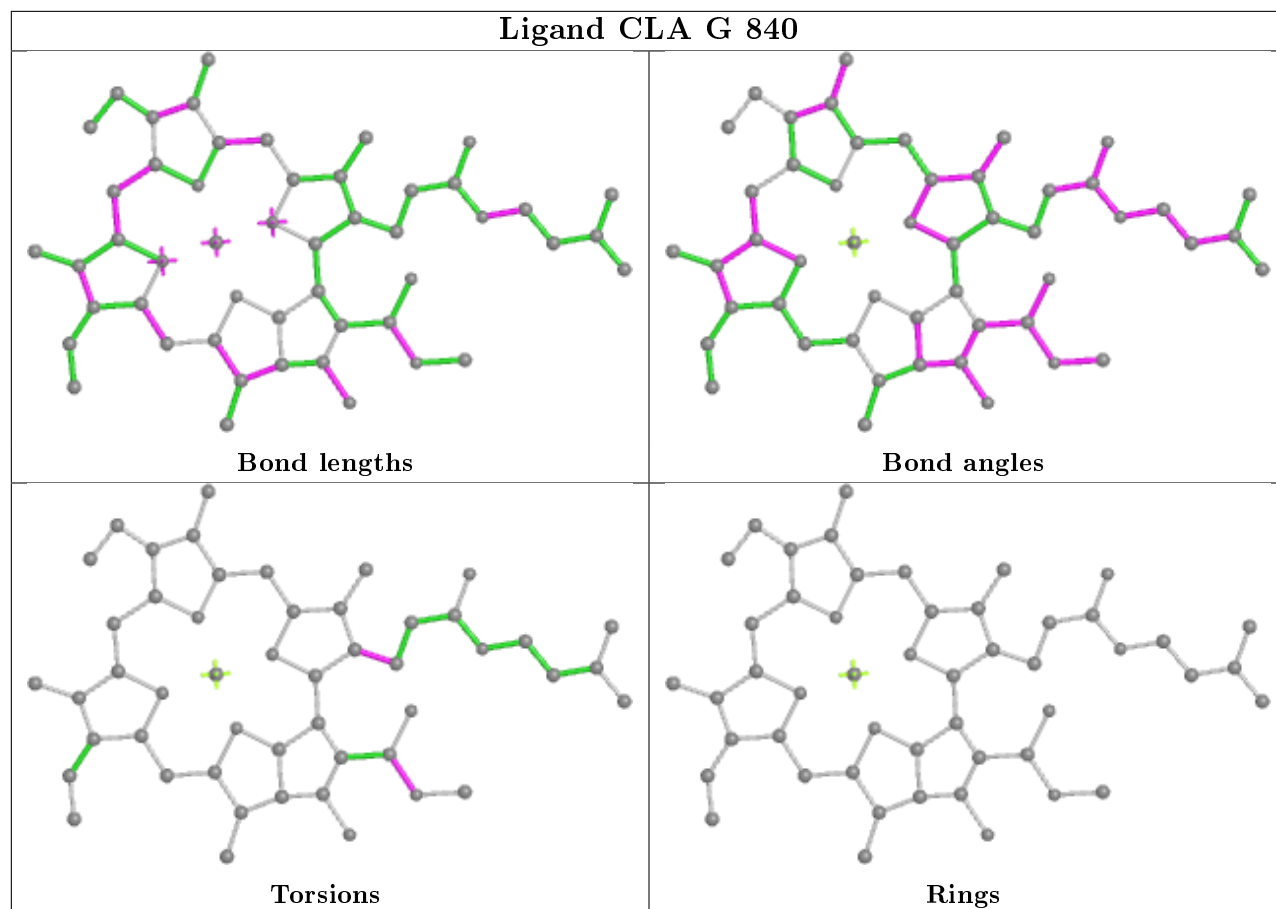


## Ligand CLA A 809

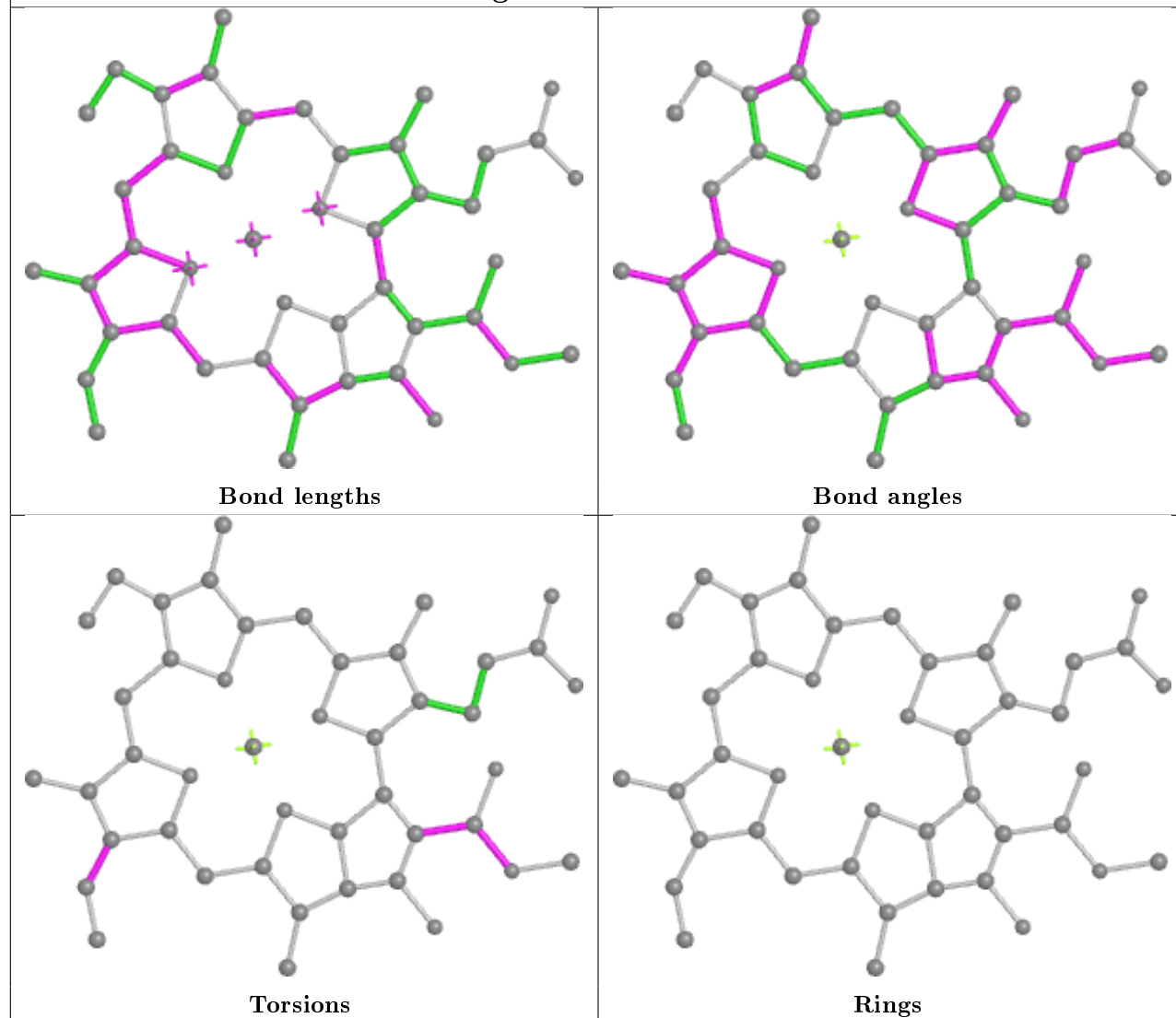


## Ligand CLA B 813

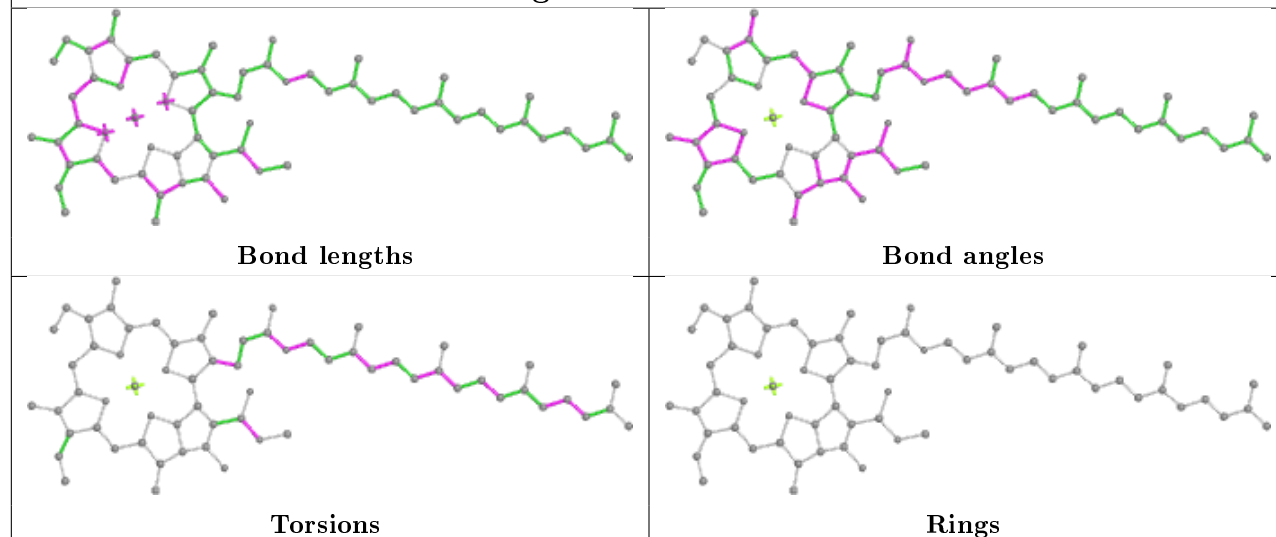




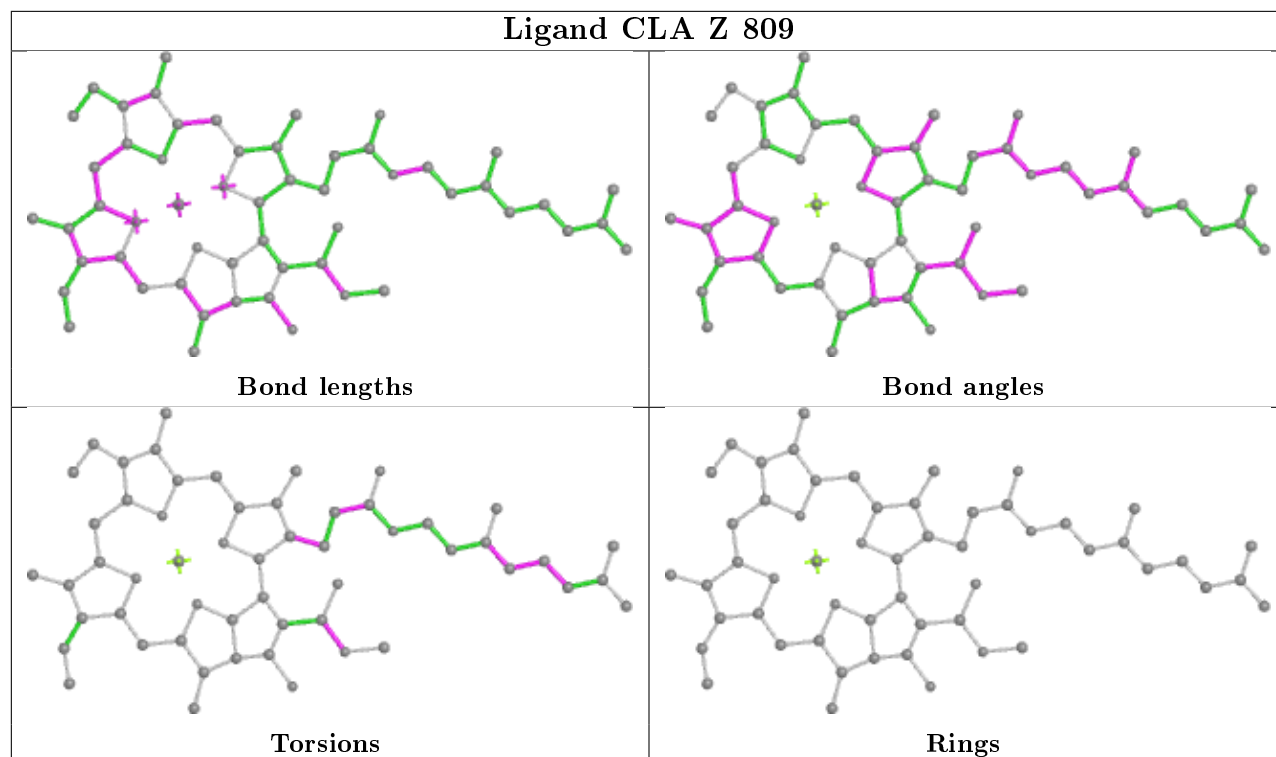
## Ligand CLA Z 834



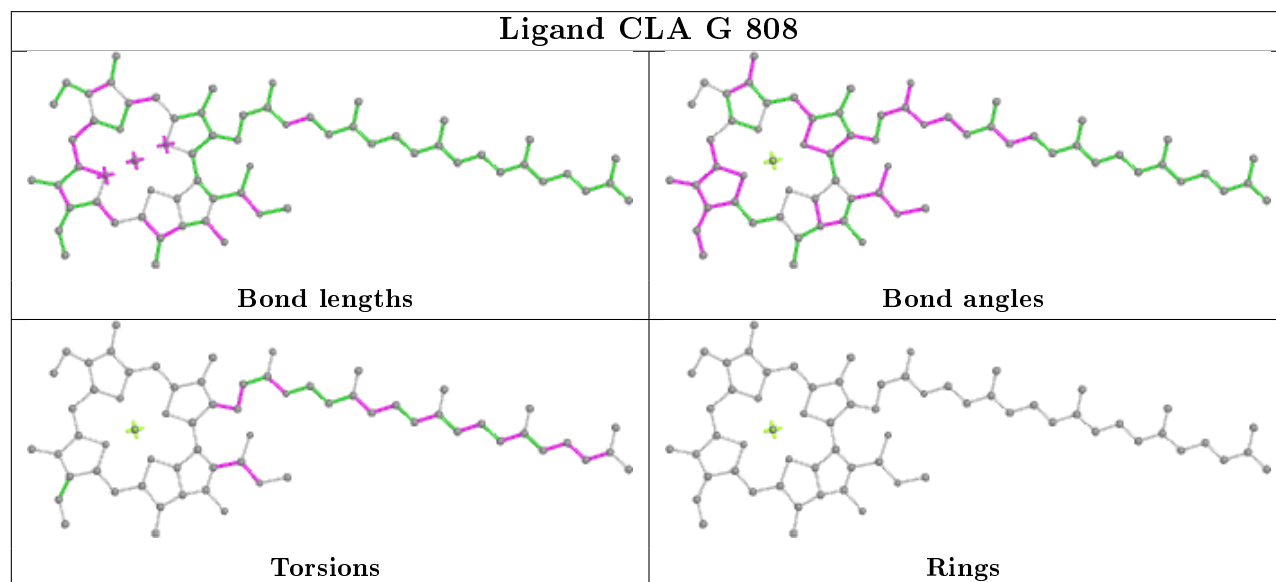
## Ligand CLA B 806



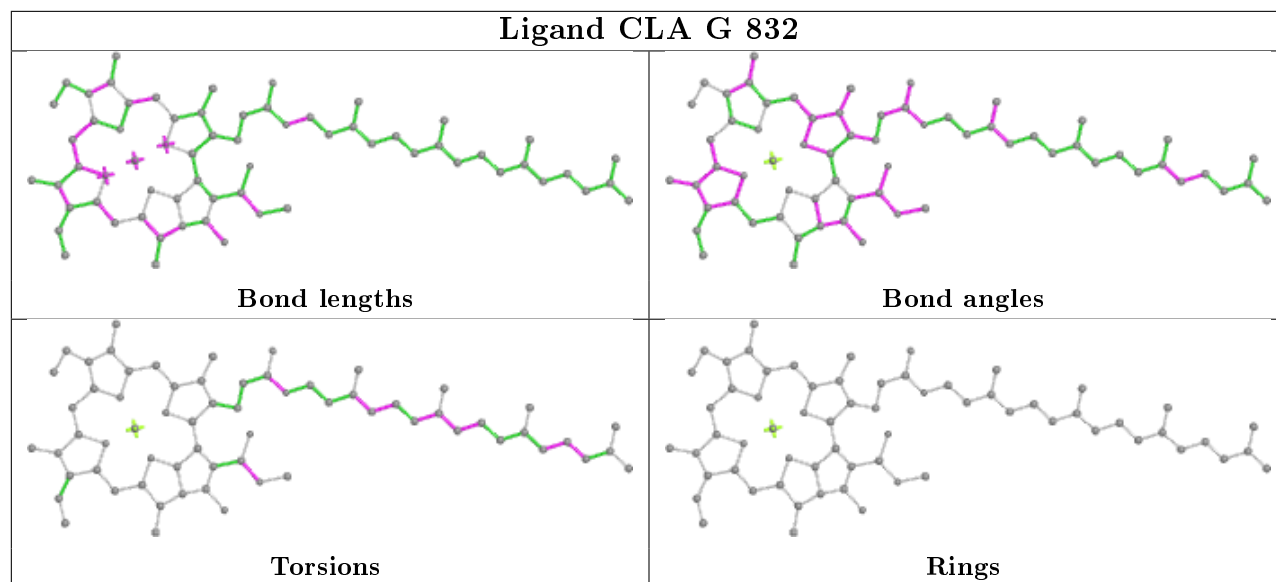
## Ligand CLA Z 809



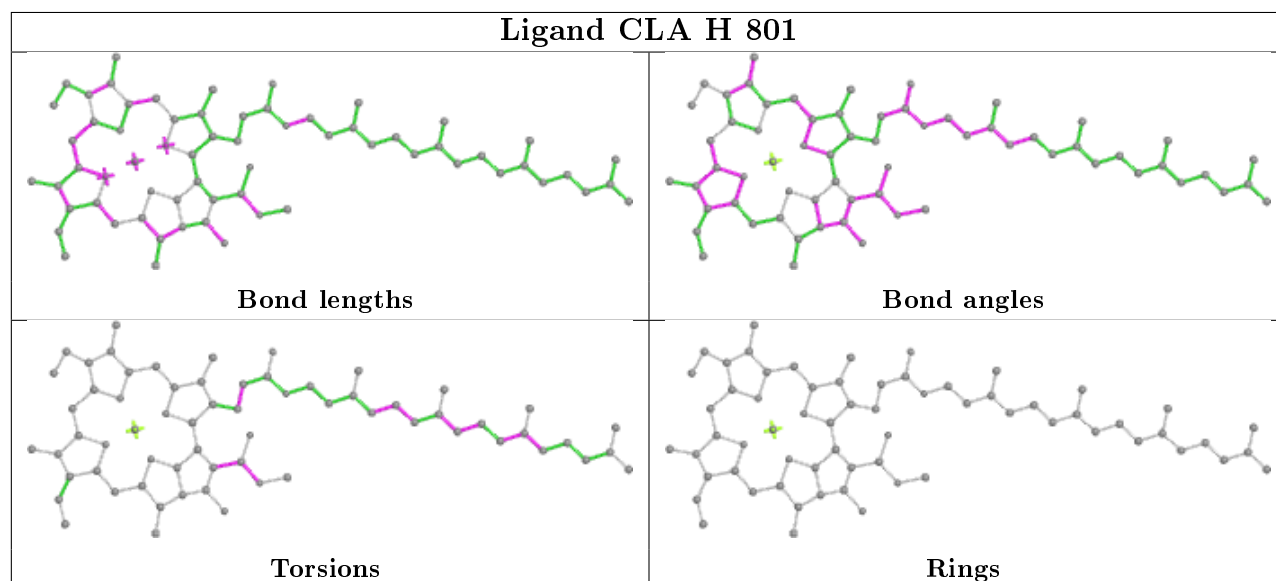
## Ligand CLA G 808



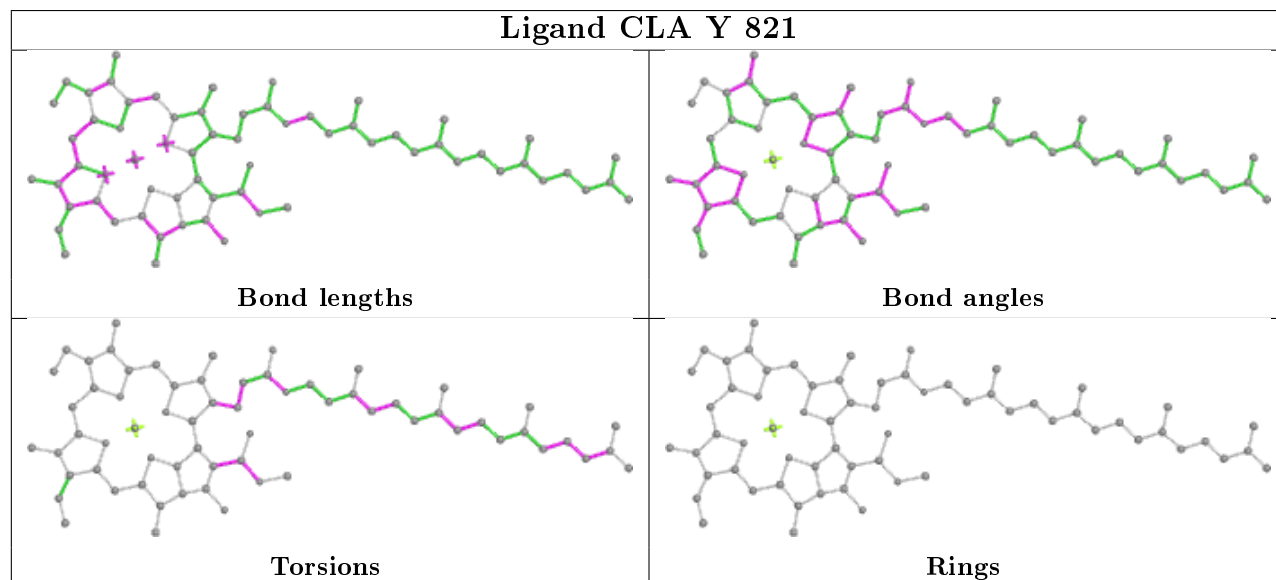
## Ligand CLA G 832



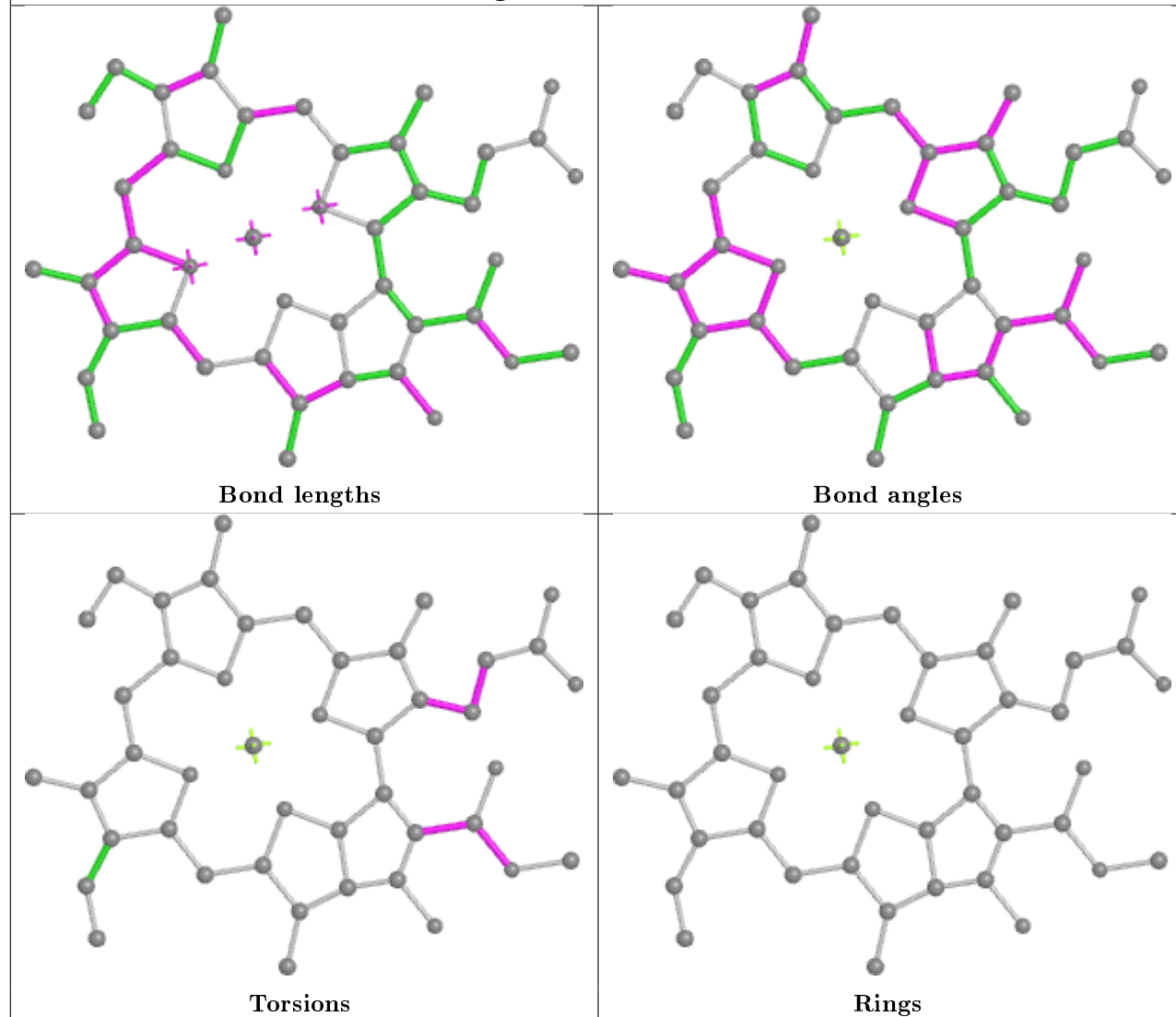
## Ligand CLA H 801



## Ligand CLA Y 821

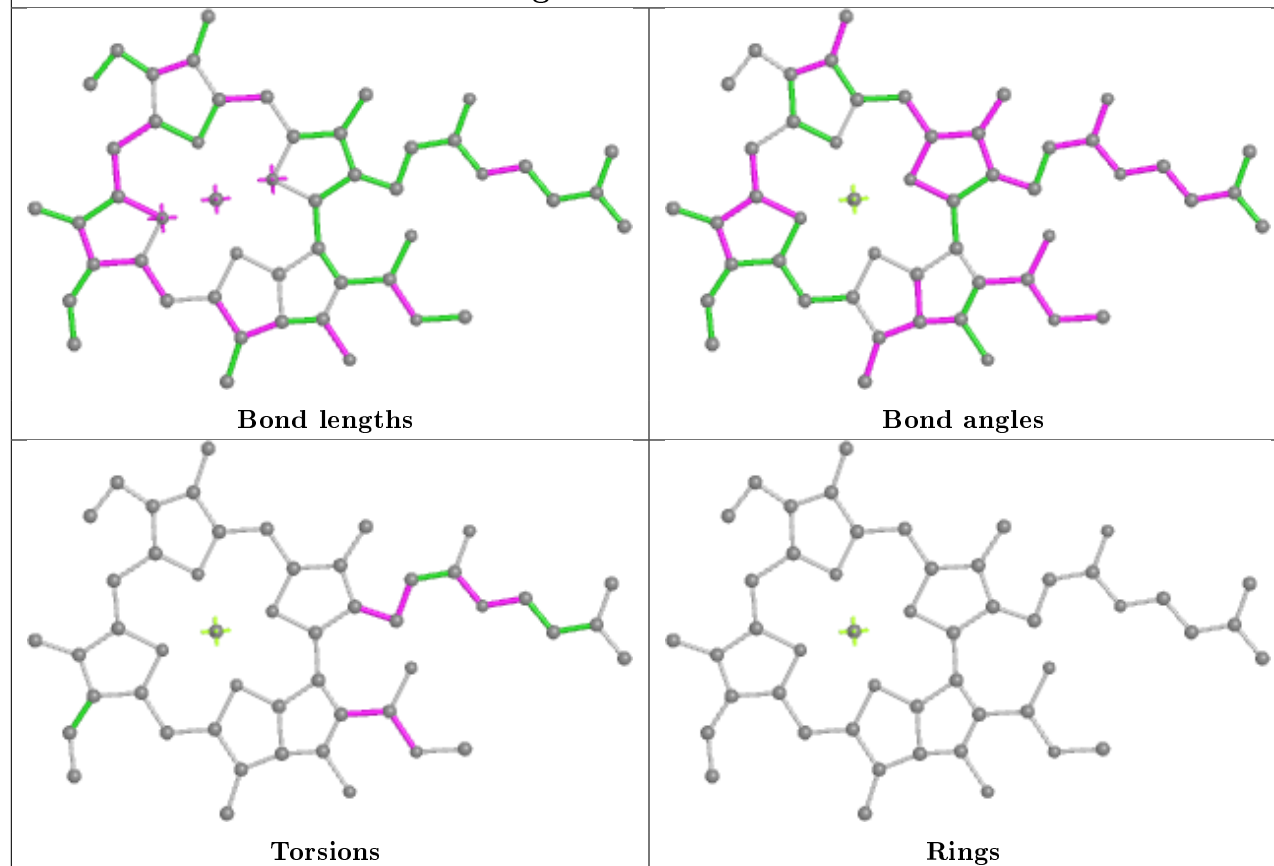


## Ligand CLA Z 828

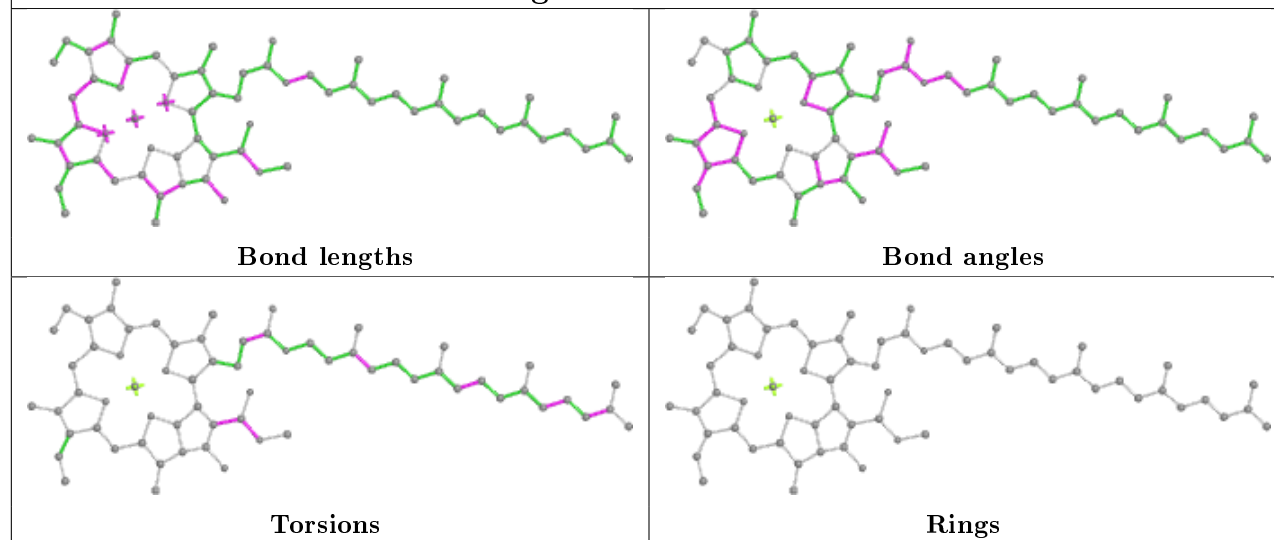




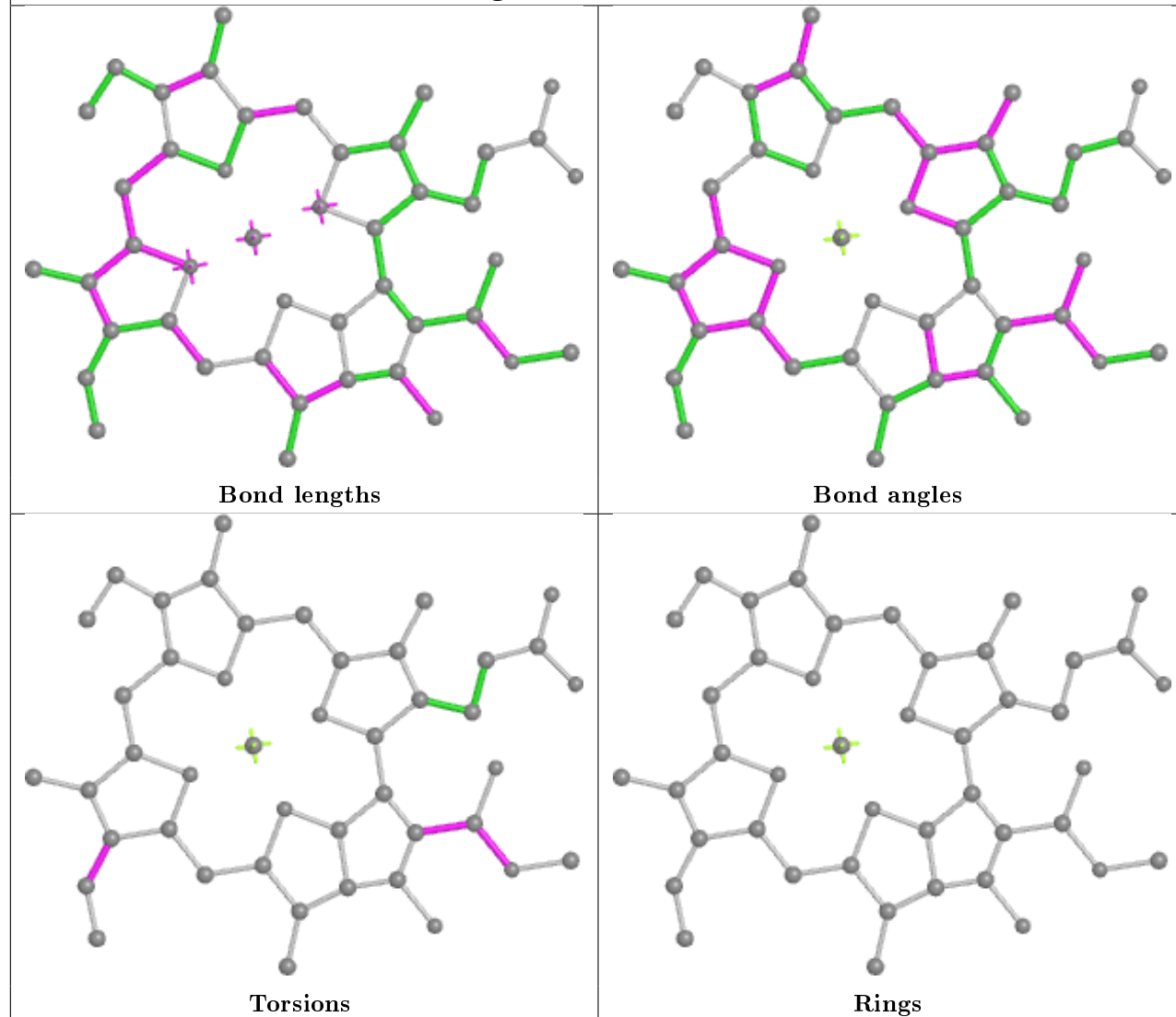
## Ligand CLA B 812



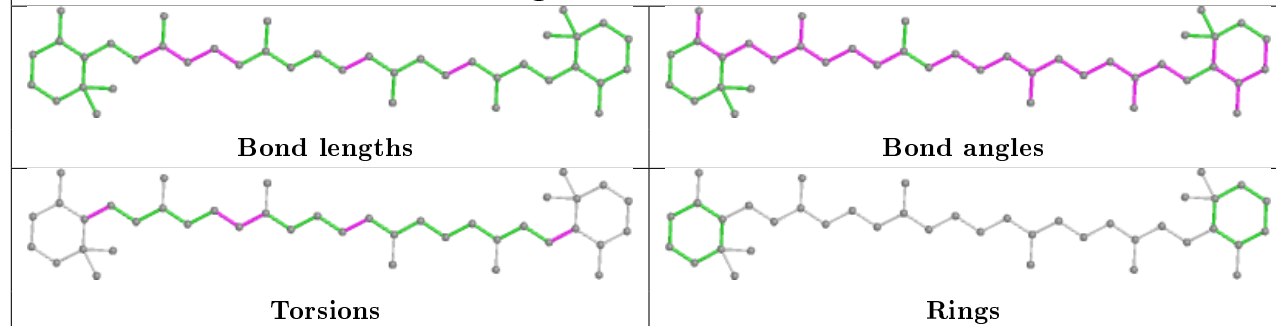
## Ligand CLA H 806



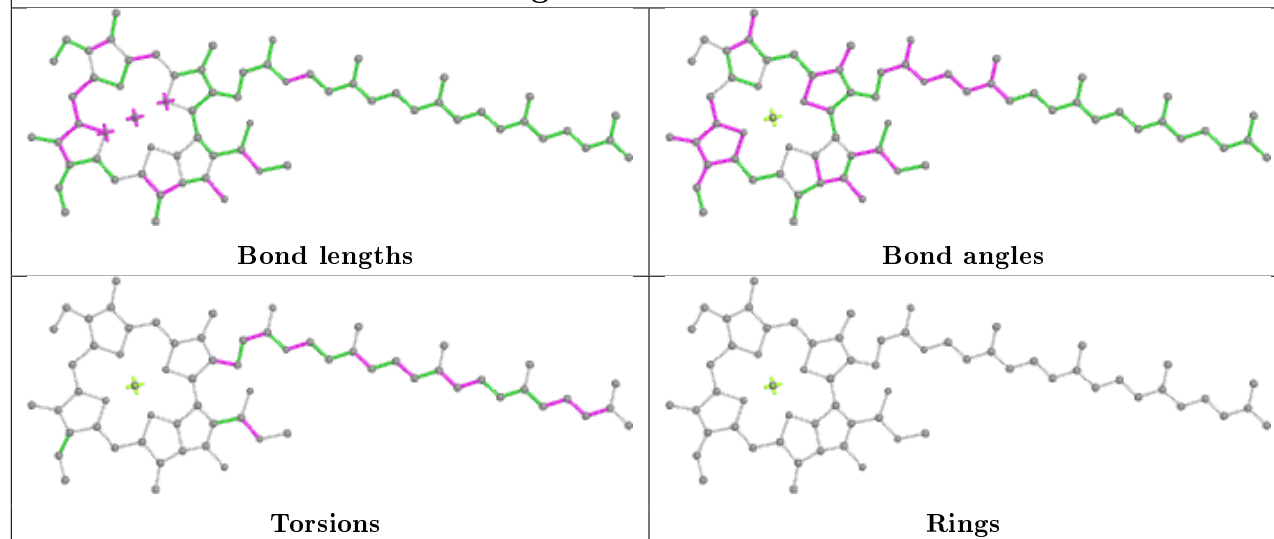
## Ligand CLA G 810



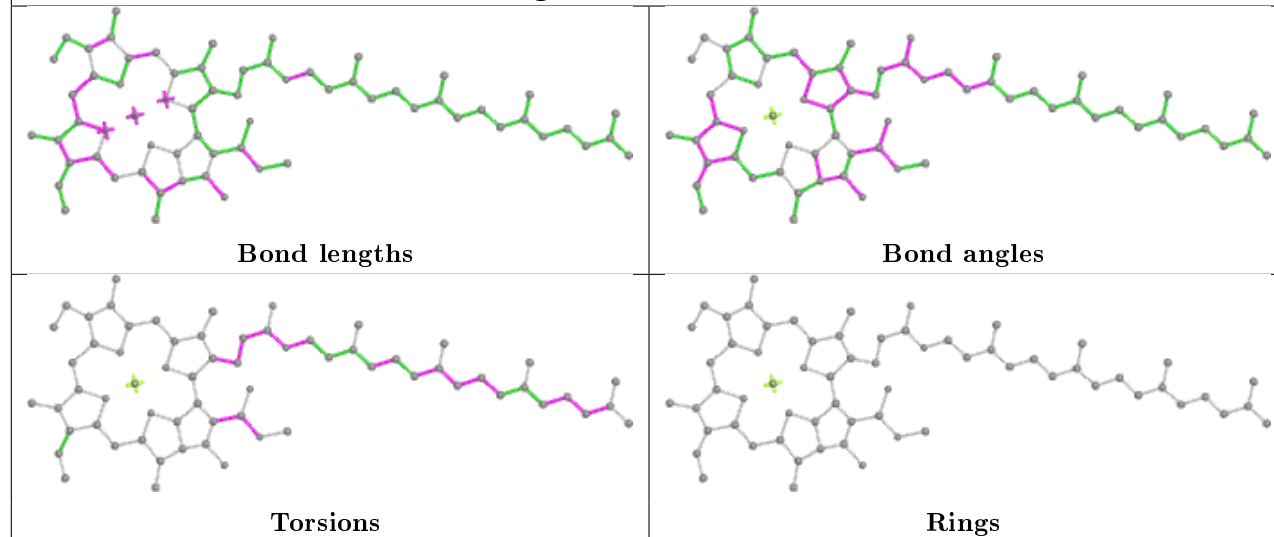
## Ligand BCR A 848



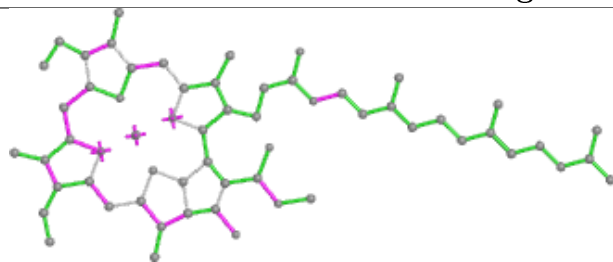
## Ligand CLA G 841



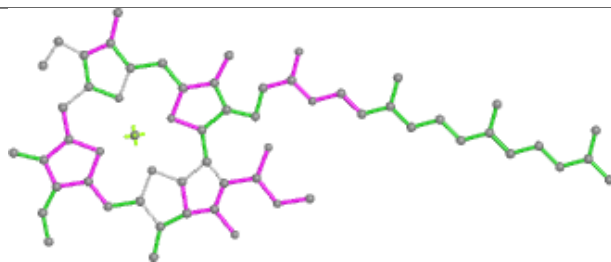
## Ligand CLA A 805



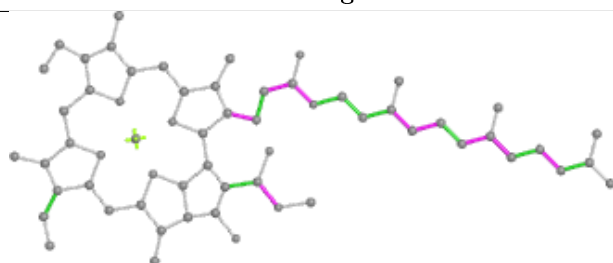
## Ligand CLA Z 817



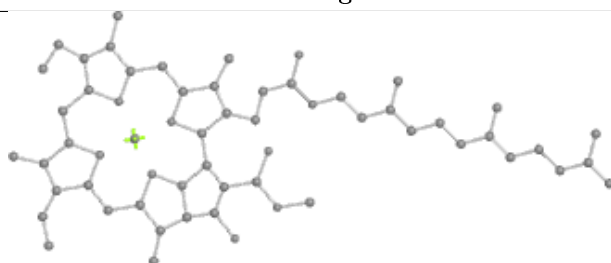
Bond lengths



Bond angles

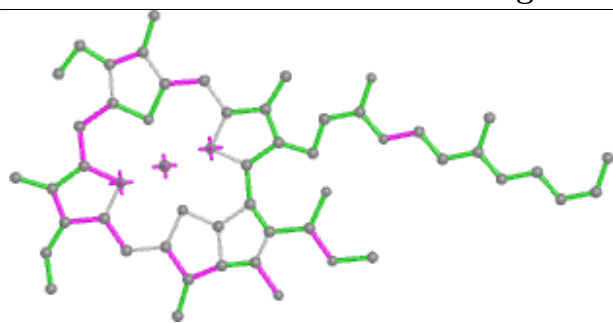


Torsions

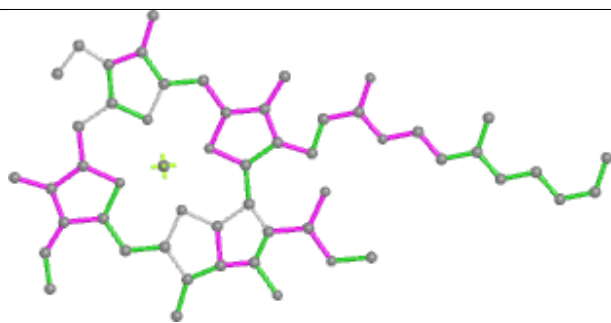


Rings

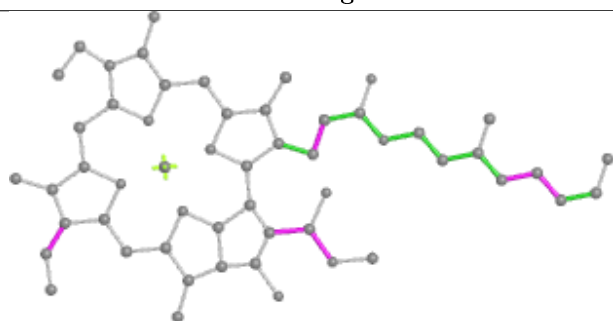
## Ligand CLA Z 803



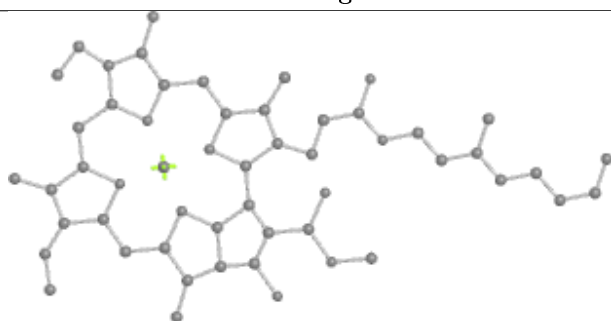
Bond lengths



Bond angles

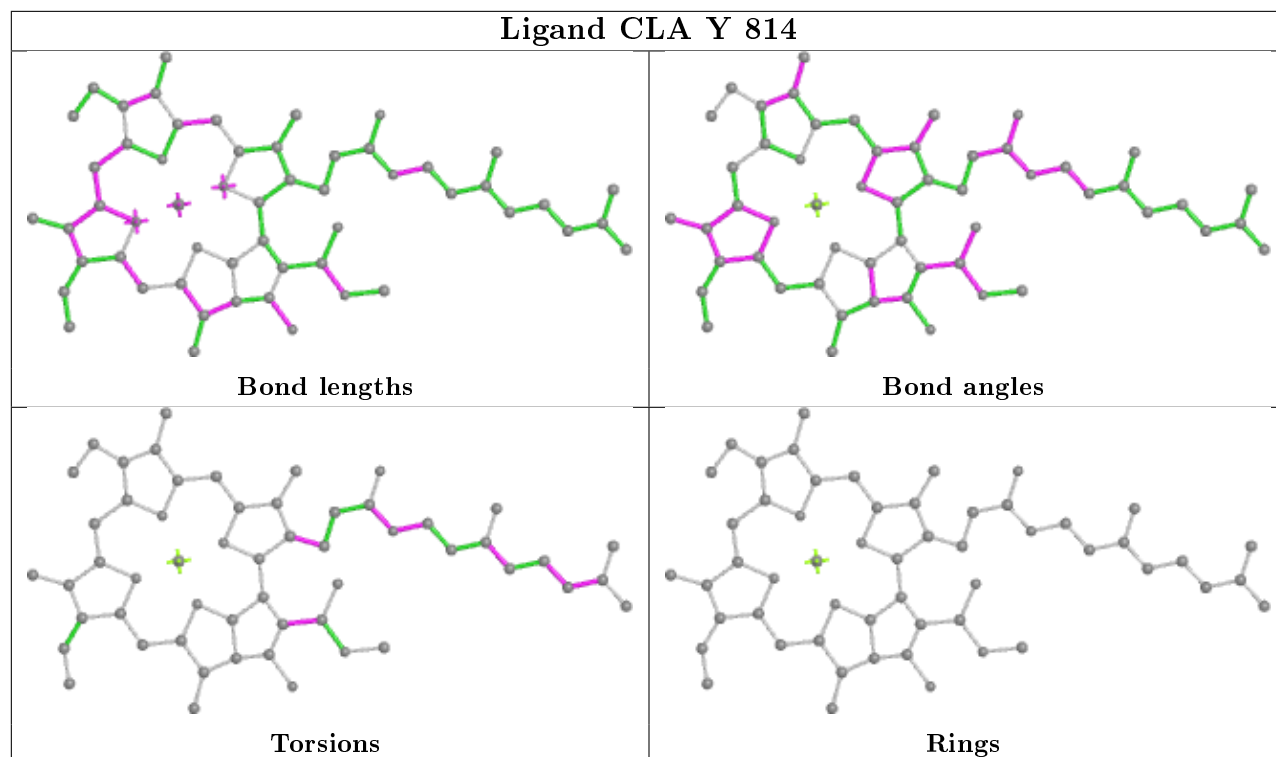


Torsions

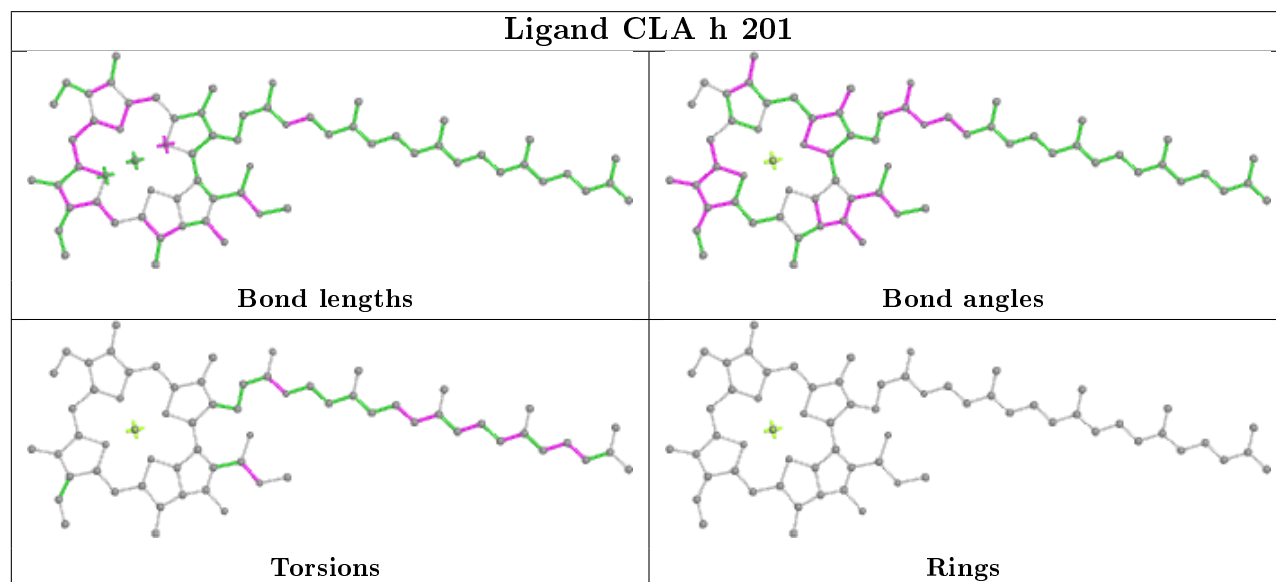


Rings

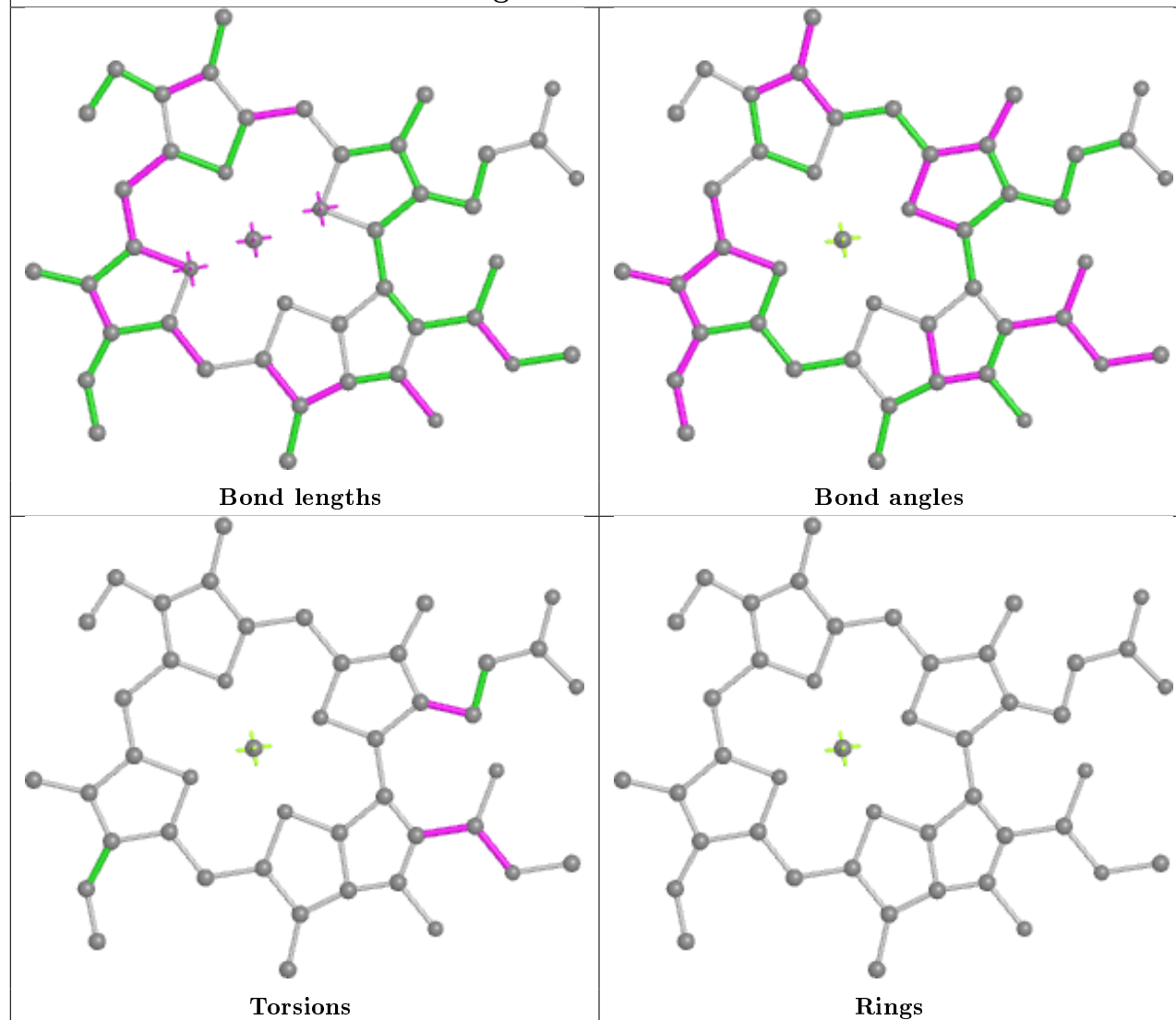
## Ligand CLA Y 814



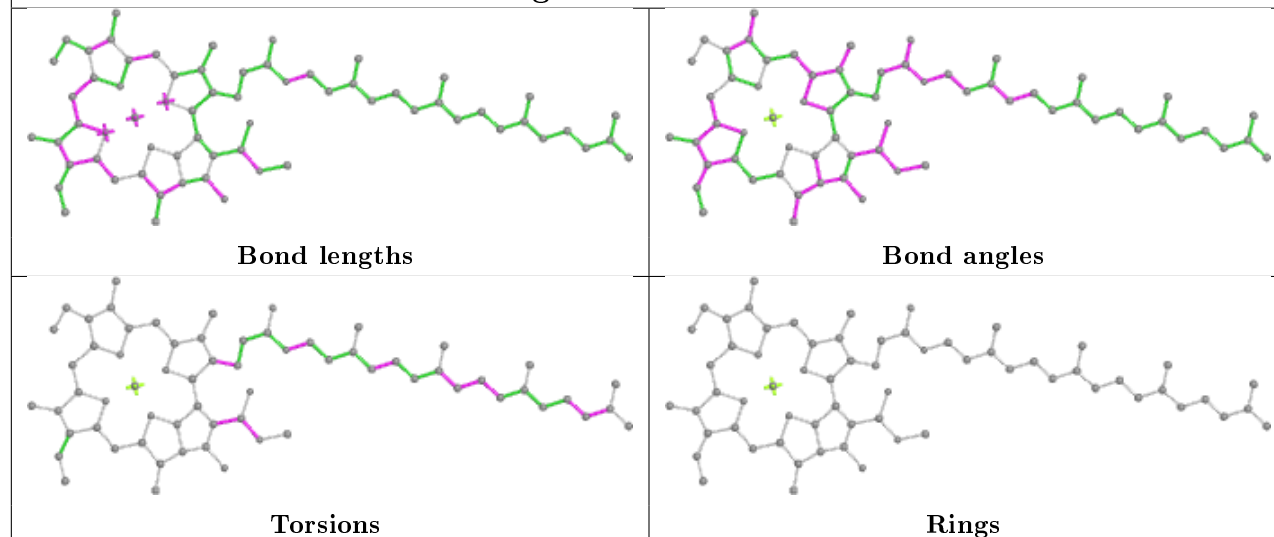
## Ligand CLA h 201

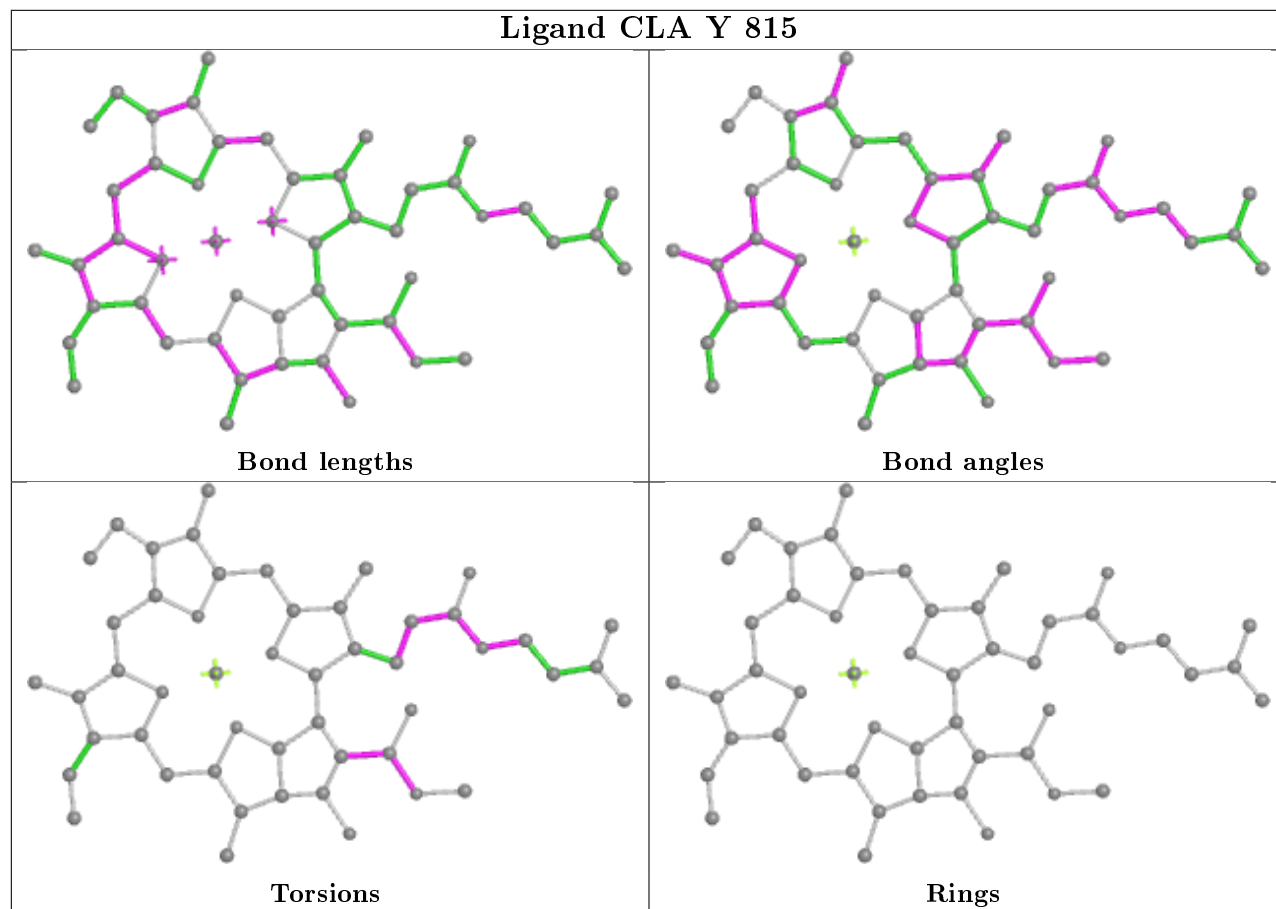
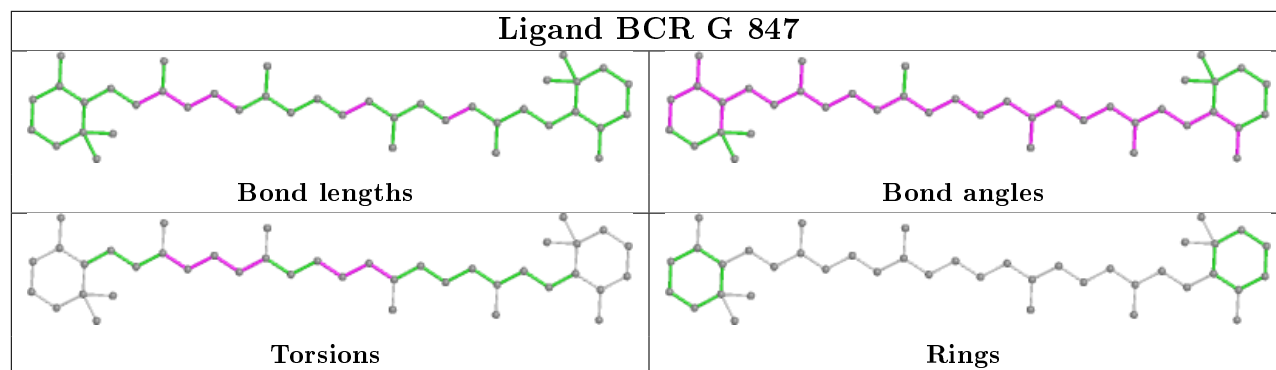
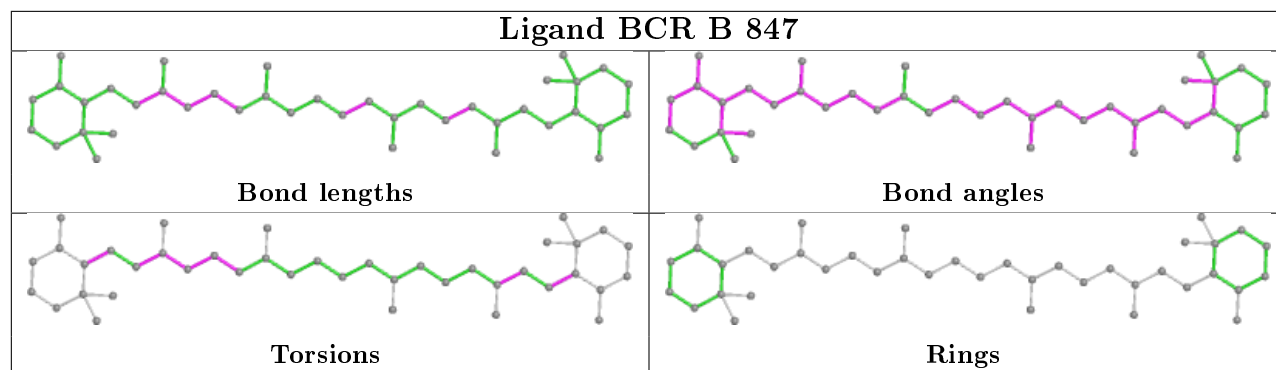


## Ligand CLA Z 819

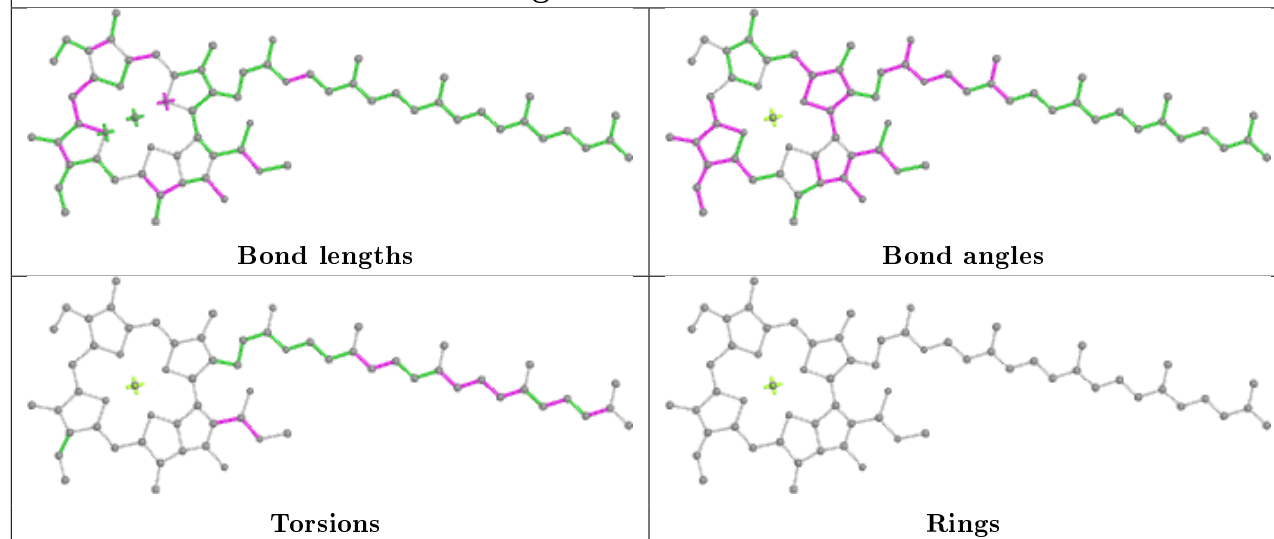


## Ligand CLA B 827

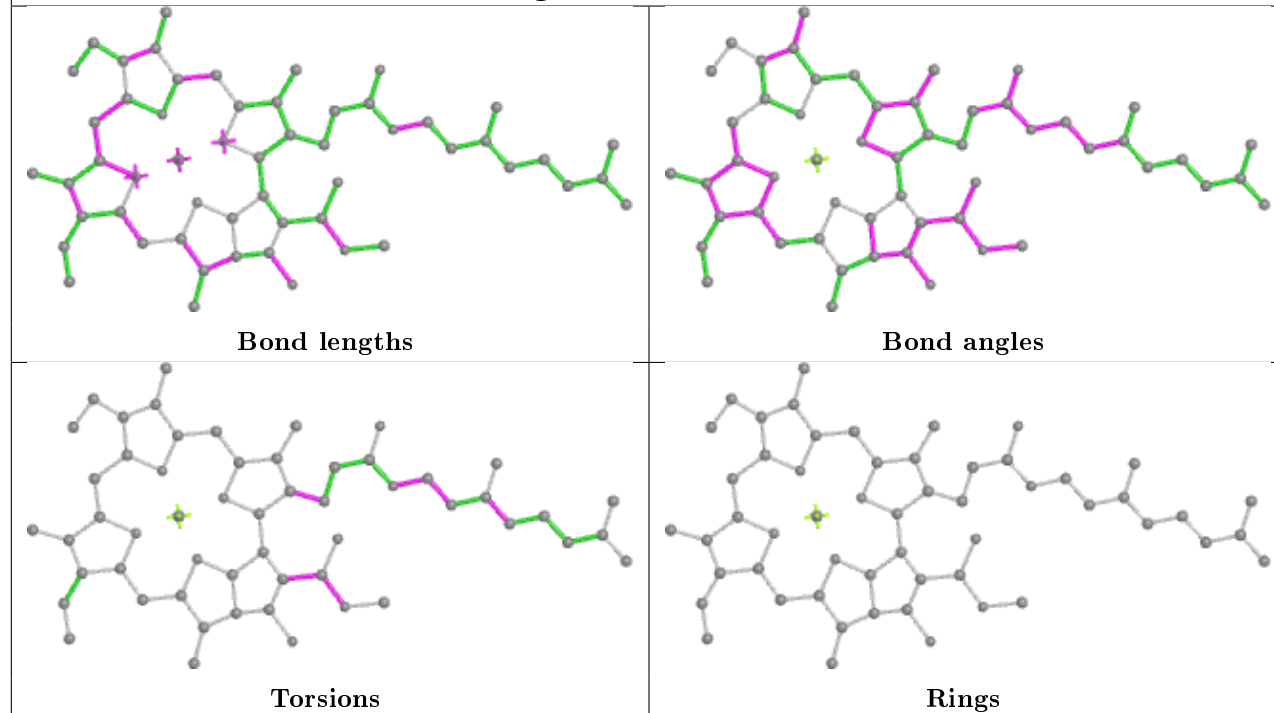




## Ligand CLA B 803

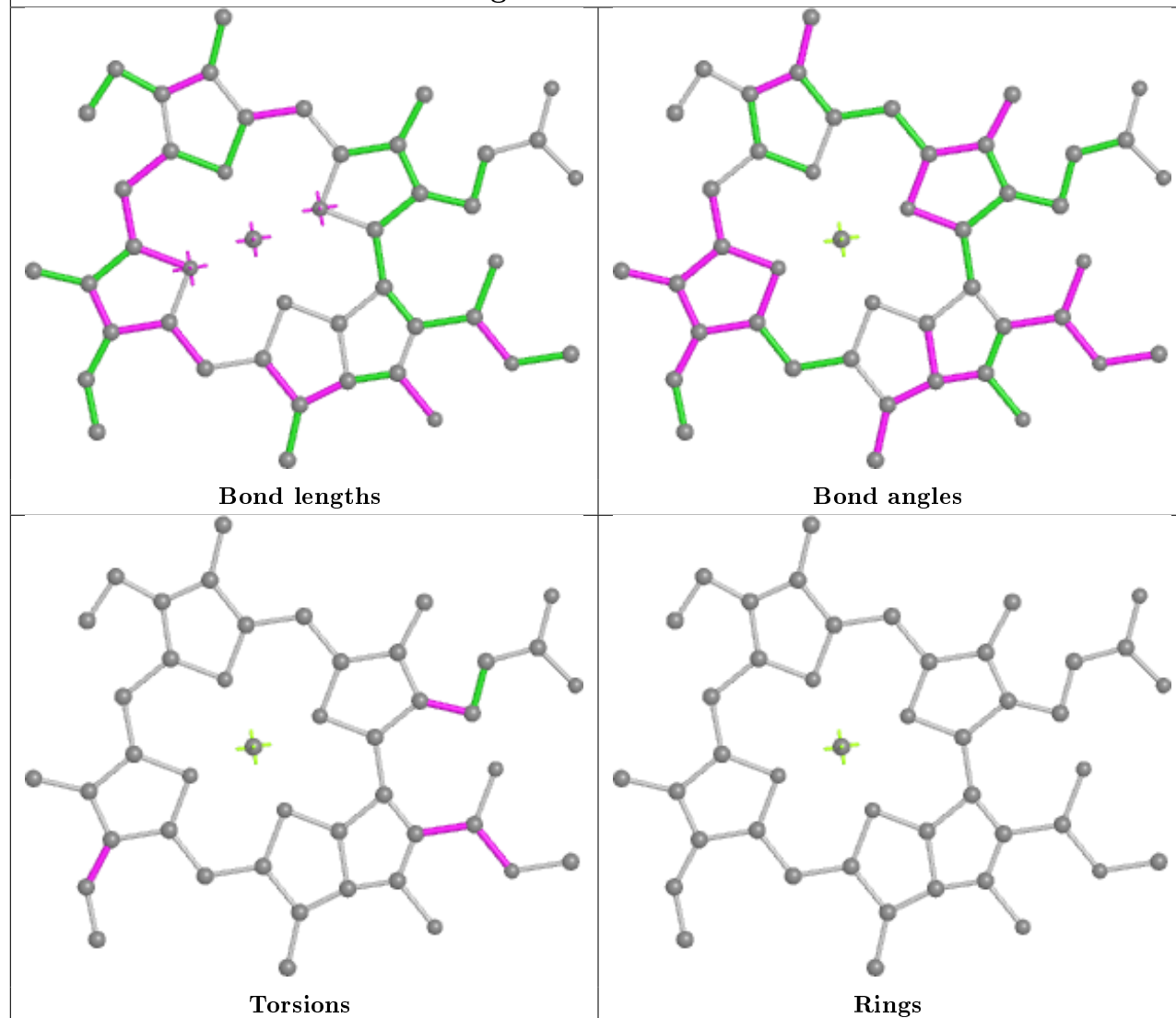


## Ligand CLA B 824

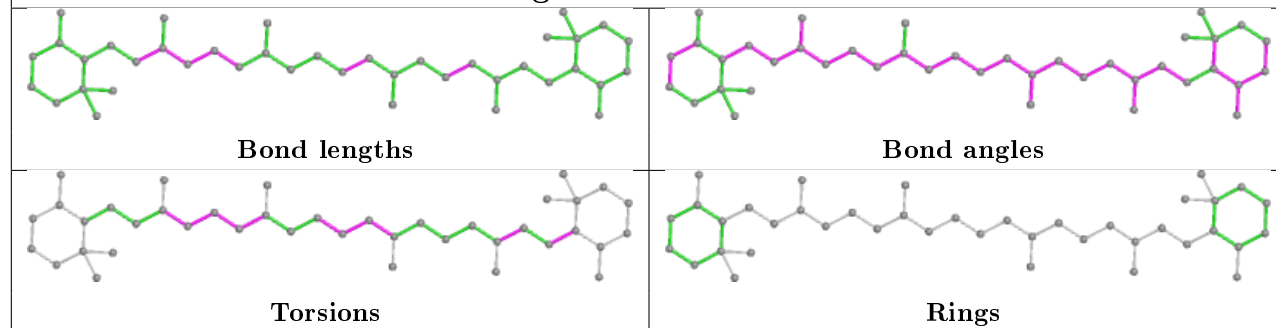


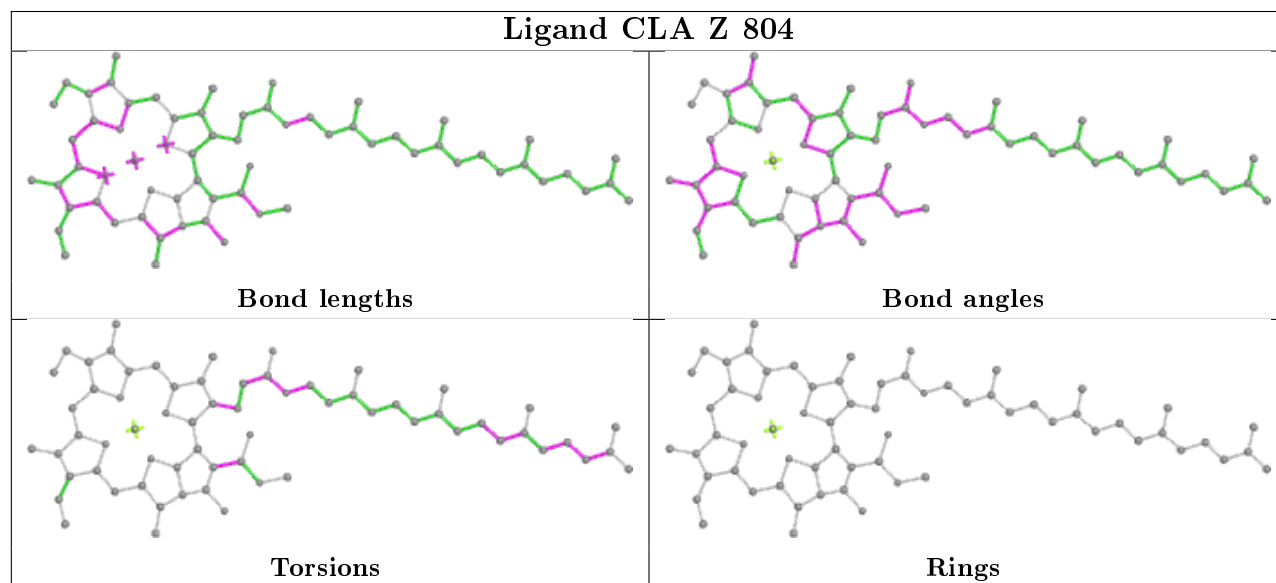
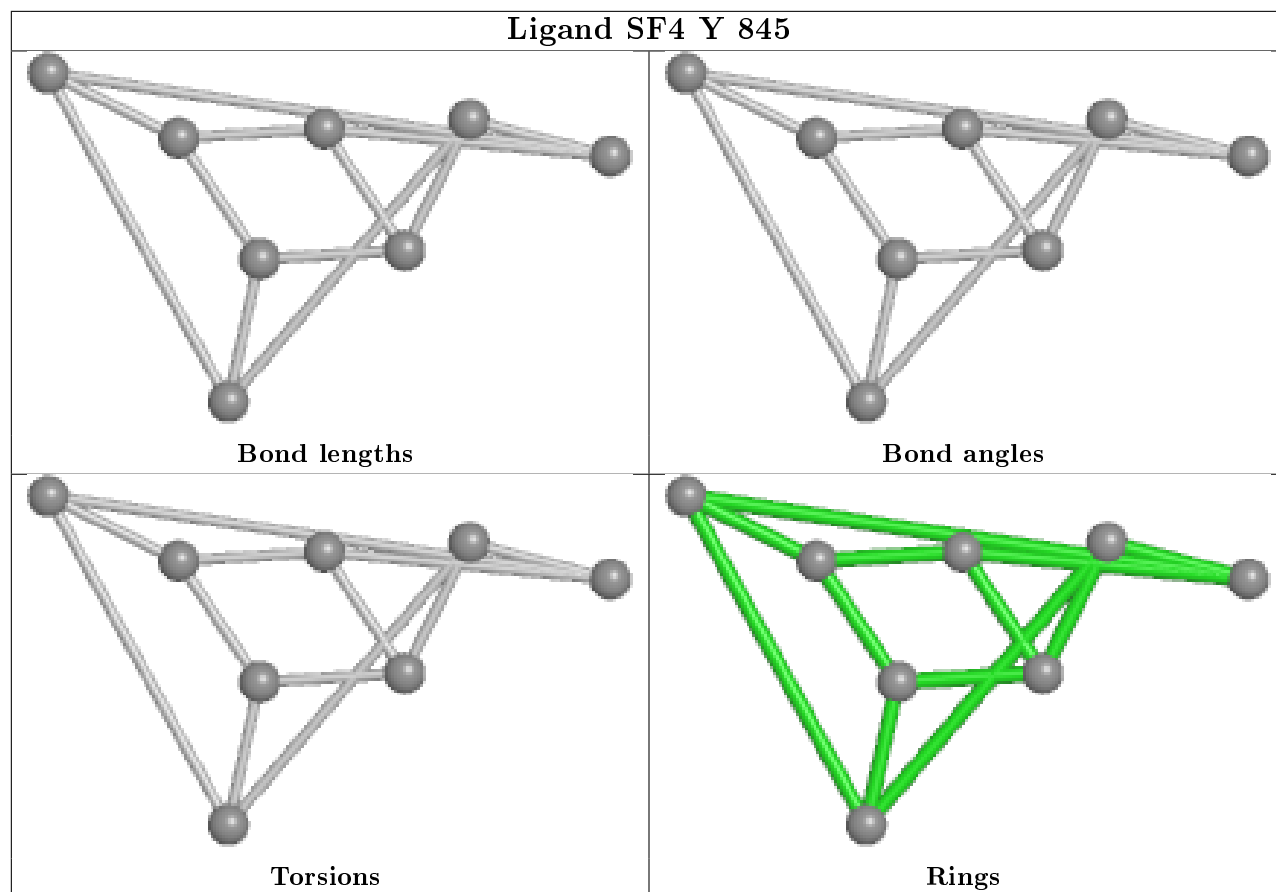


## Ligand CLA B 821

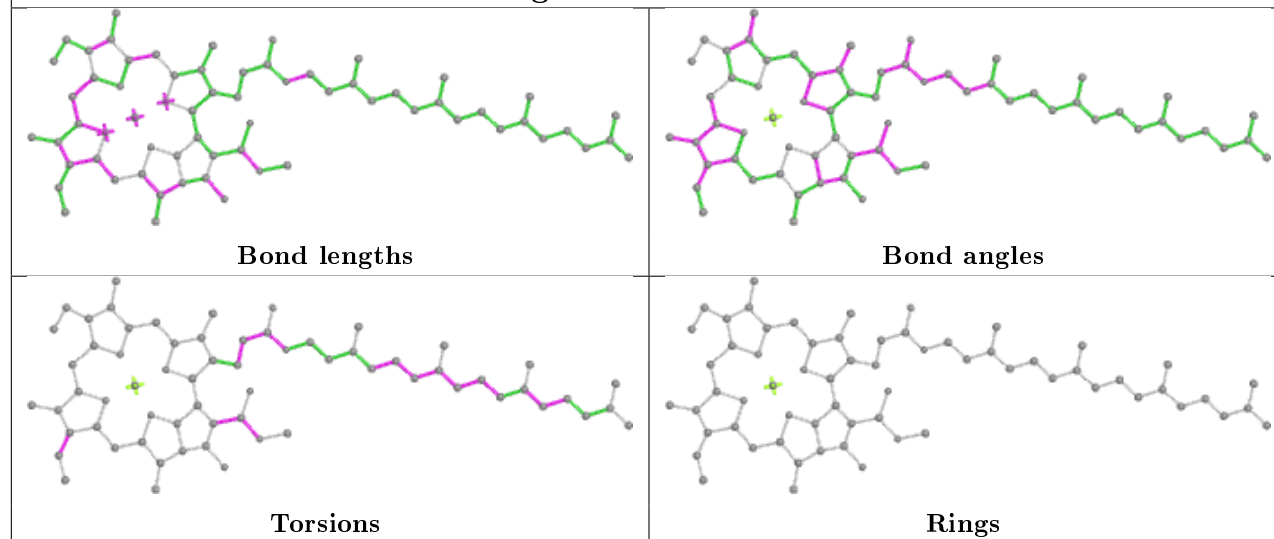


## Ligand BCR Z 841

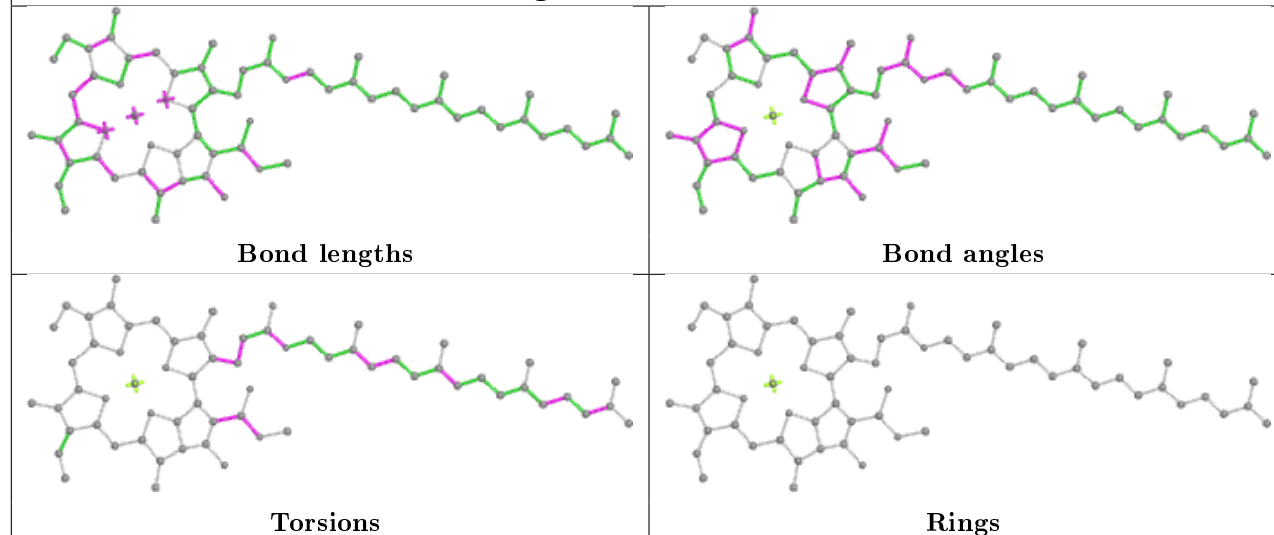




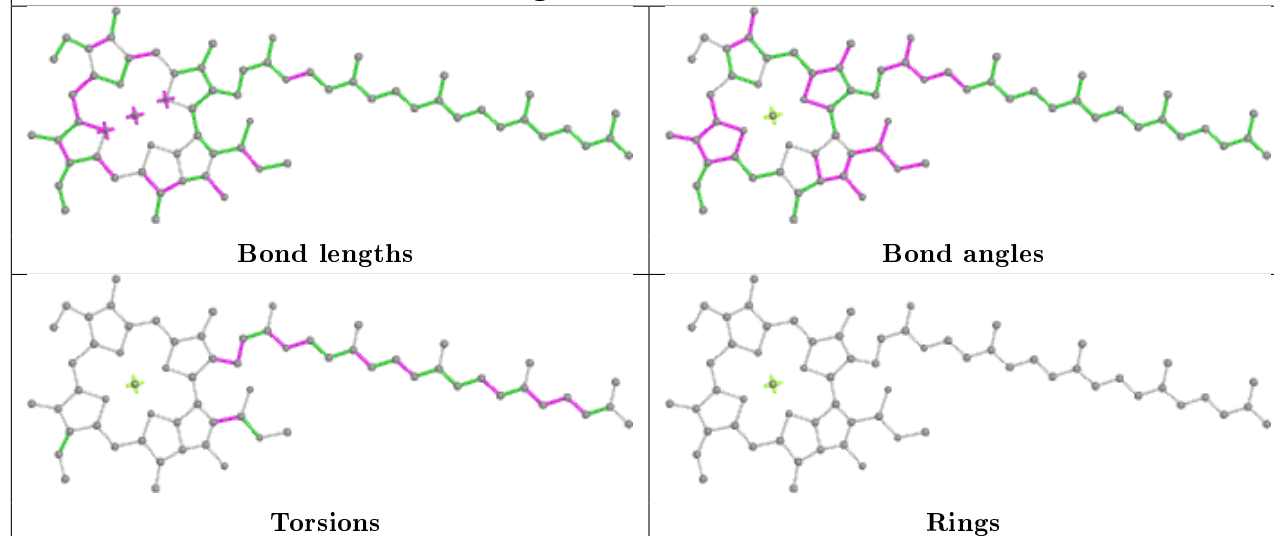
## Ligand CLA H 812

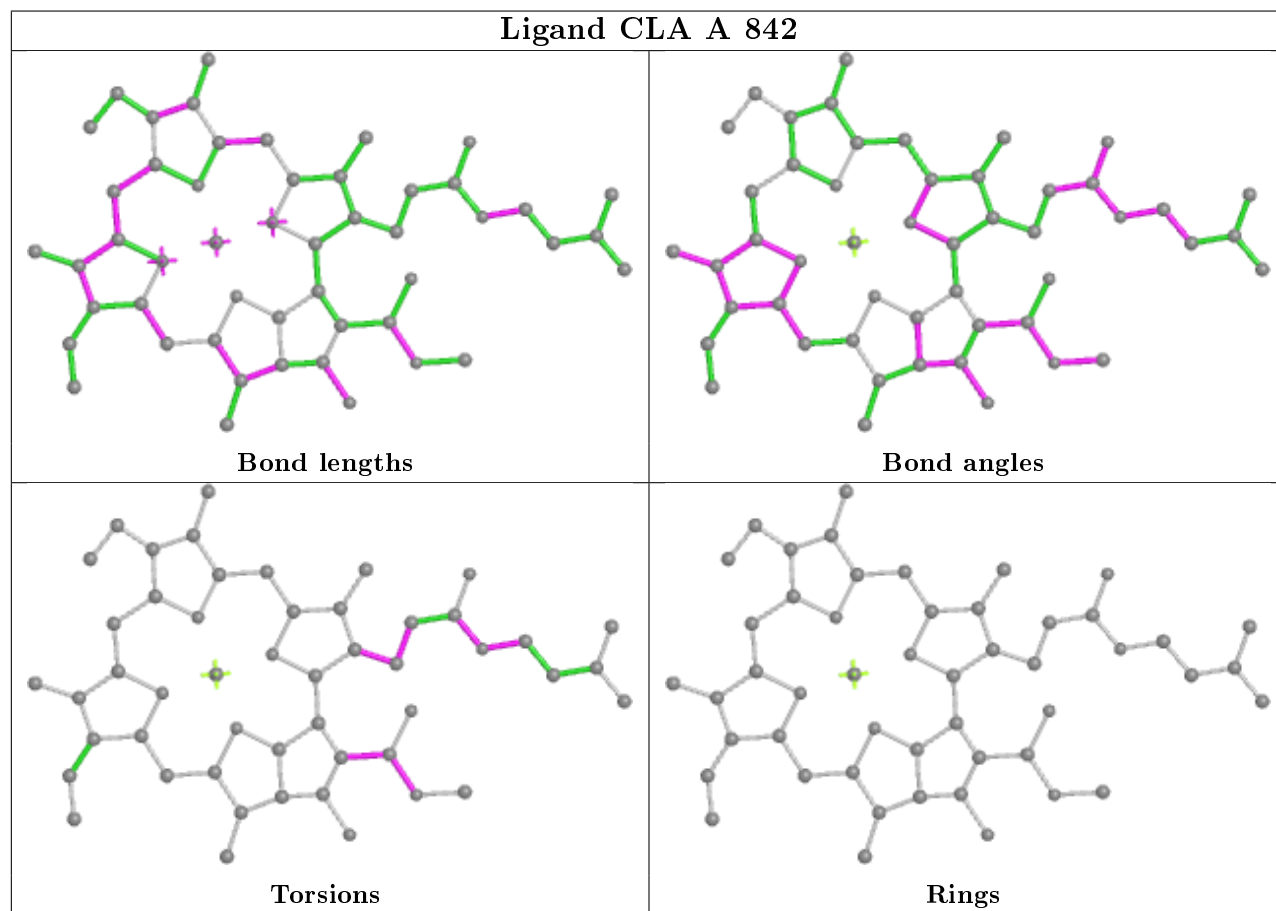
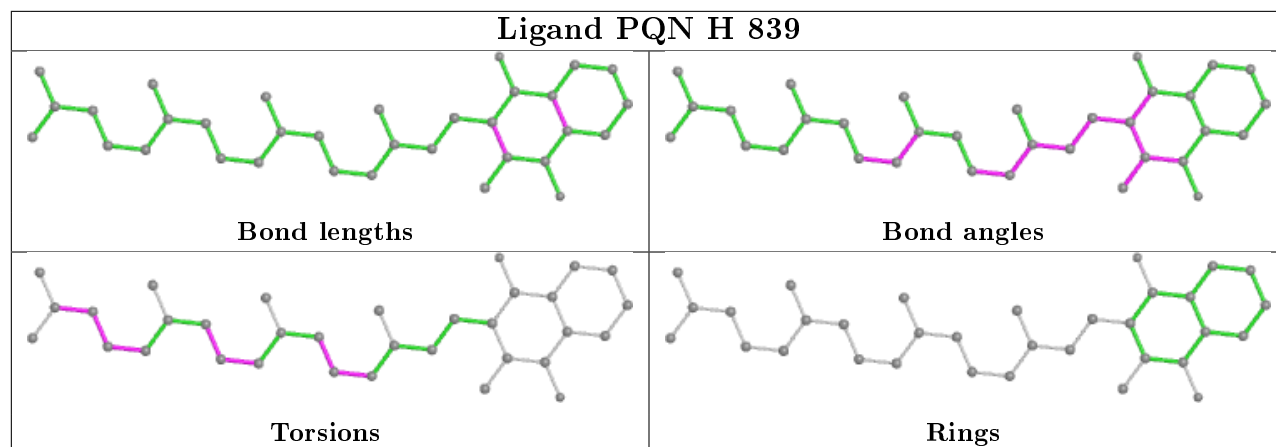


## Ligand CLA A 821

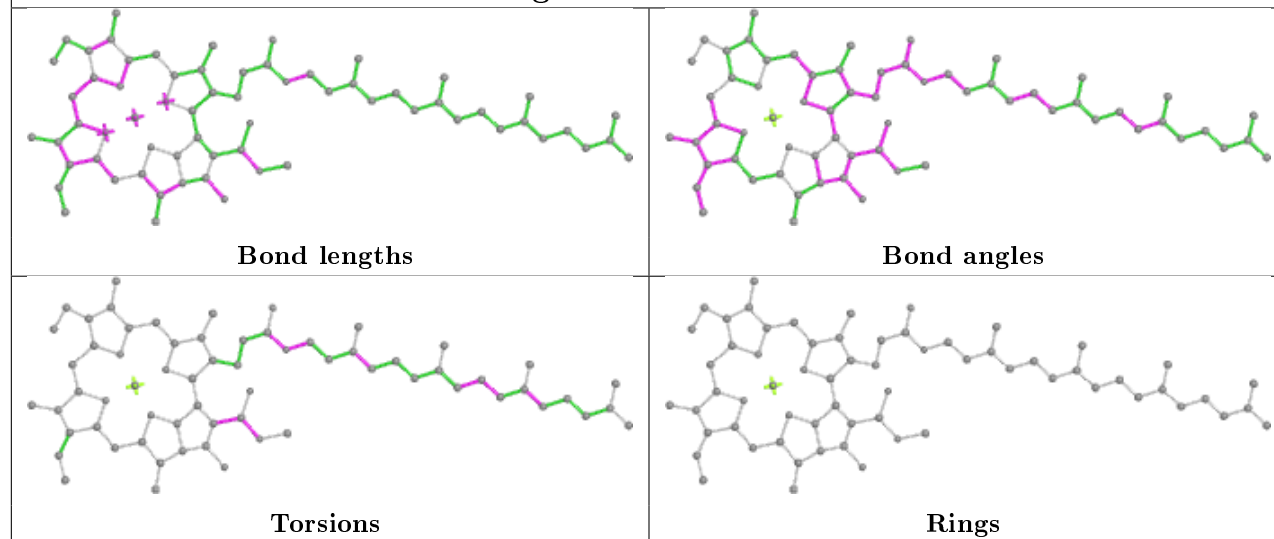


## Ligand CLA G 830

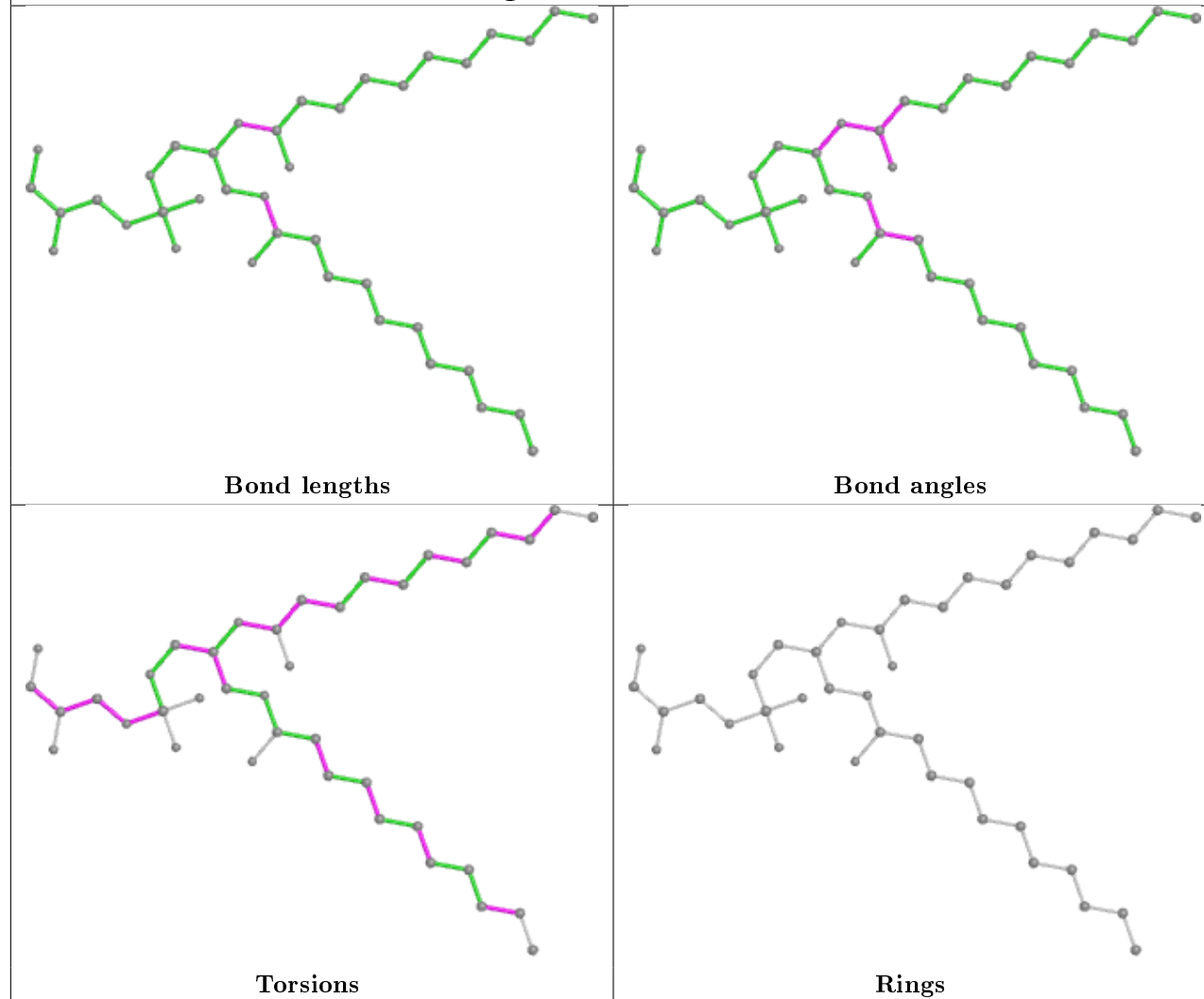




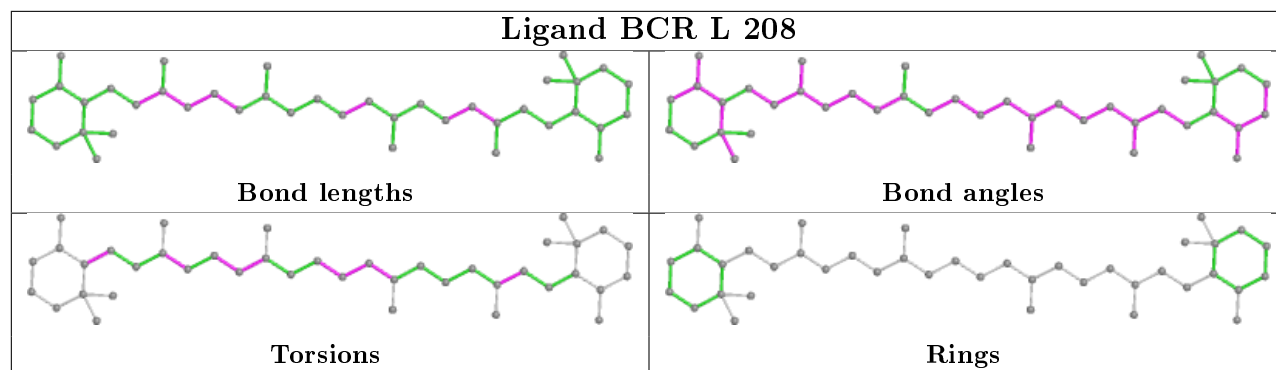
## Ligand CLA A 802



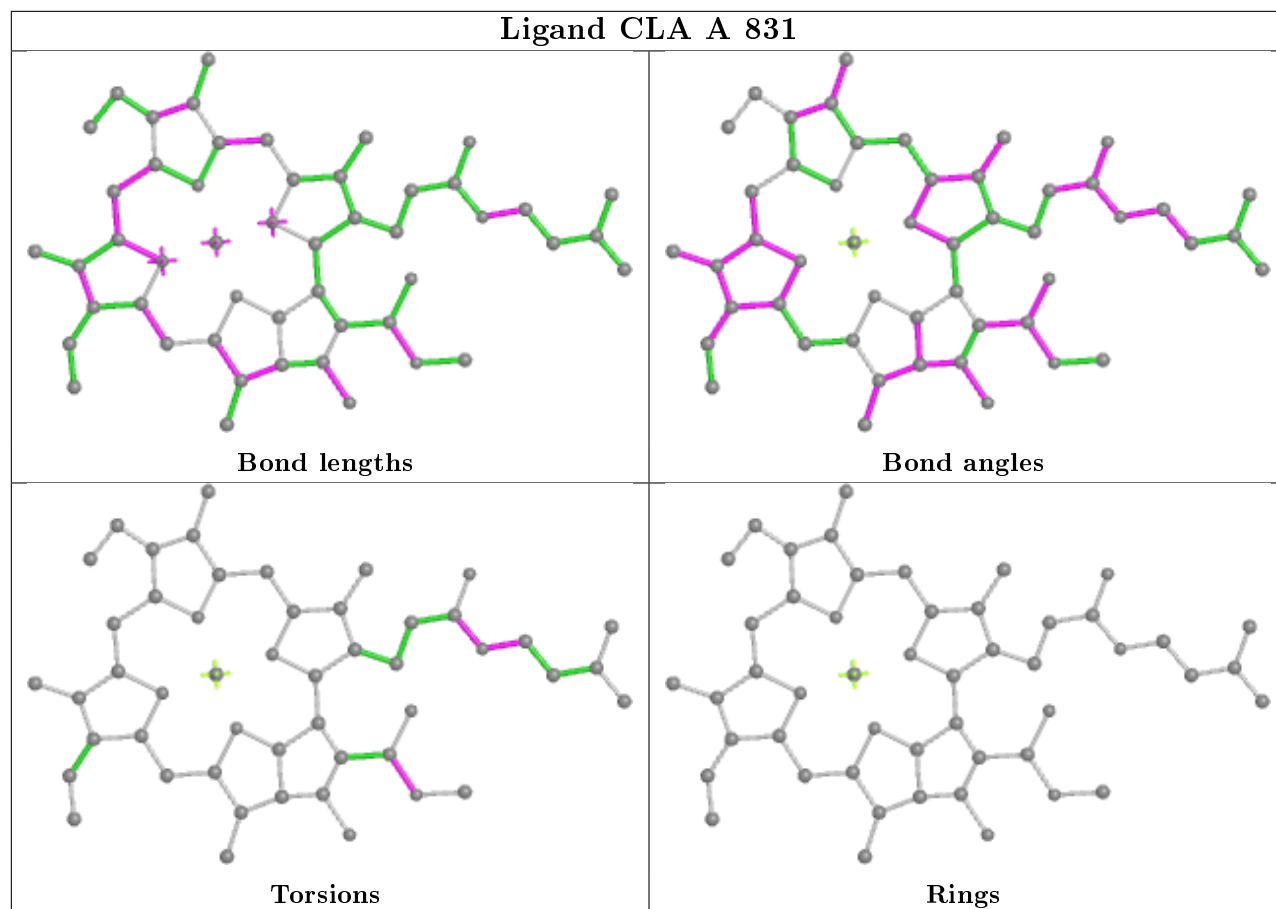
## Ligand LHG B 850



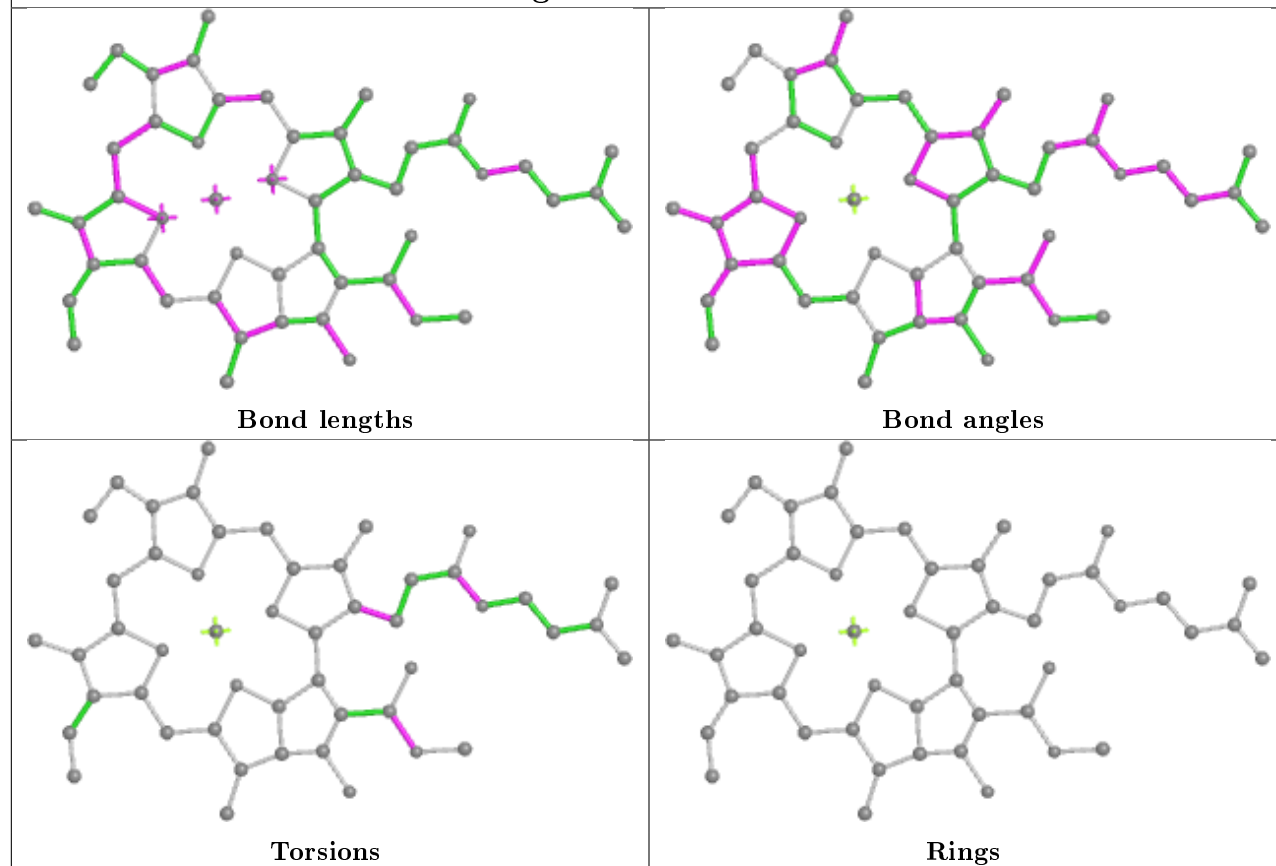
## Ligand BCR L 208



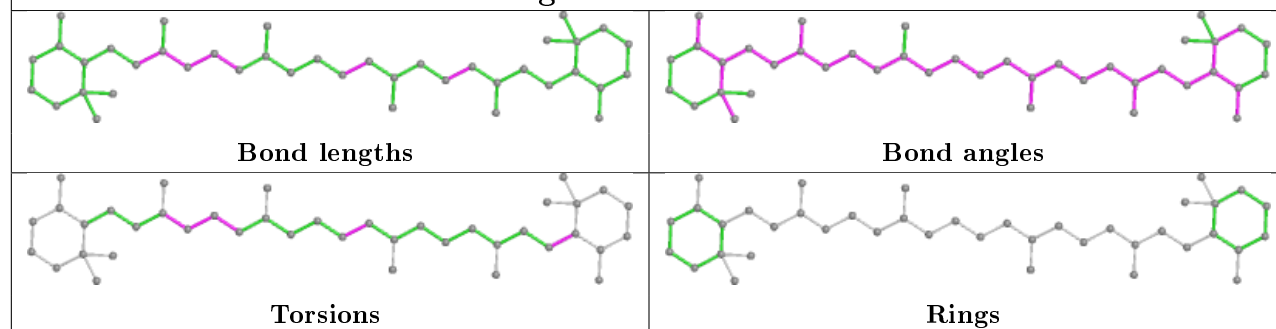
## Ligand CLA A 831



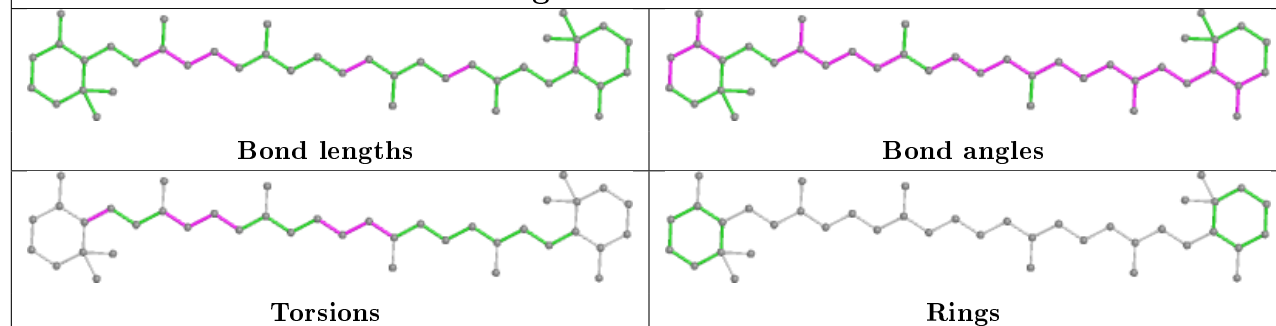
## Ligand CLA Y 823

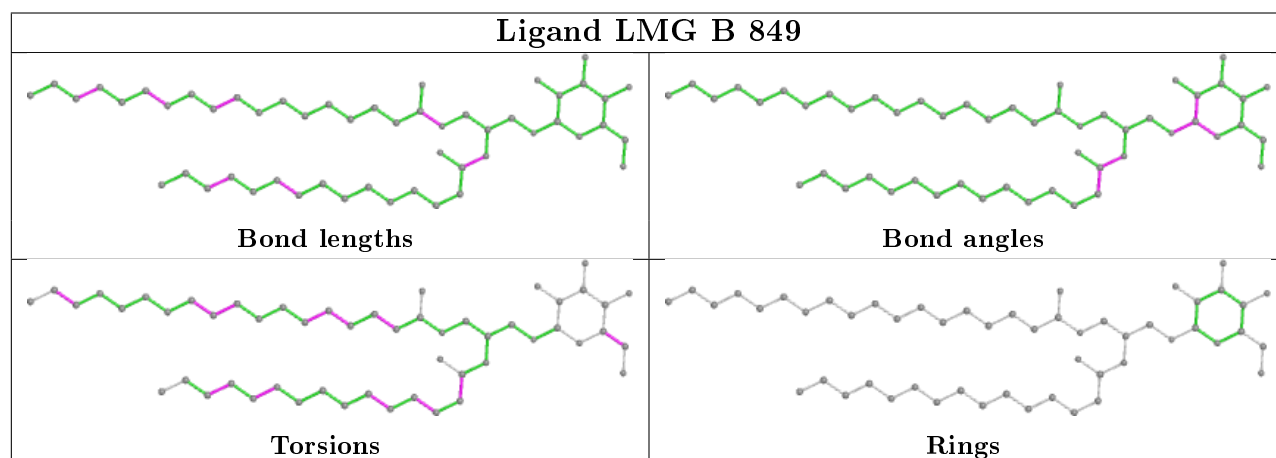
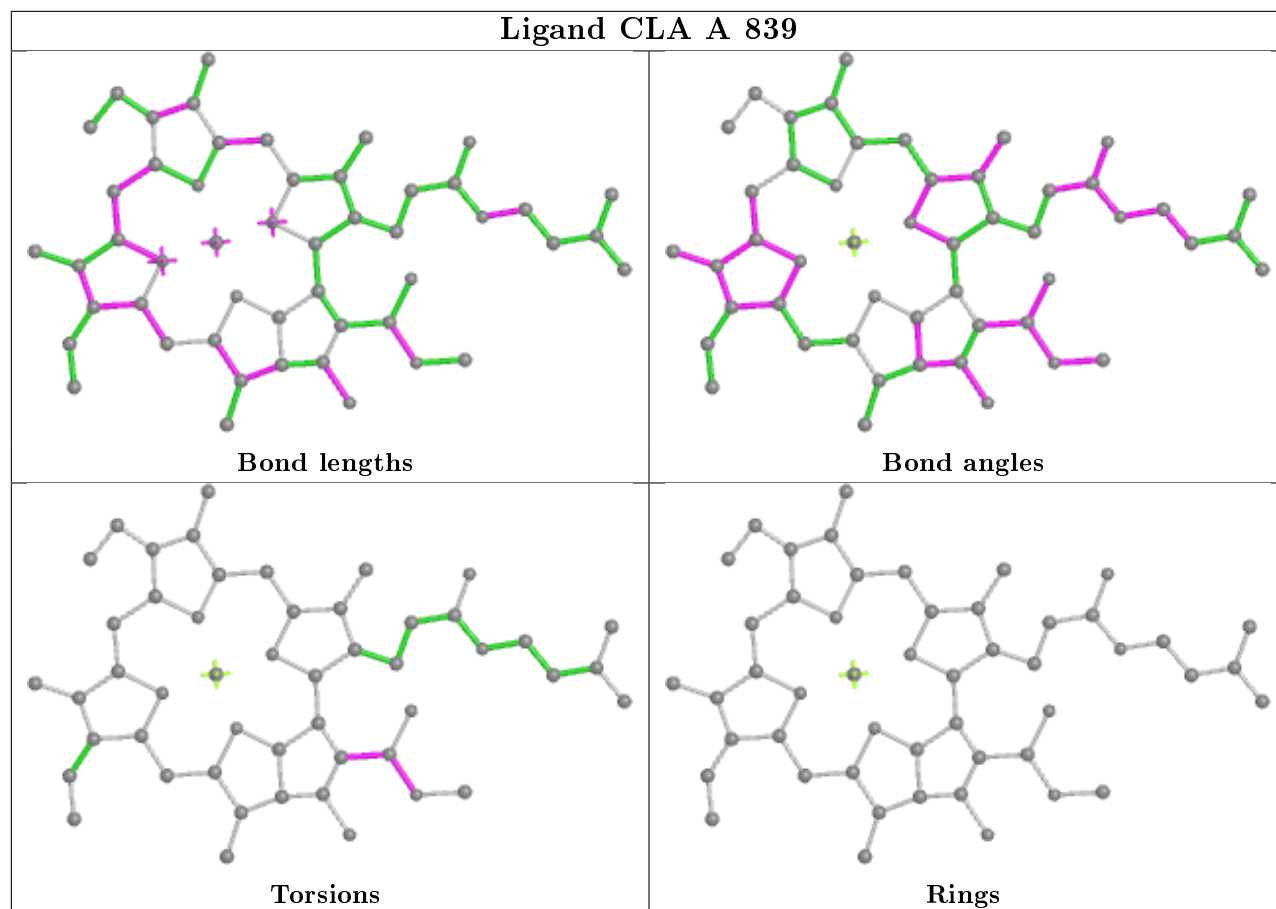
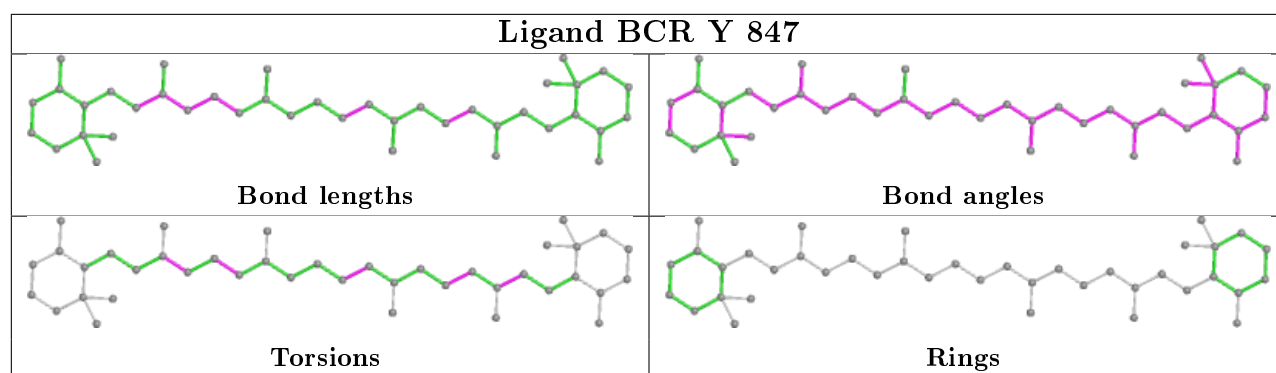


## Ligand BCR f 105



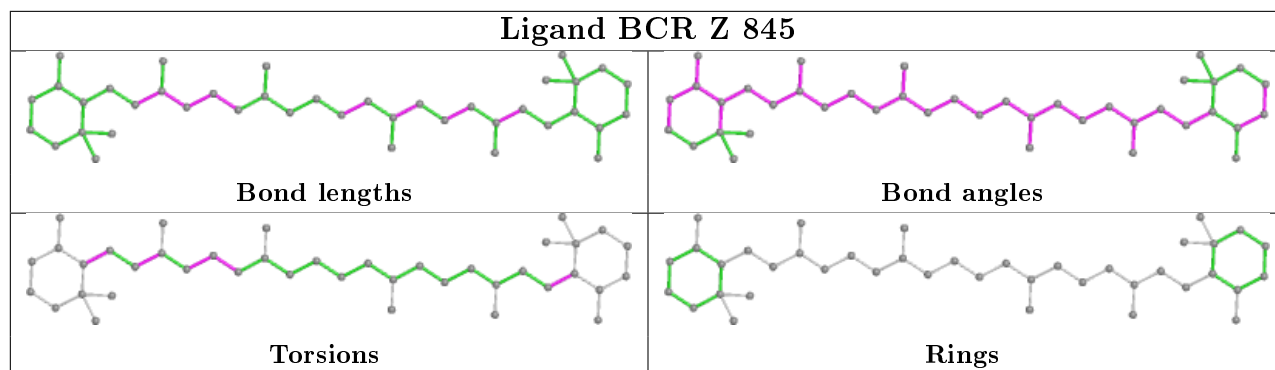
## Ligand BCR Z 846



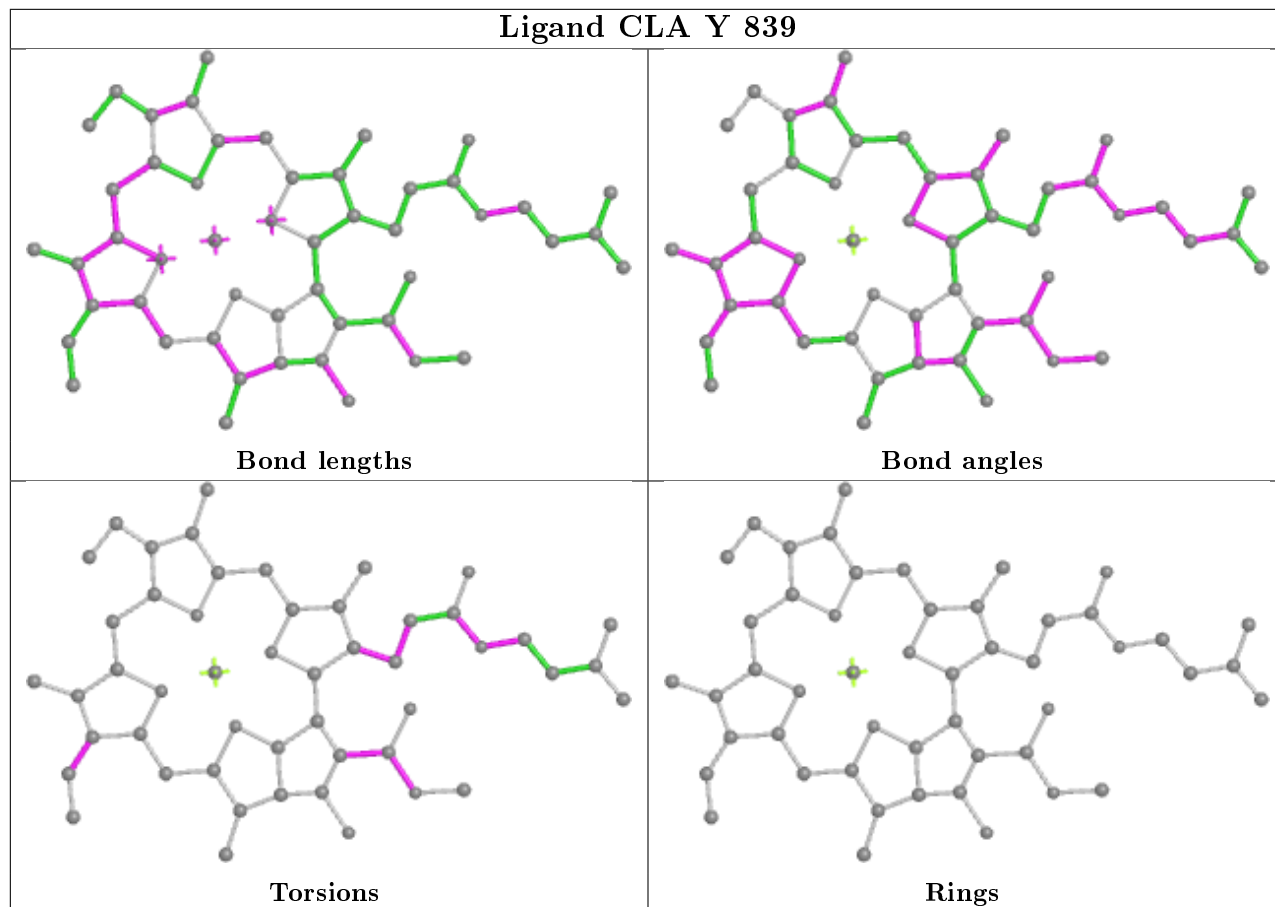




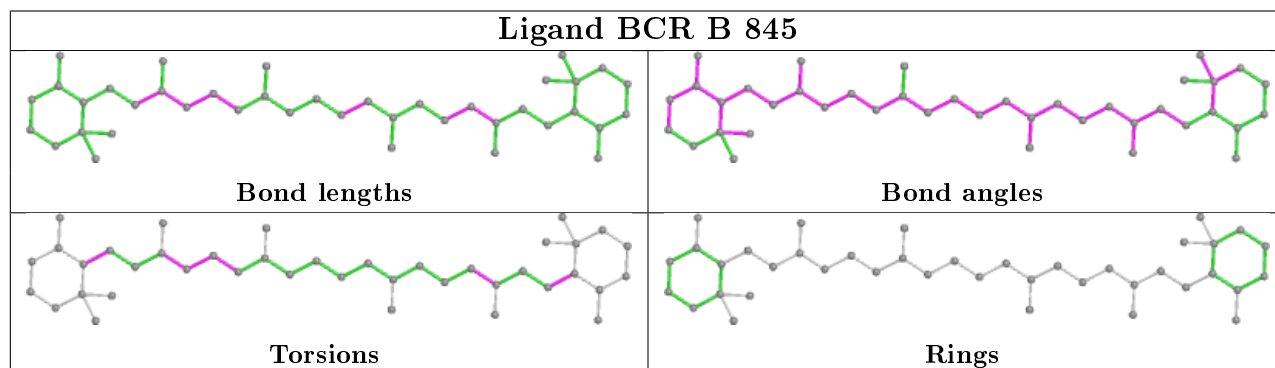
## Ligand BCR Z 845



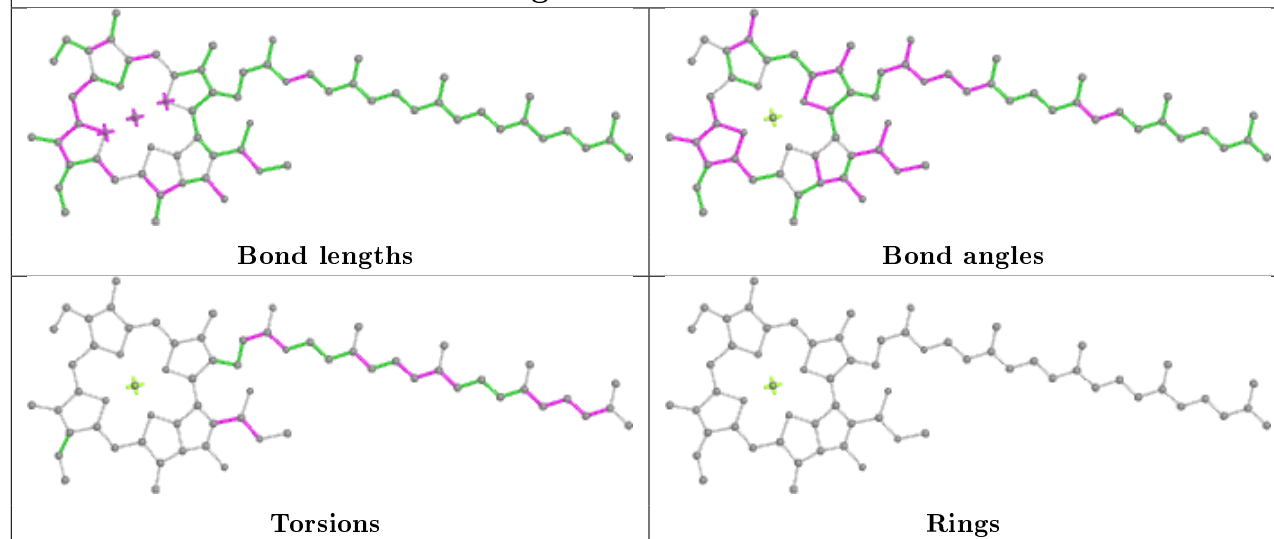
## Ligand CLA Y 839



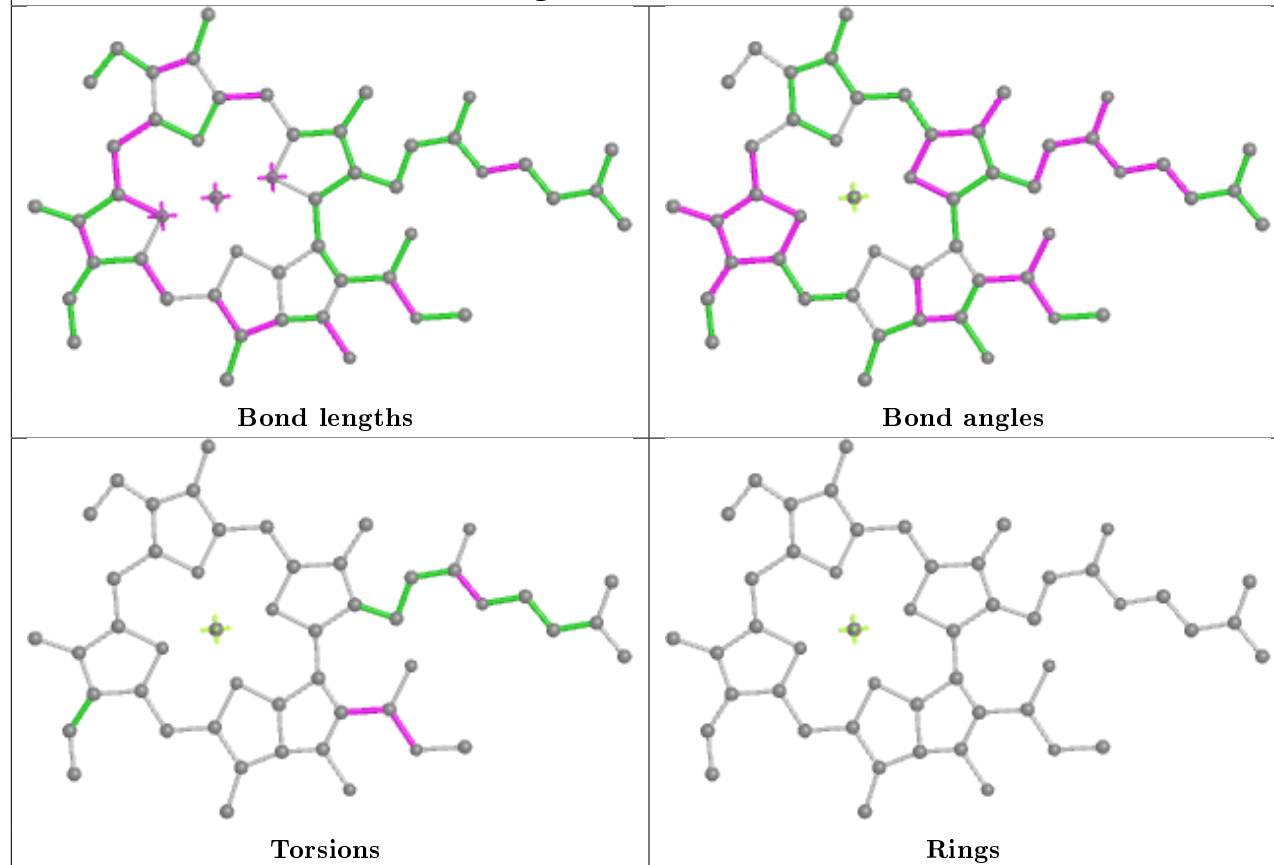
## Ligand BCR B 845



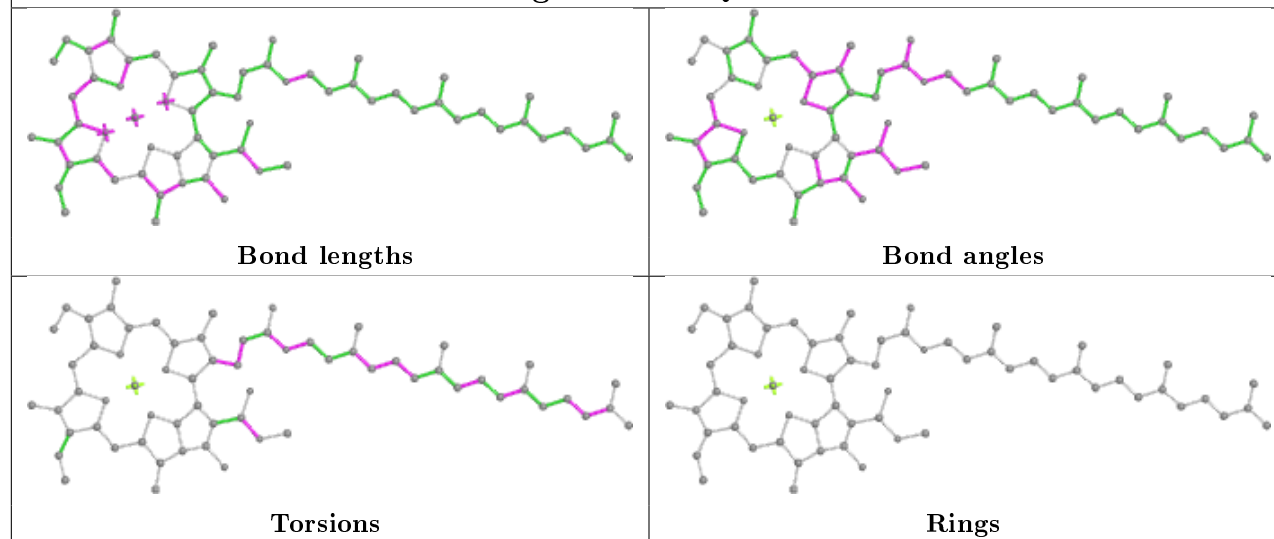
## Ligand CLA G 825



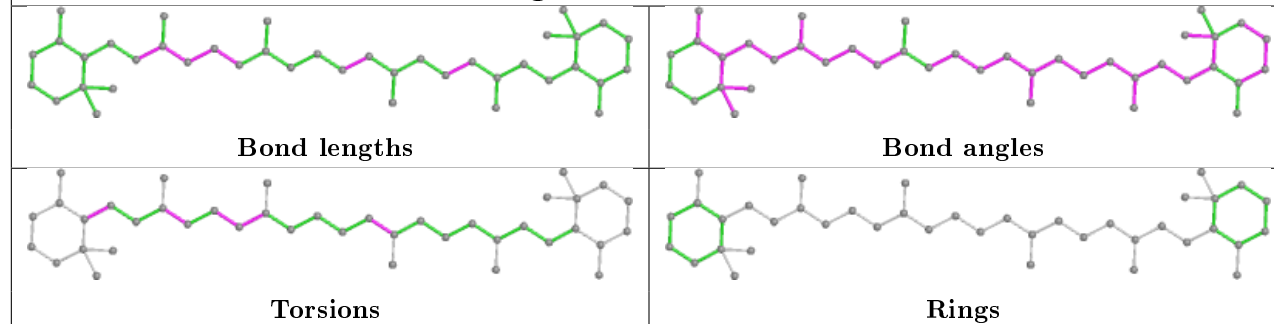
## Ligand CLA Y 816



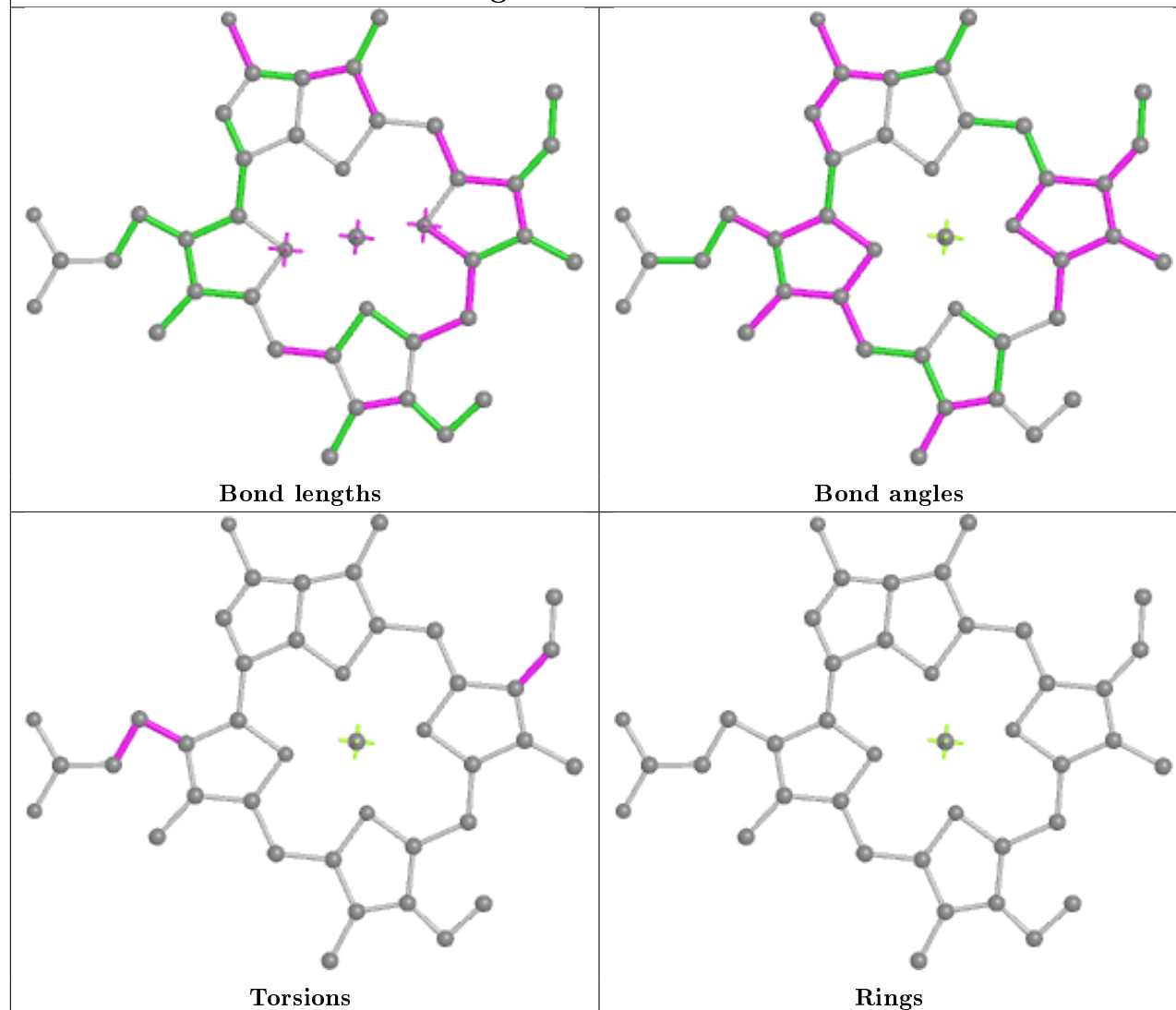
## Ligand CLA Q 201



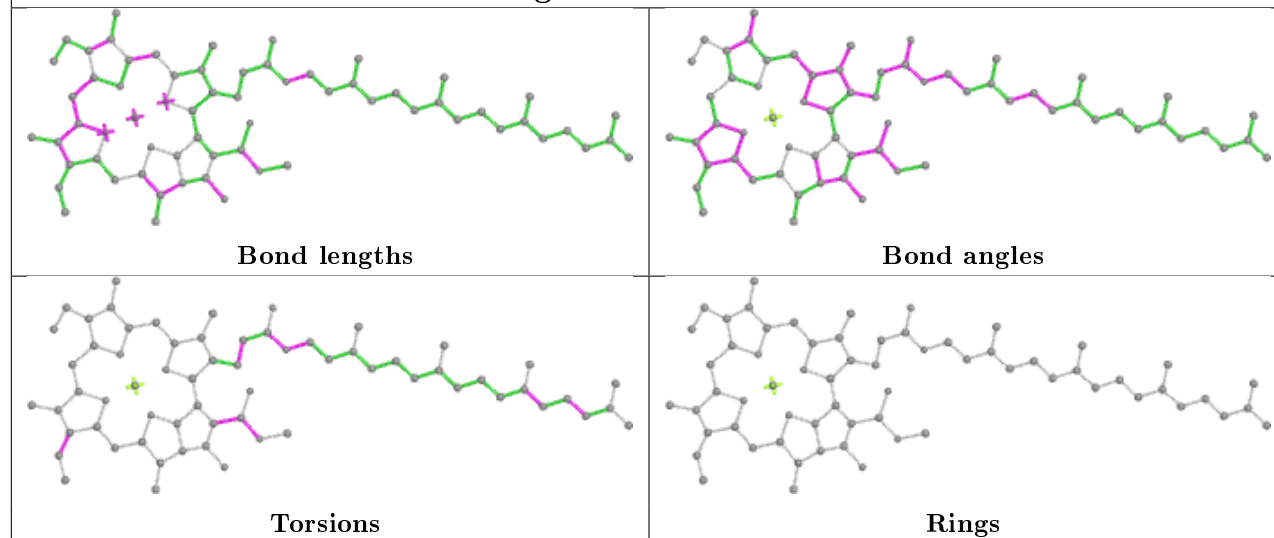
## Ligand BCR G 850



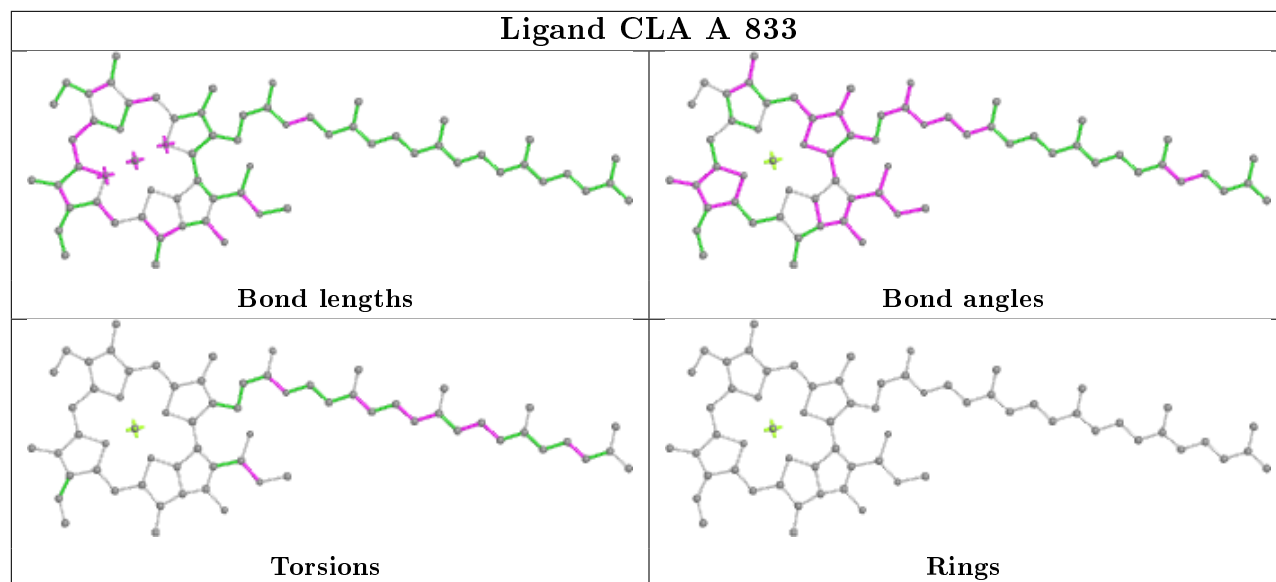
## Ligand CLA K 101



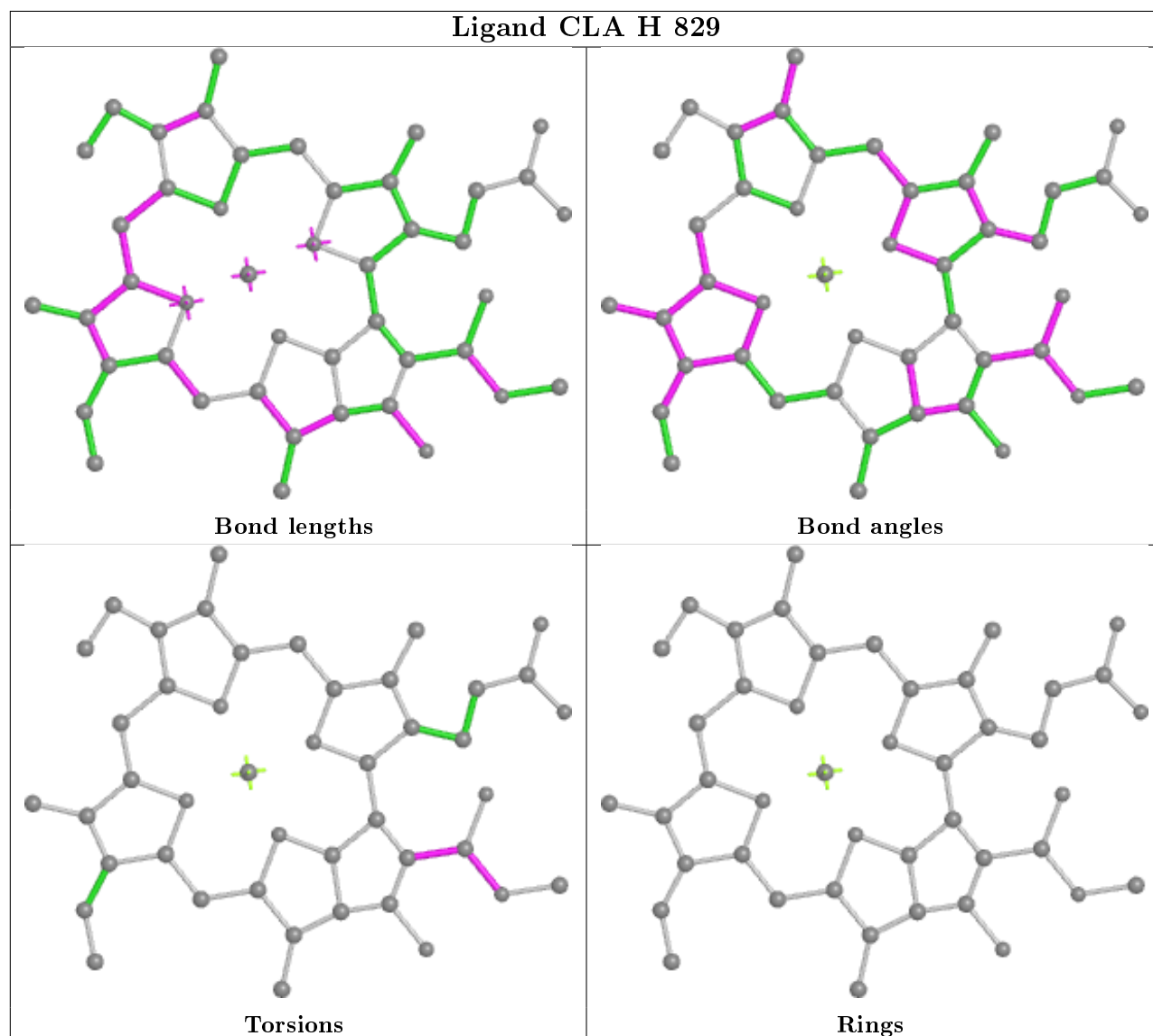
## Ligand CLA L 201



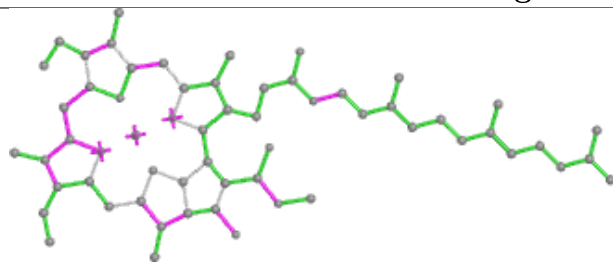
## Ligand CLA A 833



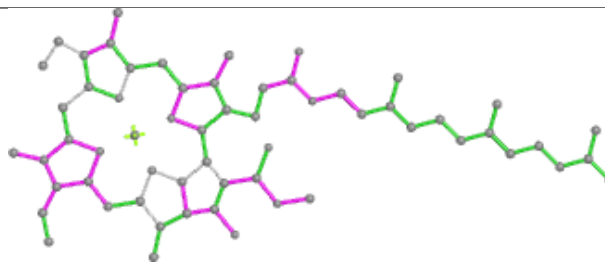
## Ligand CLA H 829



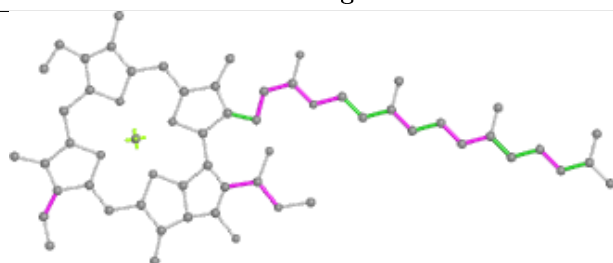
## Ligand CLA A 824



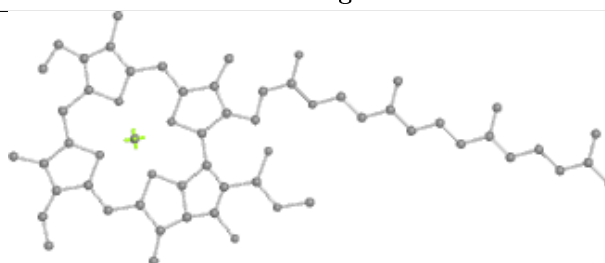
Bond lengths



Bond angles

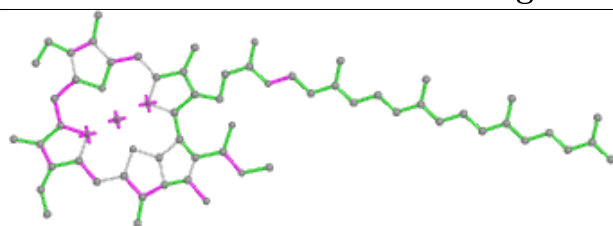


Torsions

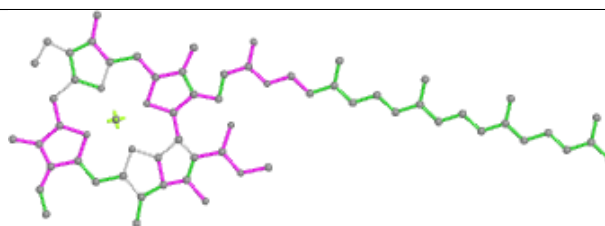


Rings

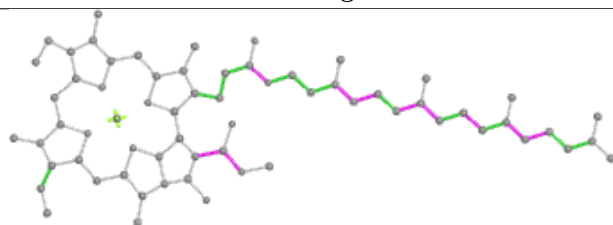
## Ligand CLA L 202



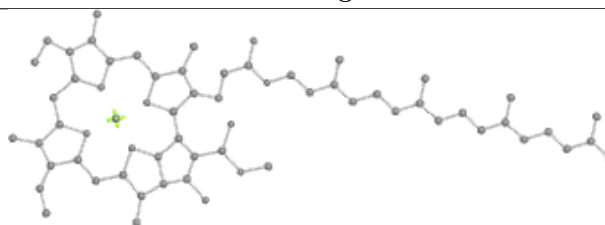
Bond lengths



Bond angles

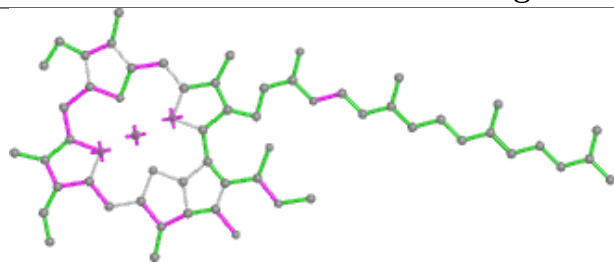


Torsions

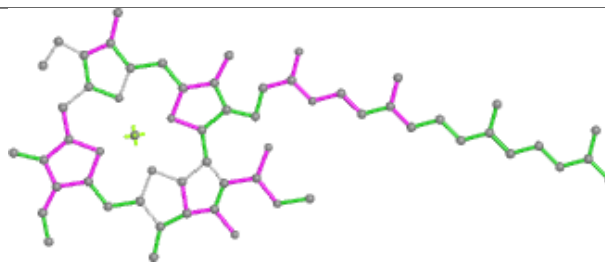


Rings

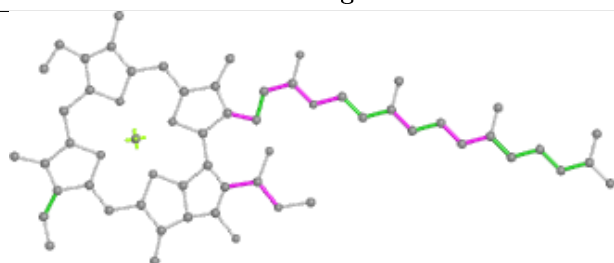
## Ligand CLA G 820



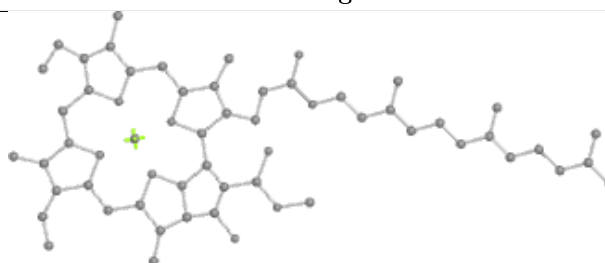
Bond lengths



Bond angles

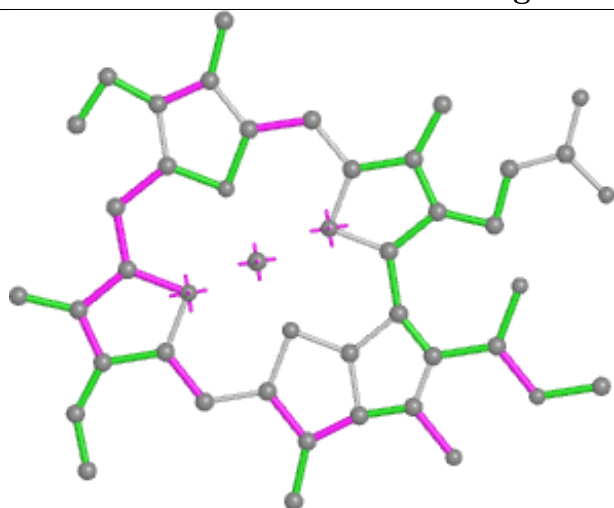


Torsions

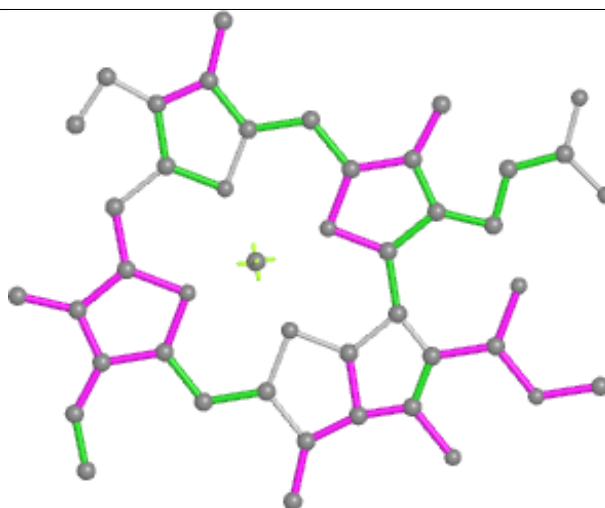


Rings

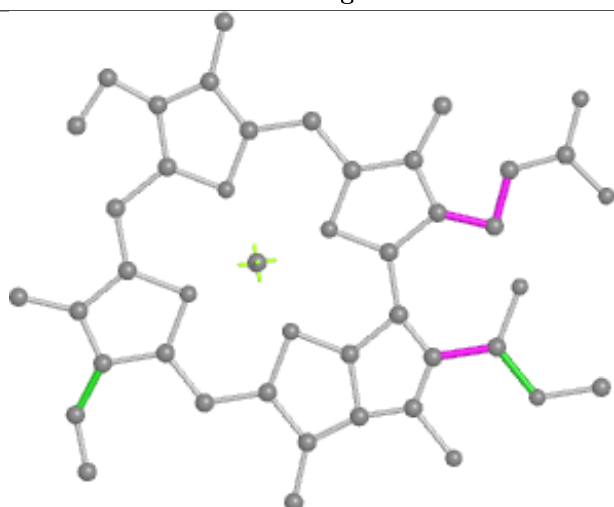
## Ligand CLA G 835



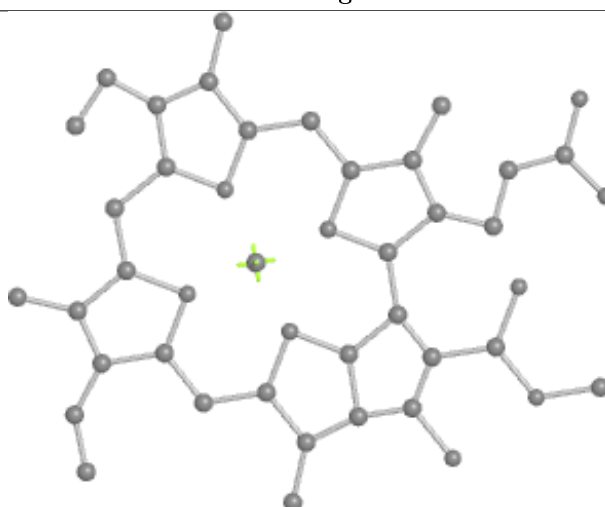
Bond lengths



Bond angles

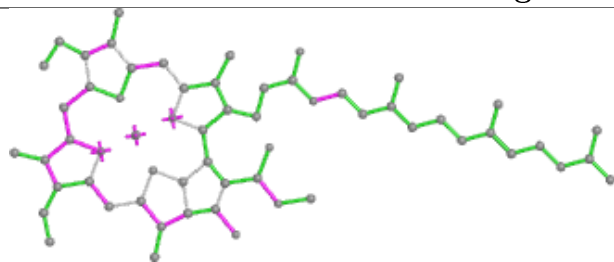


Torsions

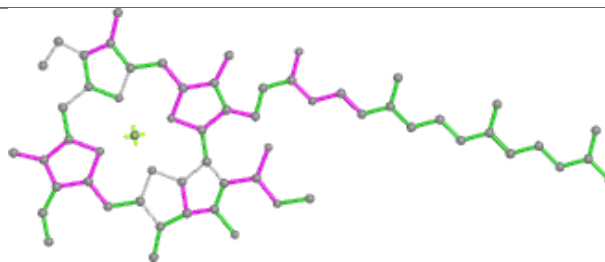


Rings

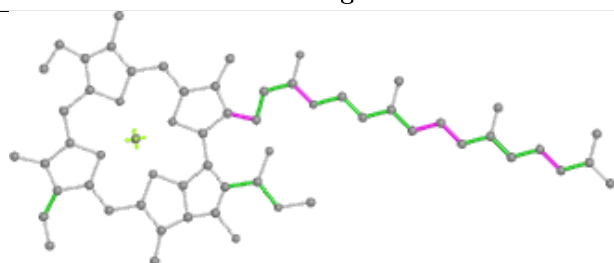
## Ligand CLA Y 826



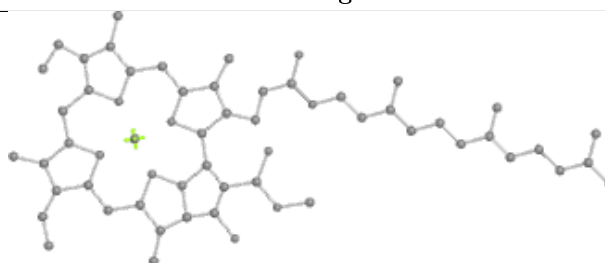
Bond lengths



Bond angles

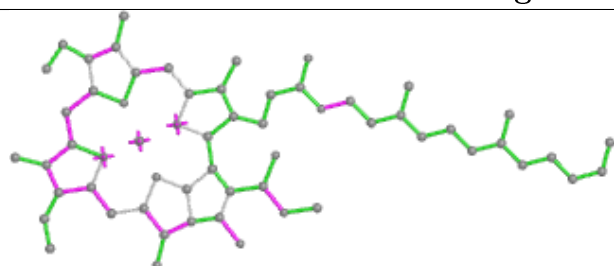


Torsions

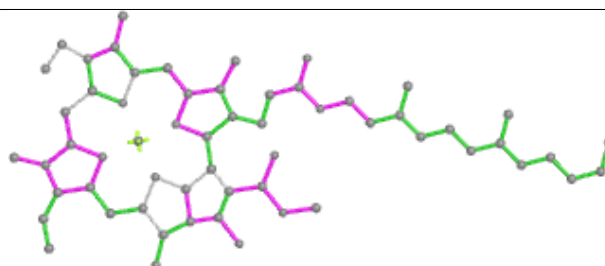


Rings

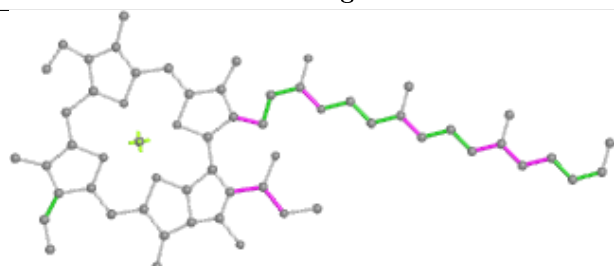
## Ligand CLA Y 804



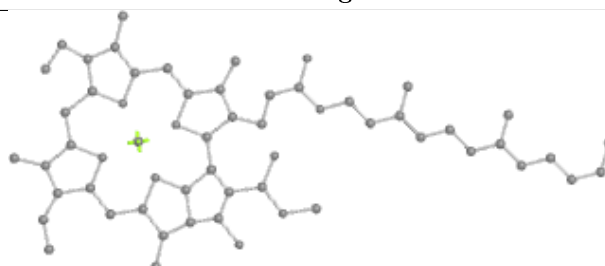
Bond lengths



Bond angles



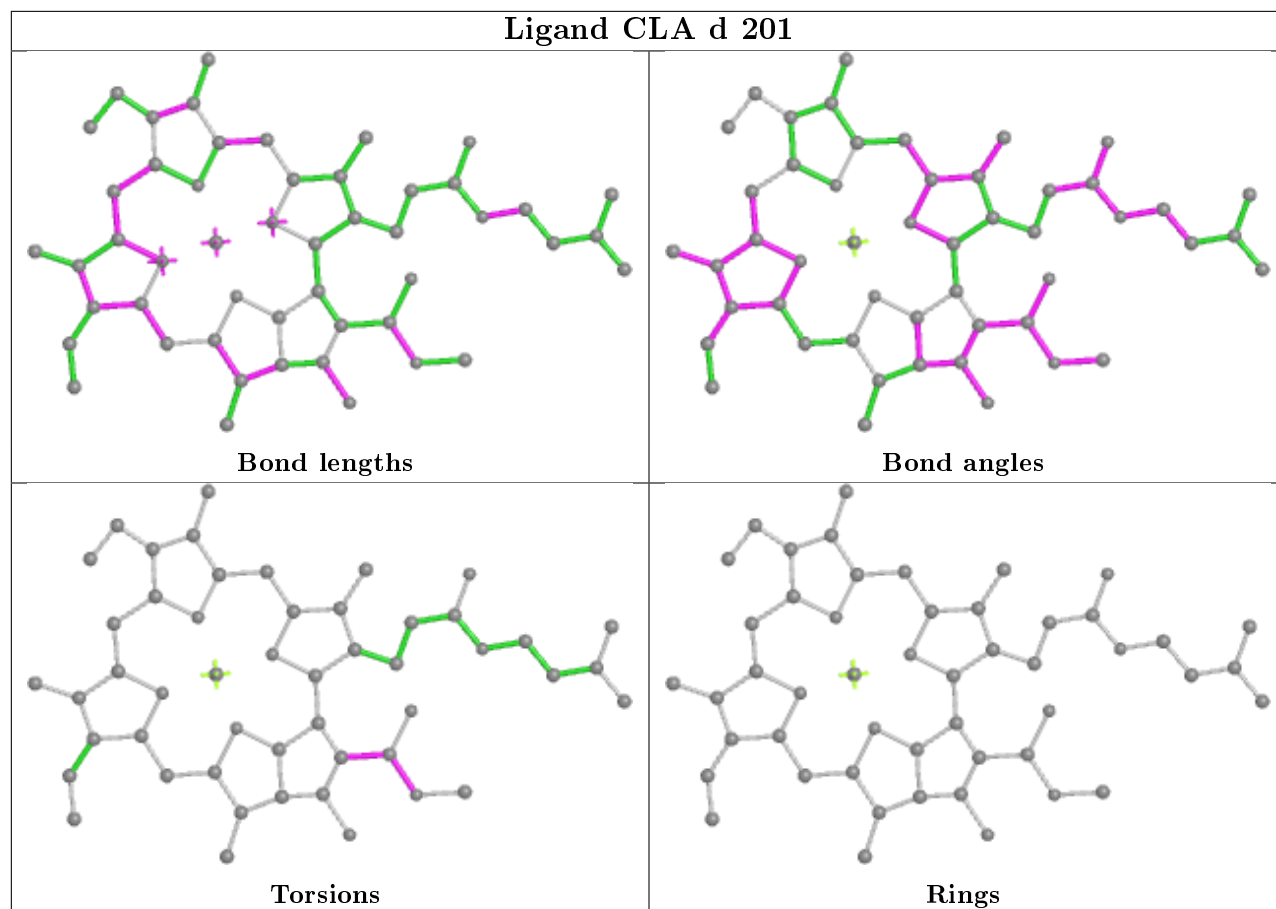
Torsions



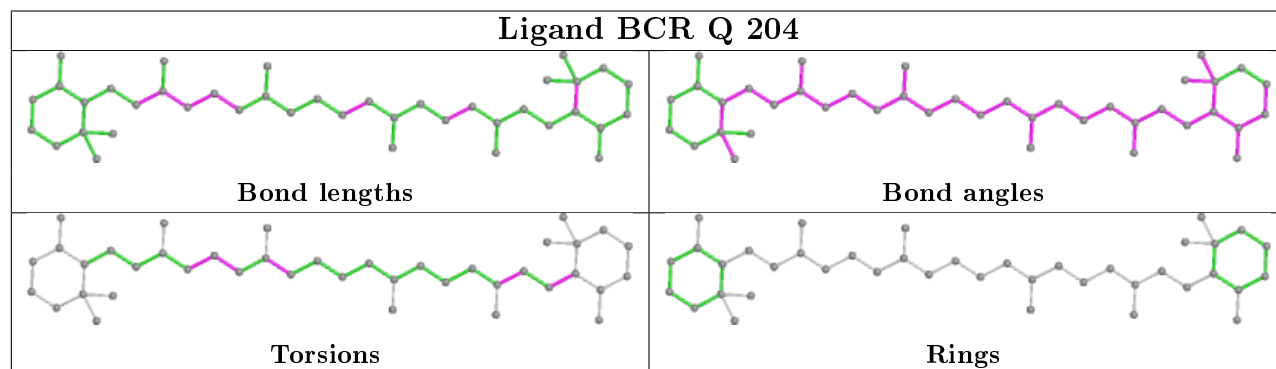
Rings



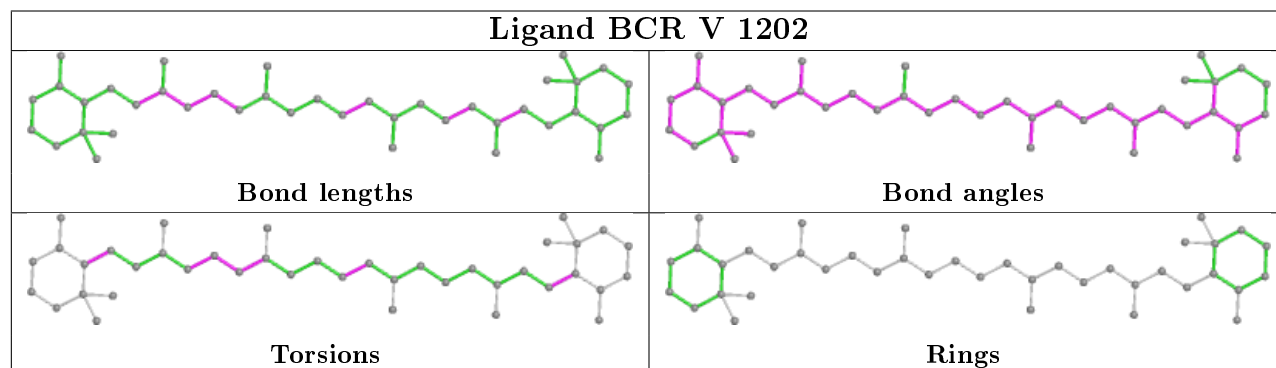
## Ligand CLA d 201



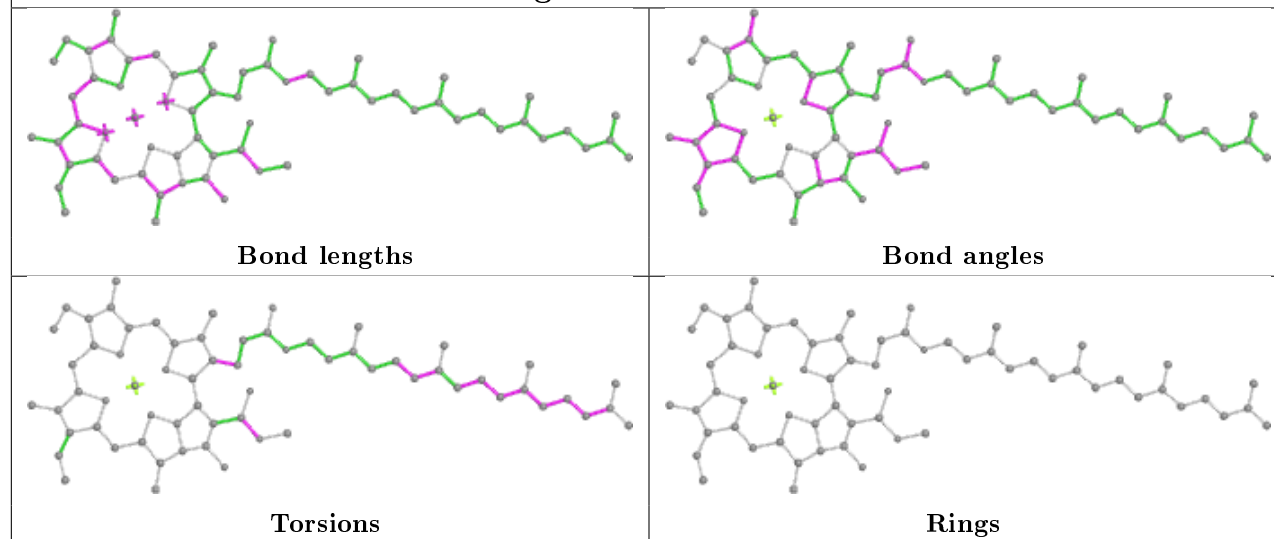
## Ligand BCR Q 204



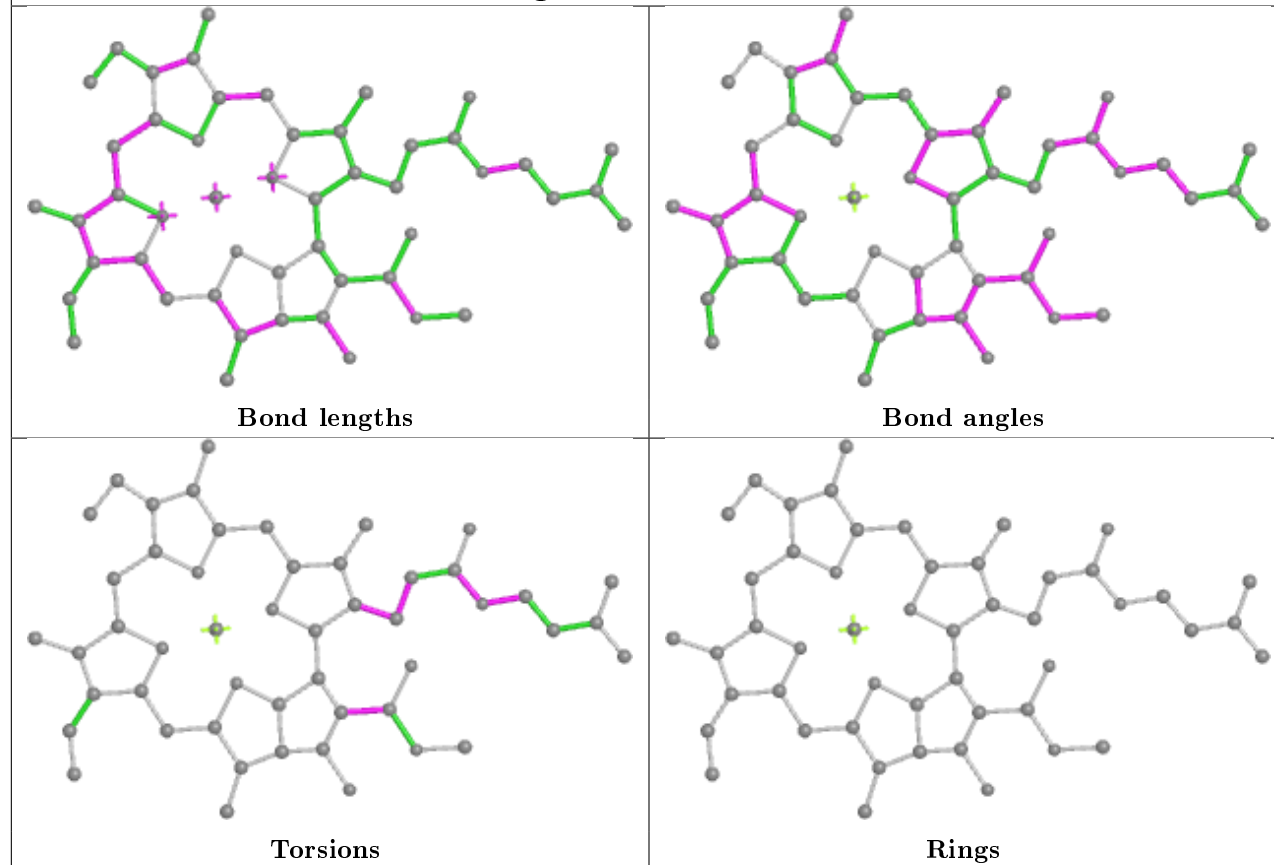
## Ligand BCR V 1202



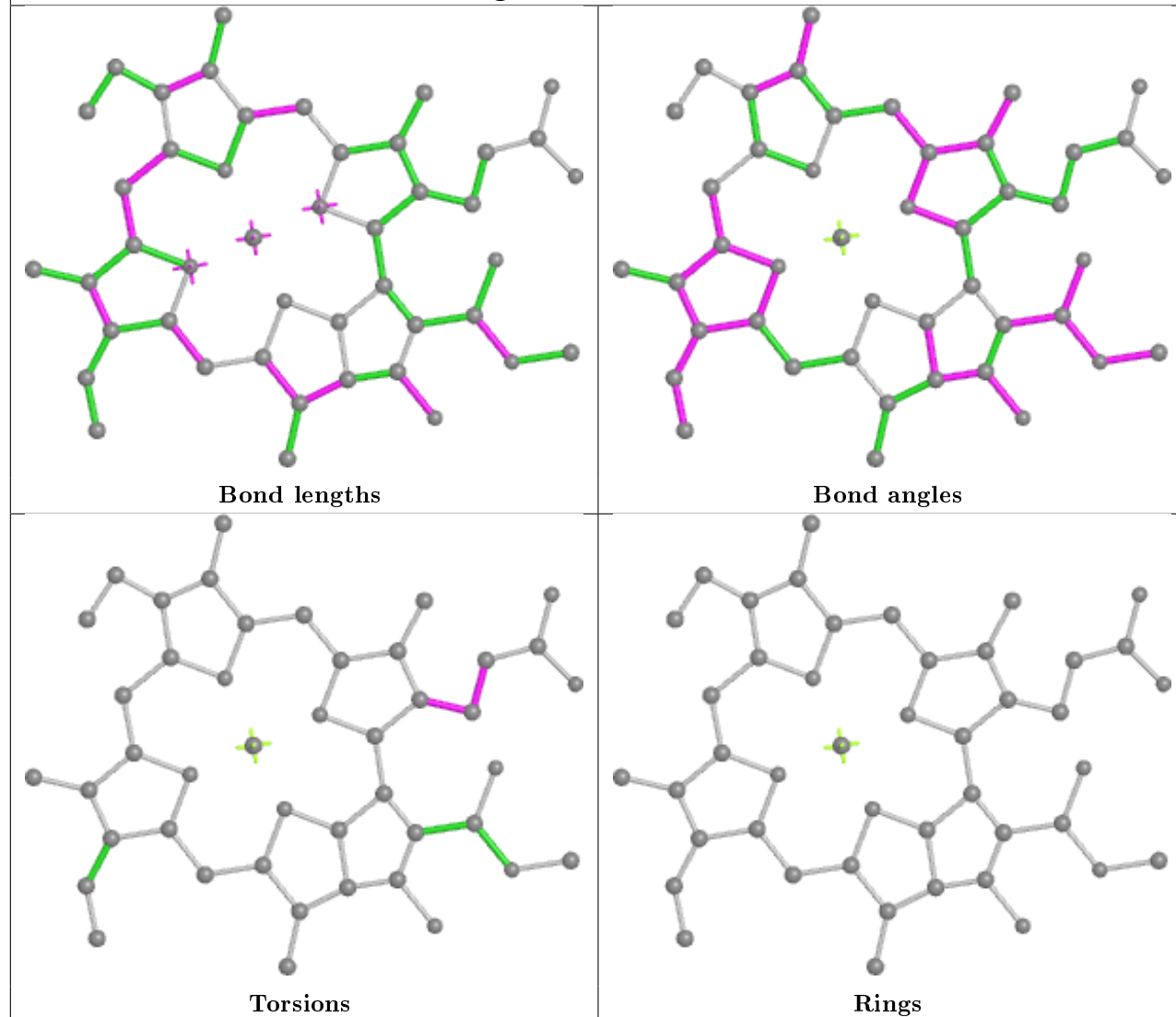
## Ligand CLA Z 825



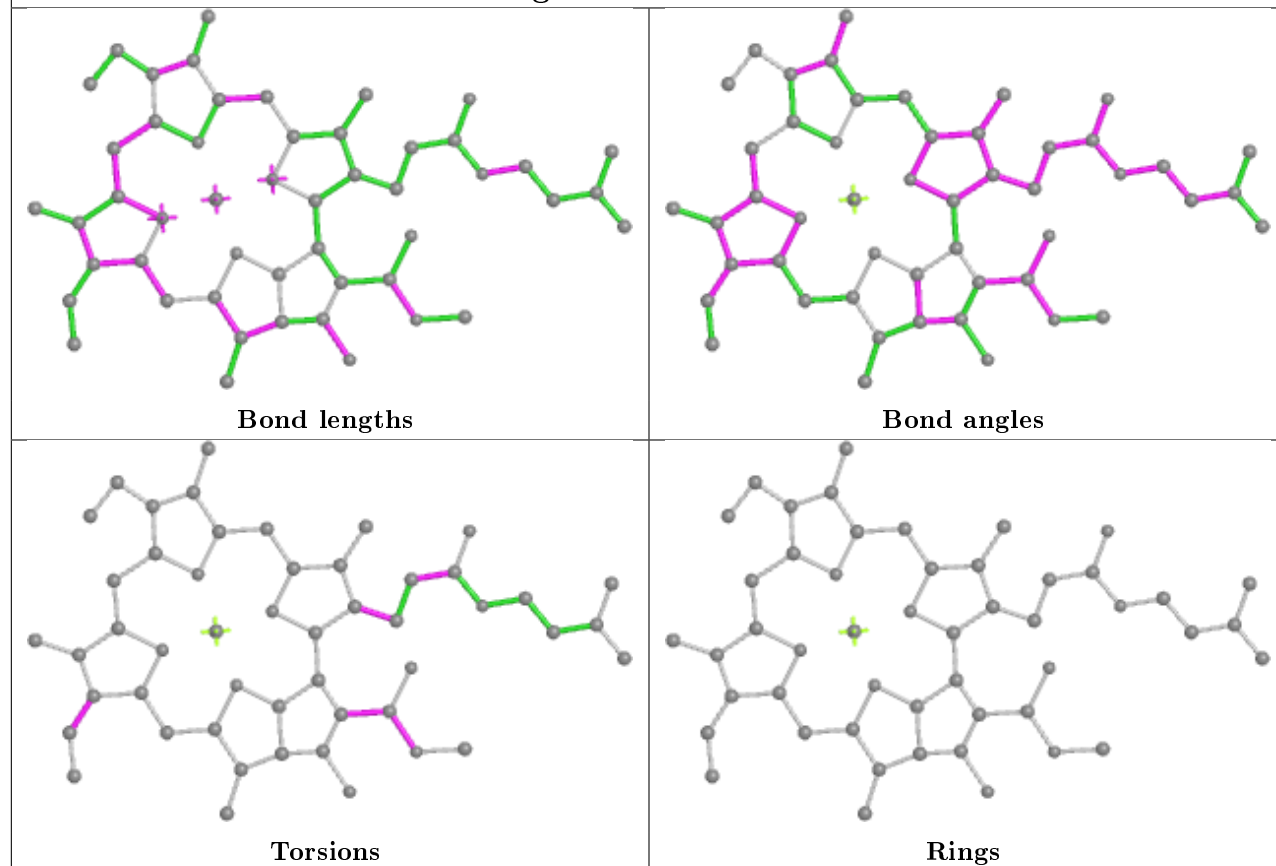
## Ligand CLA Y 837



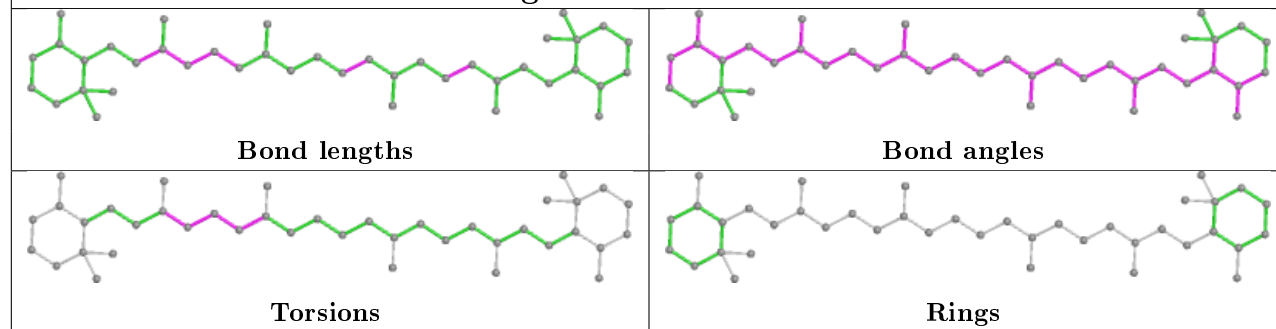
## Ligand CLA Z 818



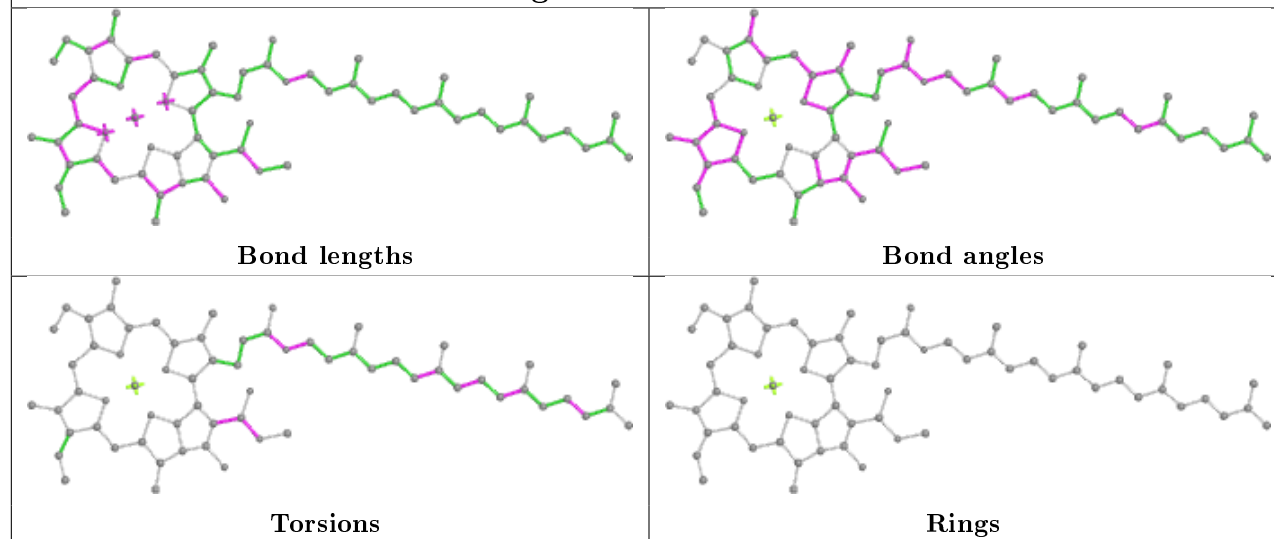
## Ligand CLA A 814



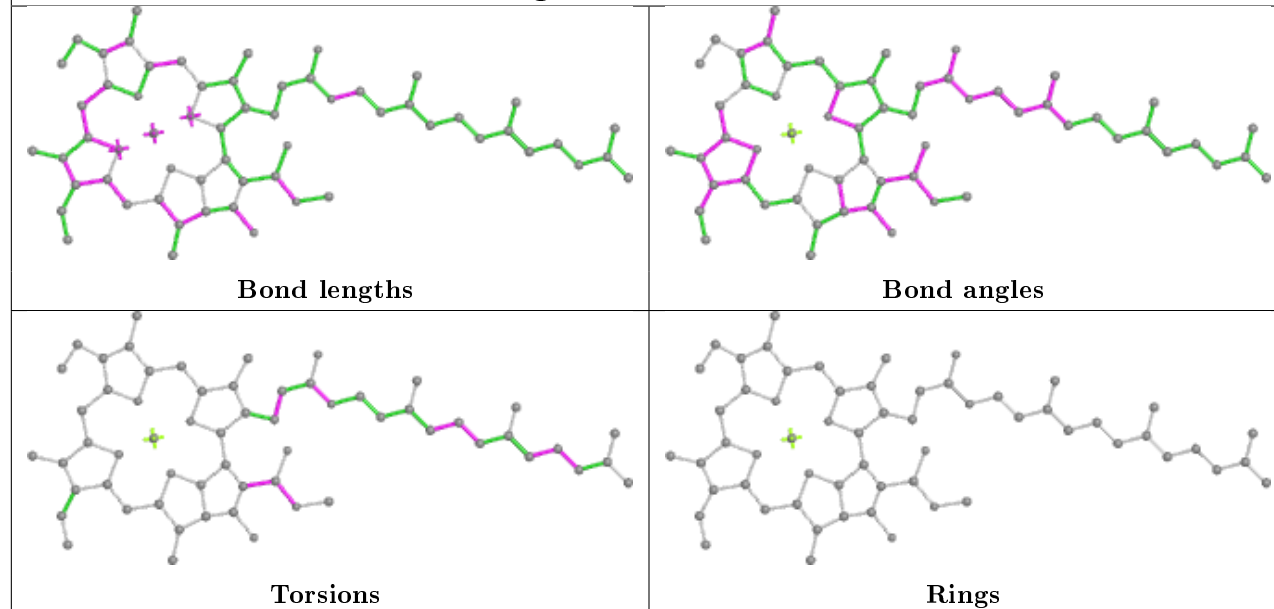
## Ligand BCR U 1008

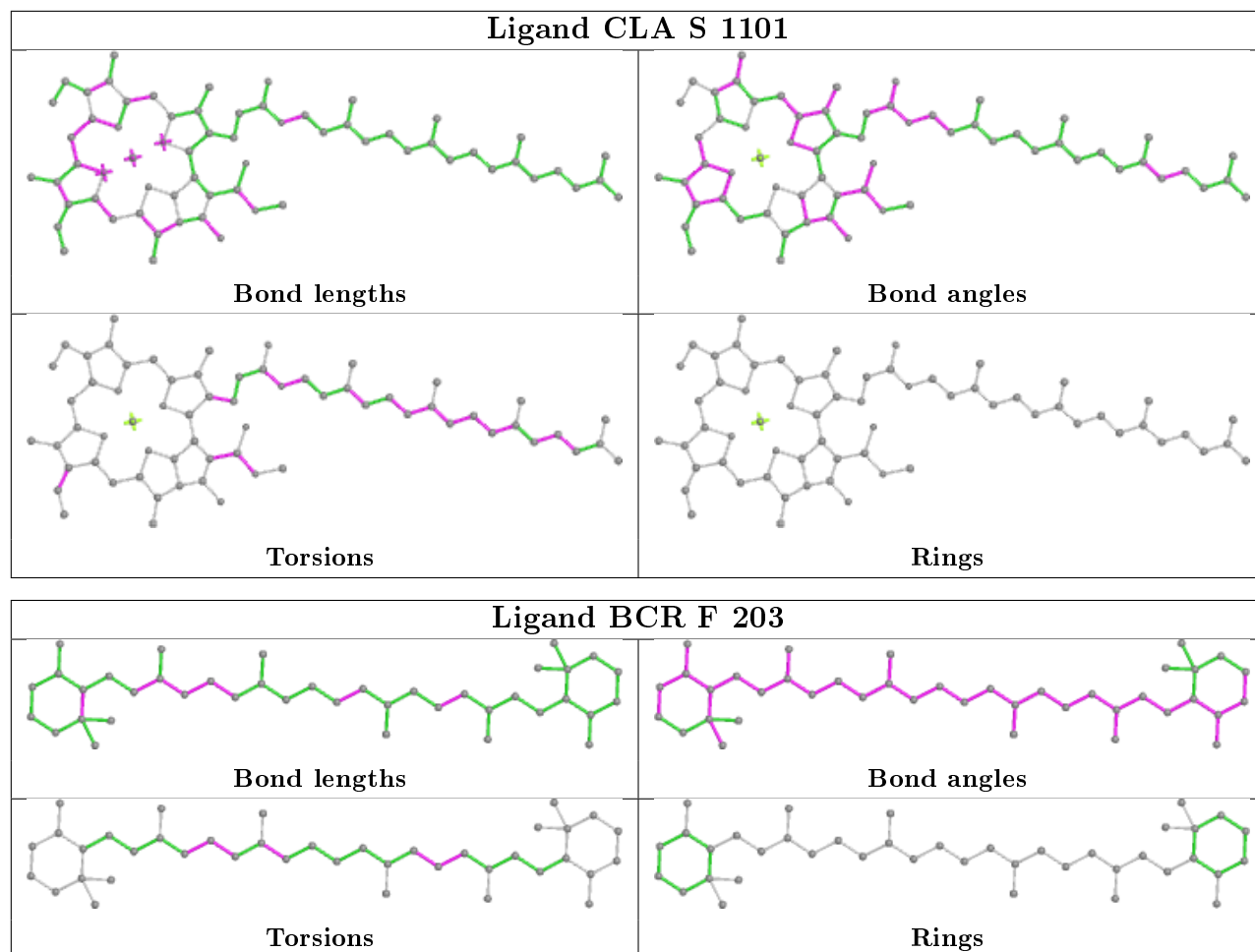


## Ligand CLA G 803

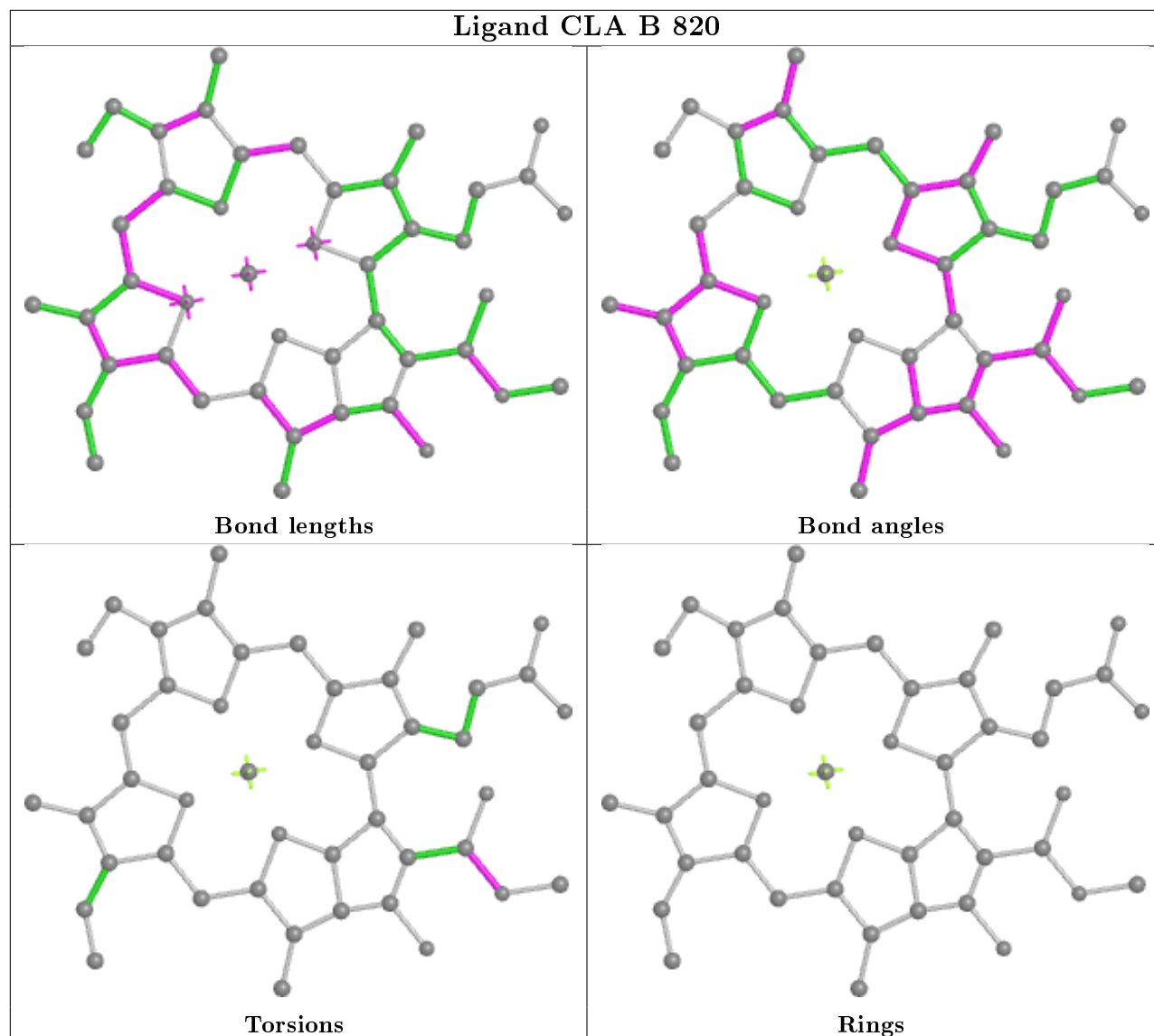


## Ligand CLA Y 813

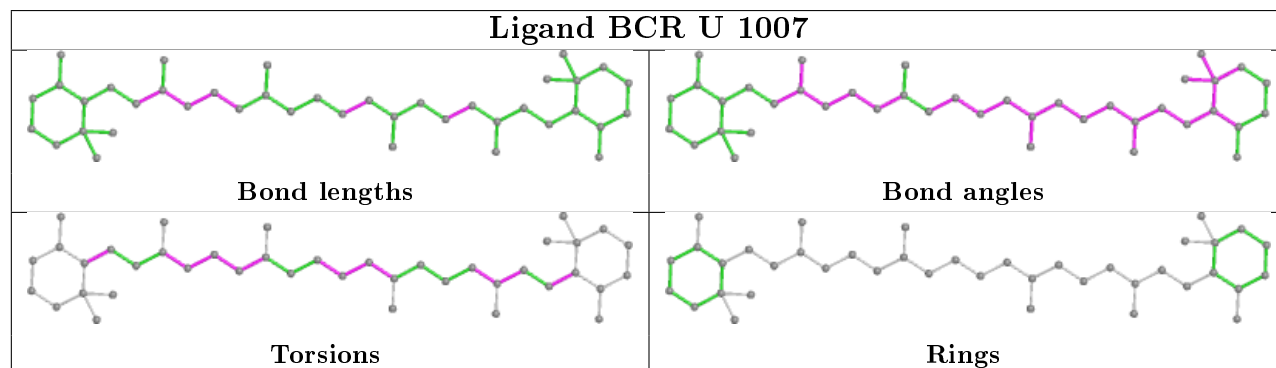




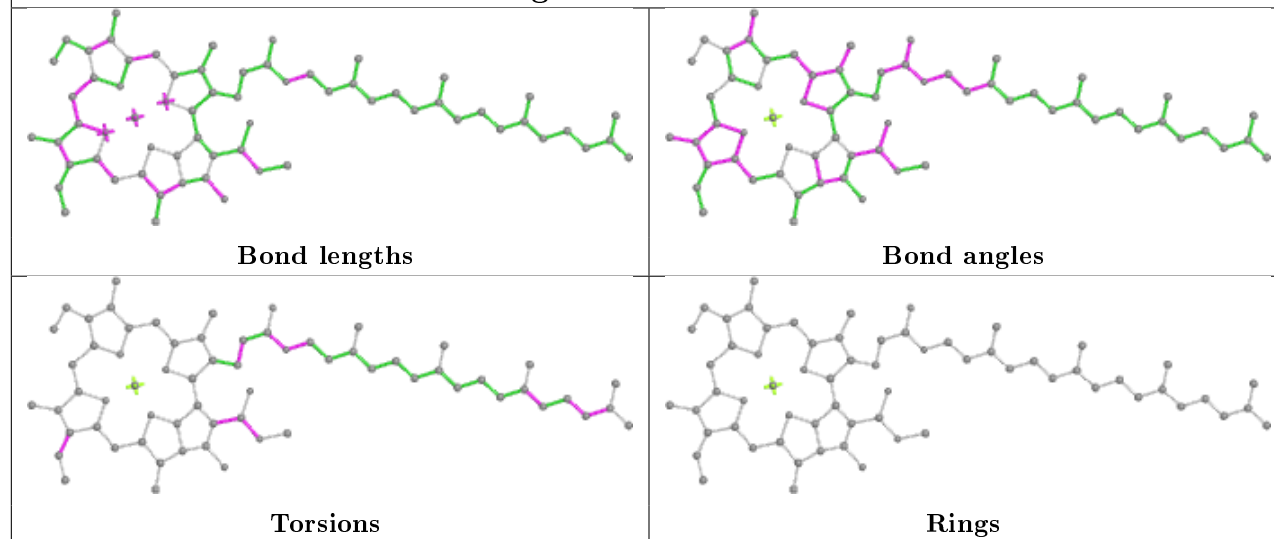
## Ligand CLA B 820



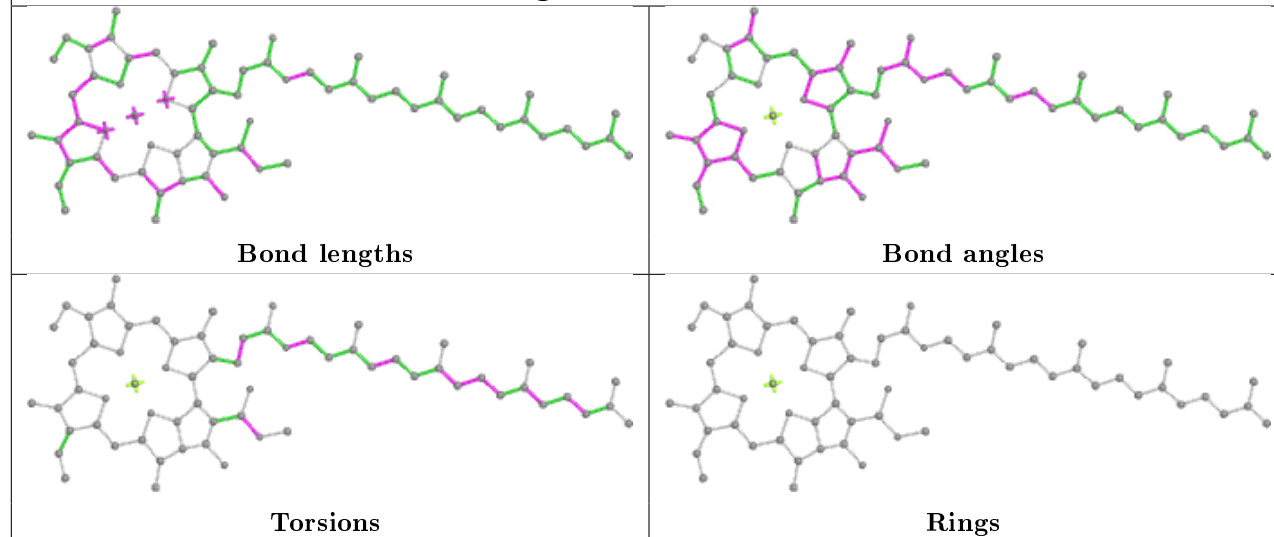
## Ligand BCR U 1007



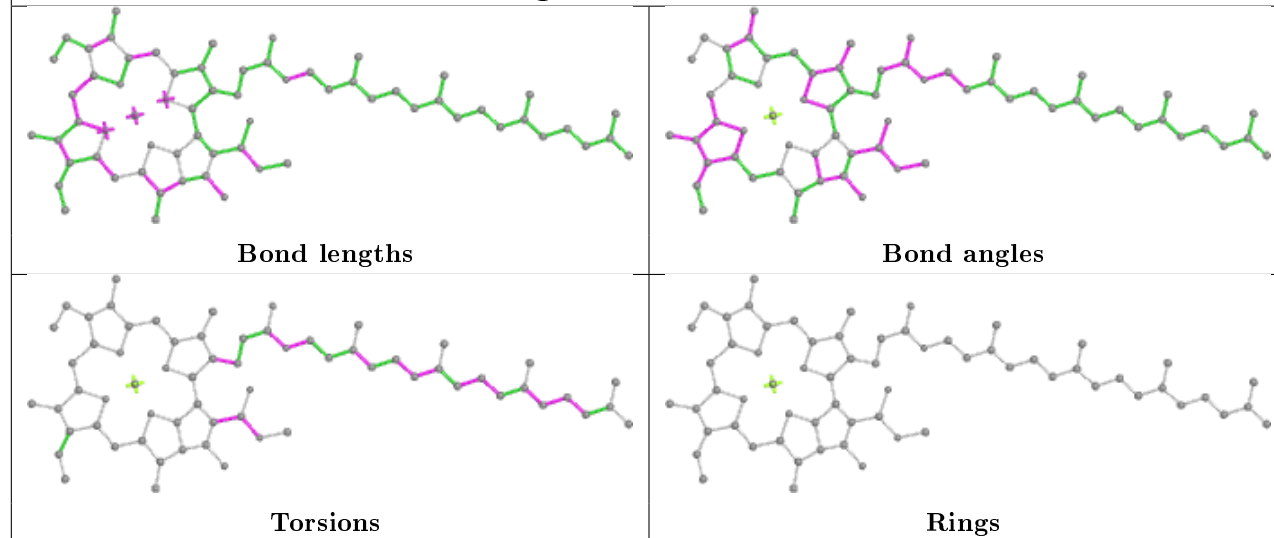
## Ligand CLA G 833



## Ligand CLA Z 838

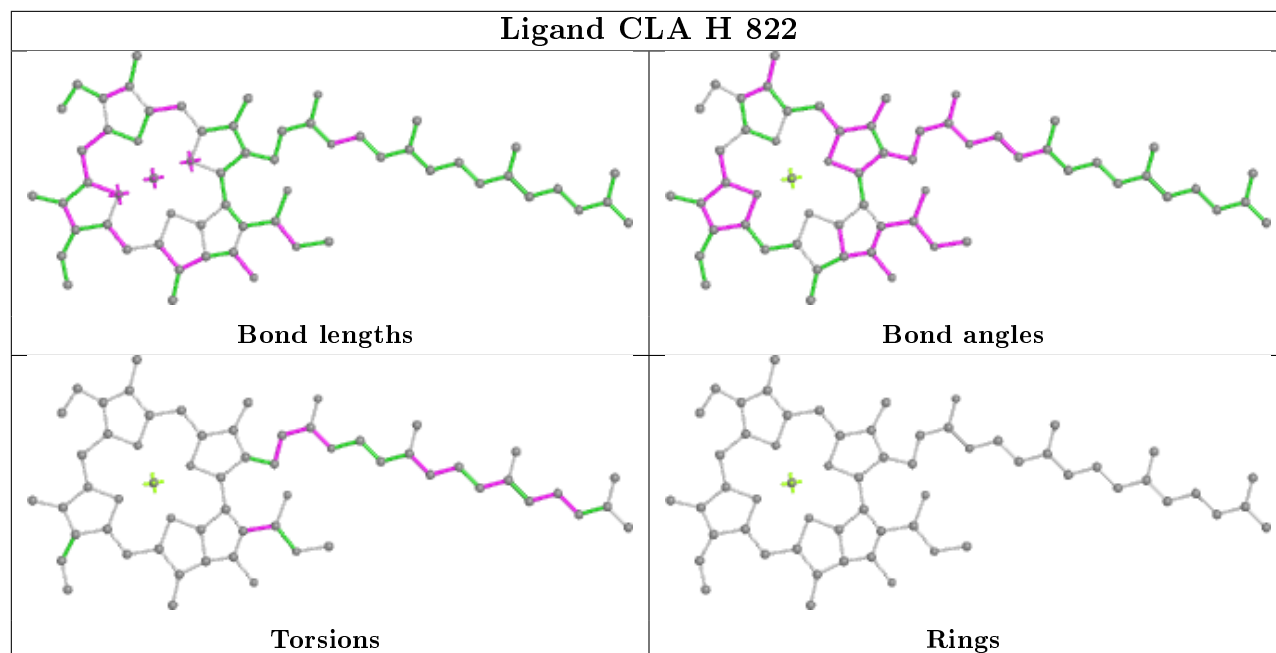


## Ligand CLA Z 811

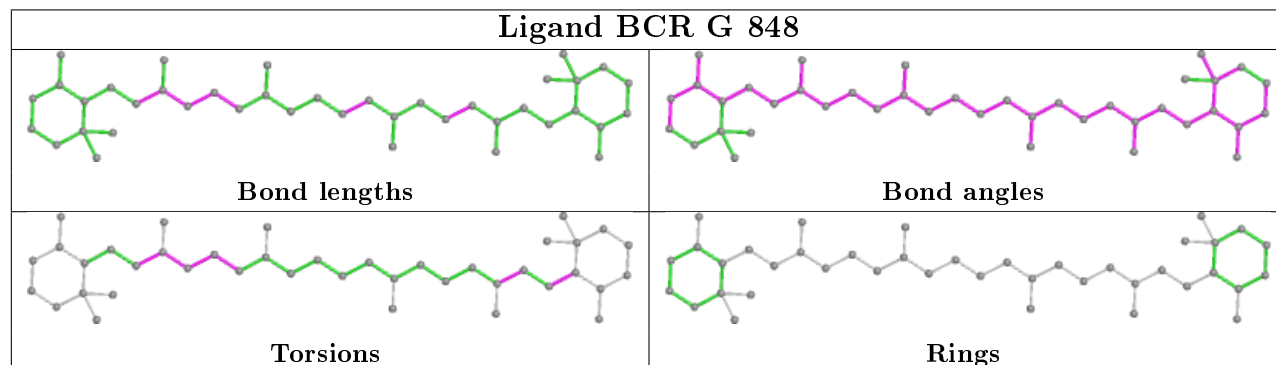




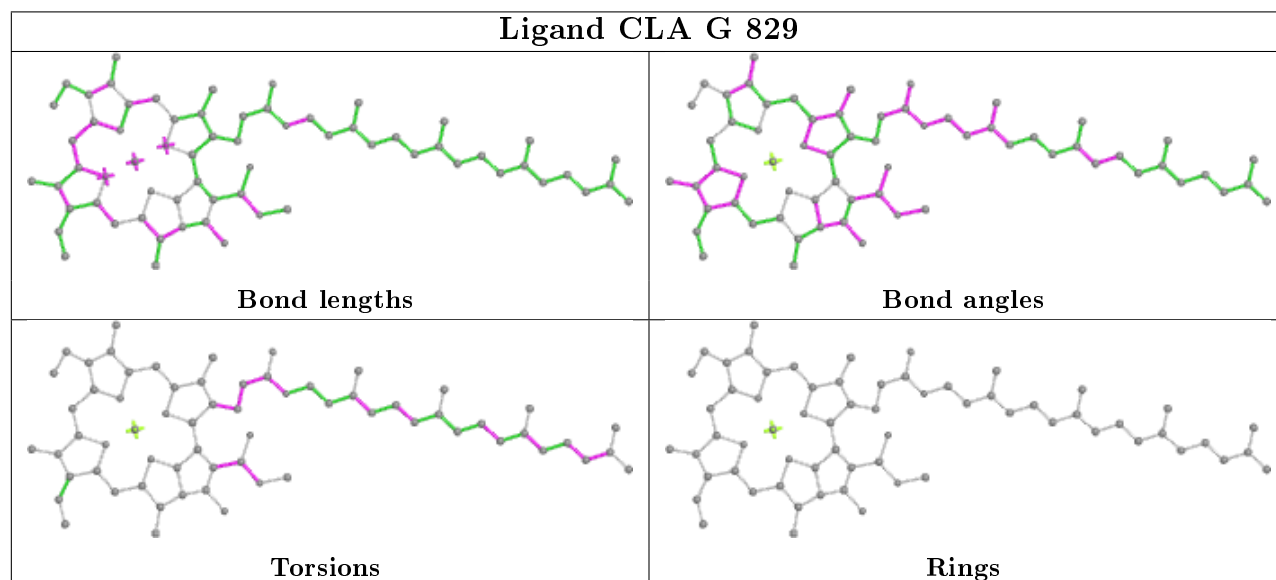
## Ligand CLA H 822



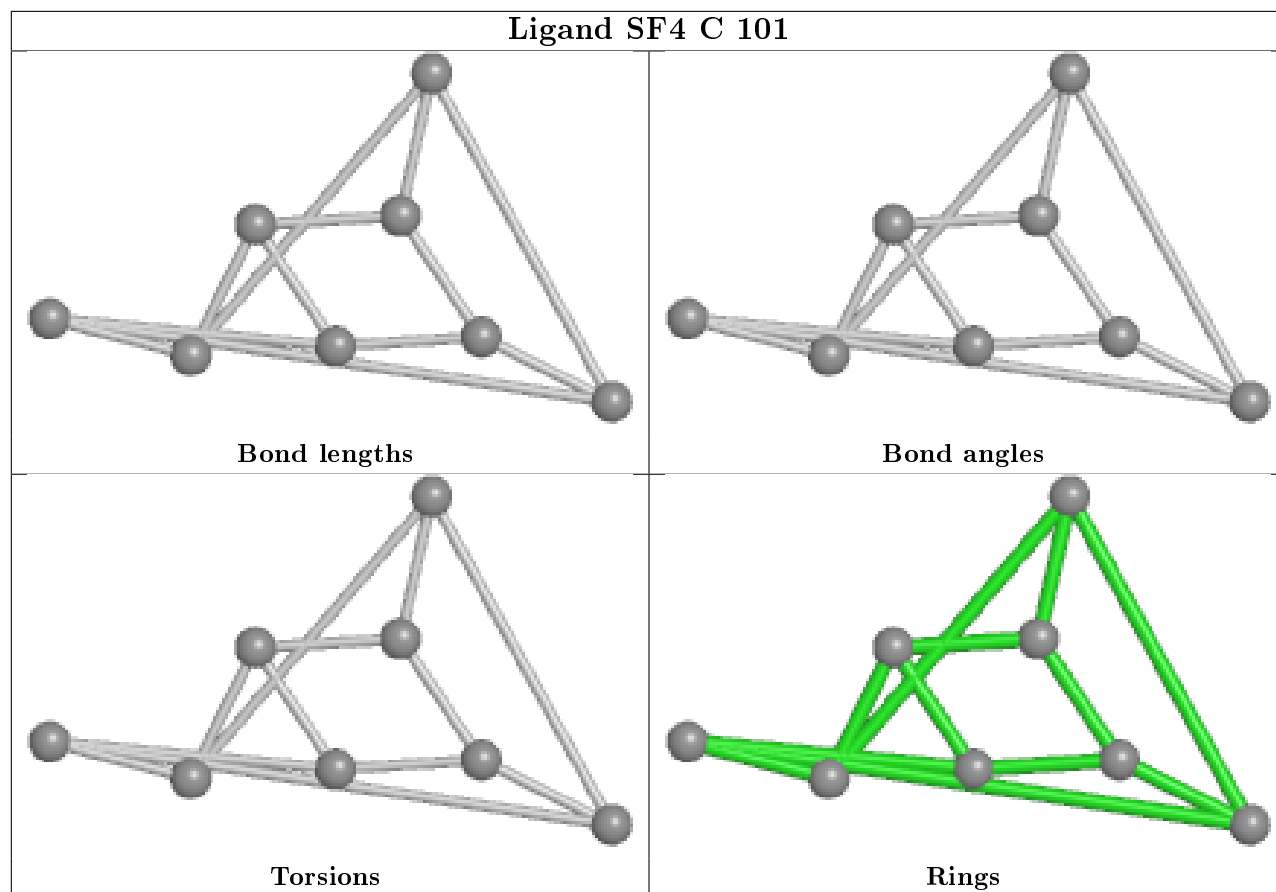
## Ligand BCR G 848



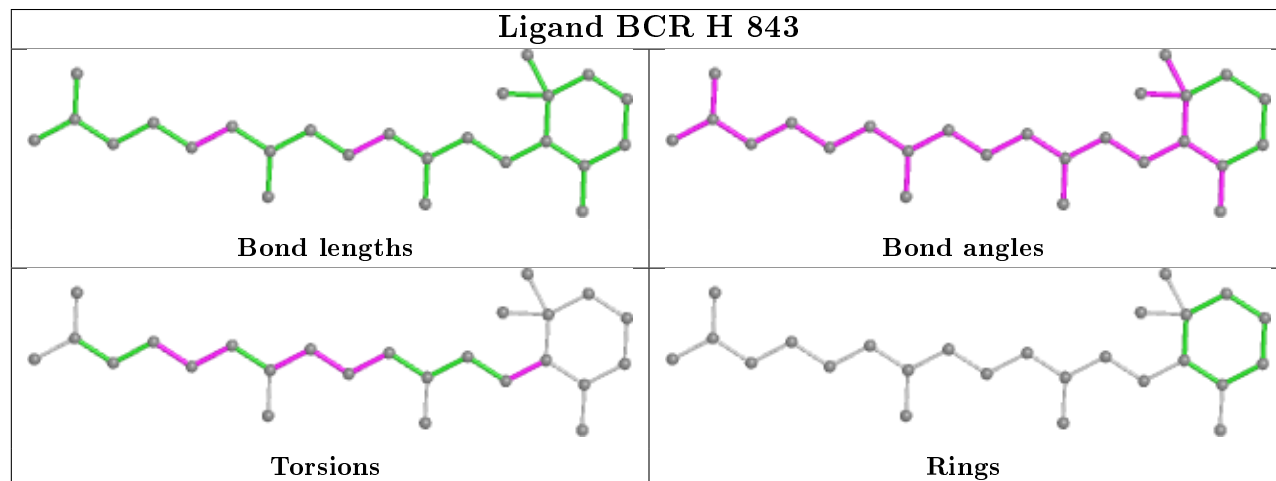
## Ligand CLA G 829



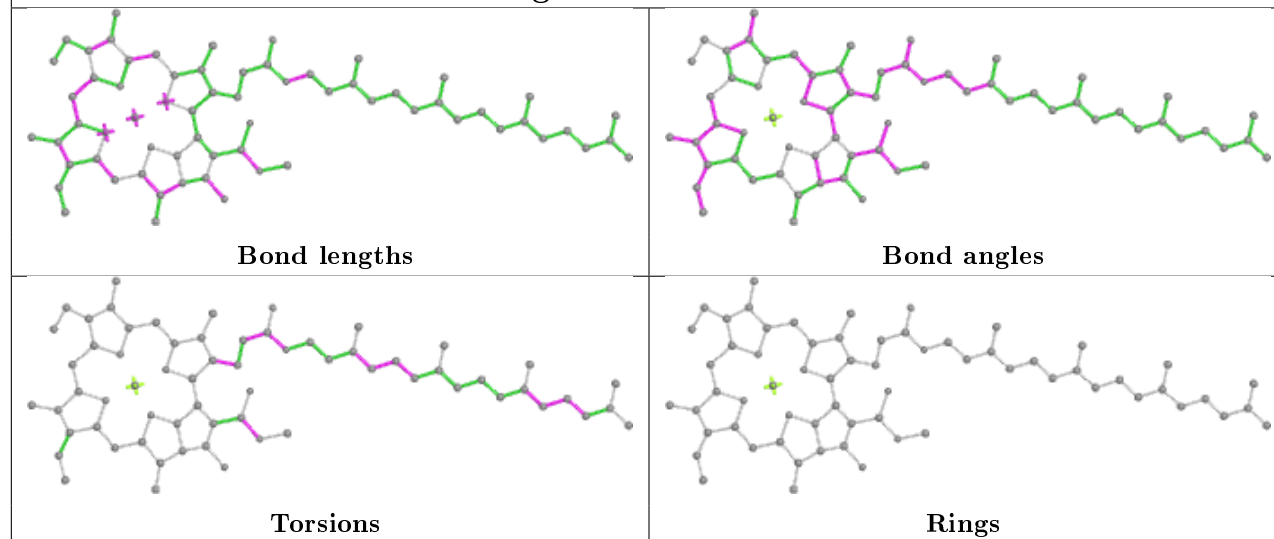
## Ligand SF4 C 101



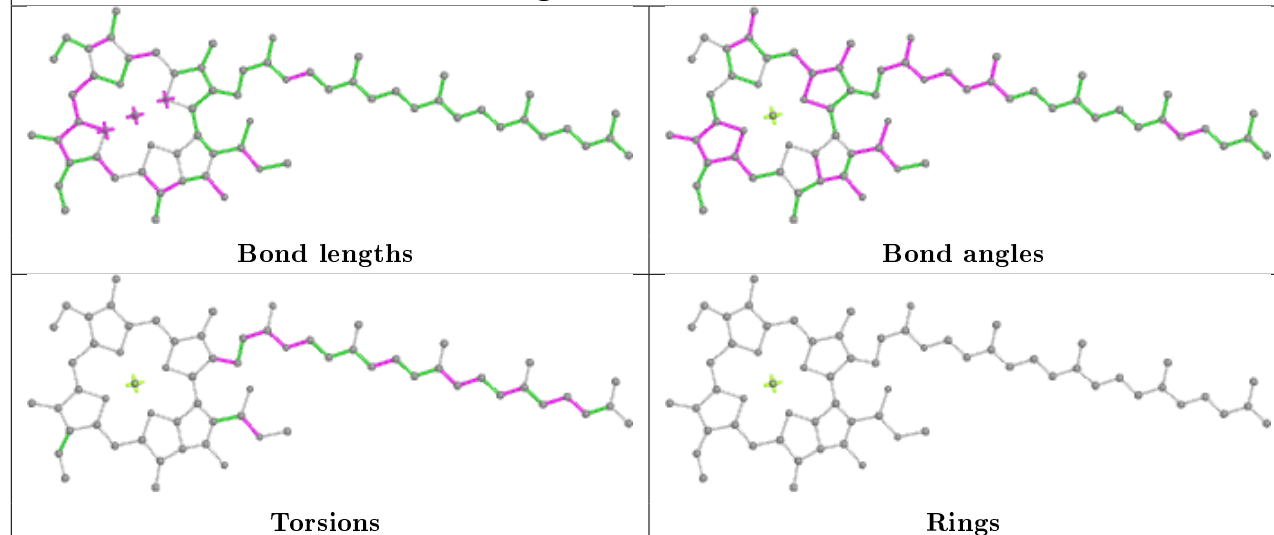
## Ligand BCR H 843



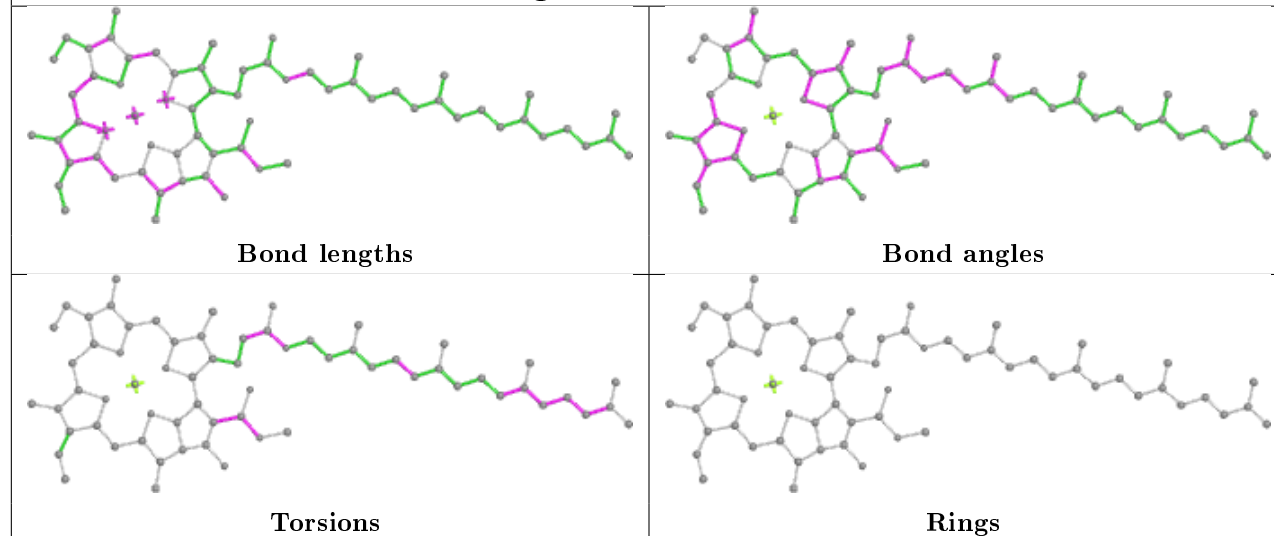
## Ligand CLA Y 806



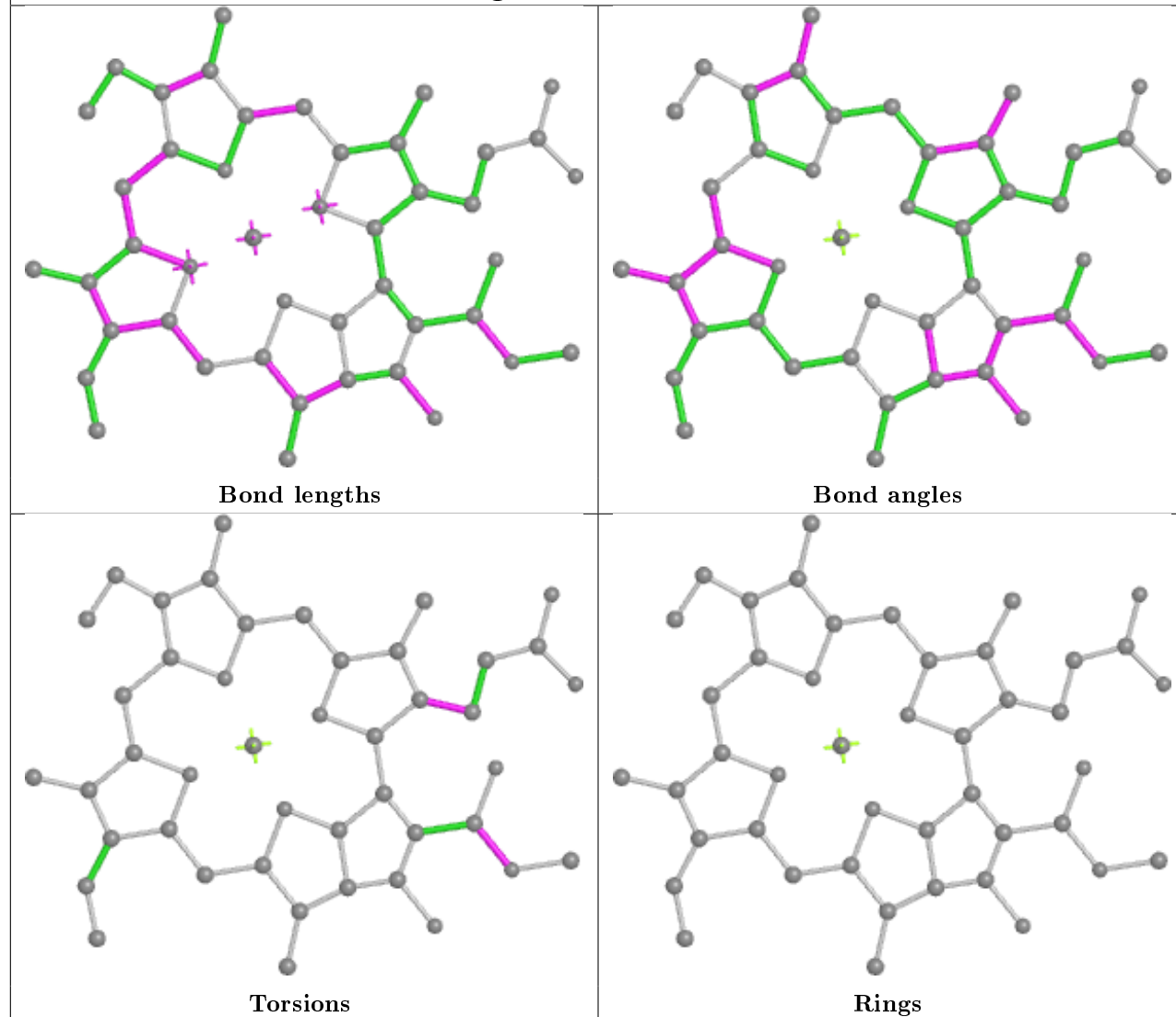
## Ligand CLA h 207



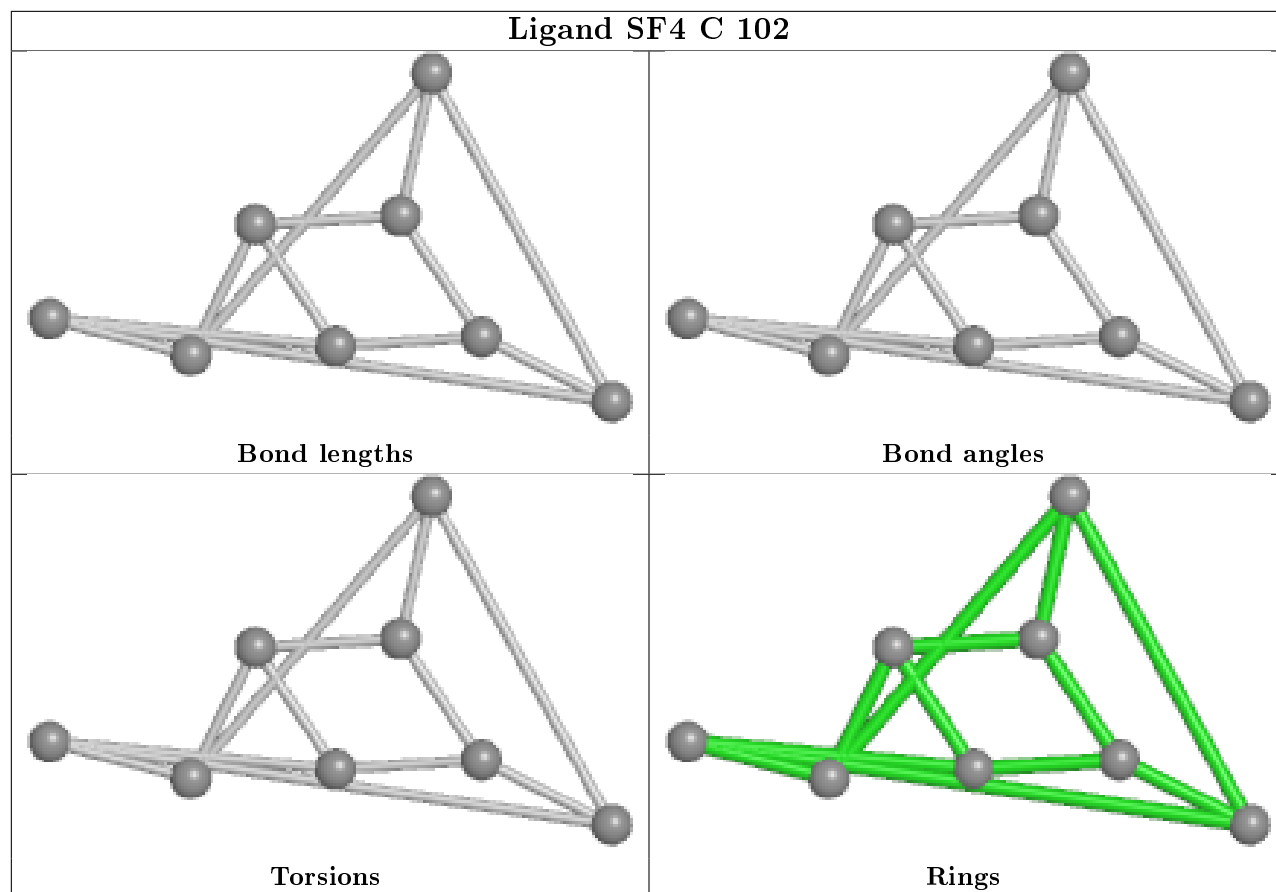
## Ligand CLA Y 829



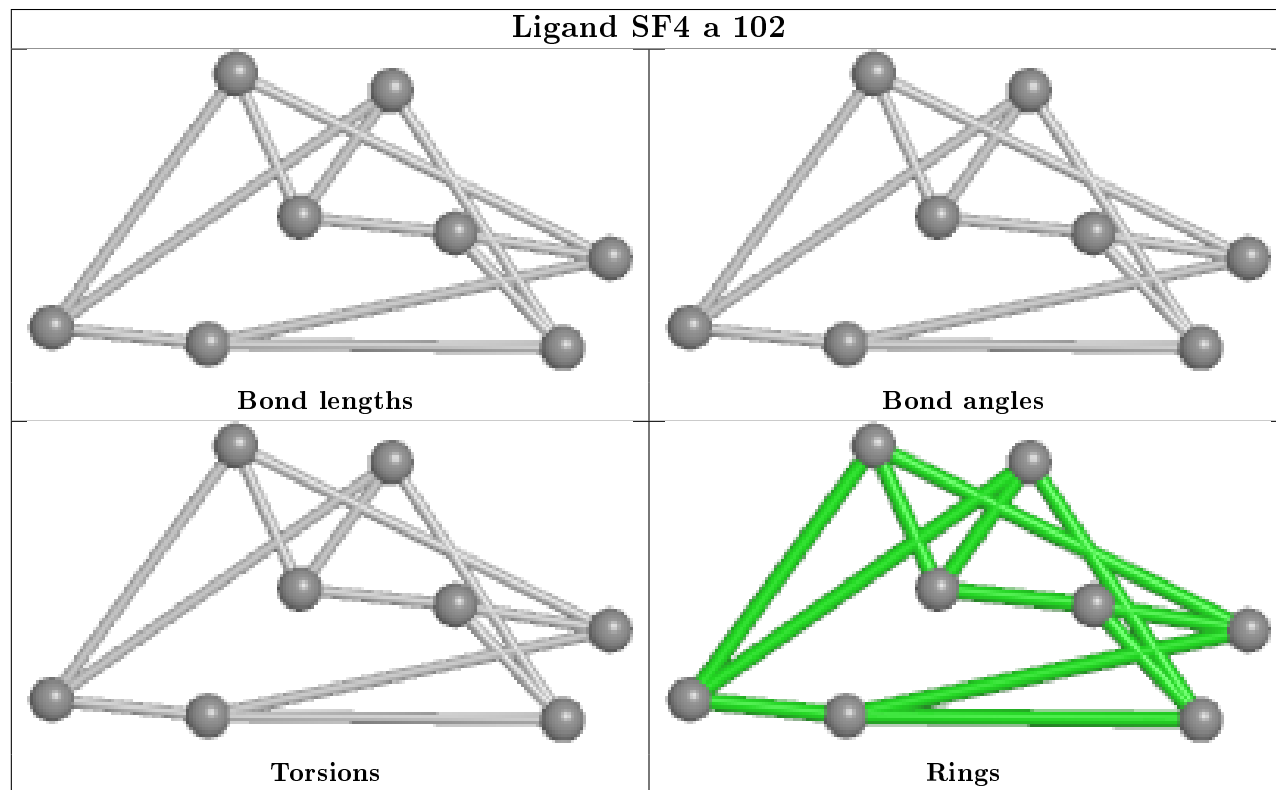
## Ligand CLA G 853



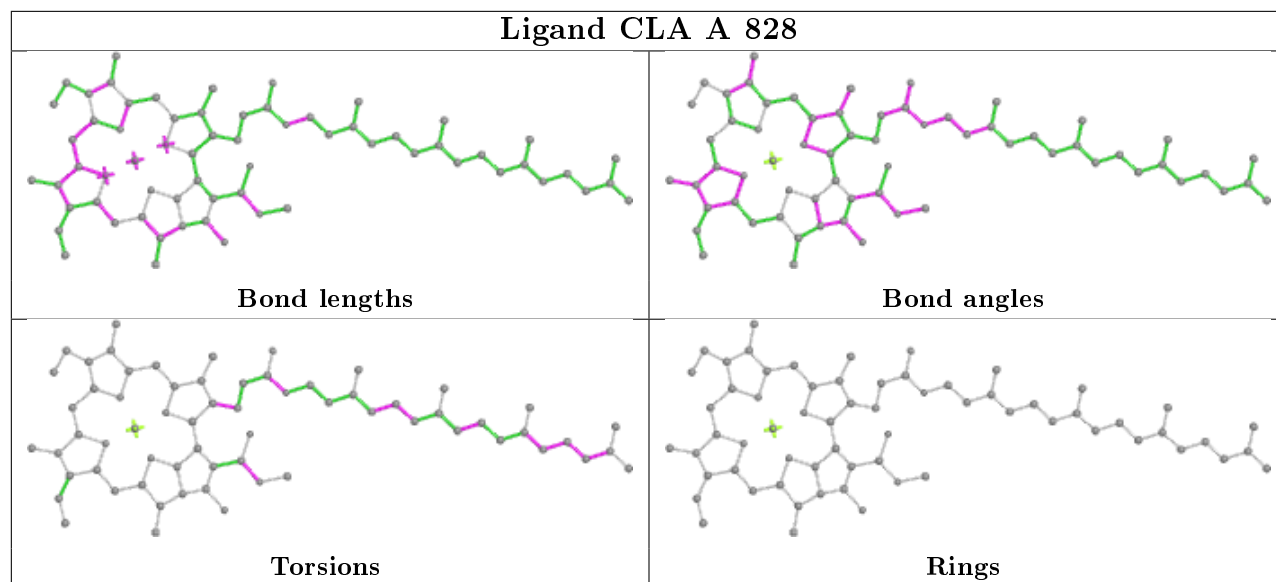
## Ligand SF4 C 102



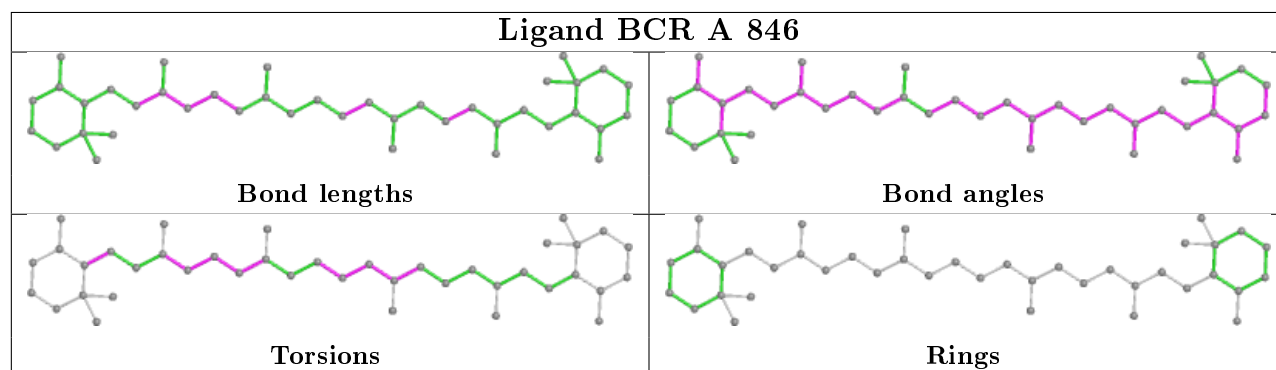
## Ligand SF4 a 102



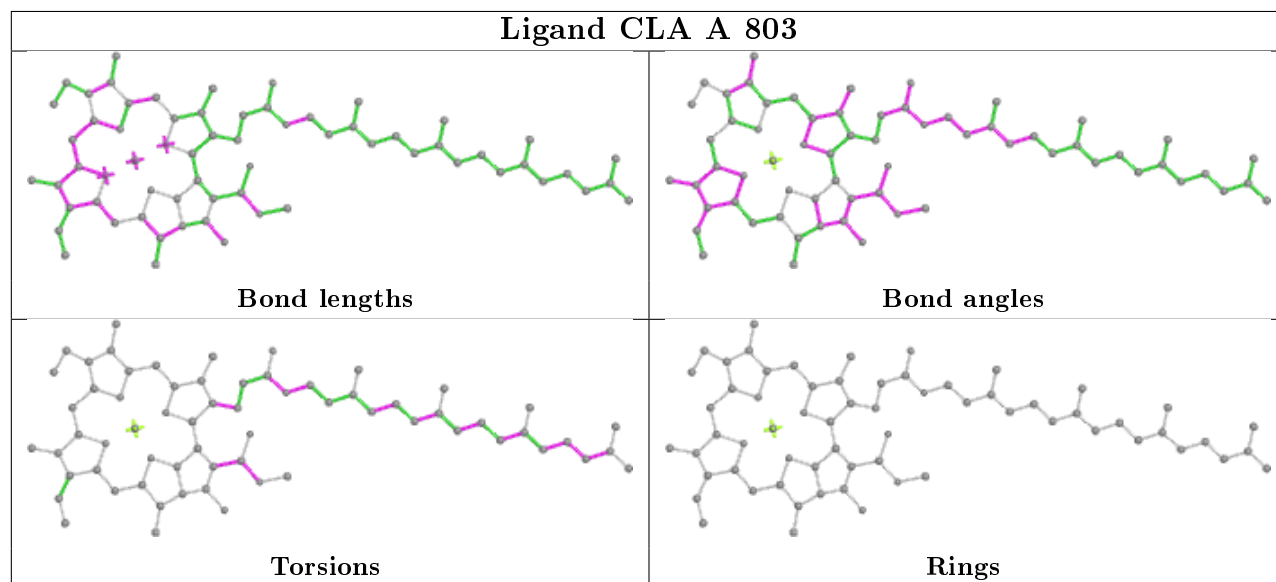
## Ligand CLA A 828



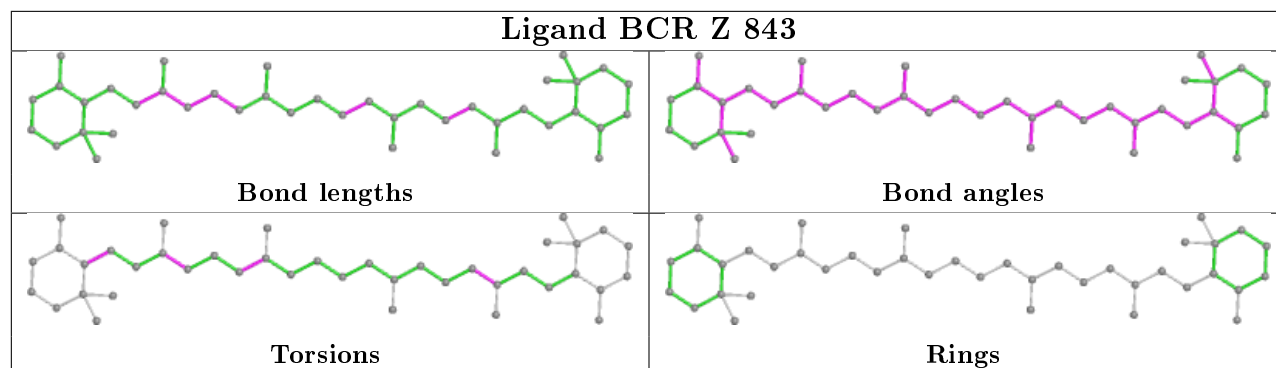
## Ligand BCR A 846



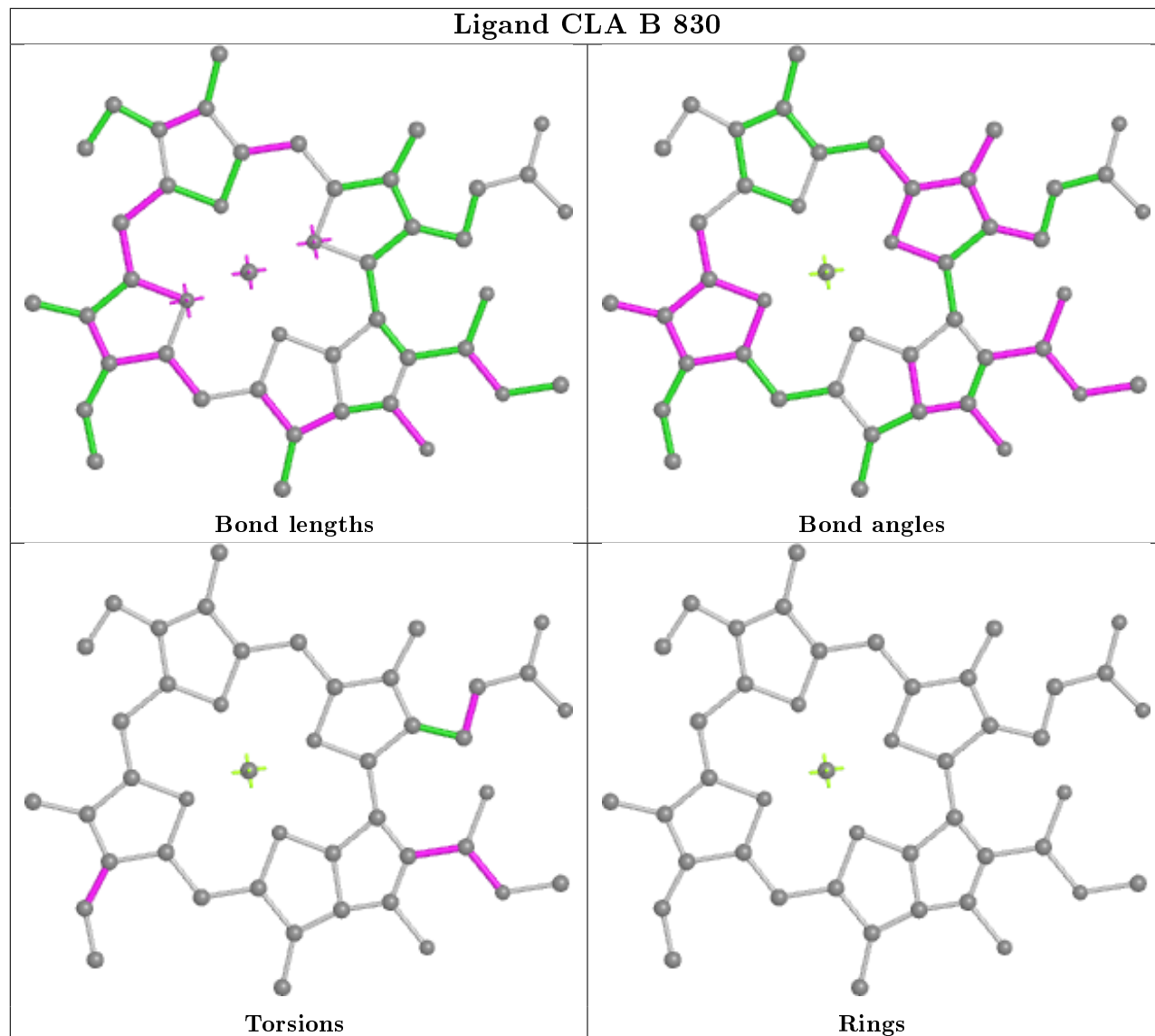
## Ligand CLA A 803



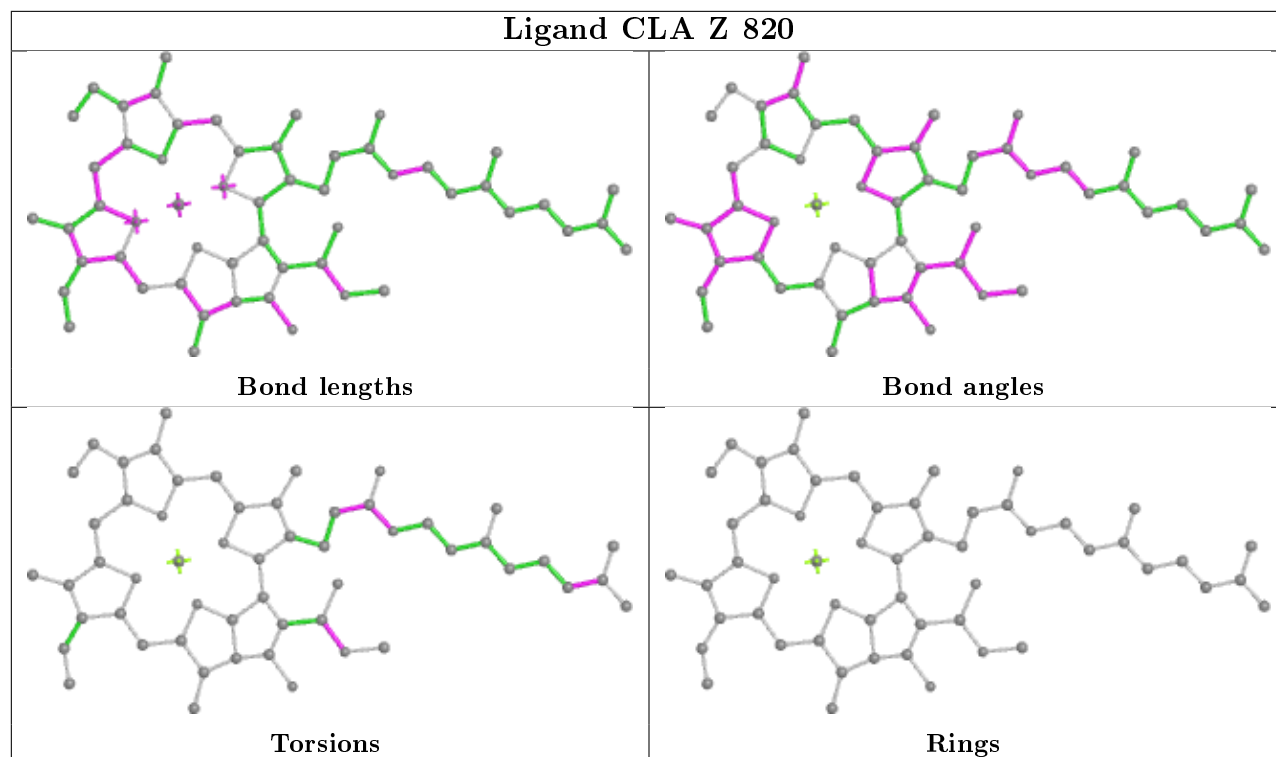
## Ligand BCR Z 843



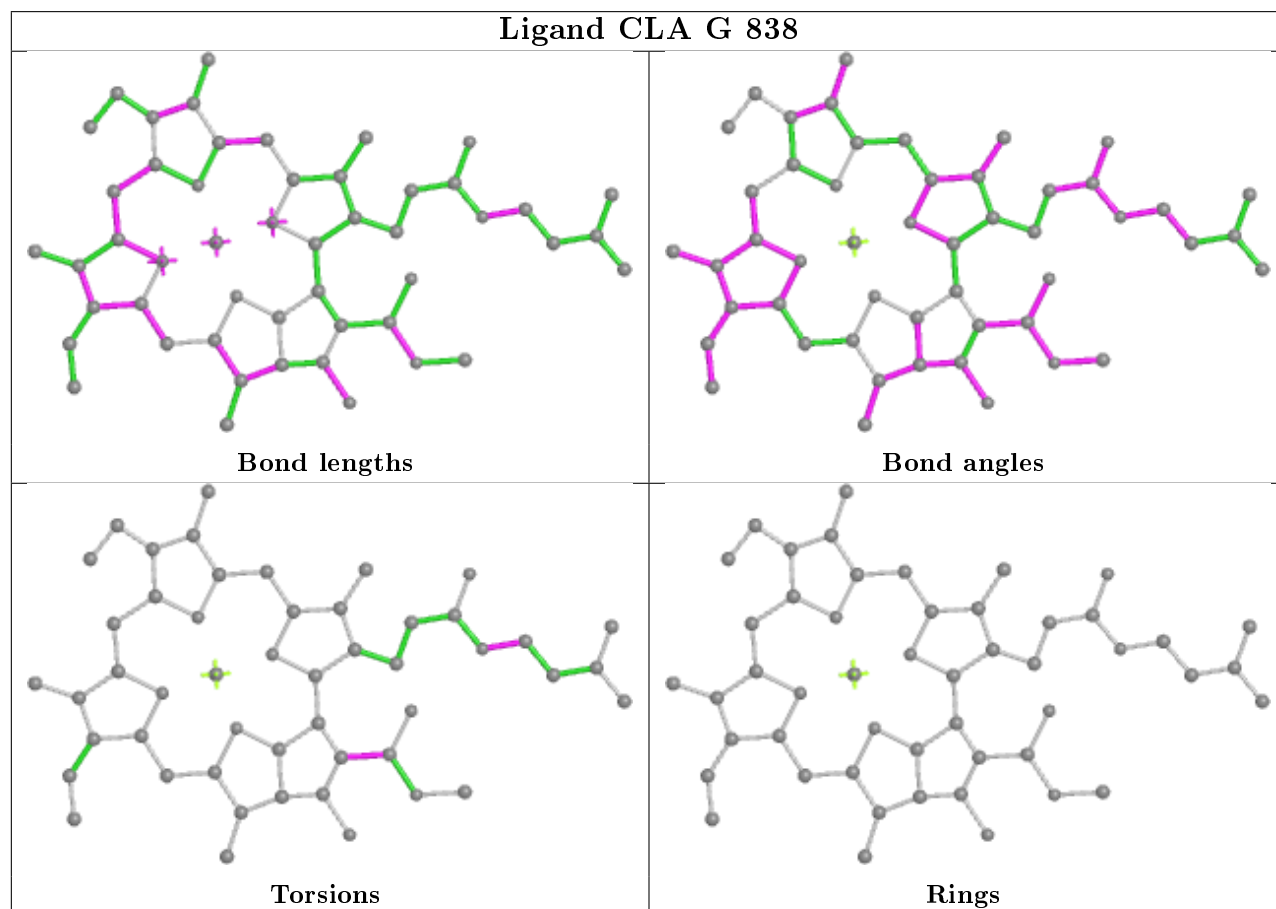
## Ligand CLA B 830



## Ligand CLA Z 820

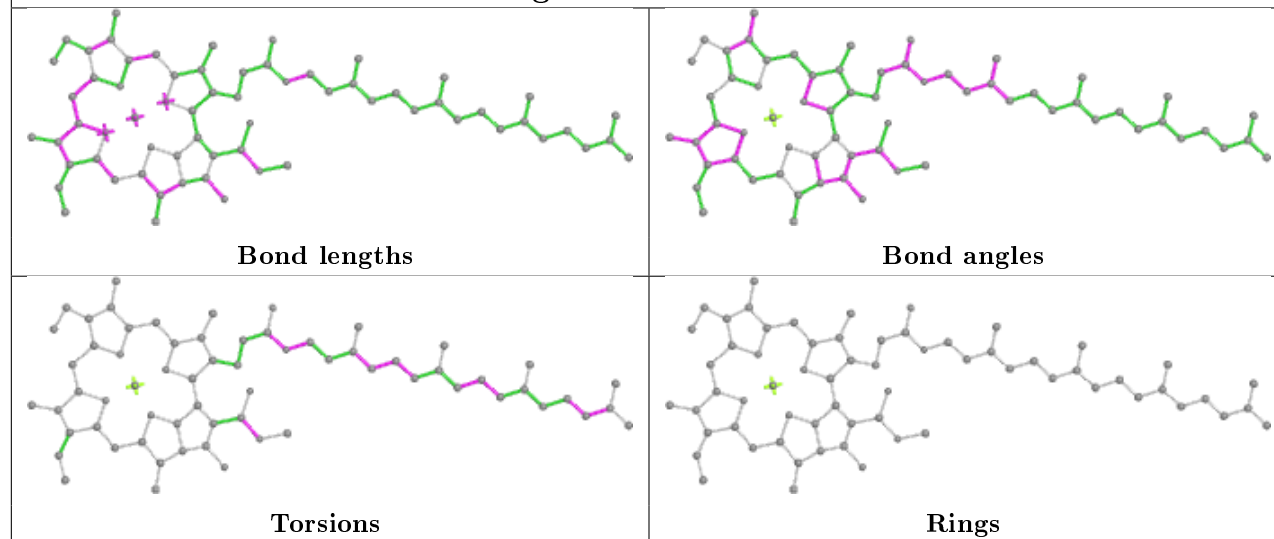


## Ligand CLA G 838

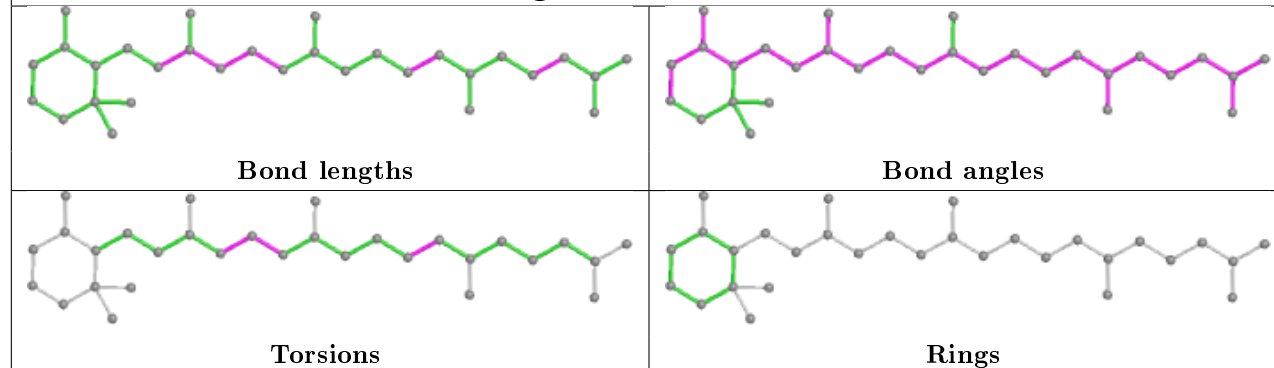




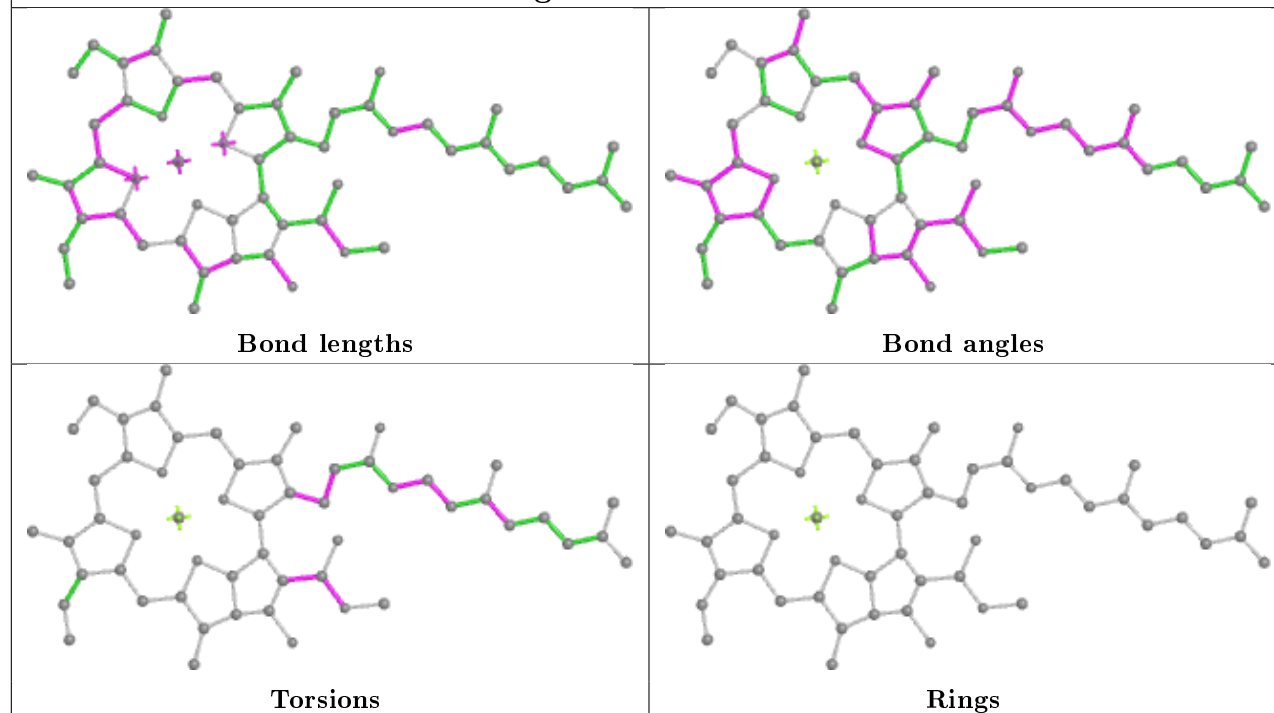
## Ligand CLA Y 841

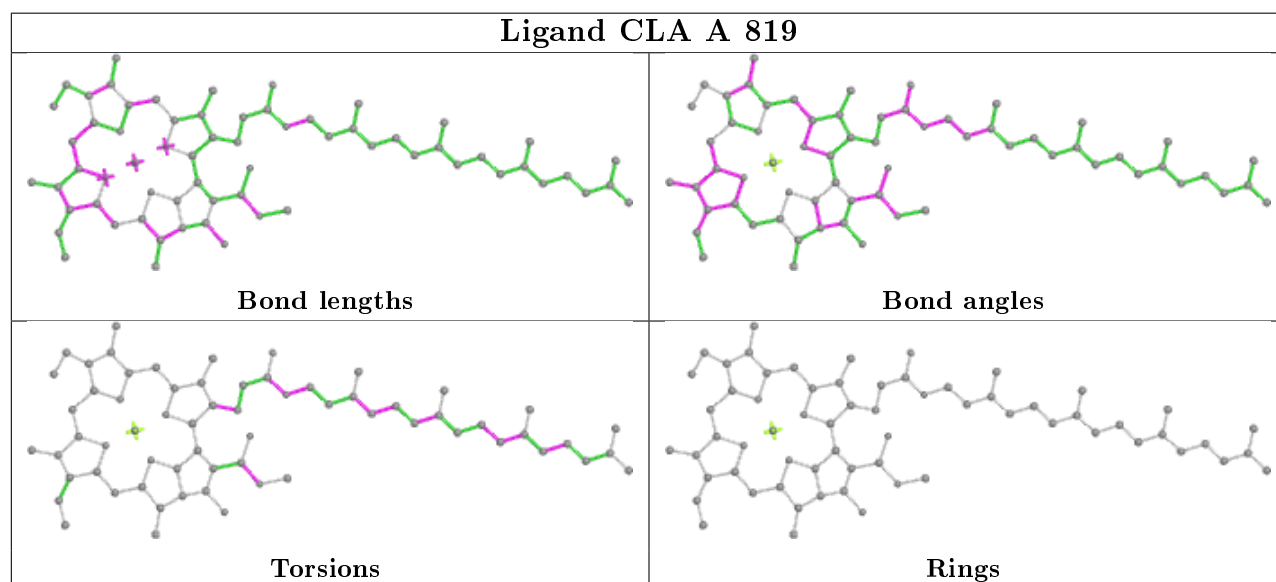
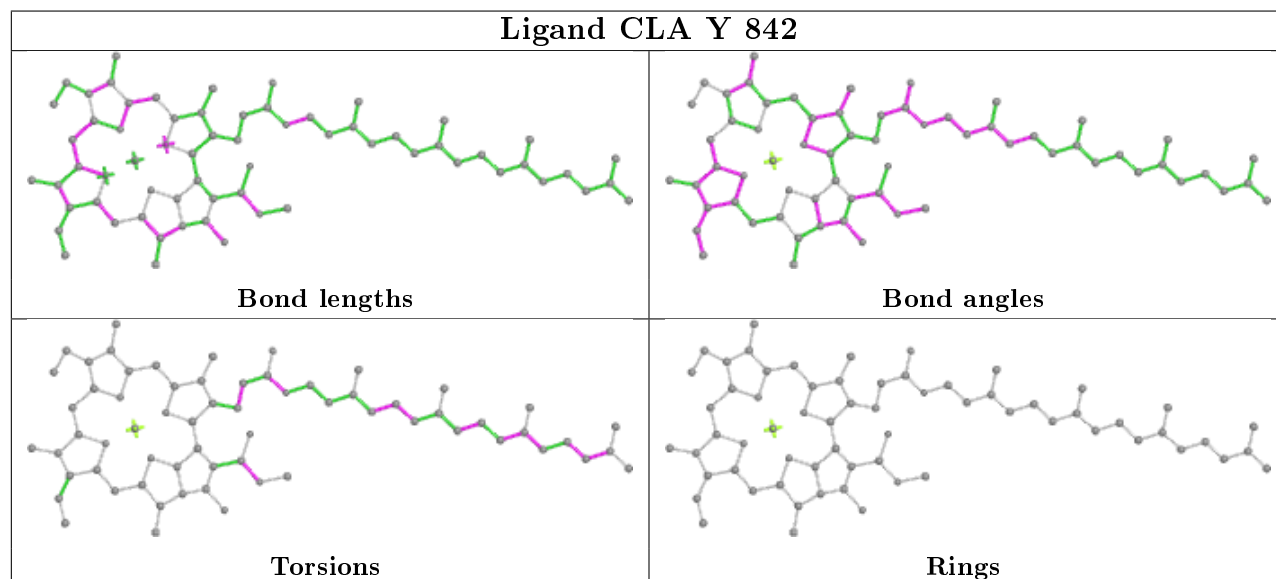
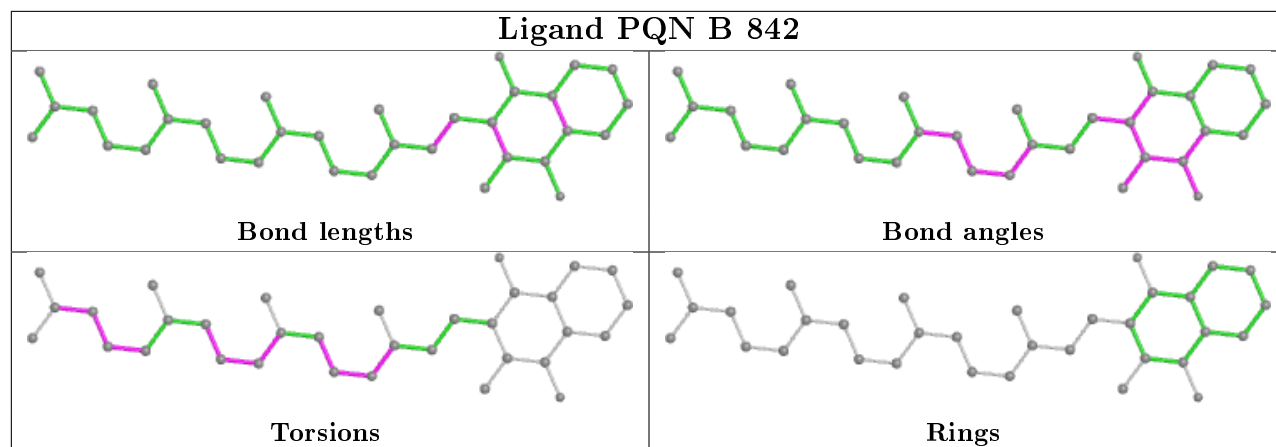


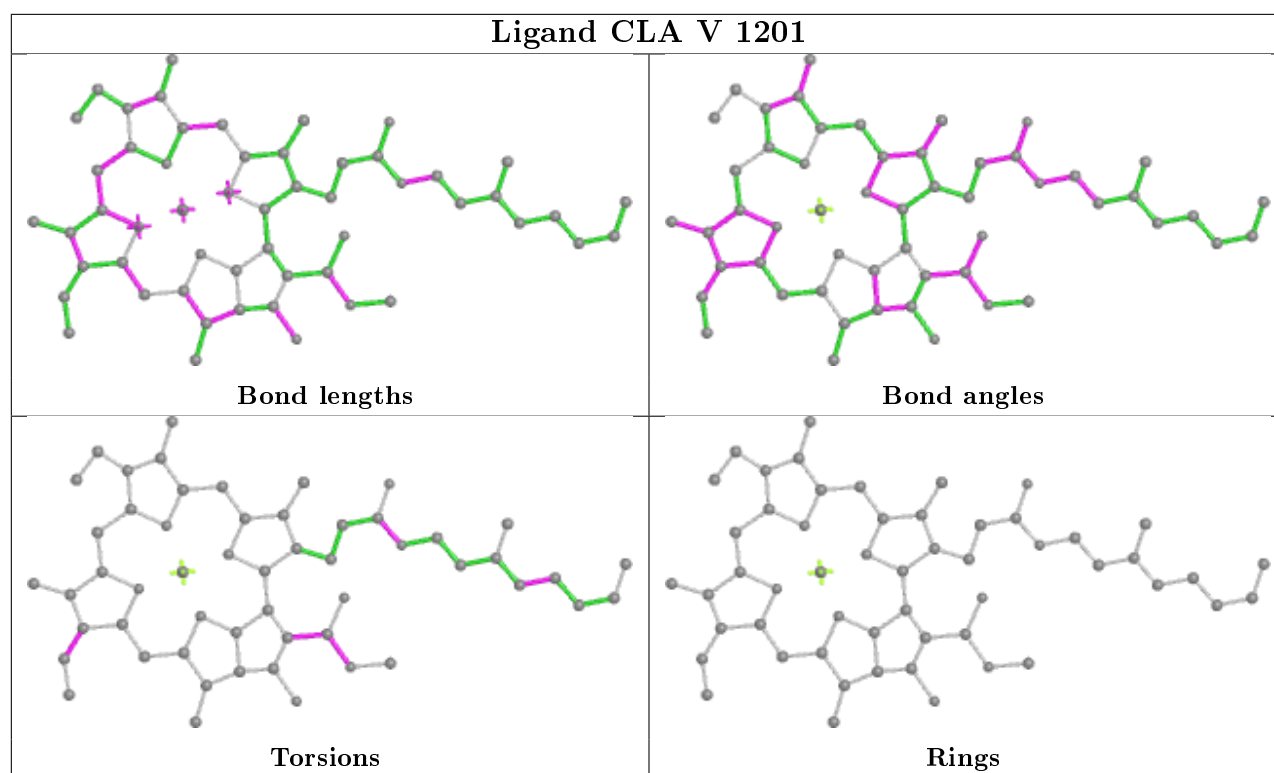
## Ligand BCR B 843



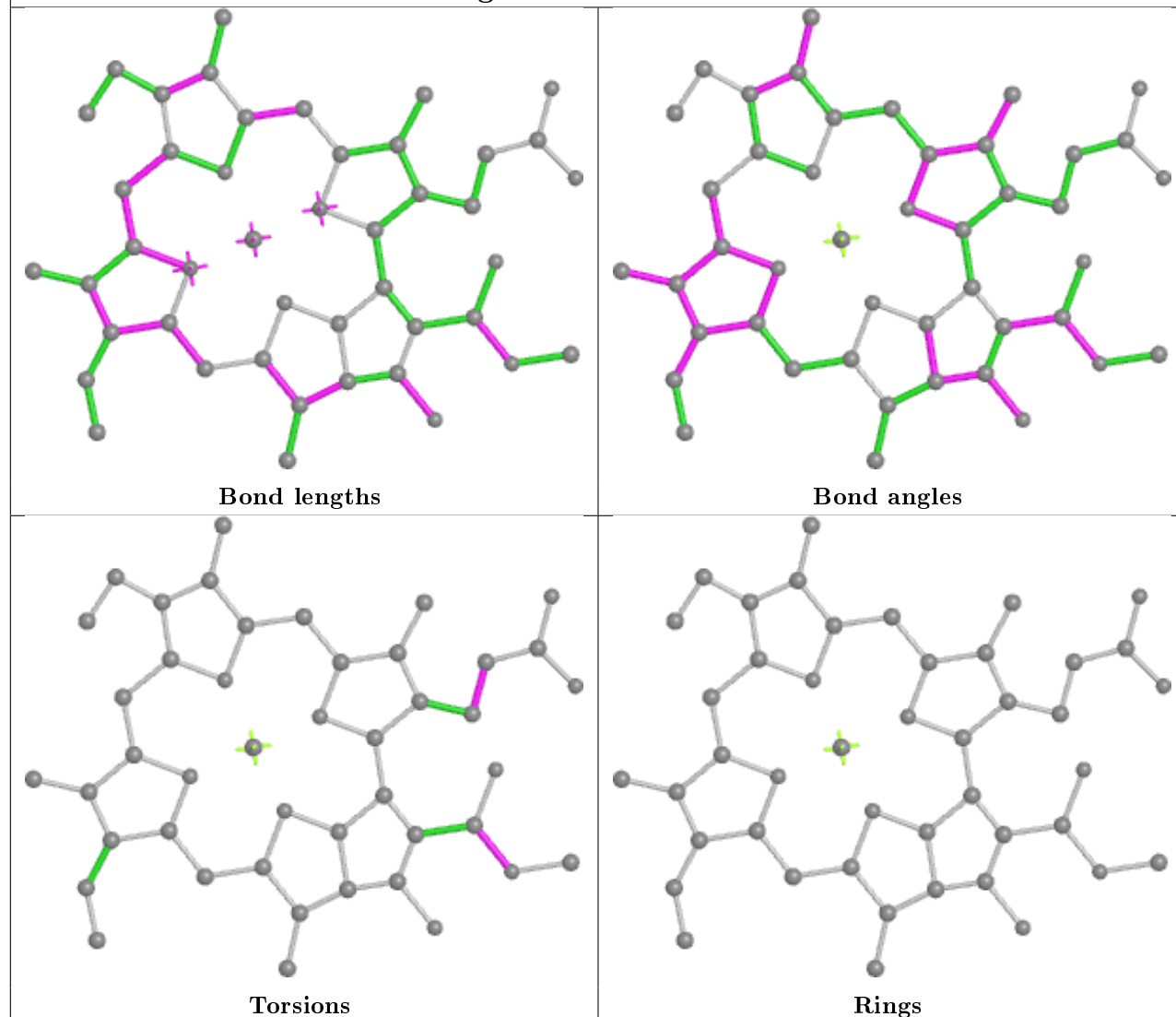
## Ligand CLA Z 822



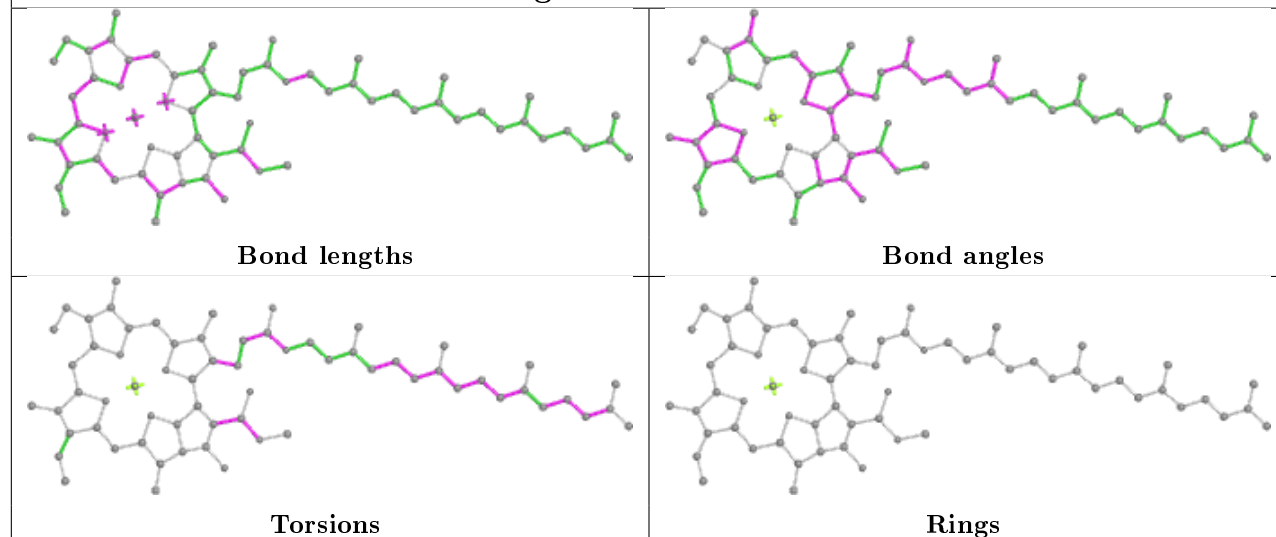




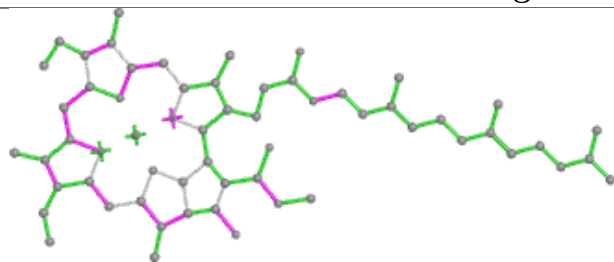
## Ligand CLA W 1701



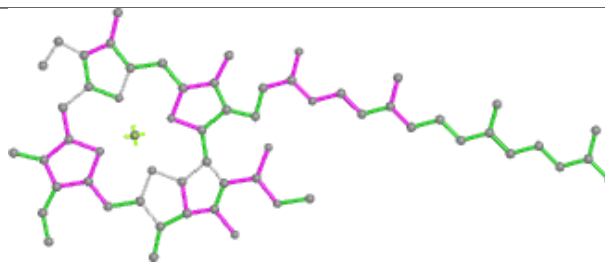
## Ligand CLA Z 802



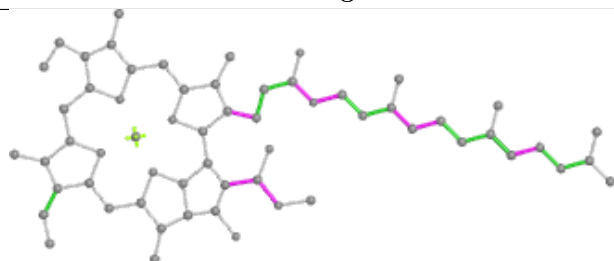
## Ligand CLA H 834



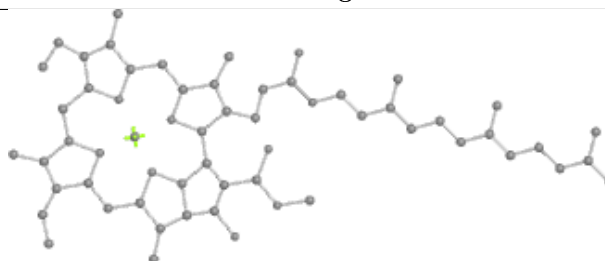
Bond lengths



Bond angles

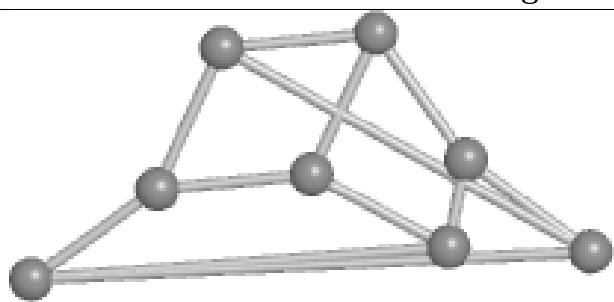


Torsions

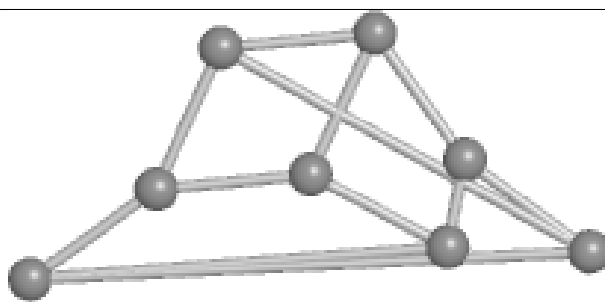


Rings

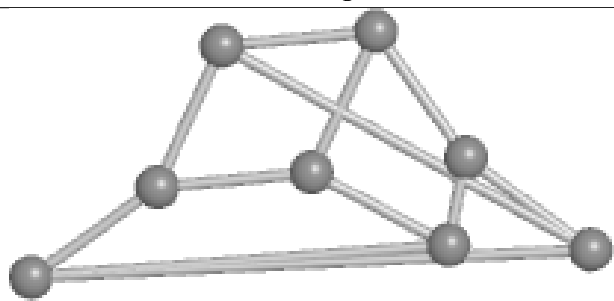
## Ligand SF4 A 844



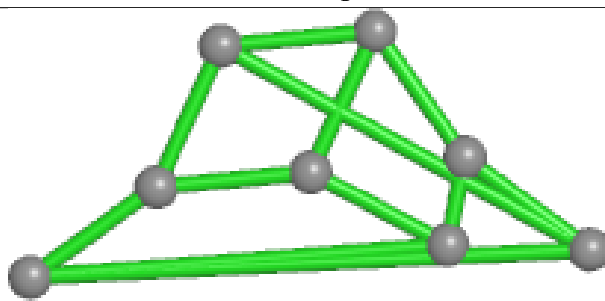
Bond lengths



Bond angles

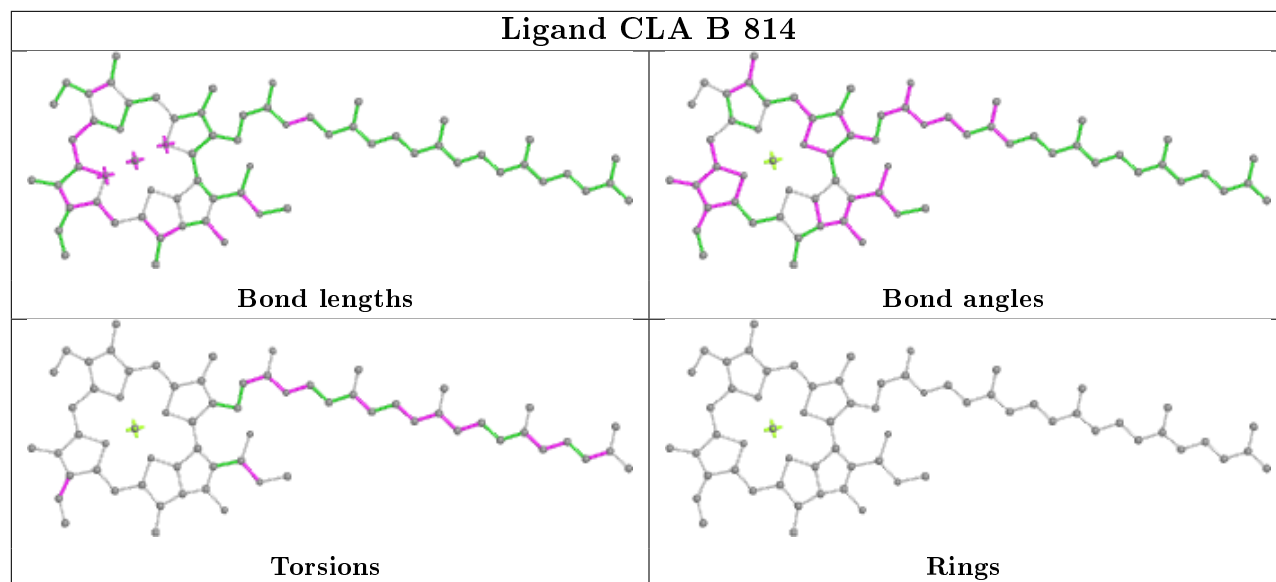


Torsions

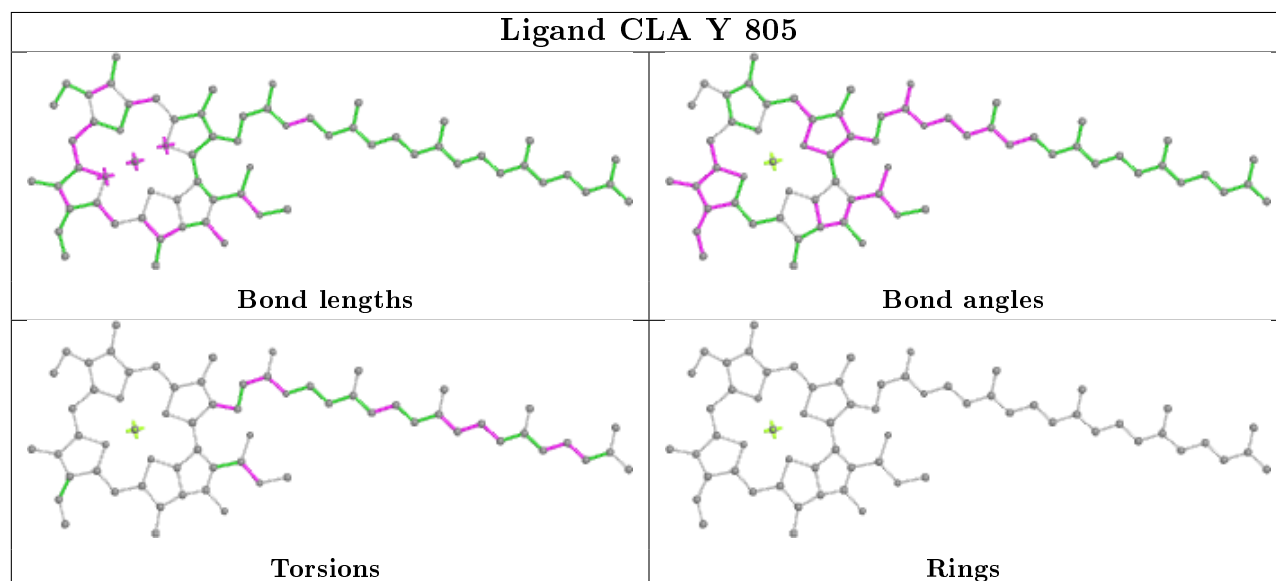


Rings

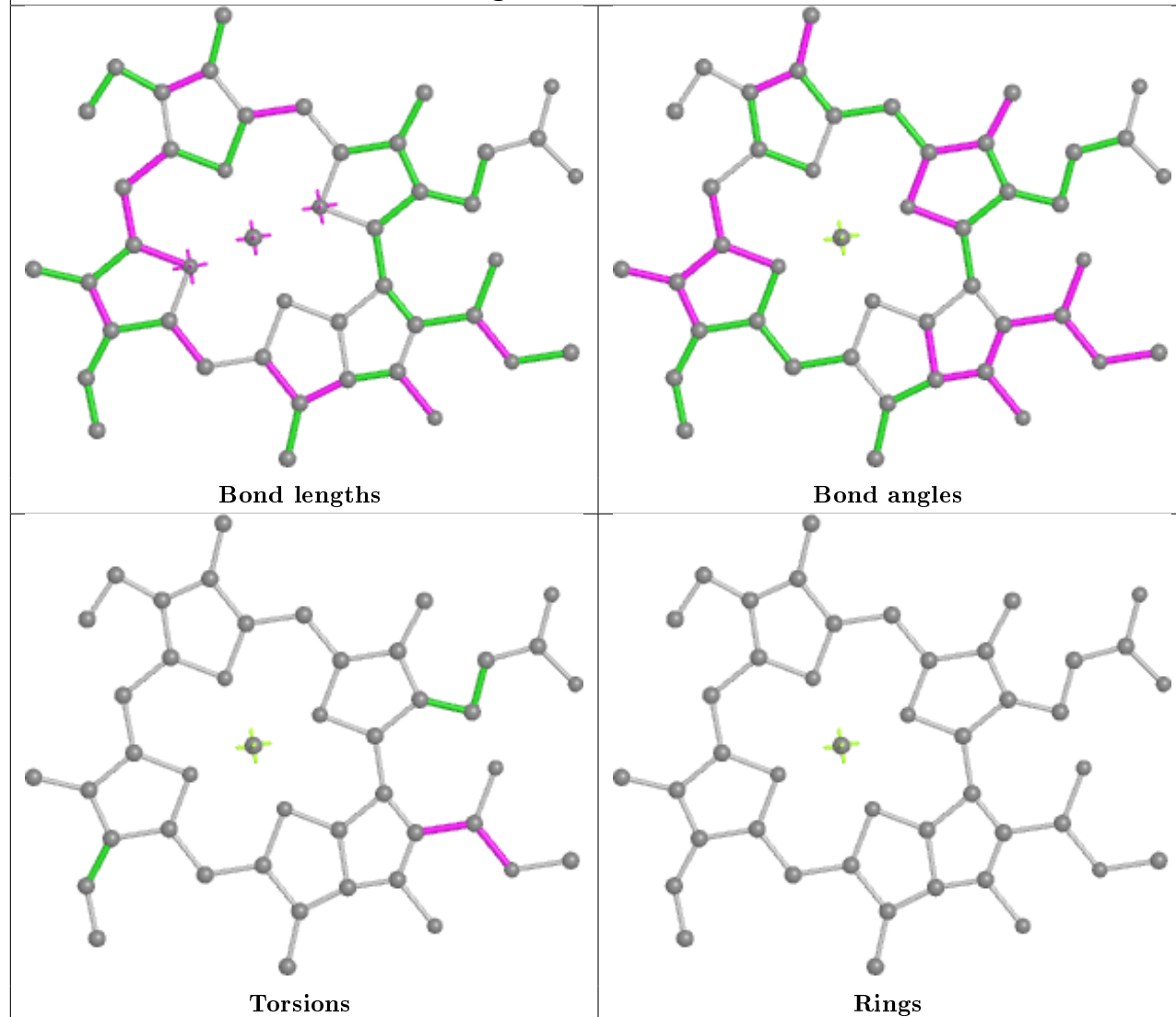
## Ligand CLA B 814



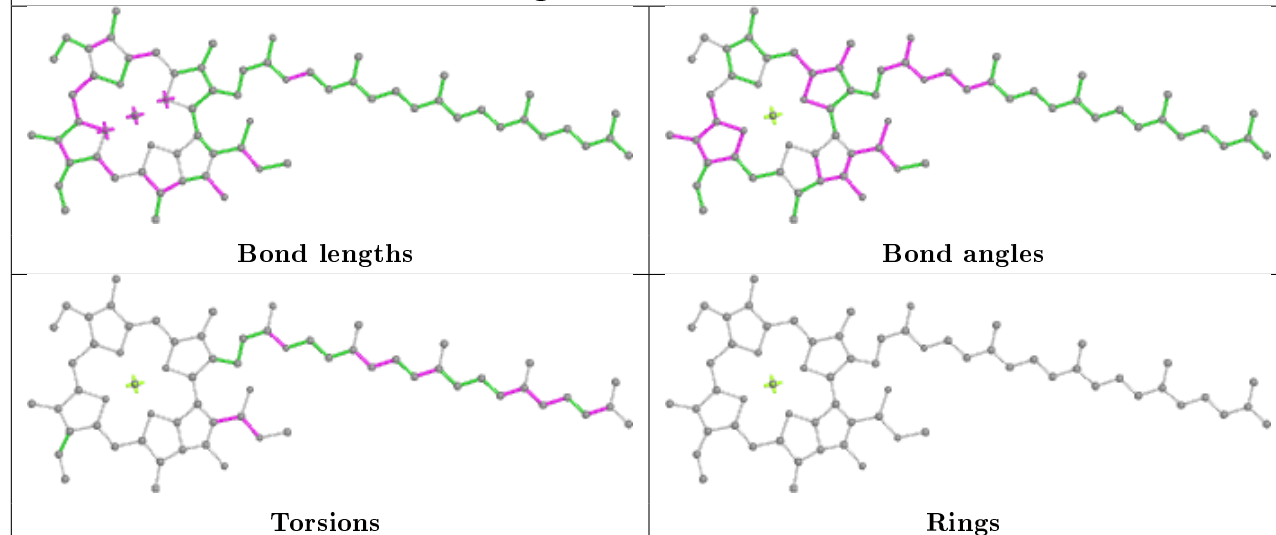
## Ligand CLA Y 805

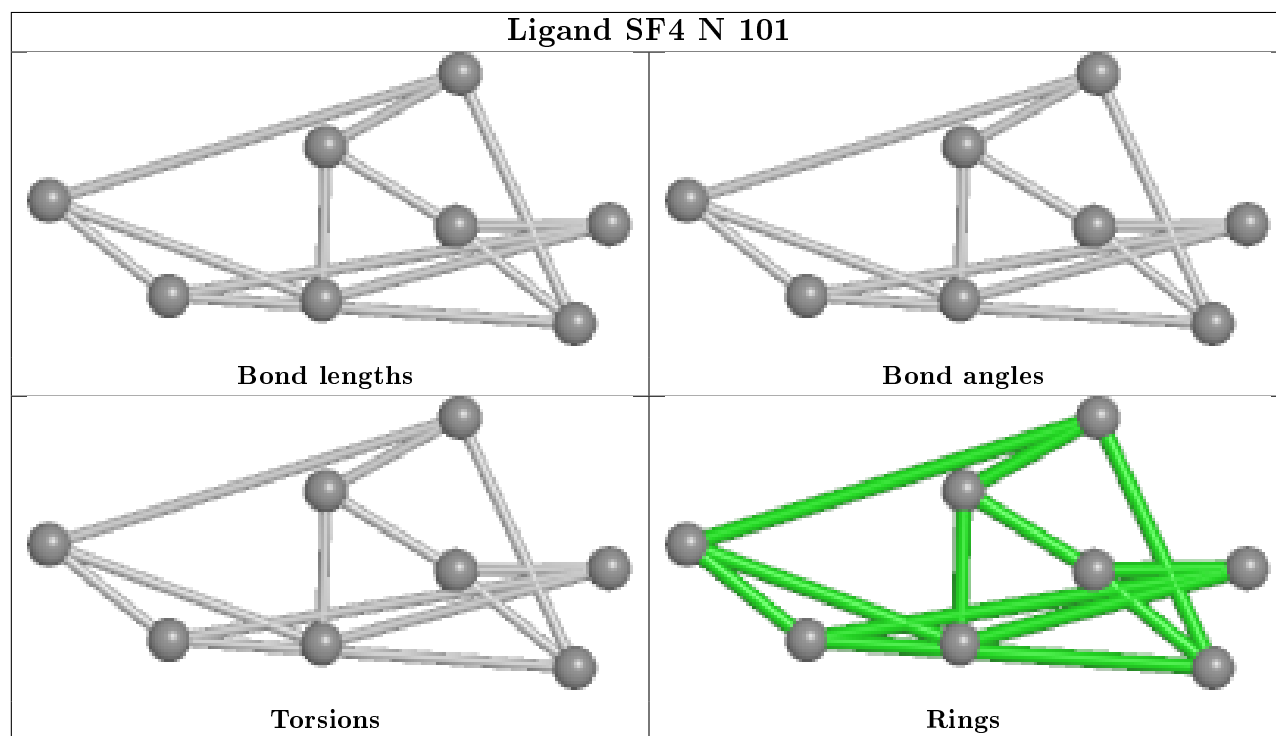
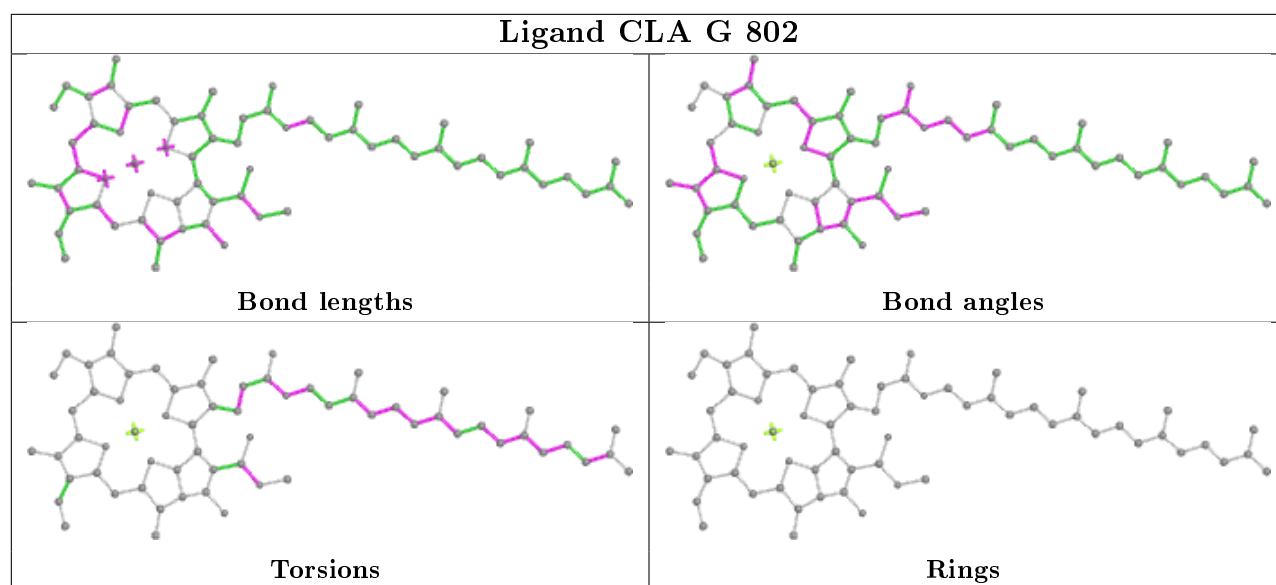


## Ligand CLA Q 203



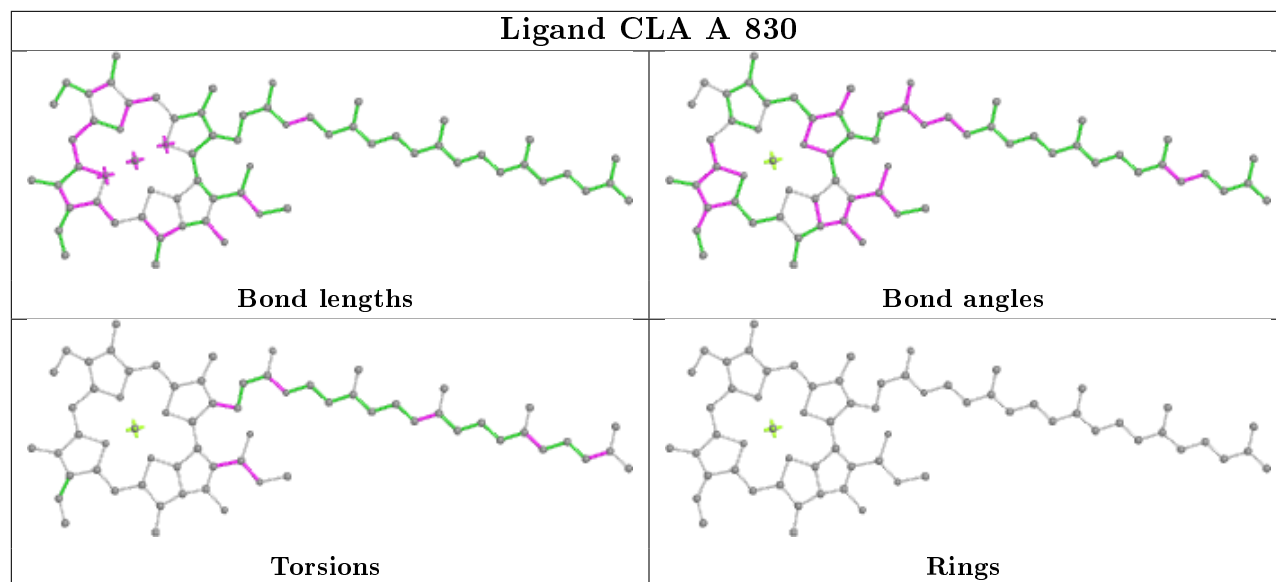
## Ligand CLA Y 854



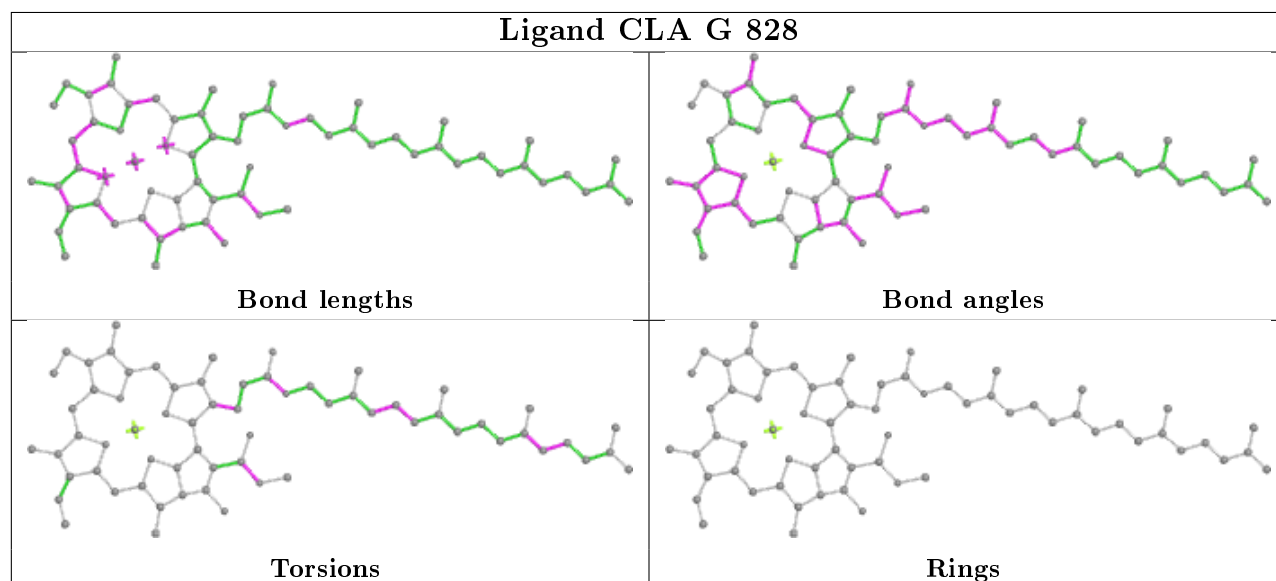




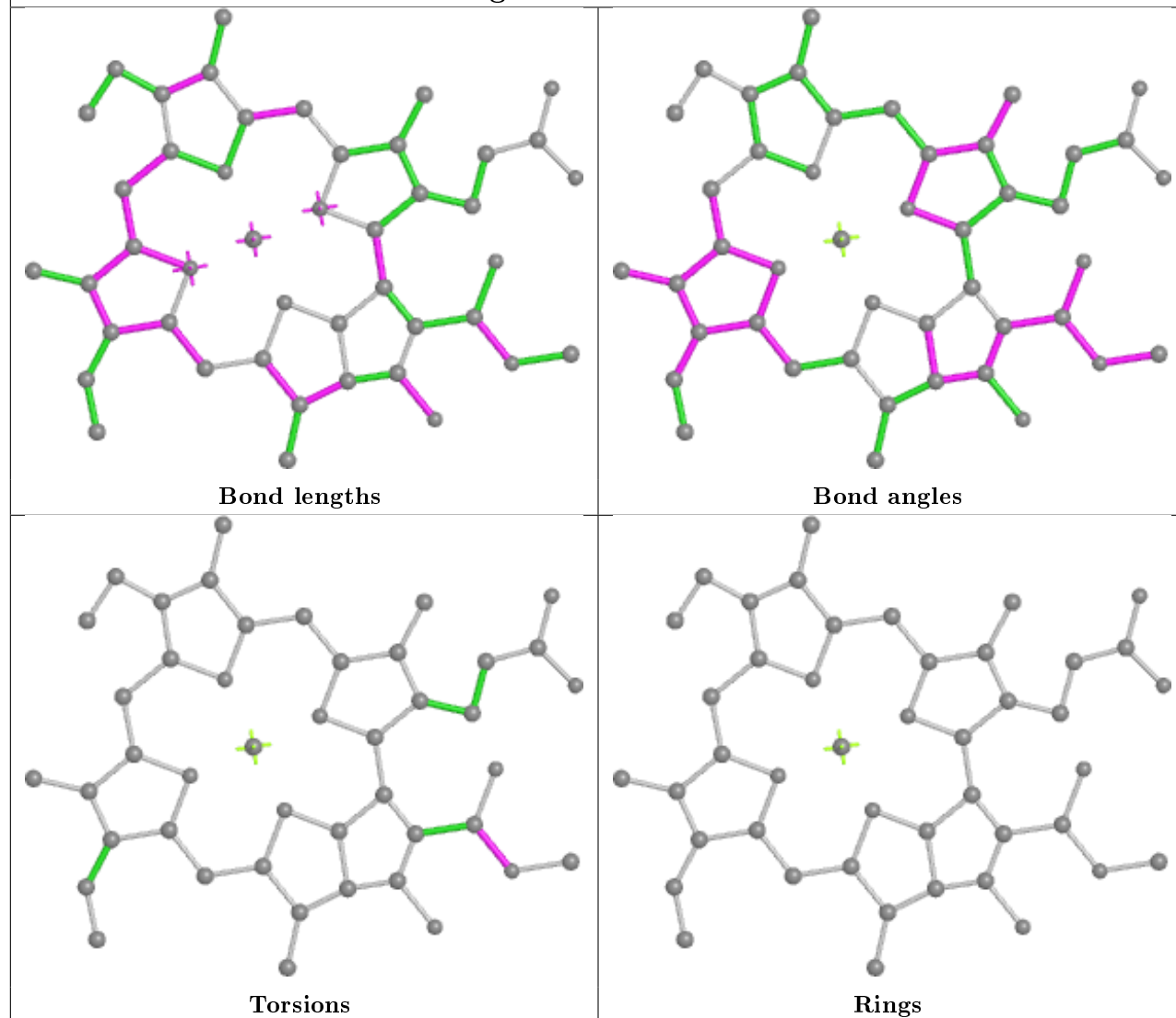
## Ligand CLA A 830



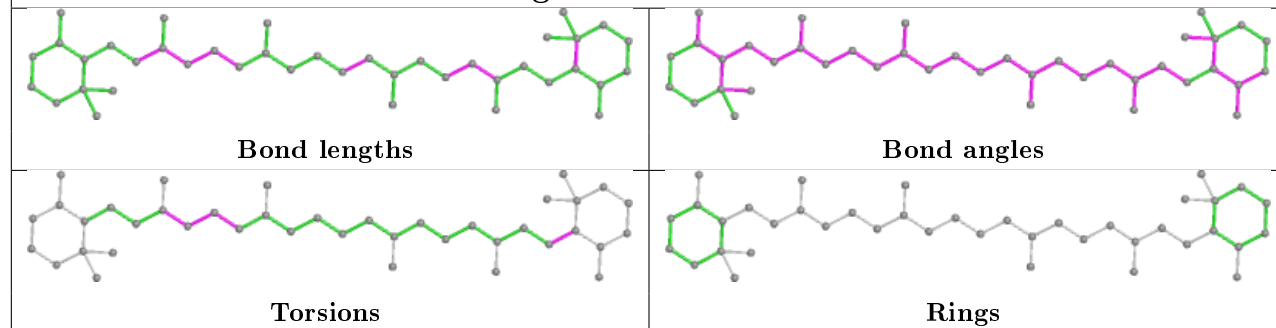
## Ligand CLA G 828



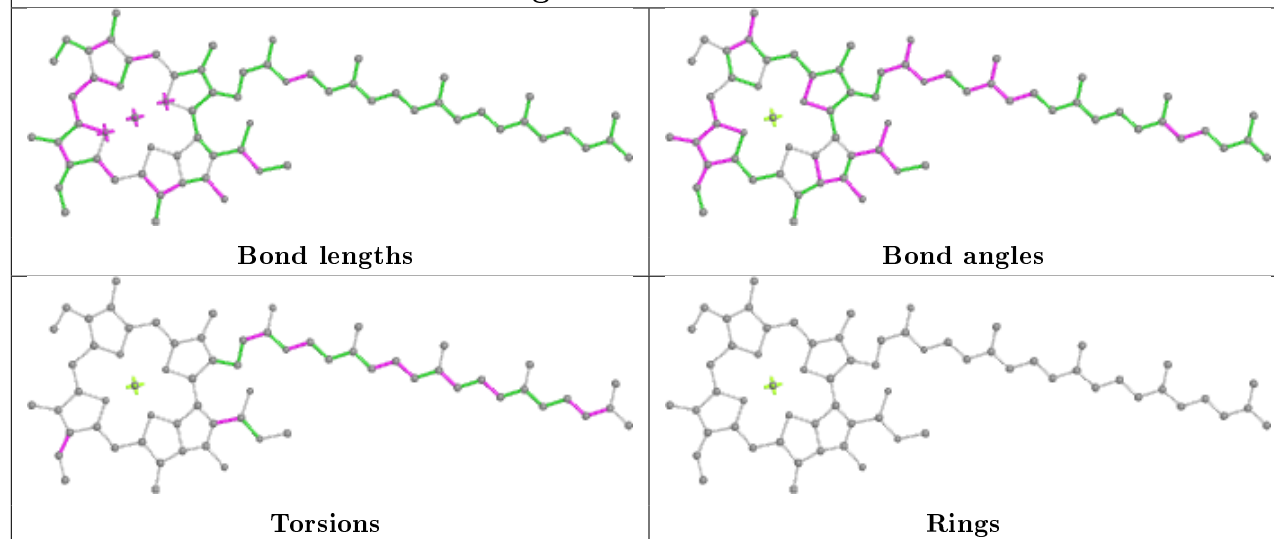
## Ligand CLA H 836



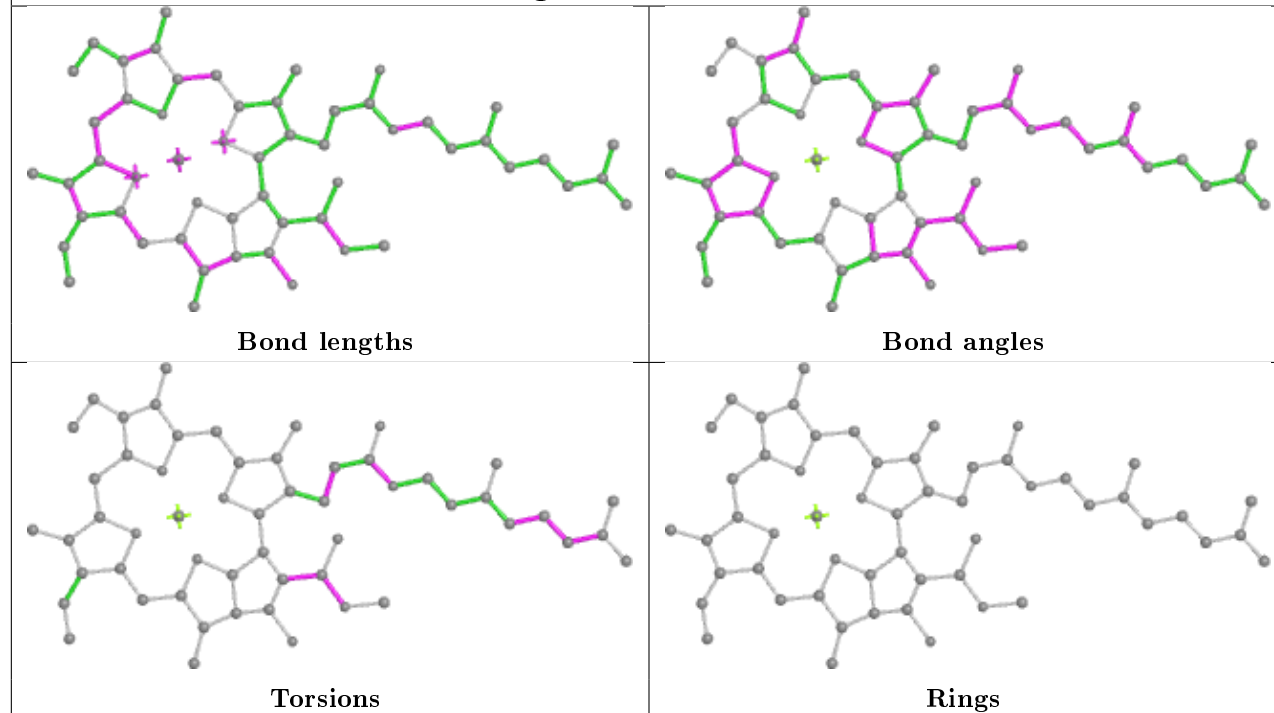
## Ligand BCR Z 842



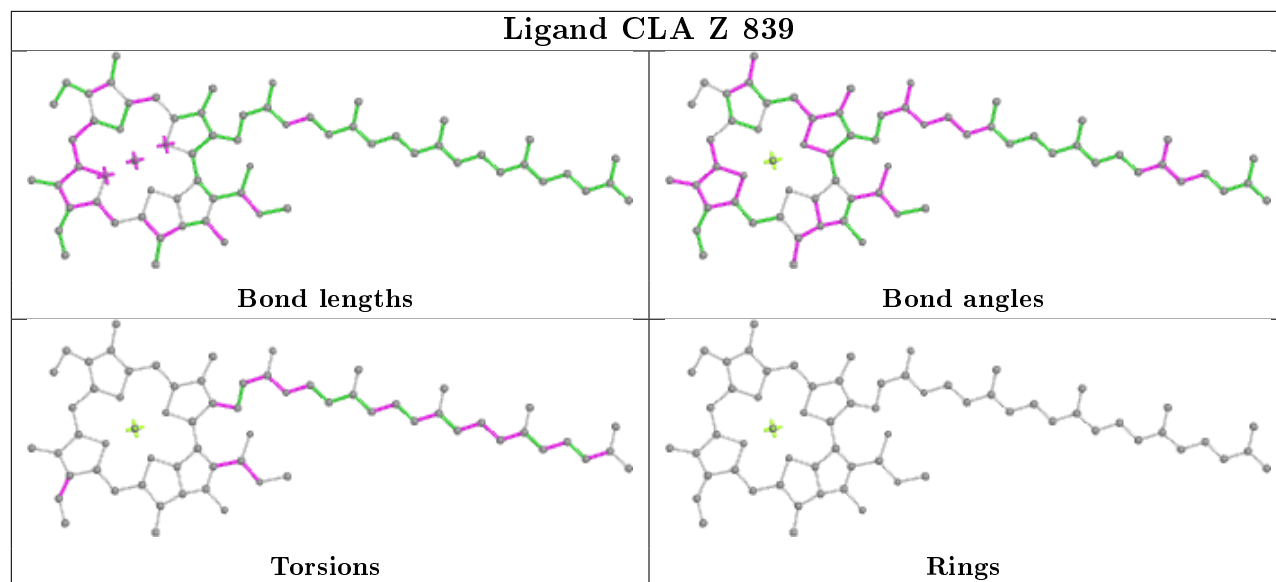
## Ligand CLA B 808



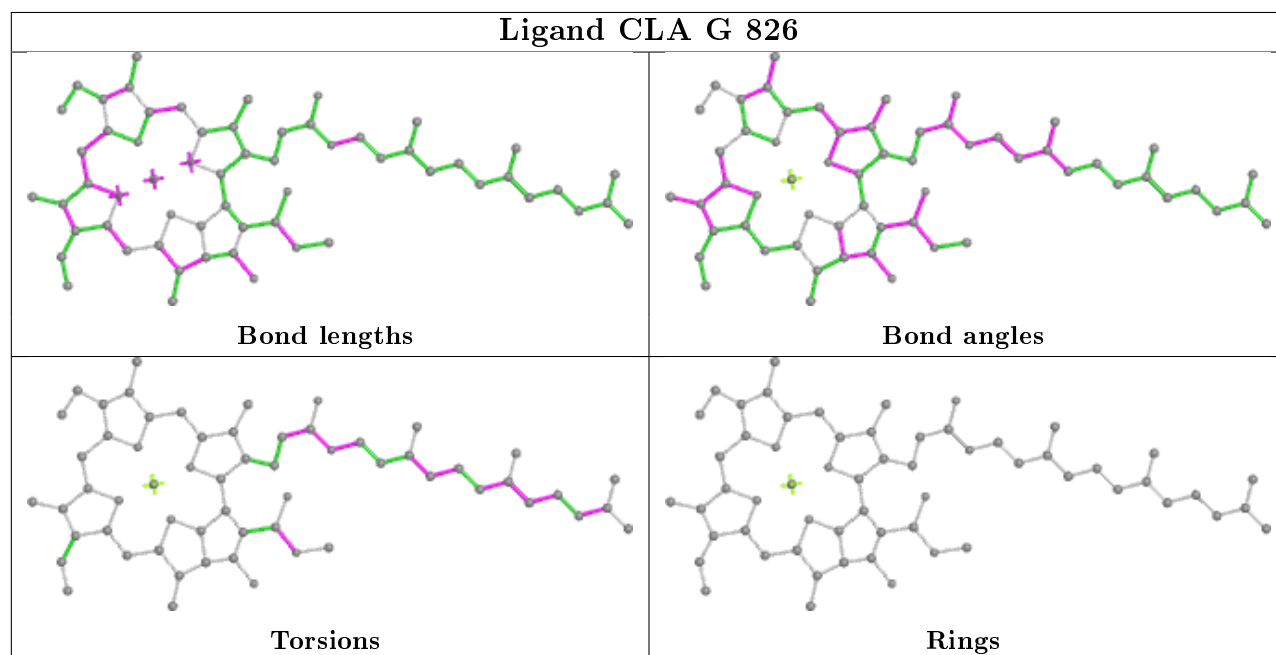
## Ligand CLA B 816



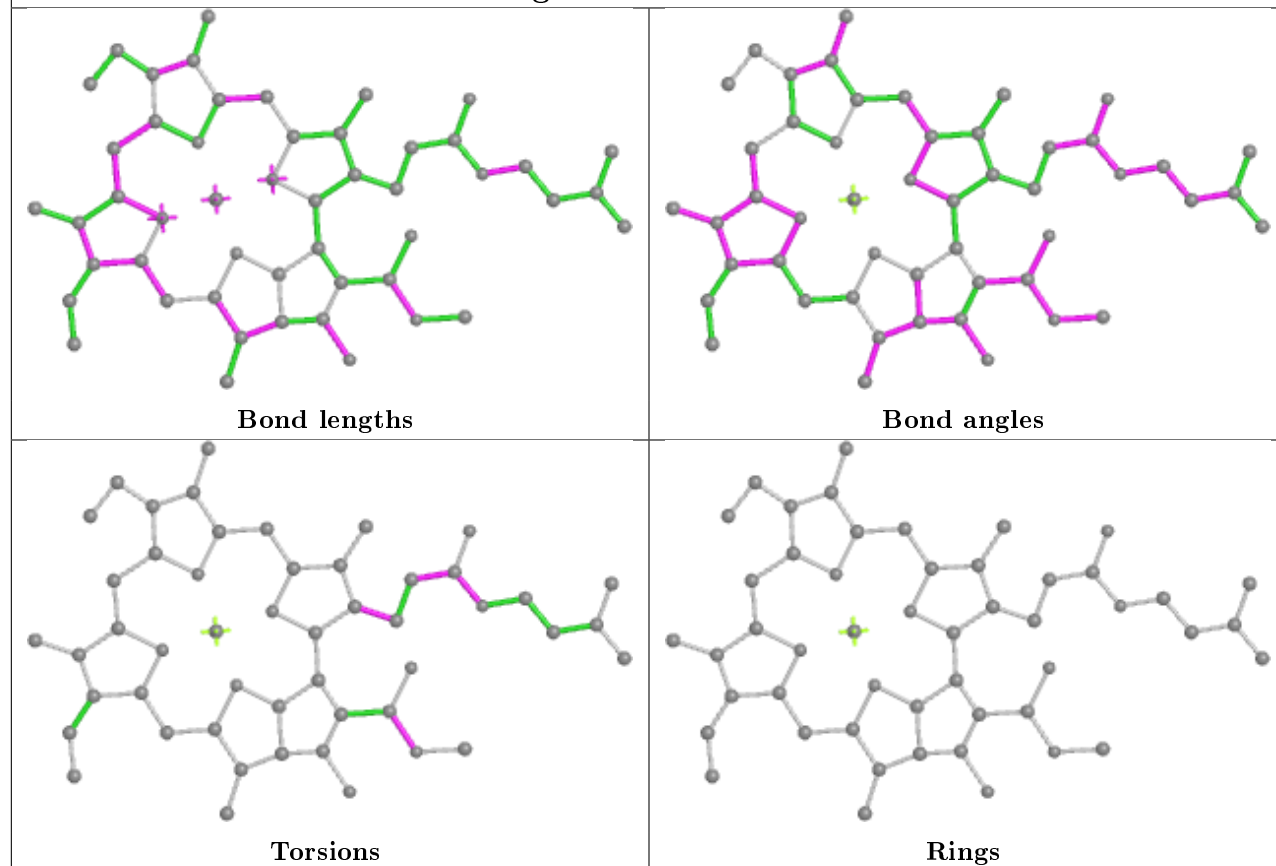
## Ligand CLA Z 839



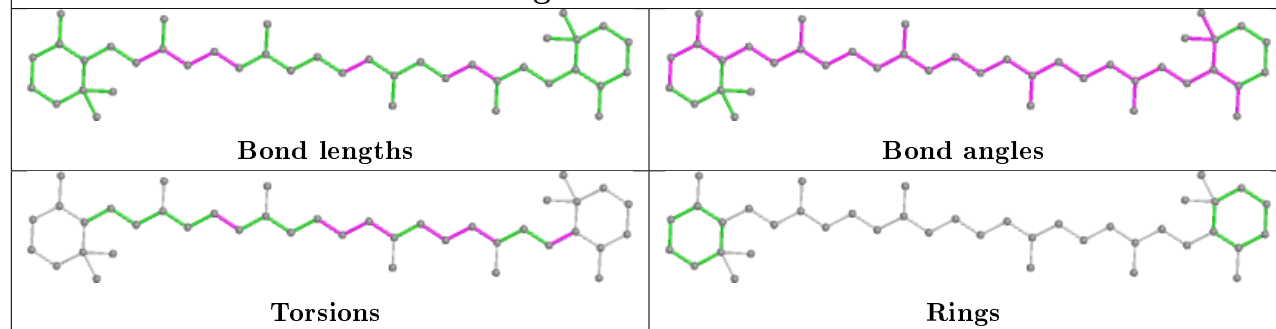
## Ligand CLA G 826



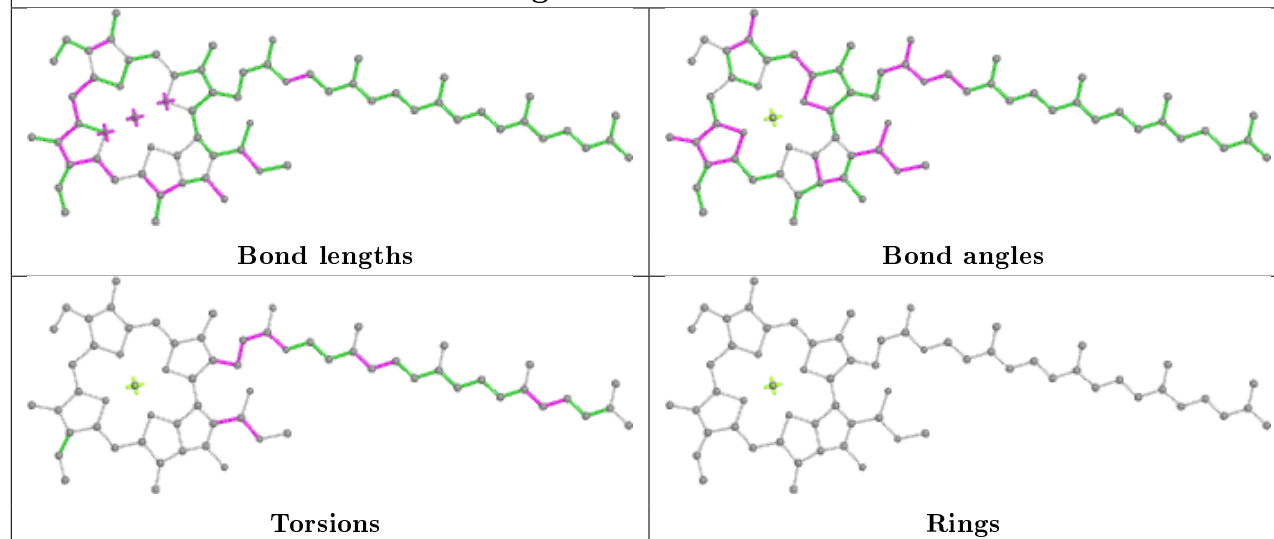
## Ligand CLA A 823



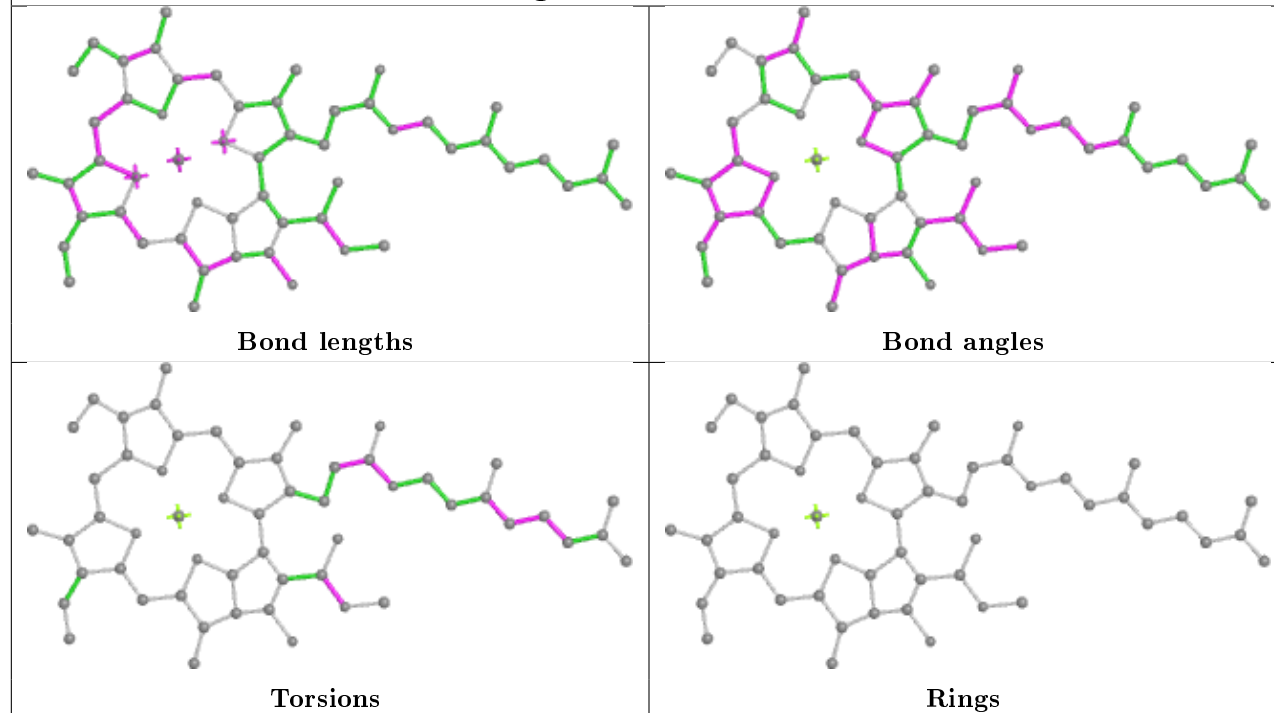
## Ligand BCR h 203

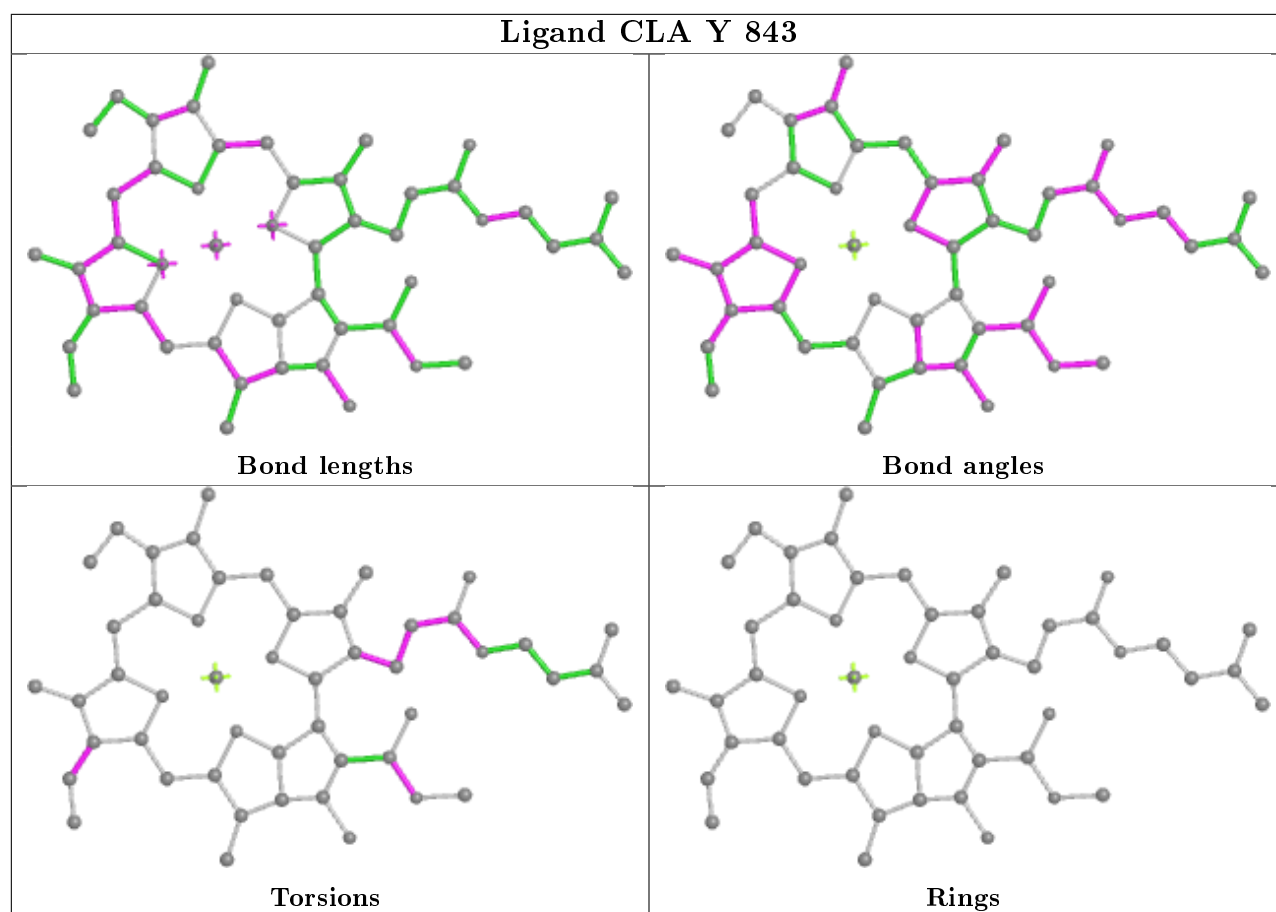


## Ligand CLA G 821

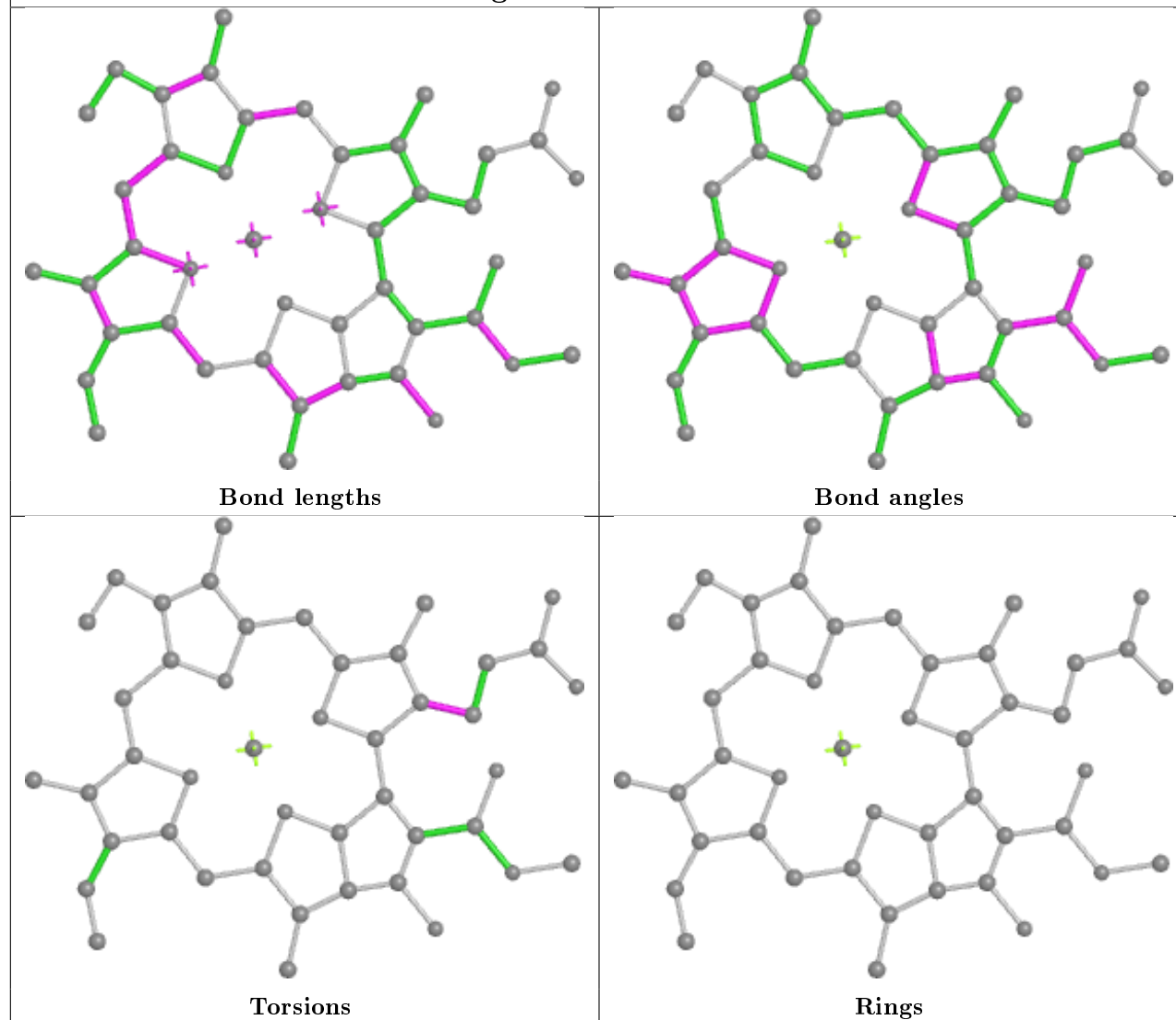


## Ligand CLA B 822

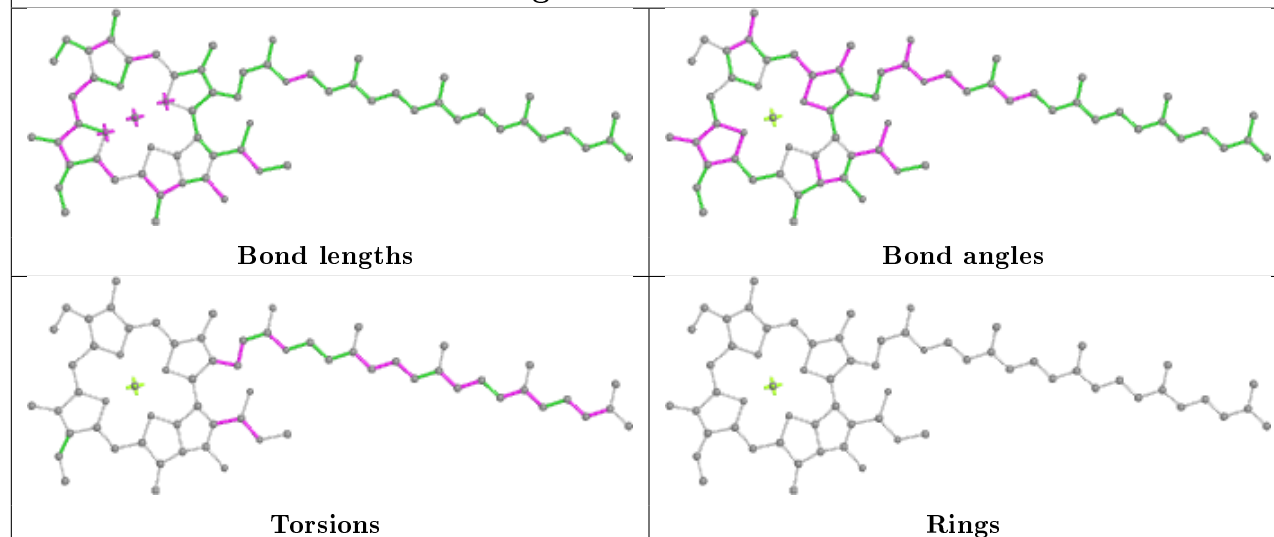




## Ligand CLA B 839

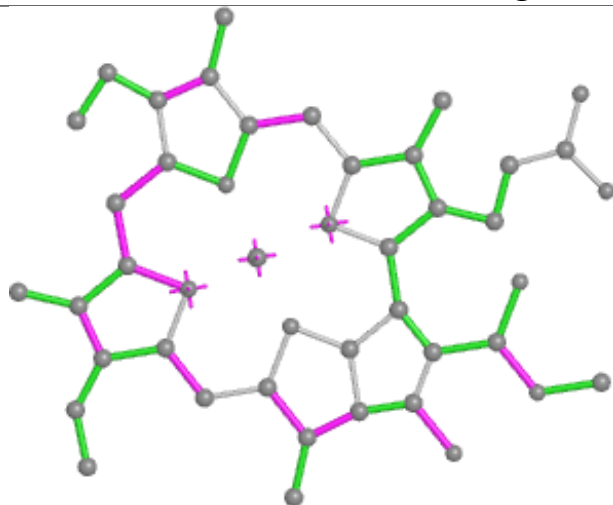


## Ligand CLA A 808

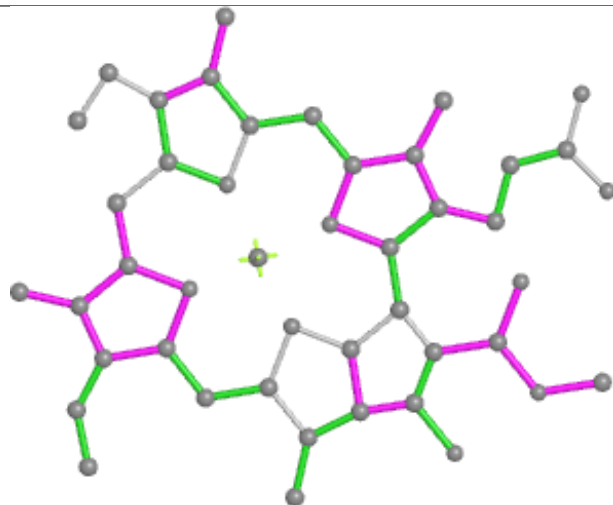




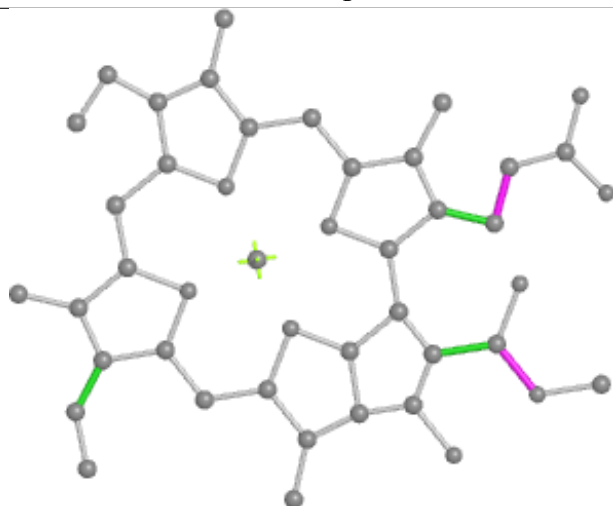
## Ligand CLA H 811



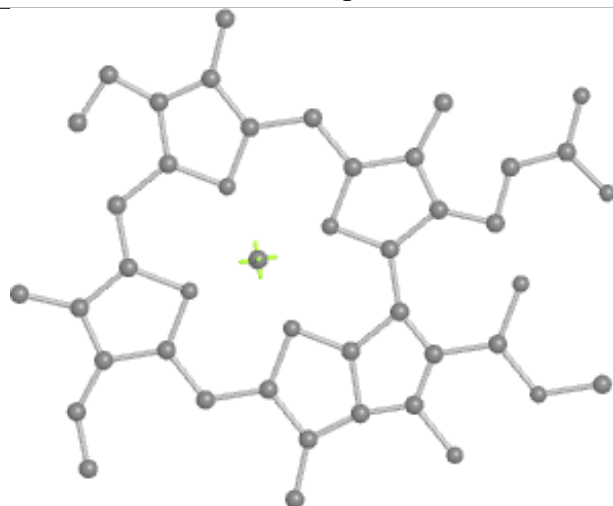
Bond lengths



Bond angles

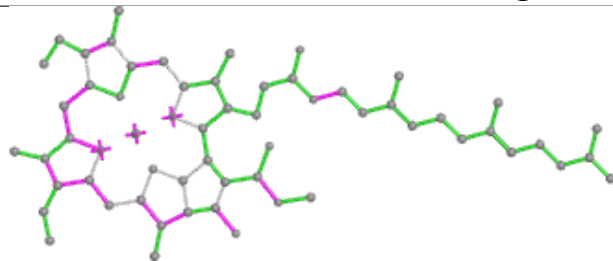


Torsions

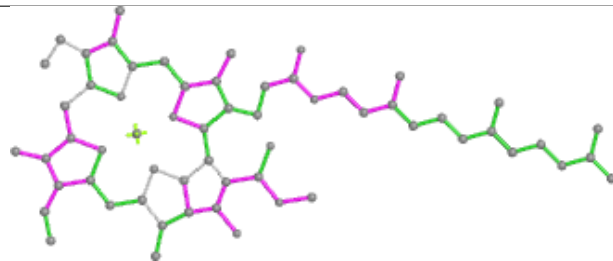


Rings

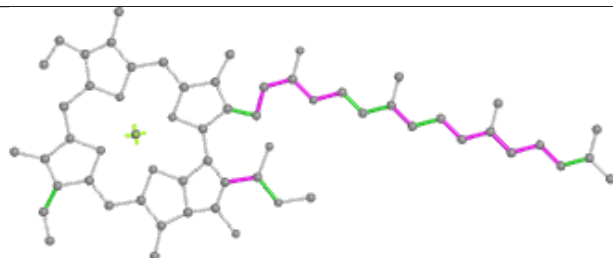
## Ligand CLA B 823



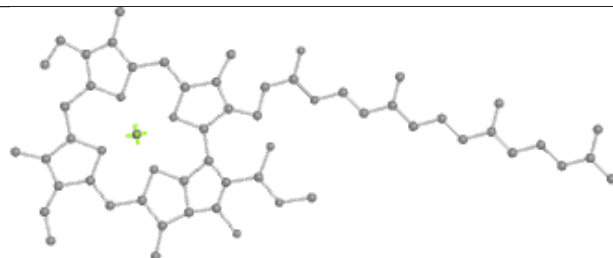
Bond lengths



Bond angles

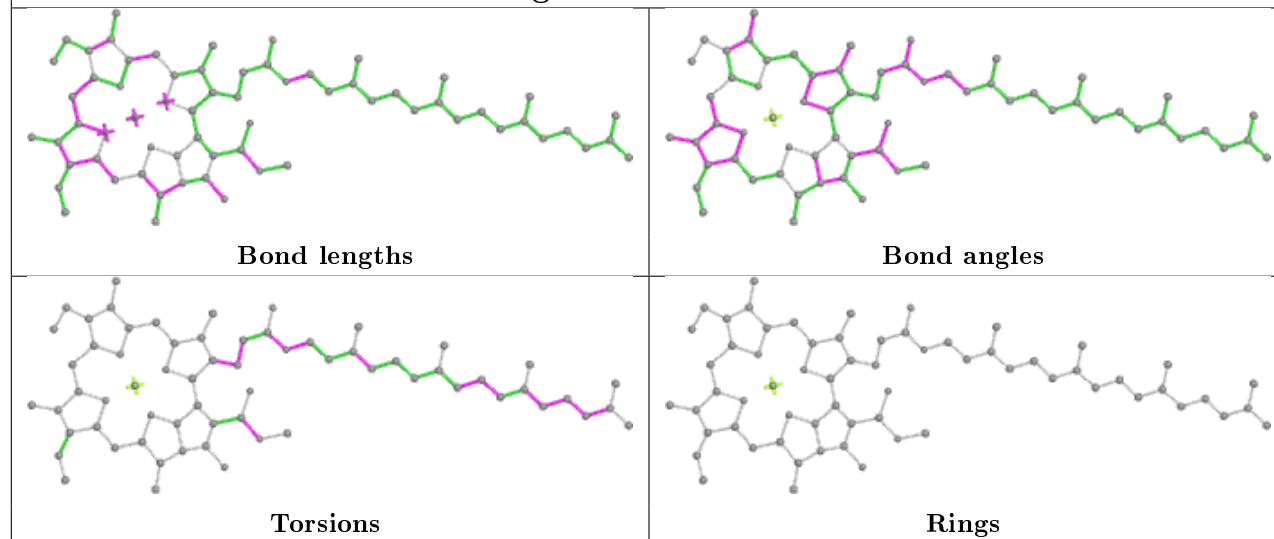


Torsions

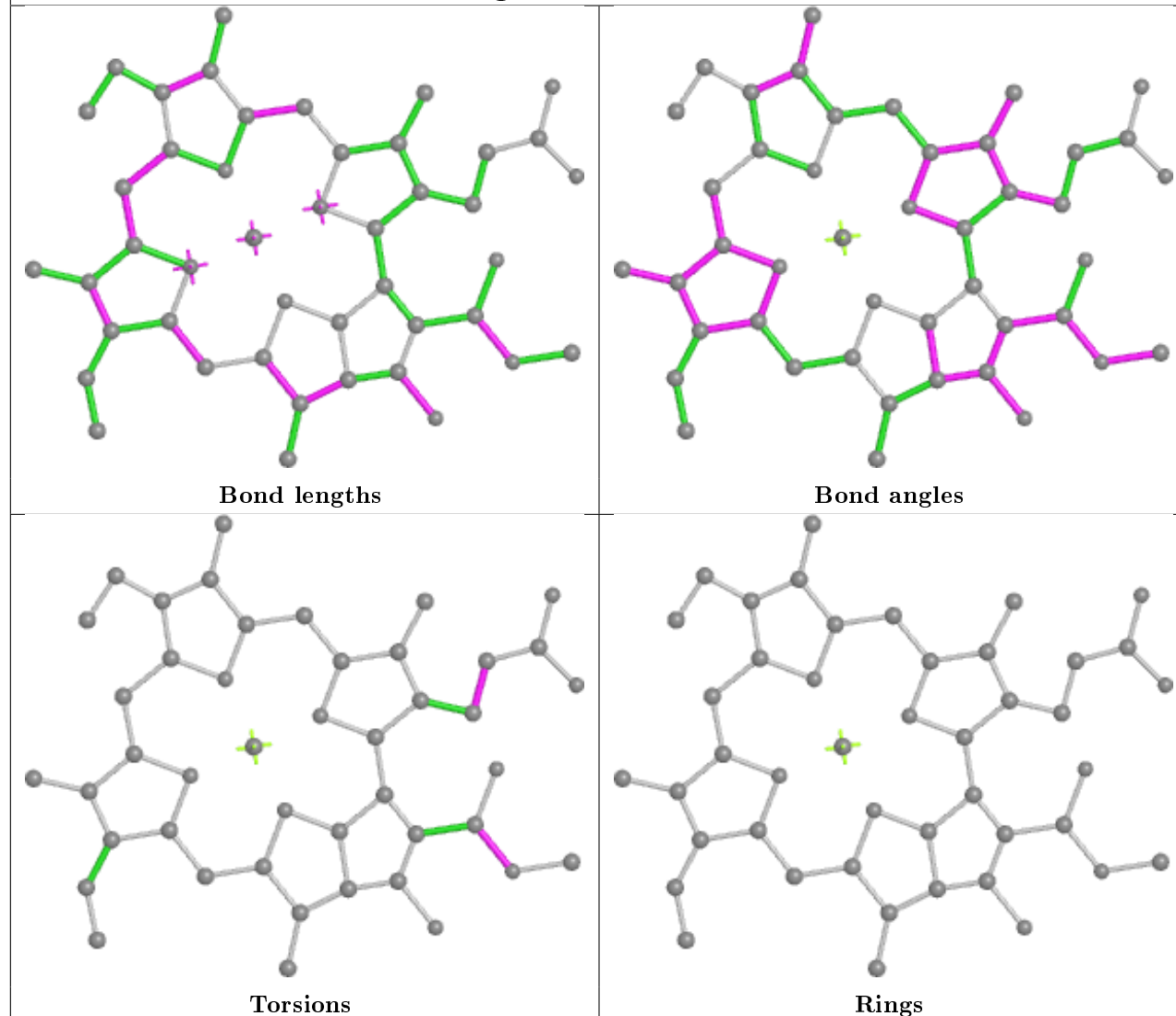


Rings

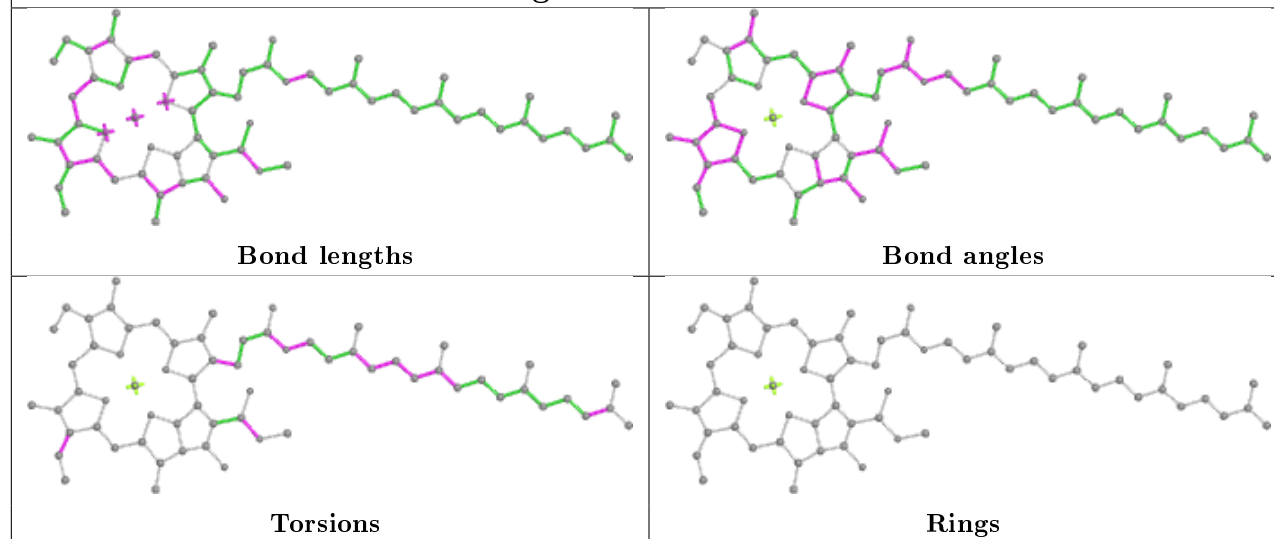
## Ligand CLA A 811



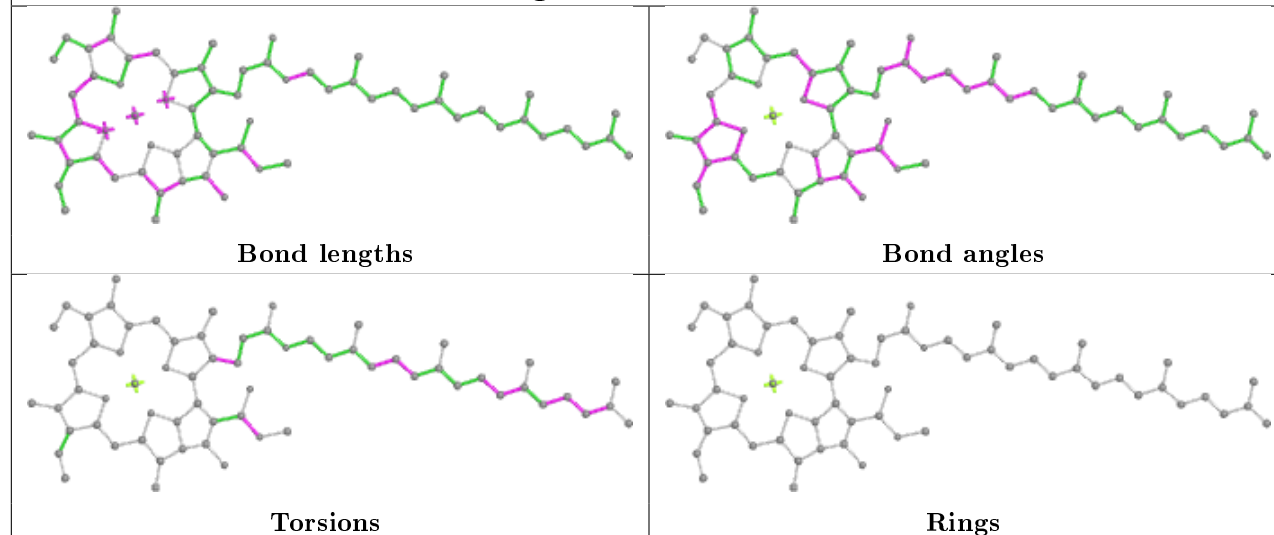
## Ligand CLA Z 810



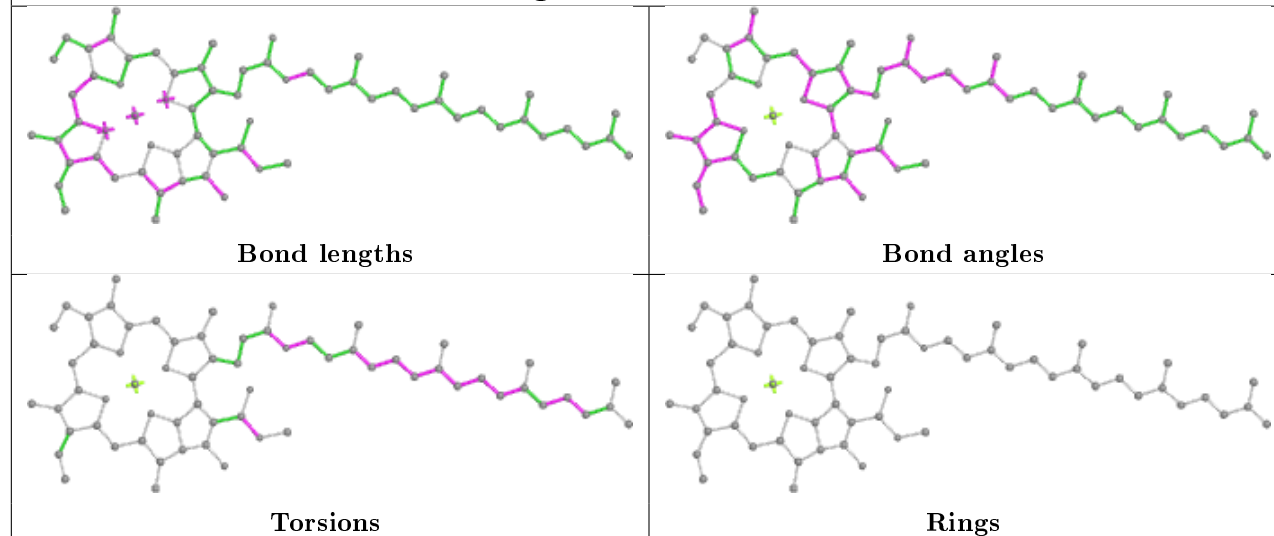
## Ligand CLA Y 803

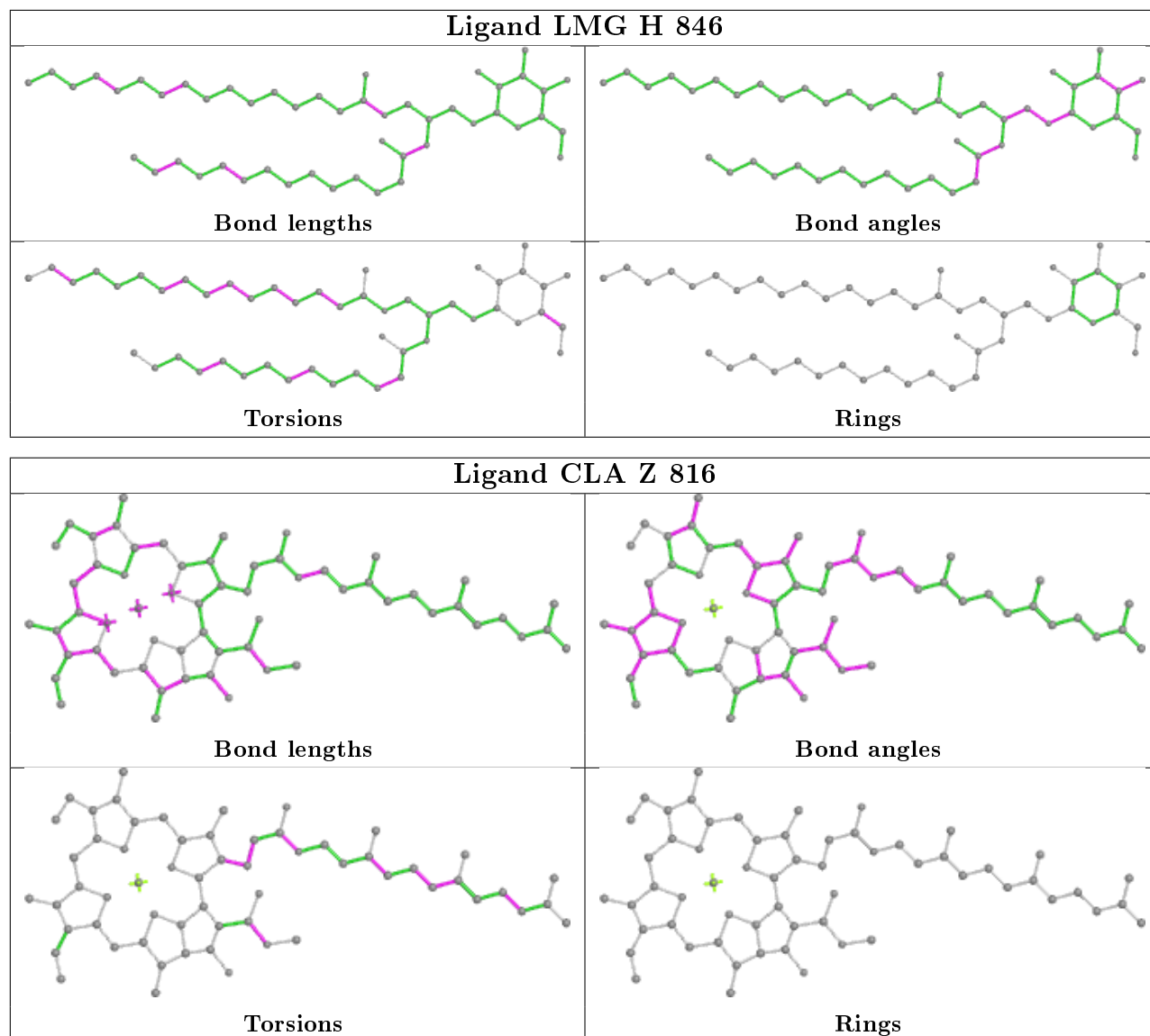


## Ligand CLA H 826

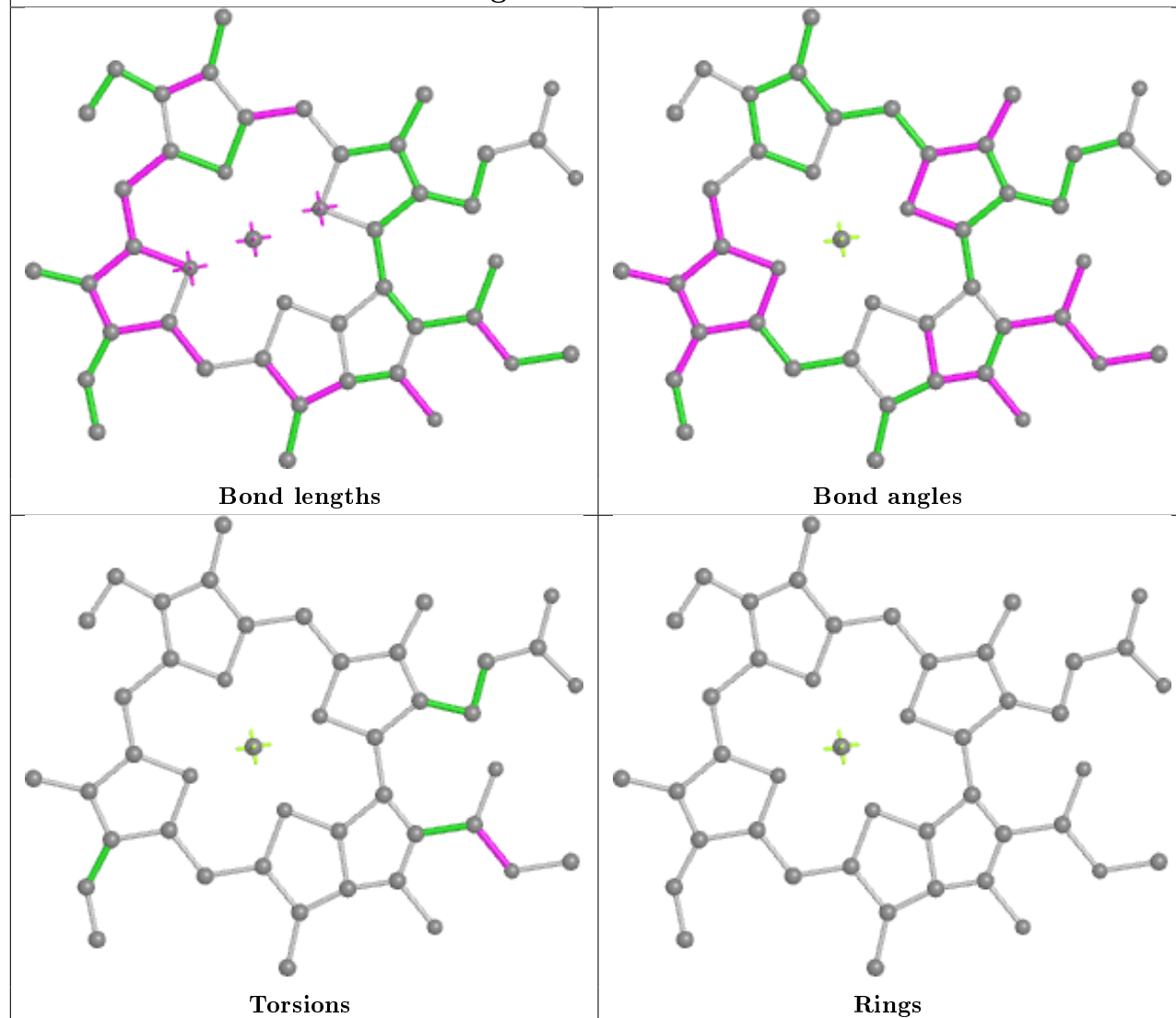


## Ligand CLA B 807

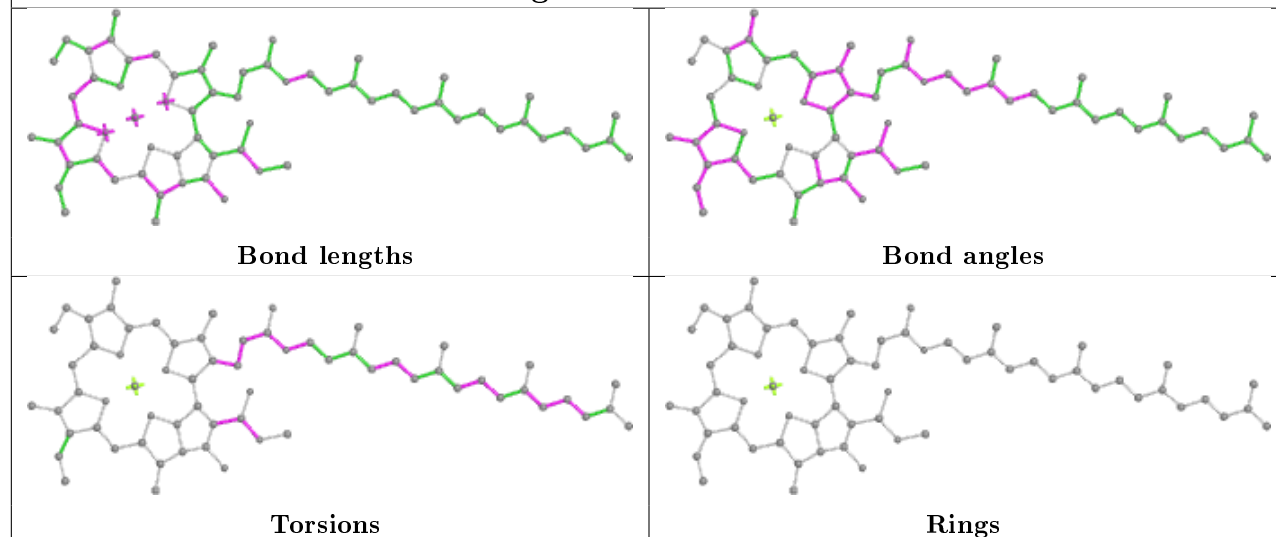


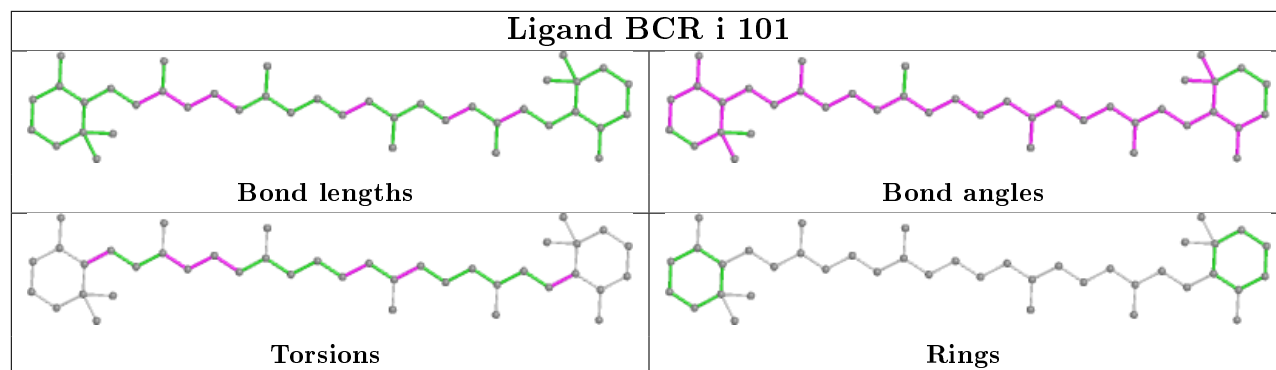
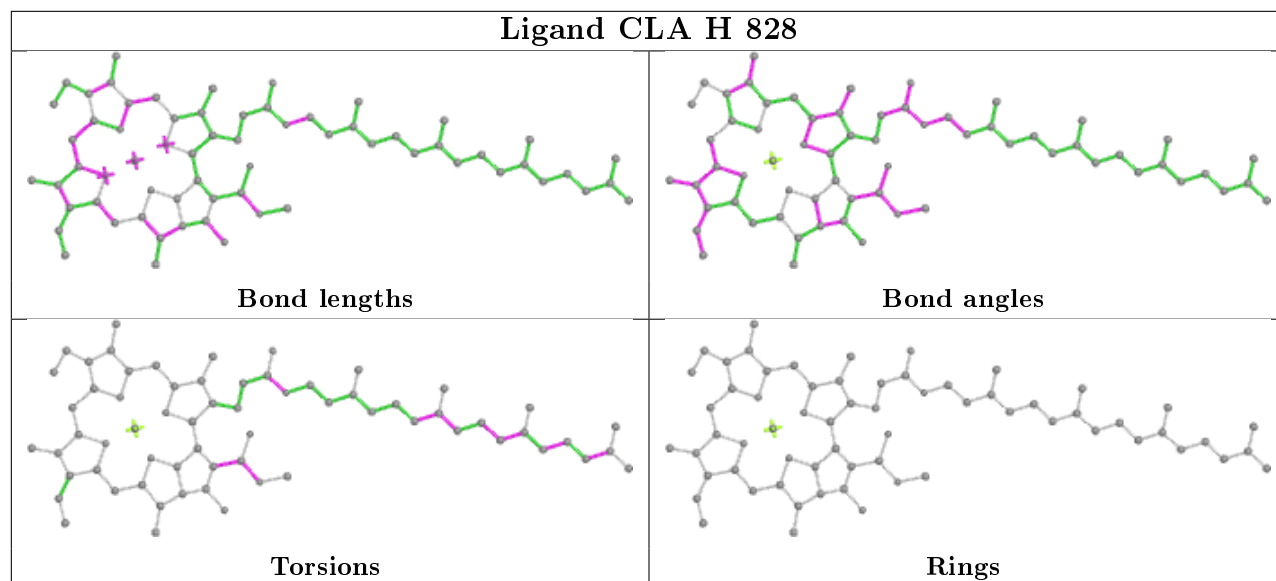


## Ligand CLA B 836

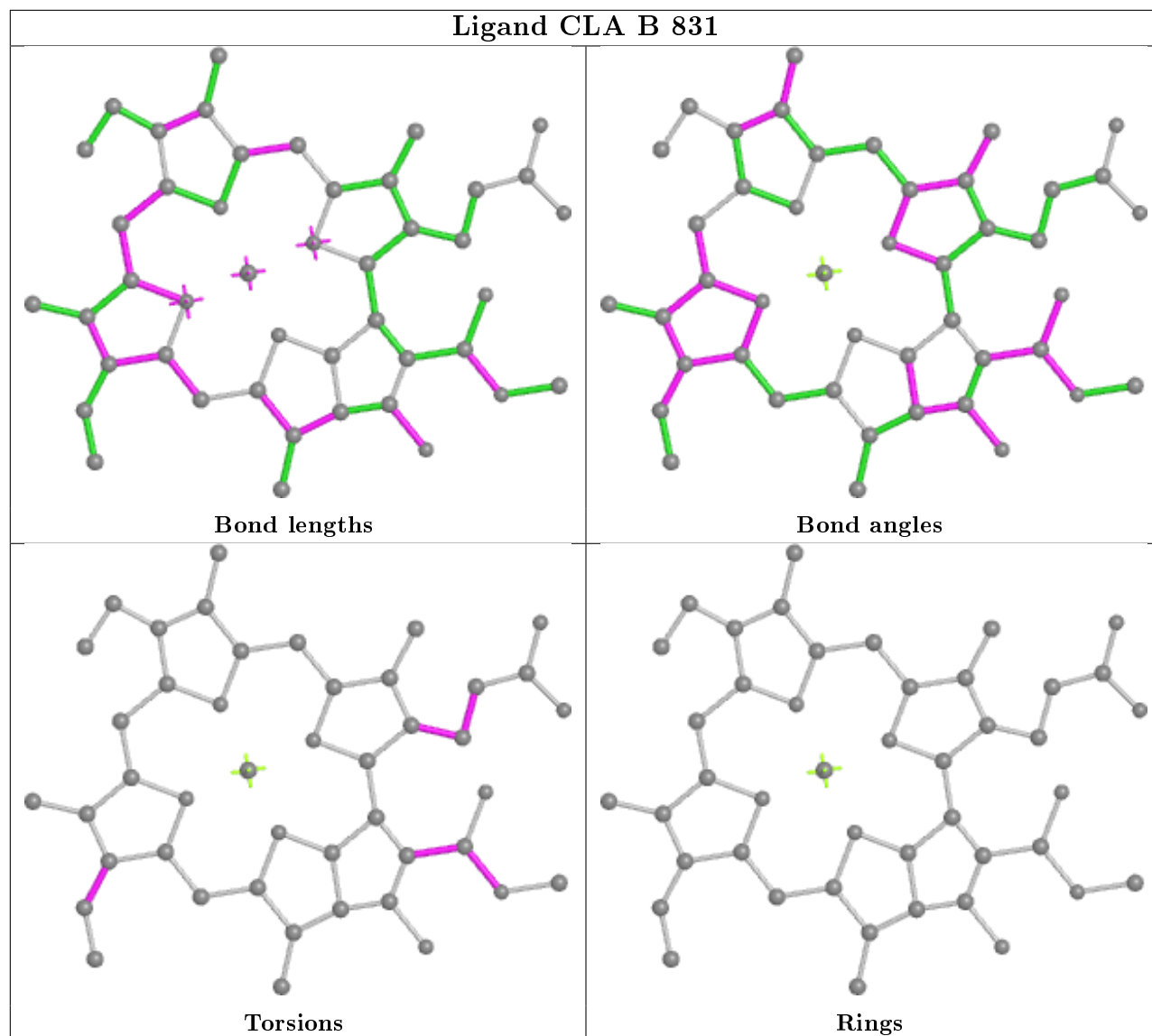


## Ligand CLA G 805

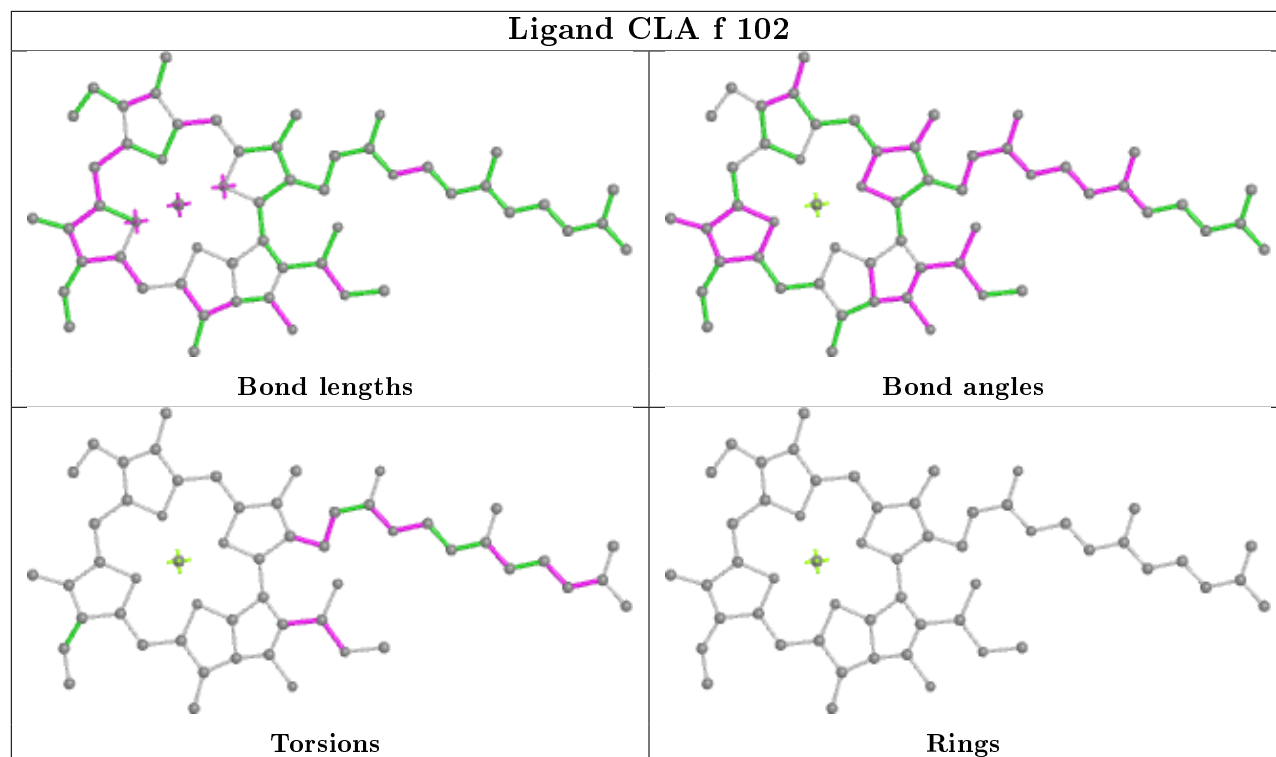


**Ligand BCR i 101****Ligand CLA H 828**

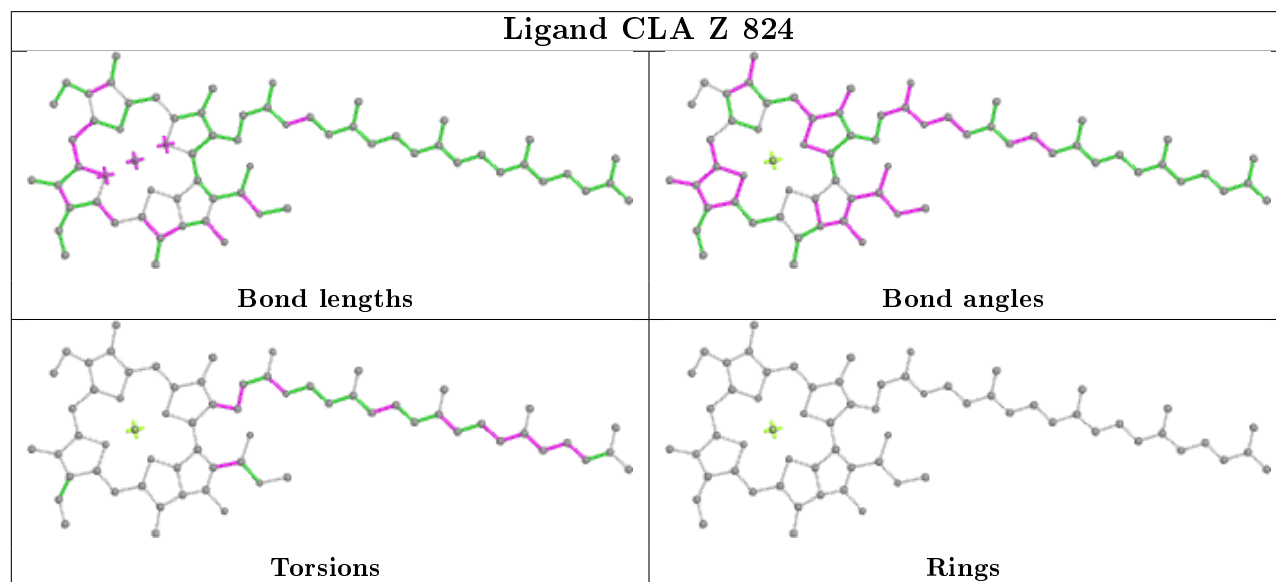
## Ligand CLA B 831



## Ligand CLA f 102

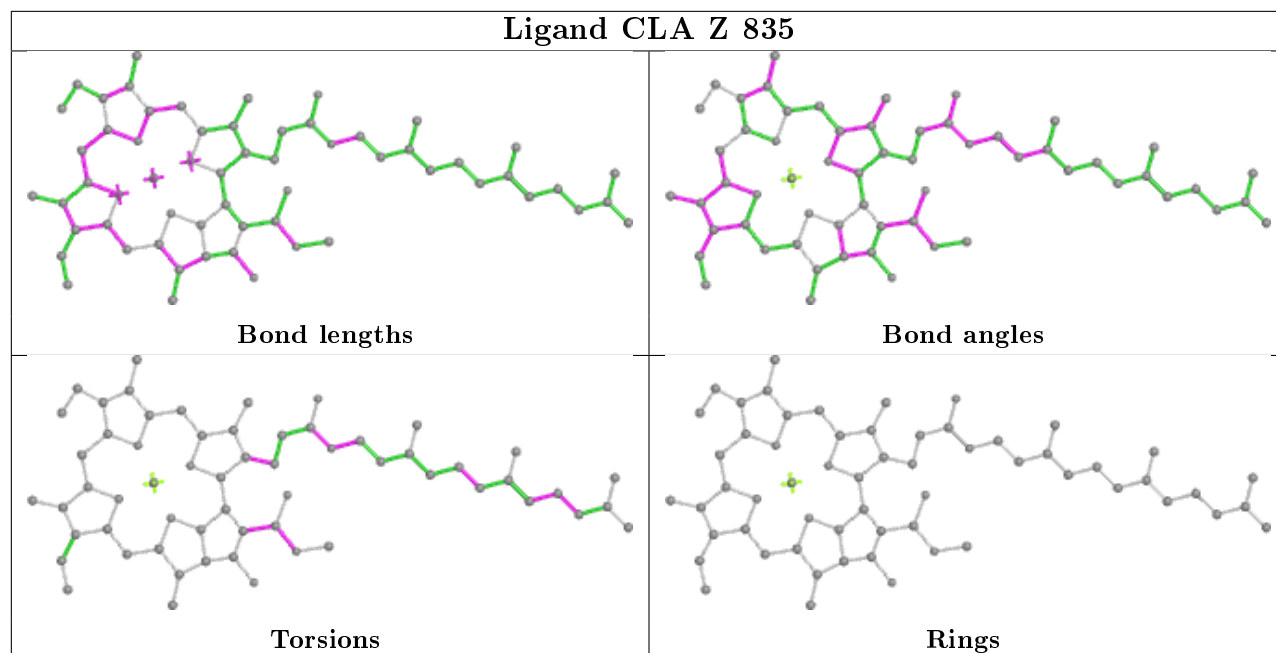


## Ligand CLA Z 824

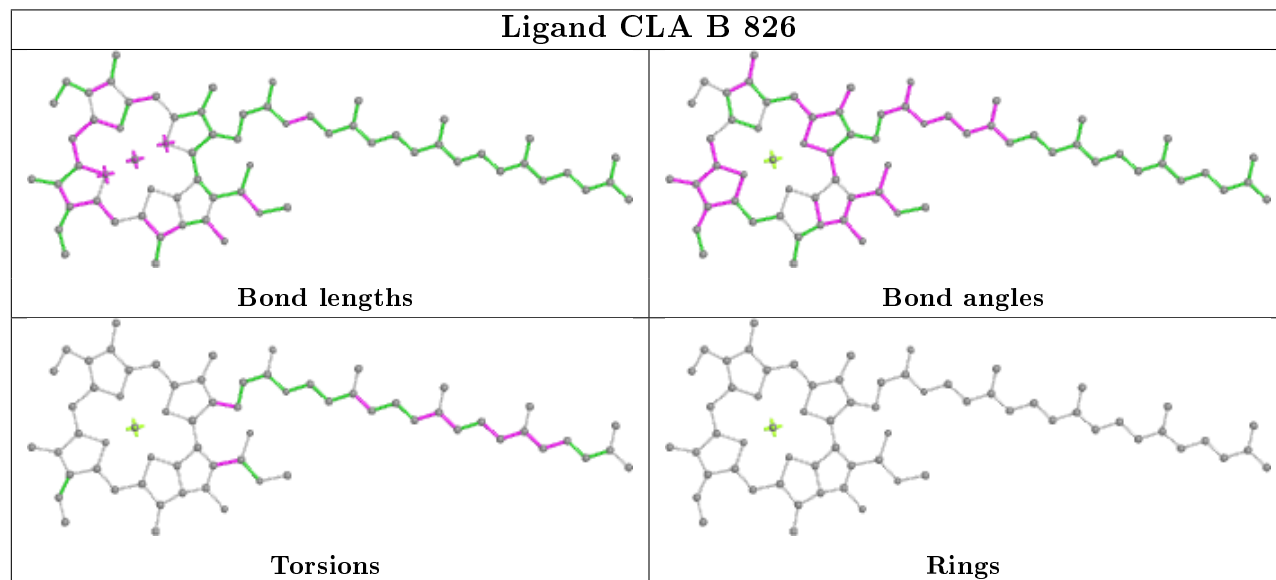




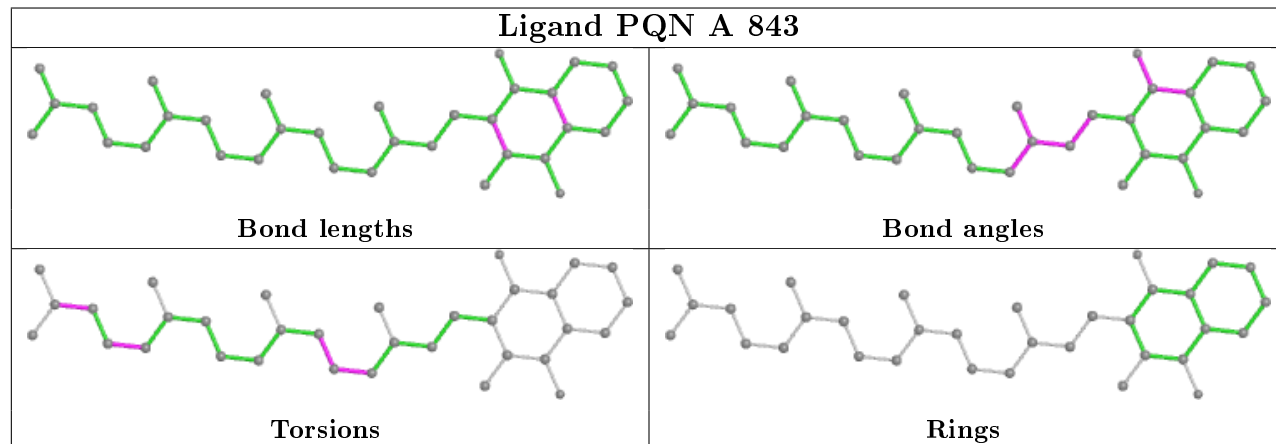
## Ligand CLA Z 835



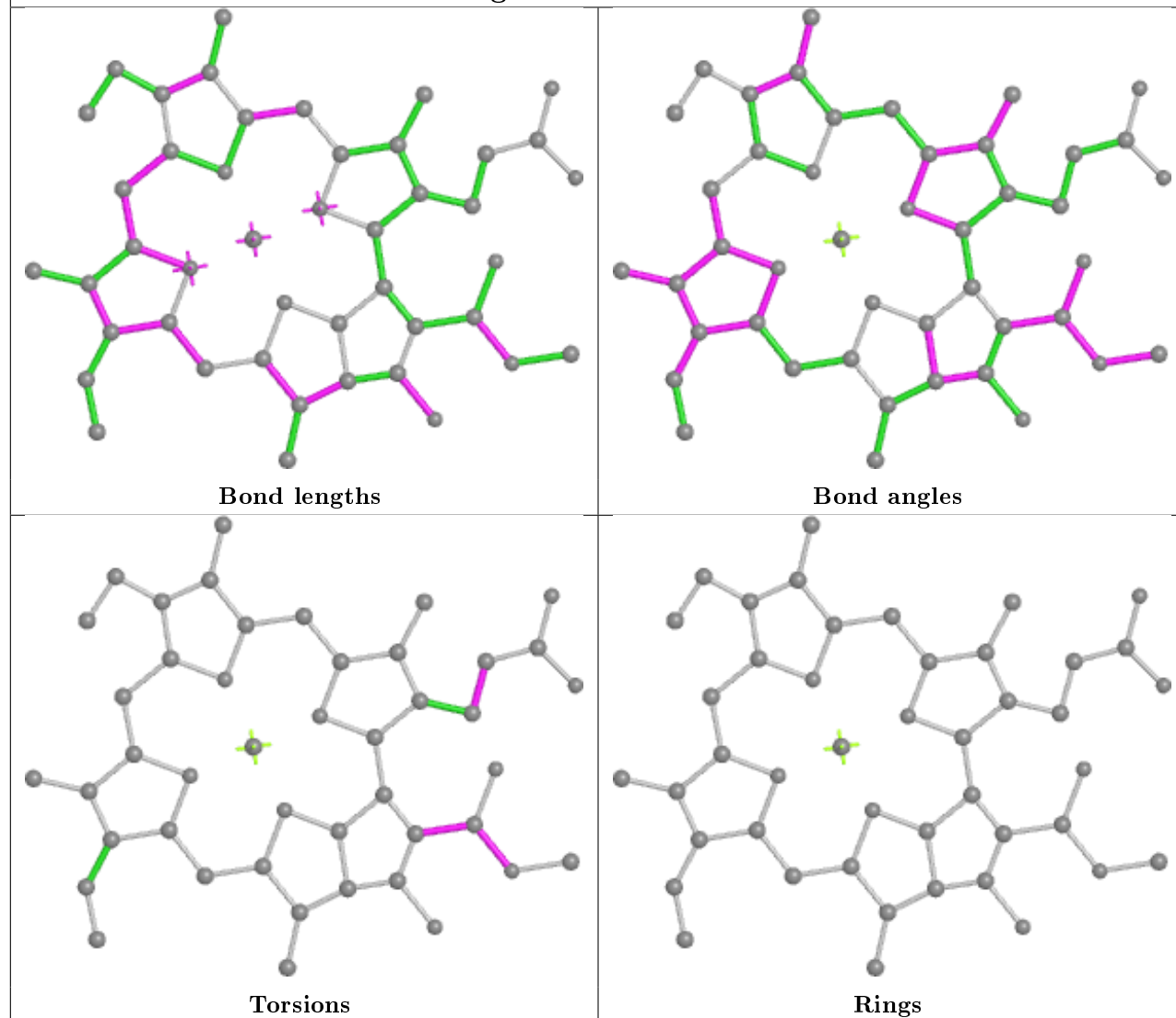
## Ligand CLA B 826



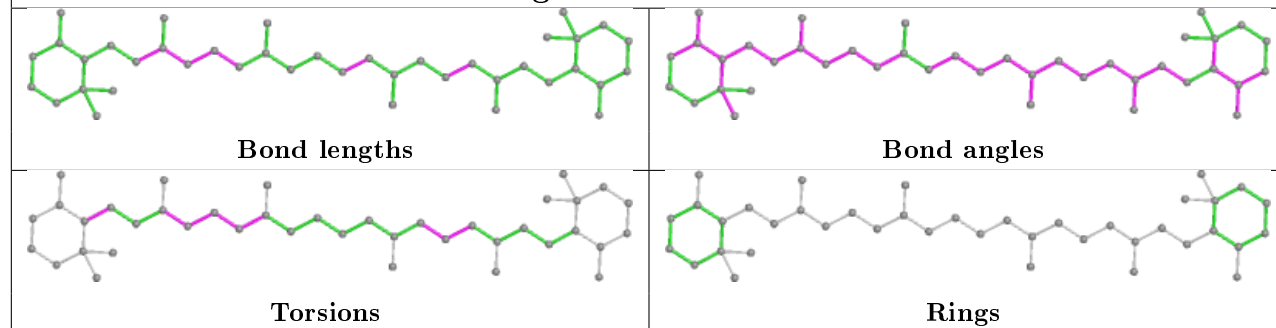
## Ligand PQN A 843



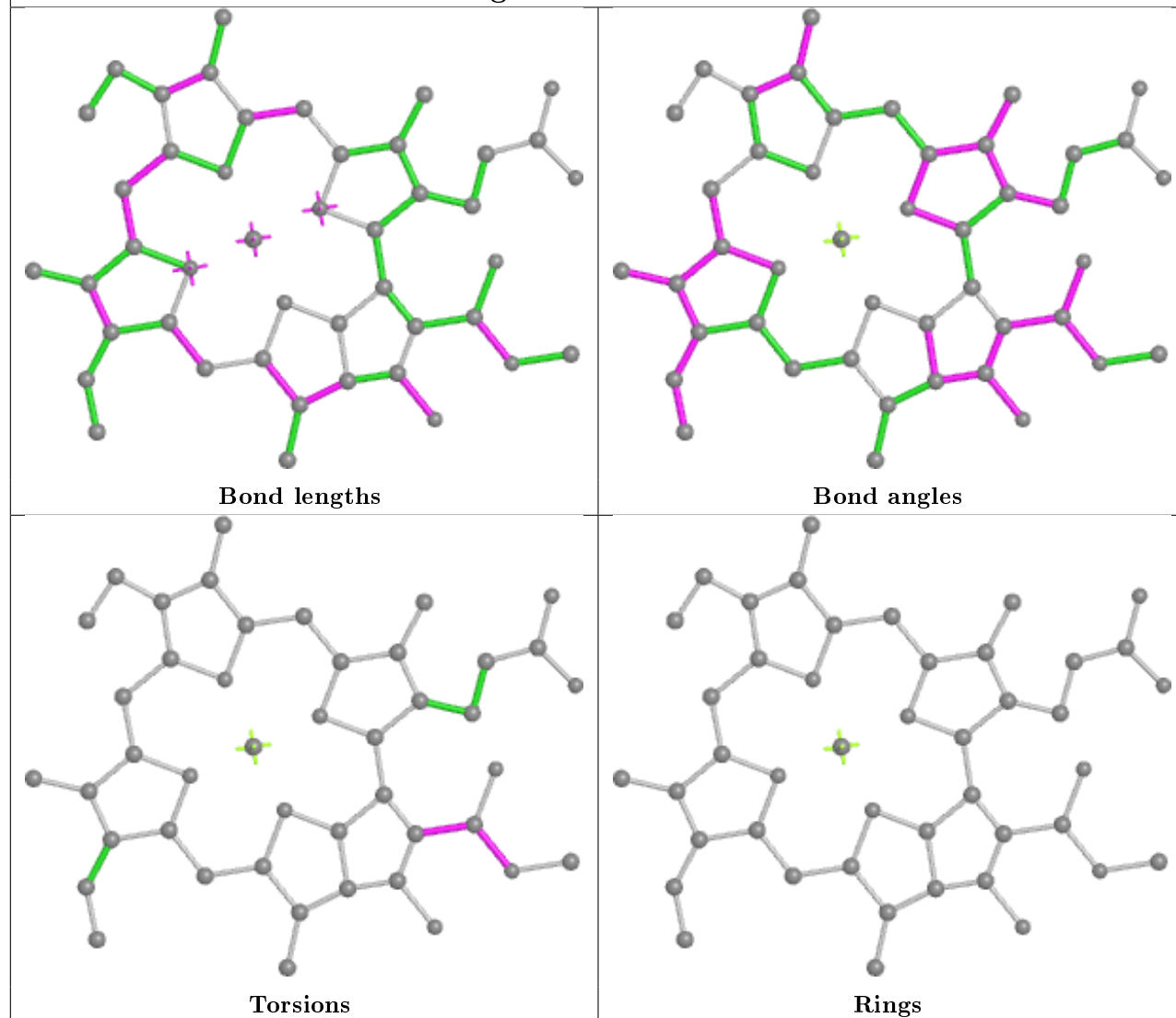
## Ligand CLA A 835



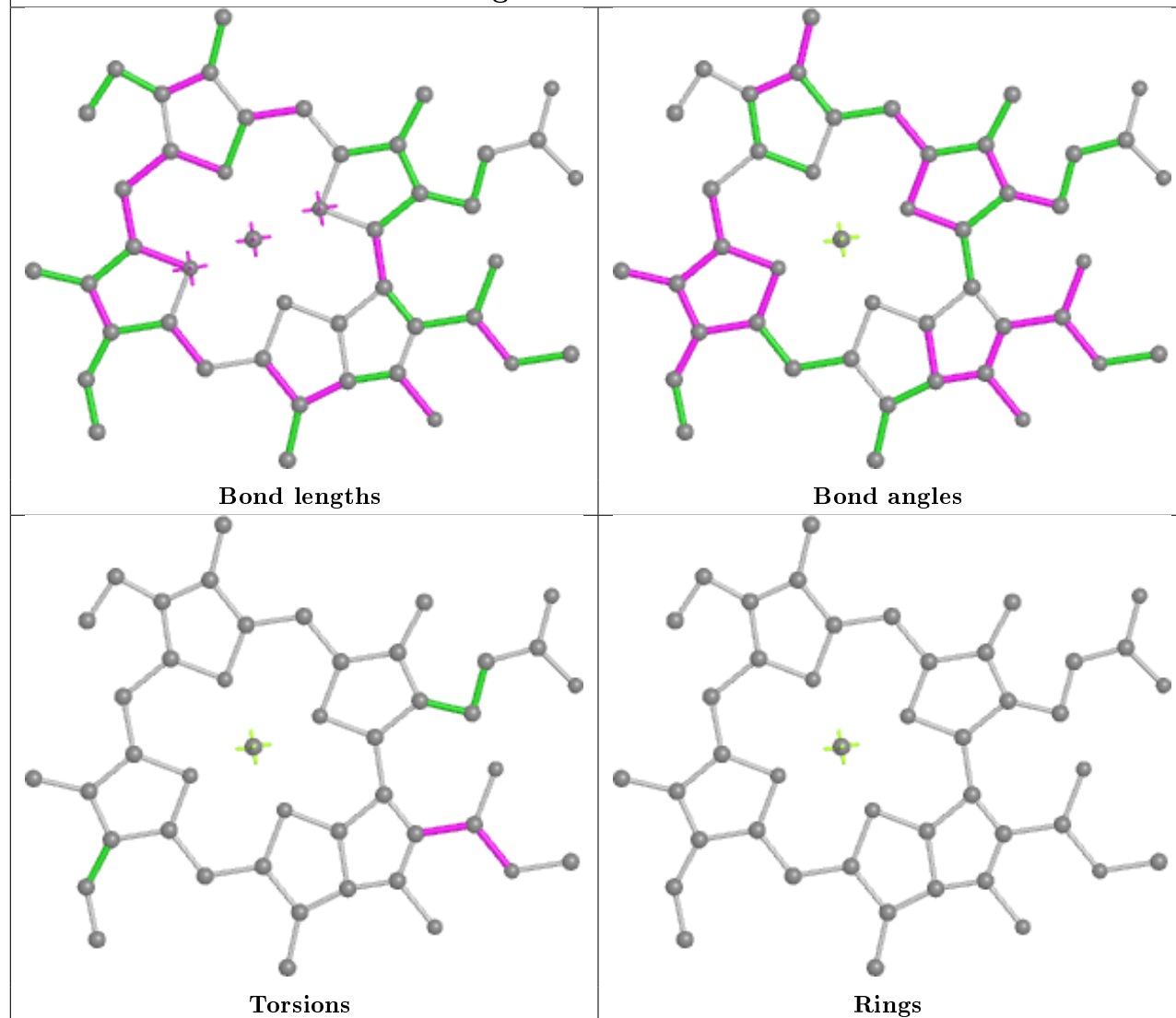
## Ligand BCR L 209



## Ligand CLA B 815



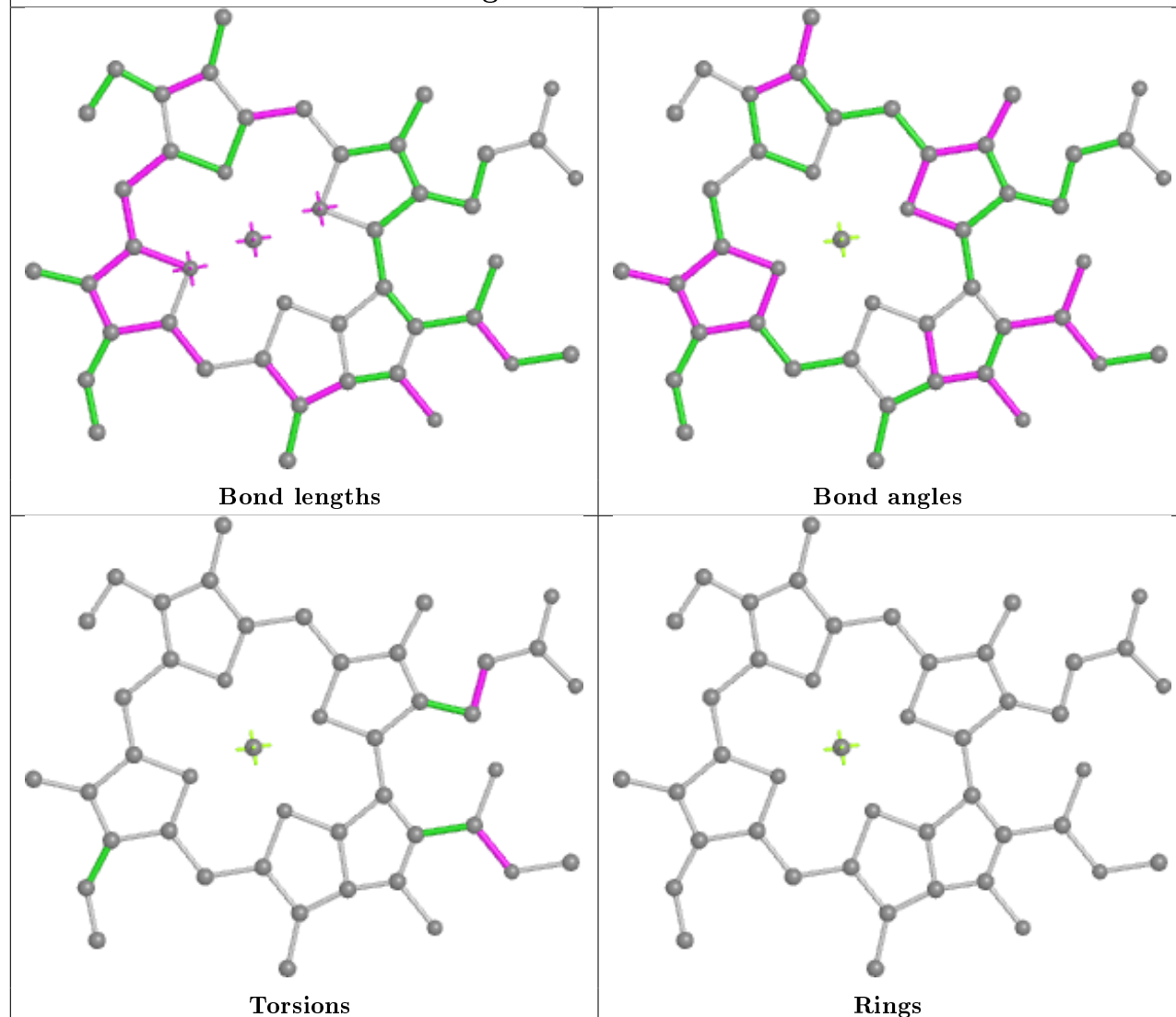
## Ligand CLA Z 813



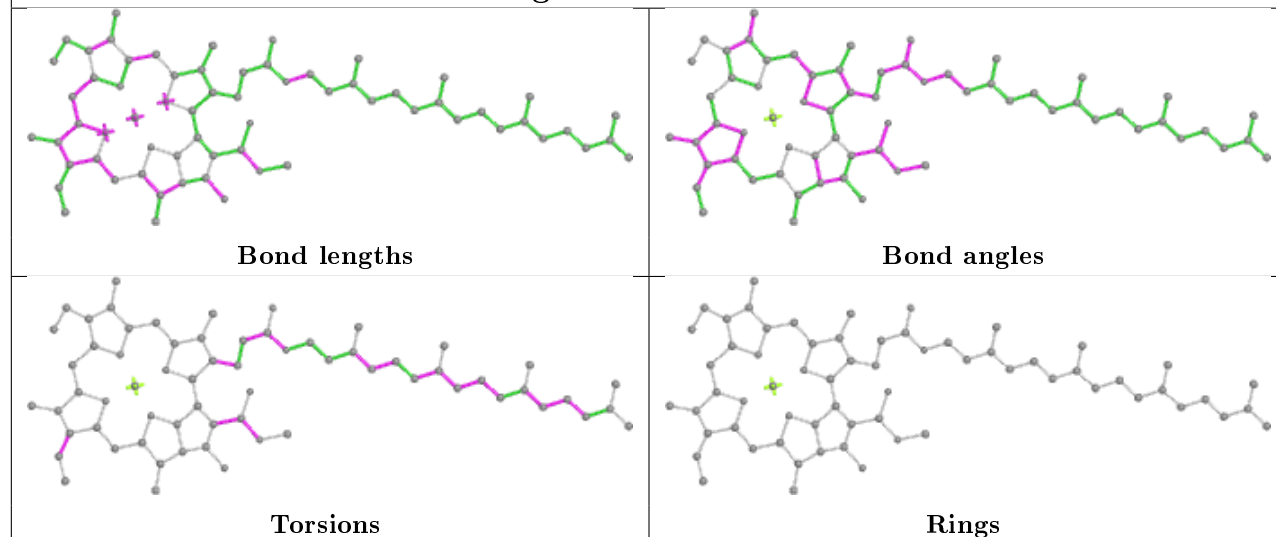
## Ligand BCR F 201



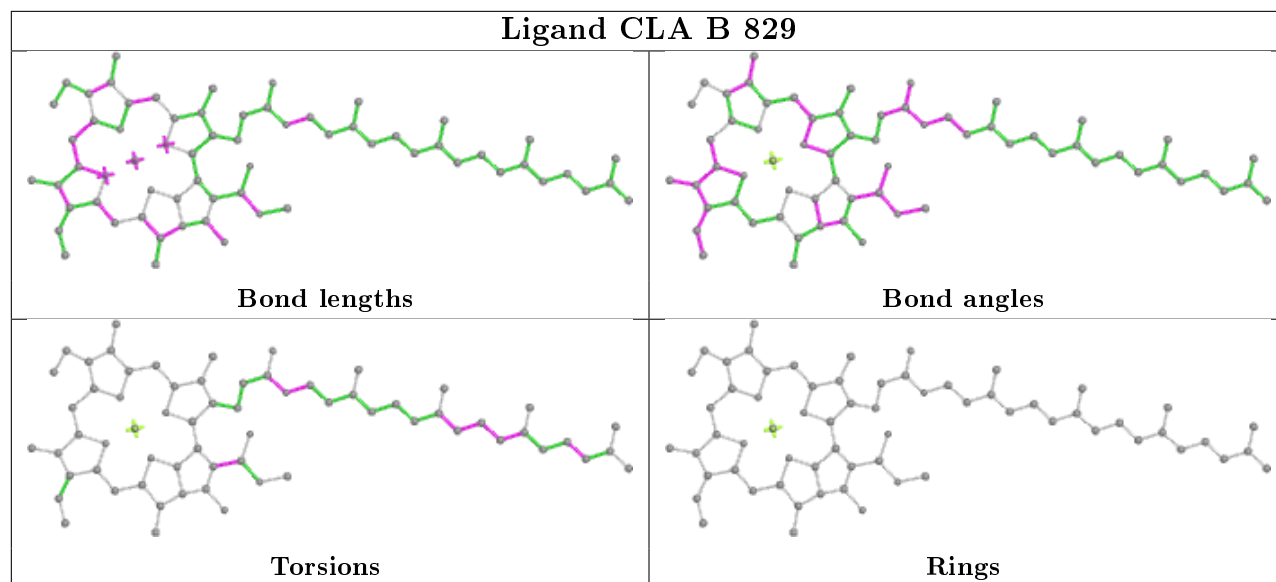
## Ligand CLA X 1701



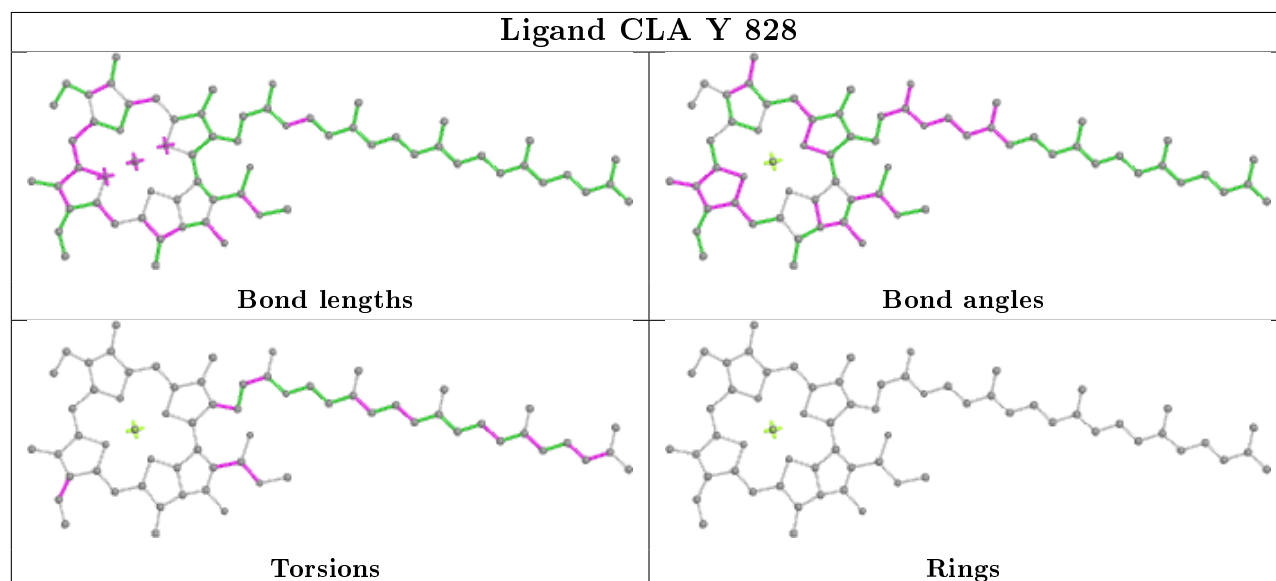
## Ligand CLA A 806



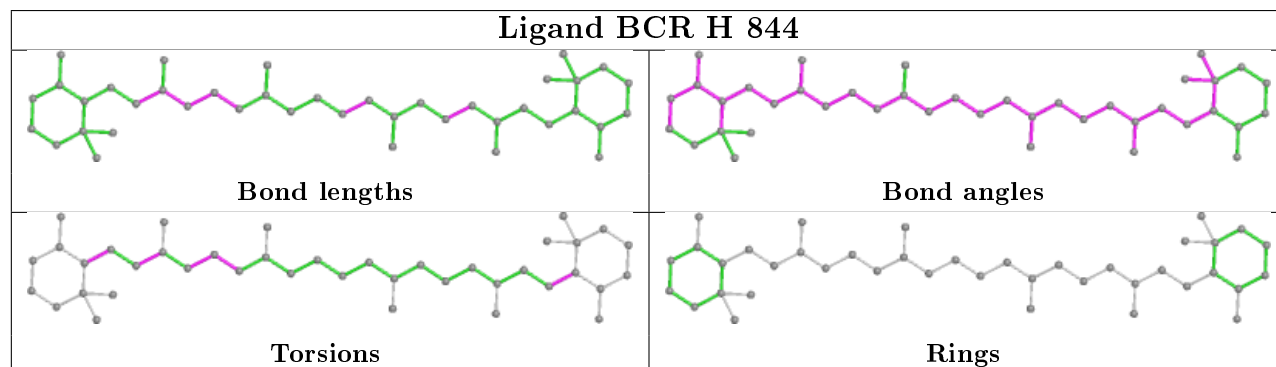
## Ligand CLA B 829



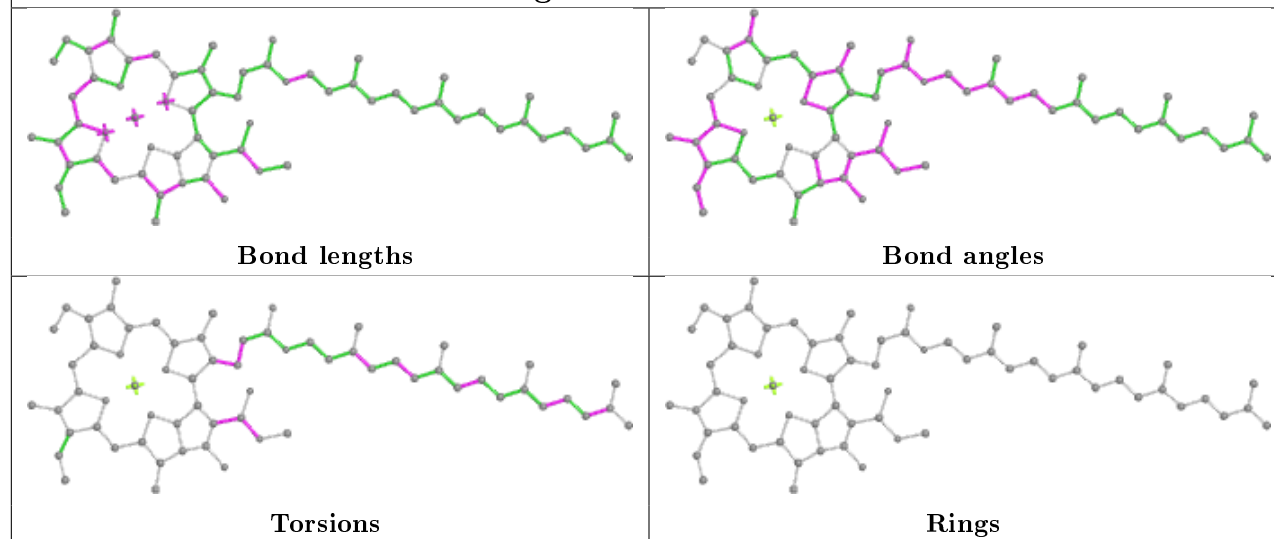
## Ligand CLA Y 828



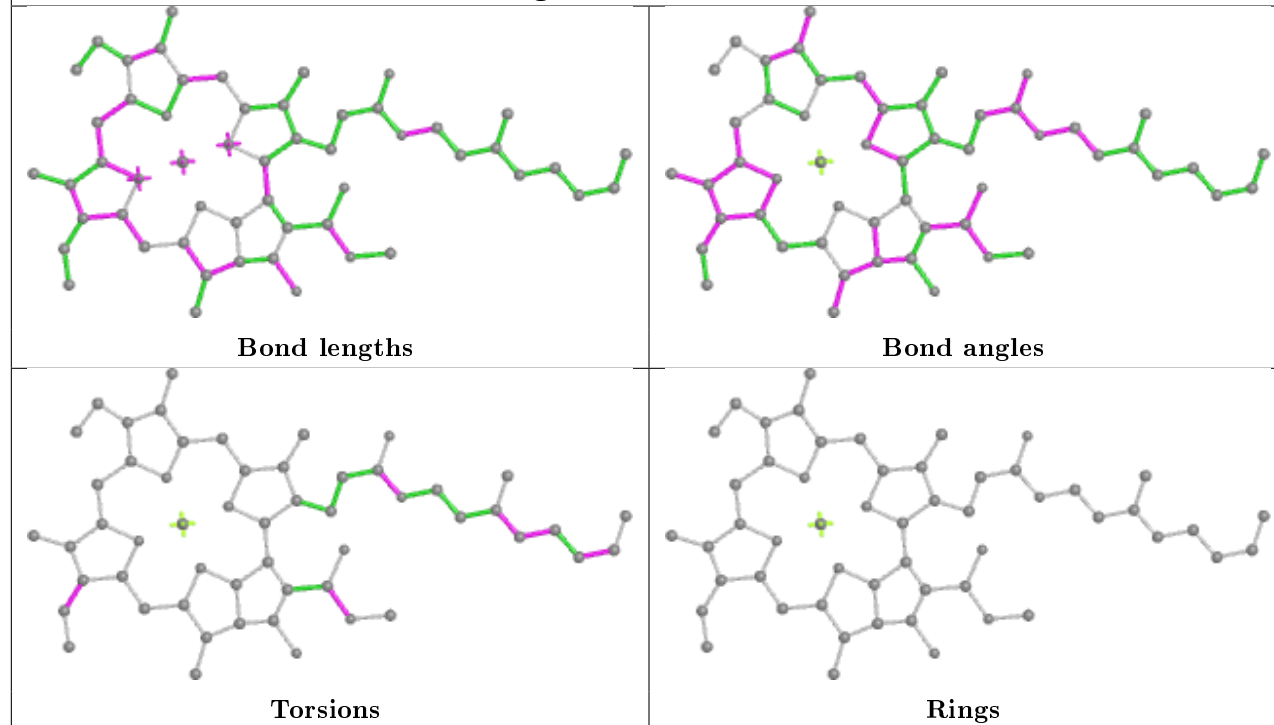
## Ligand BCR H 844

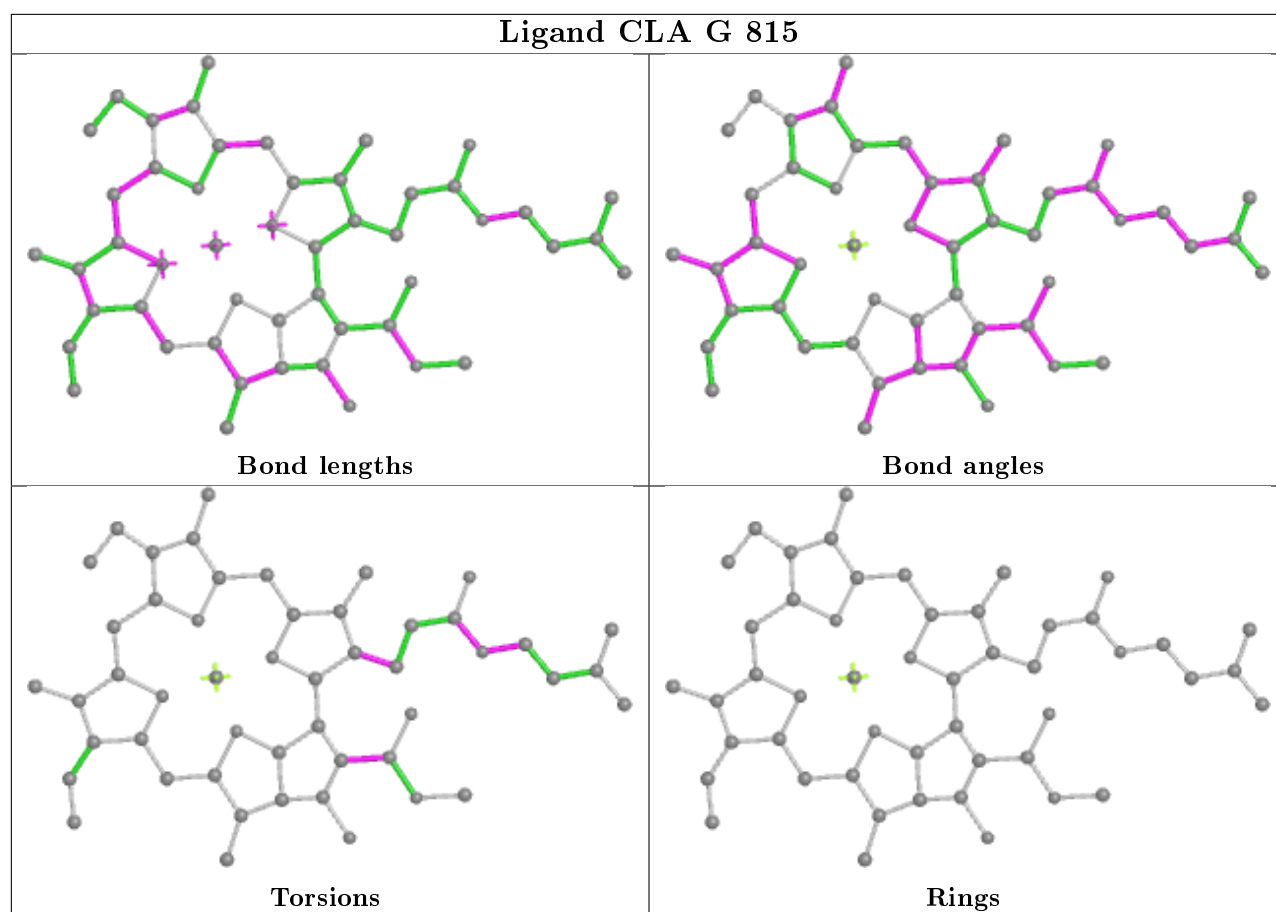


## Ligand CLA Z 826



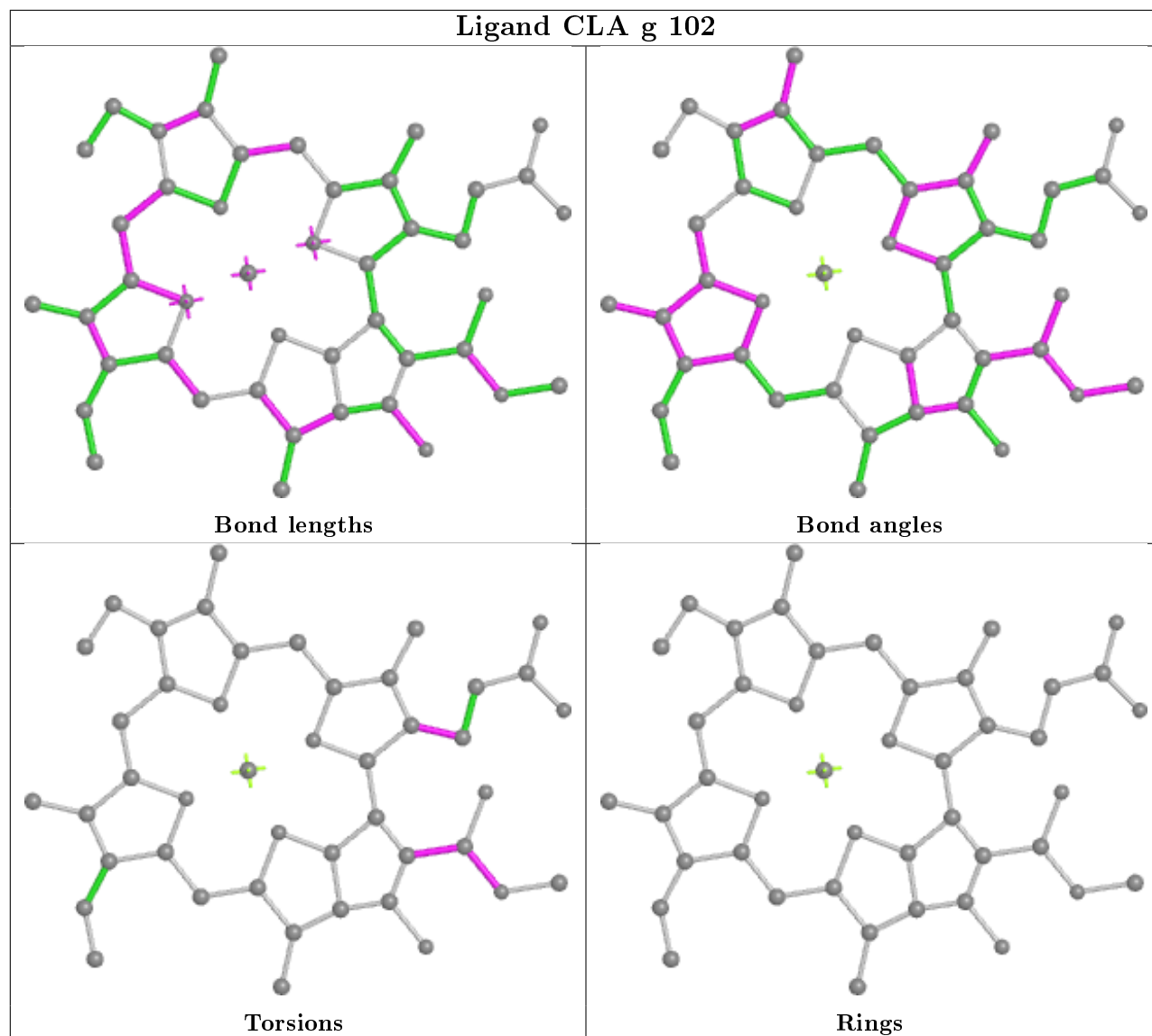
## Ligand CLA B 805



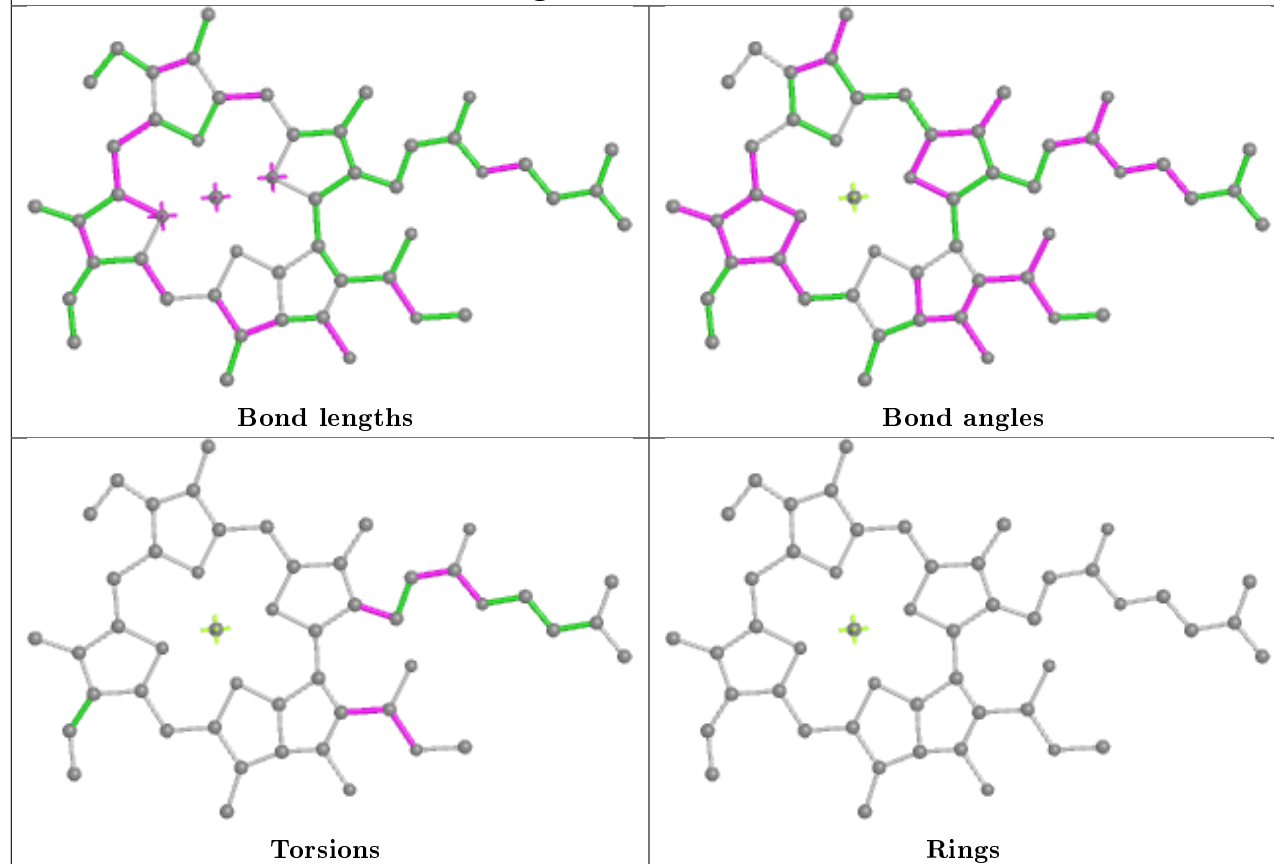




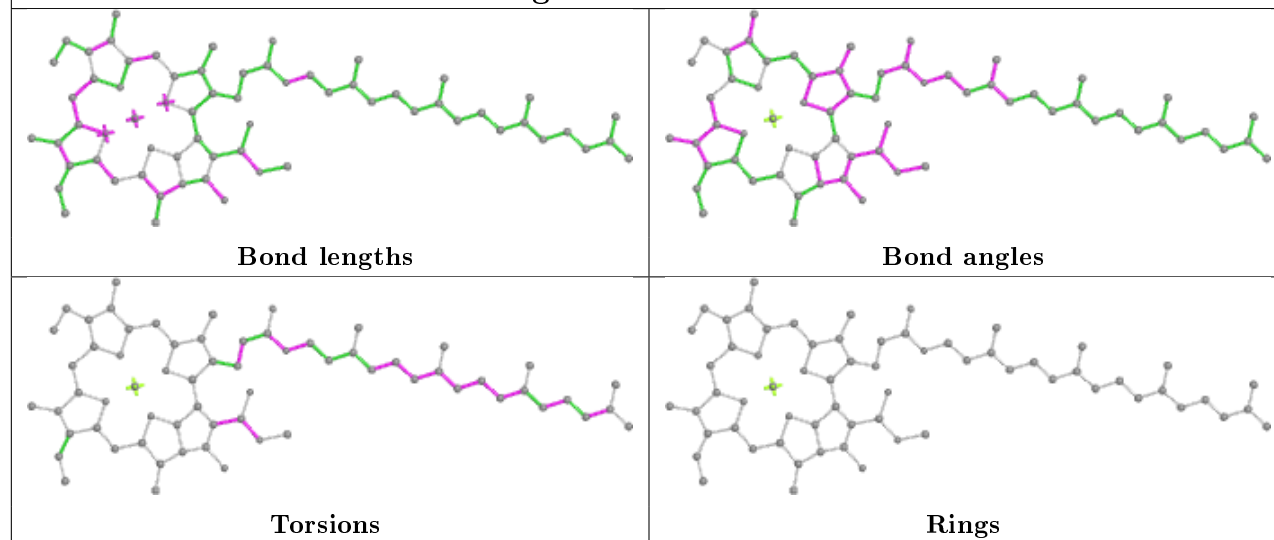
## Ligand CLA g 102

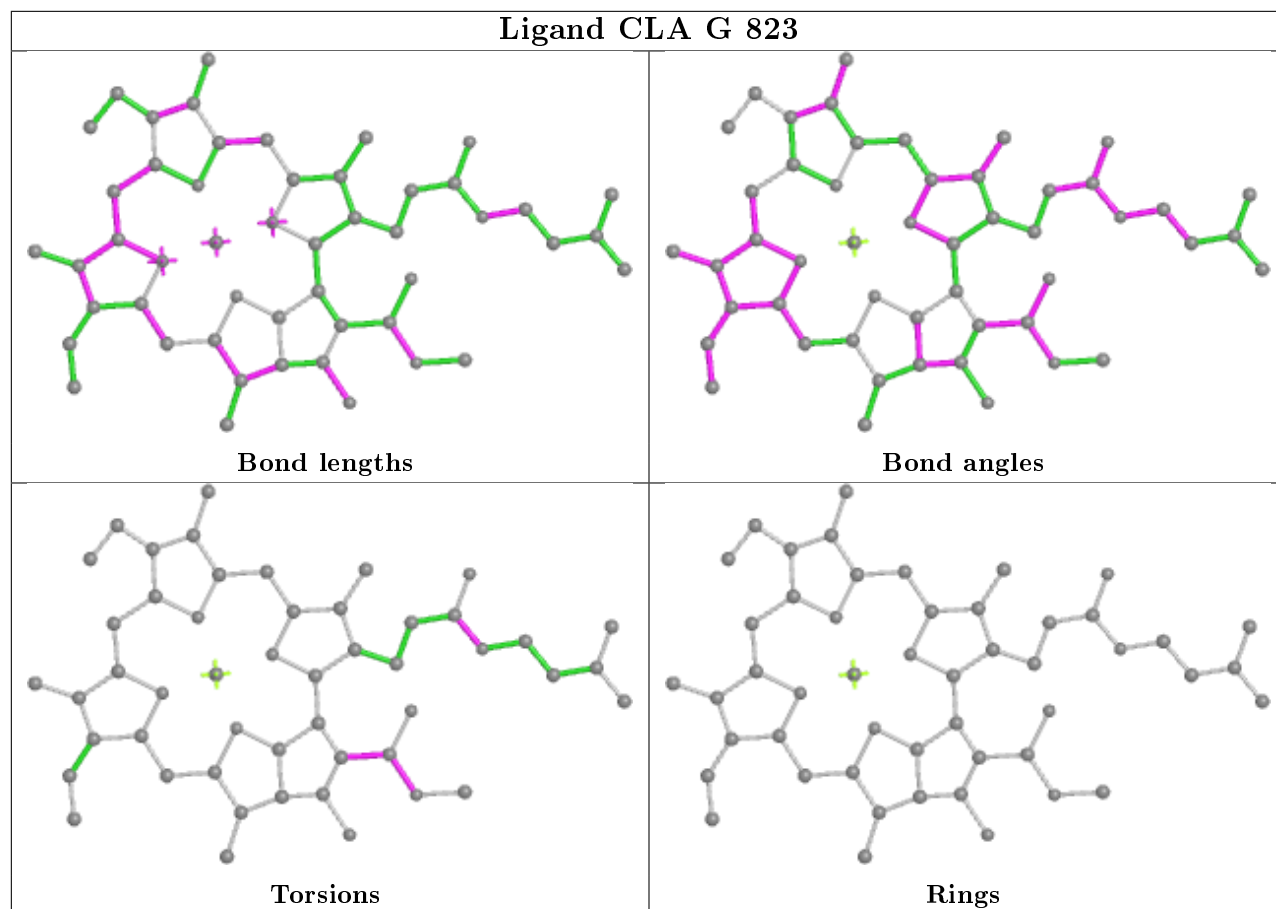
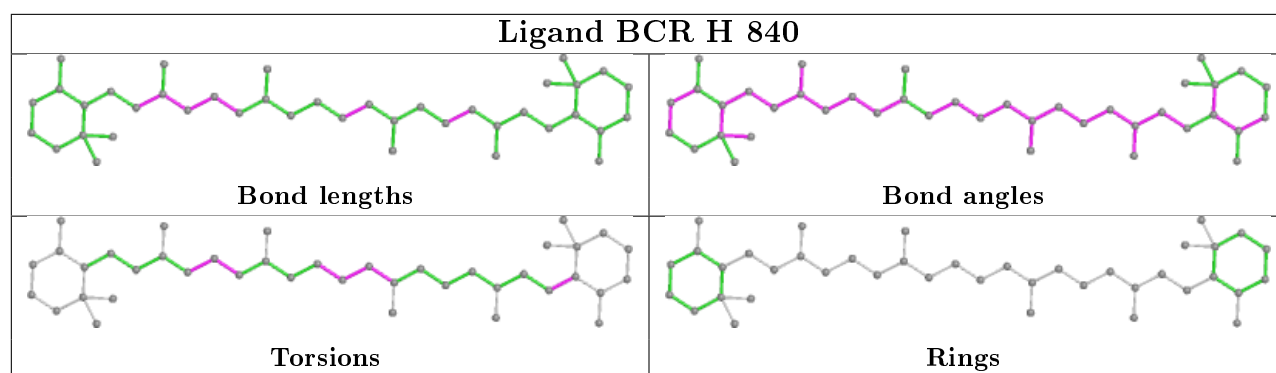


## Ligand CLA G 831

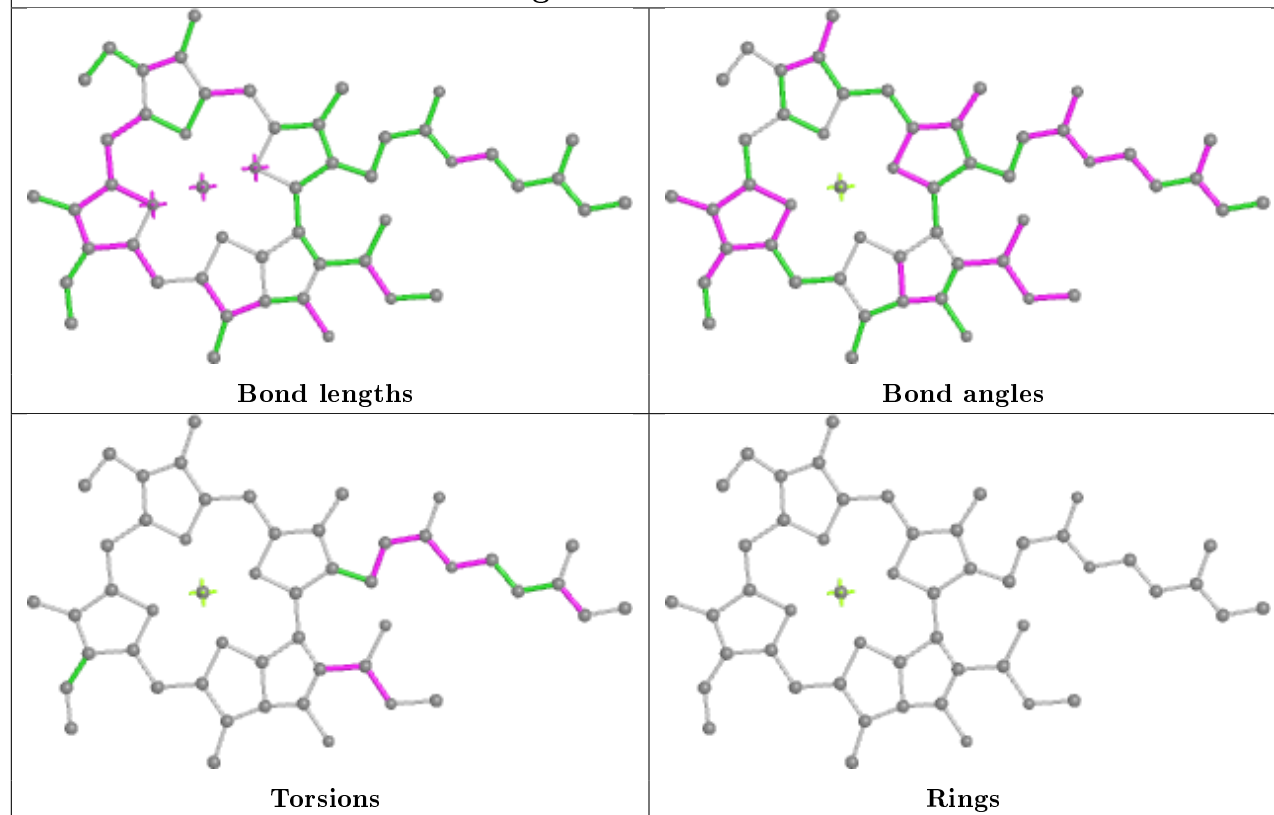


## Ligand CLA B 809

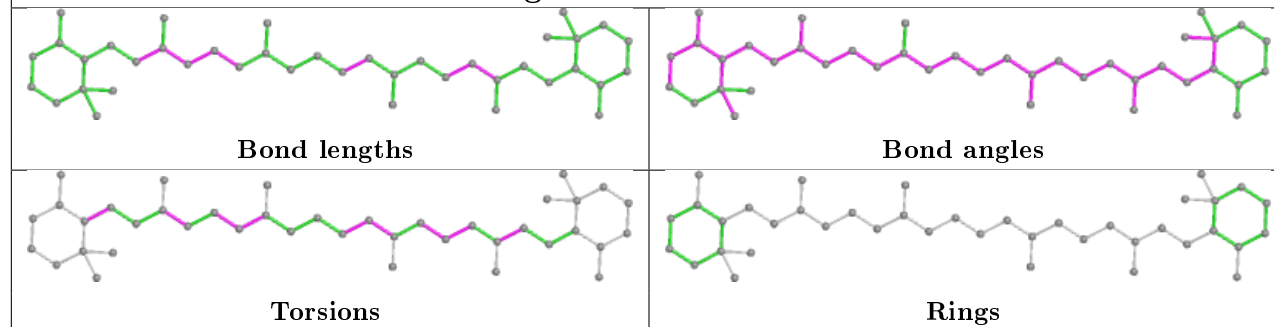




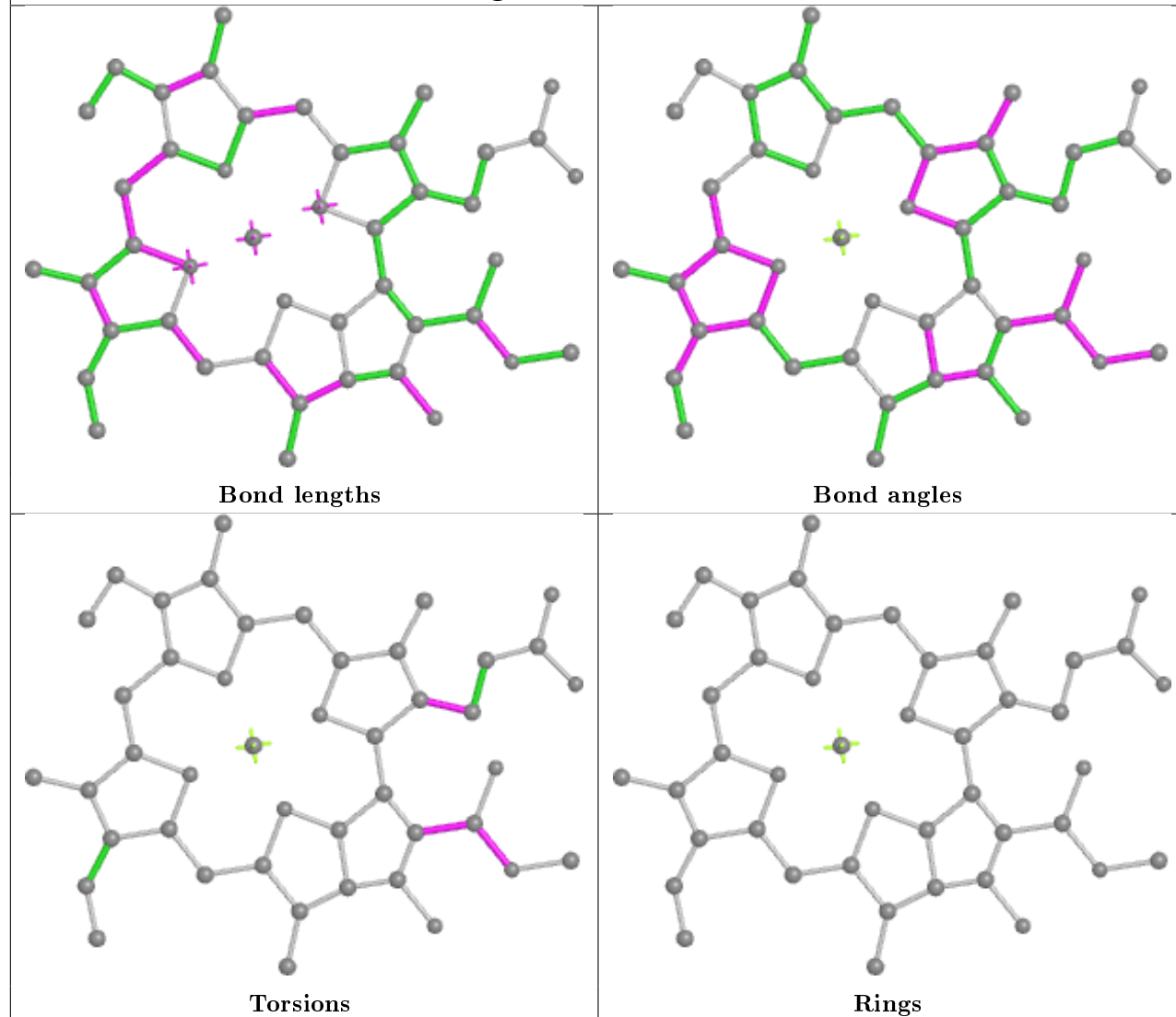
## Ligand CLA Y 807



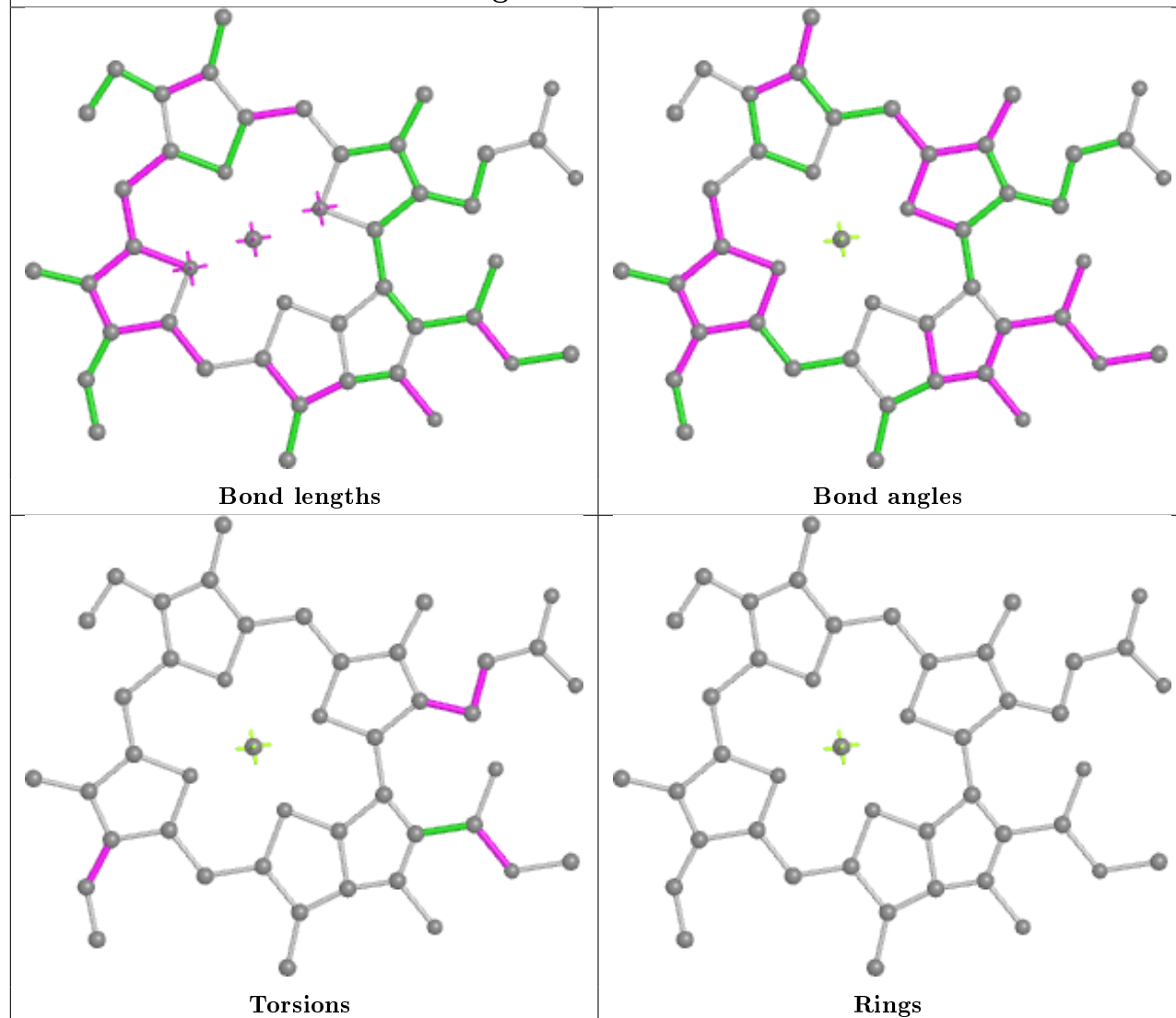
## Ligand BCR S 1104



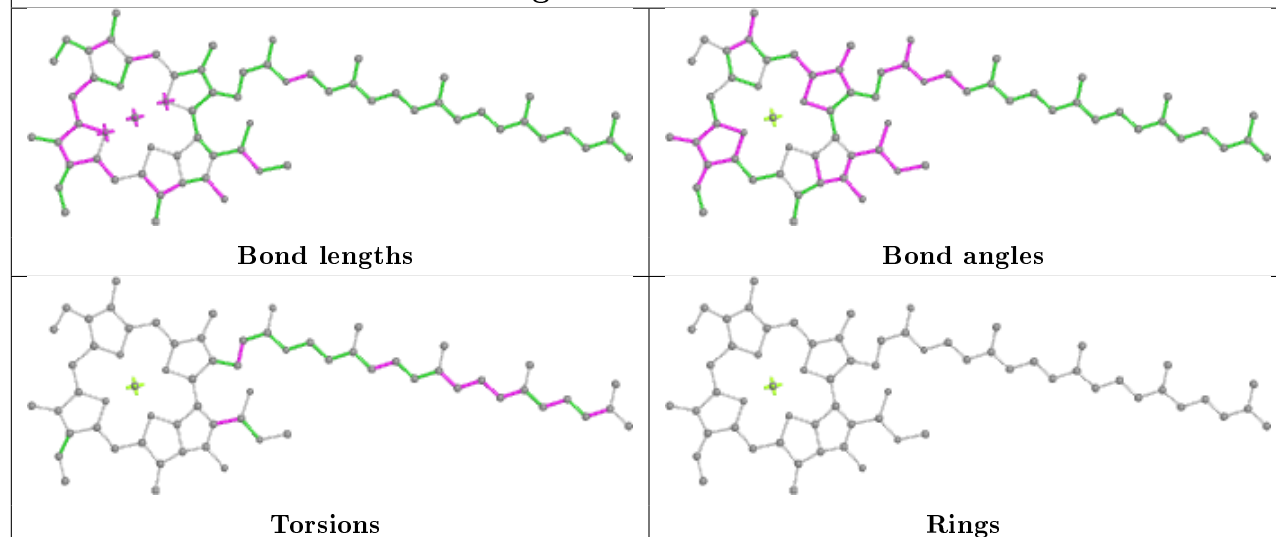
## Ligand CLA K 103



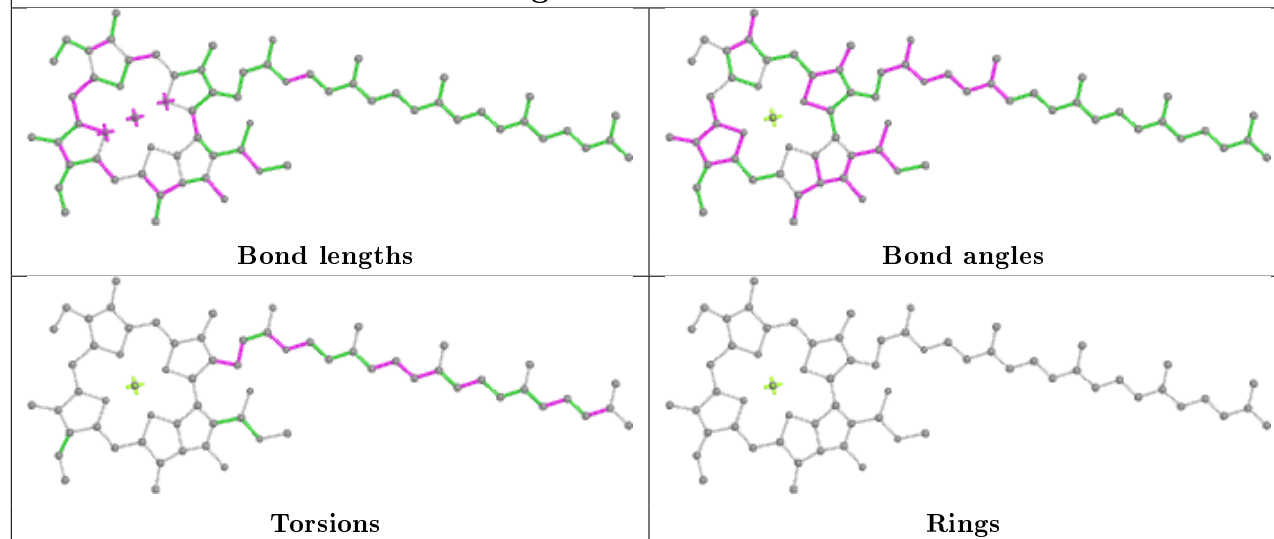
## Ligand CLA Z 829



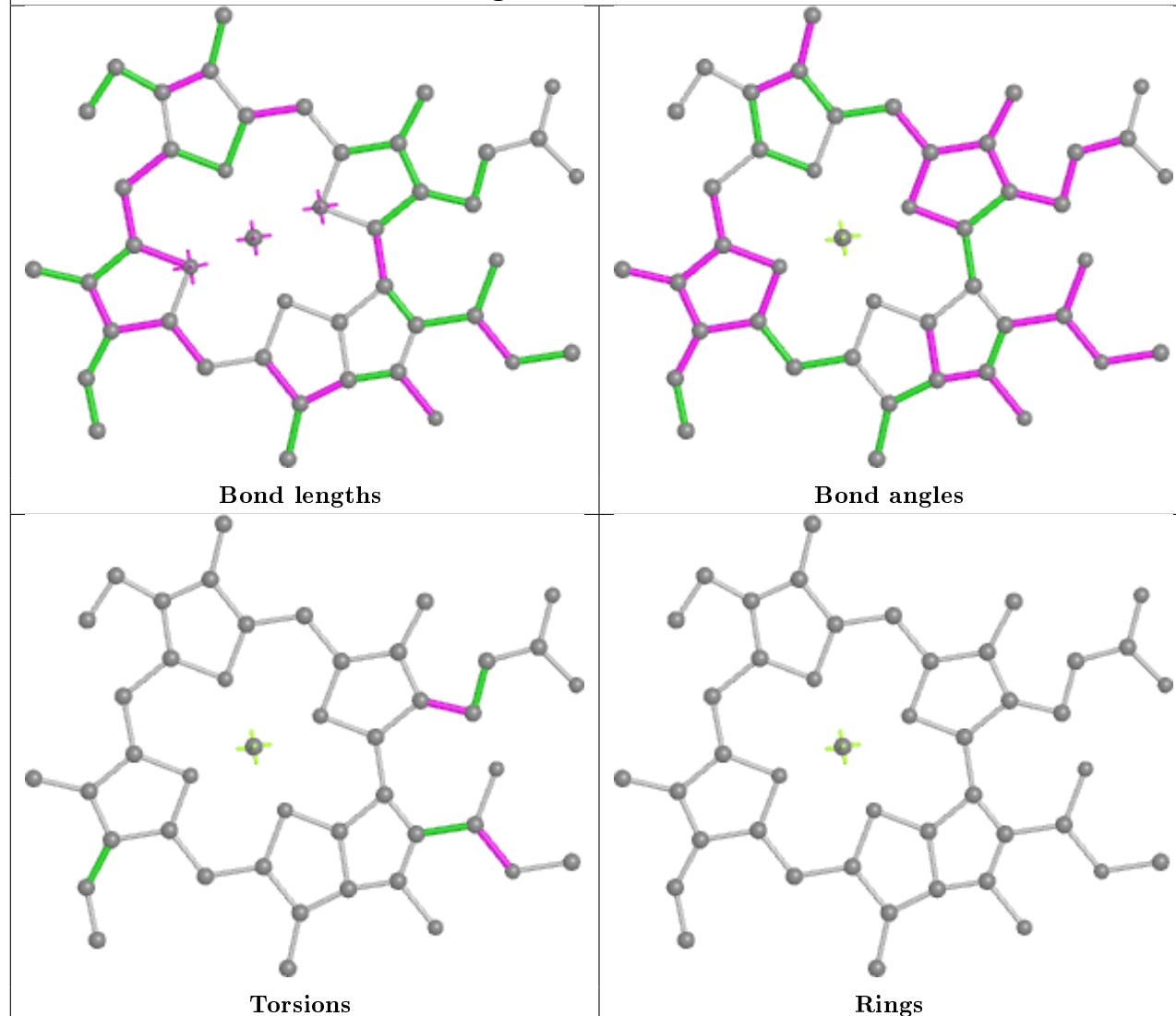
## Ligand CLA B 840



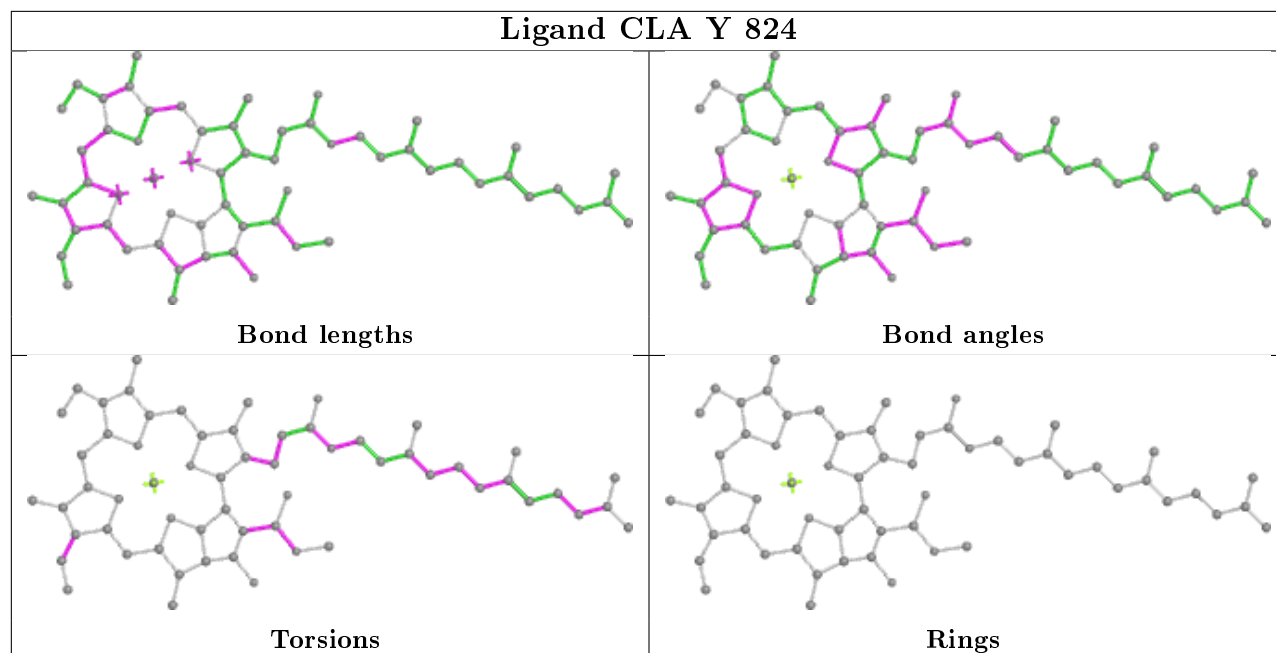
## Ligand CLA G 822



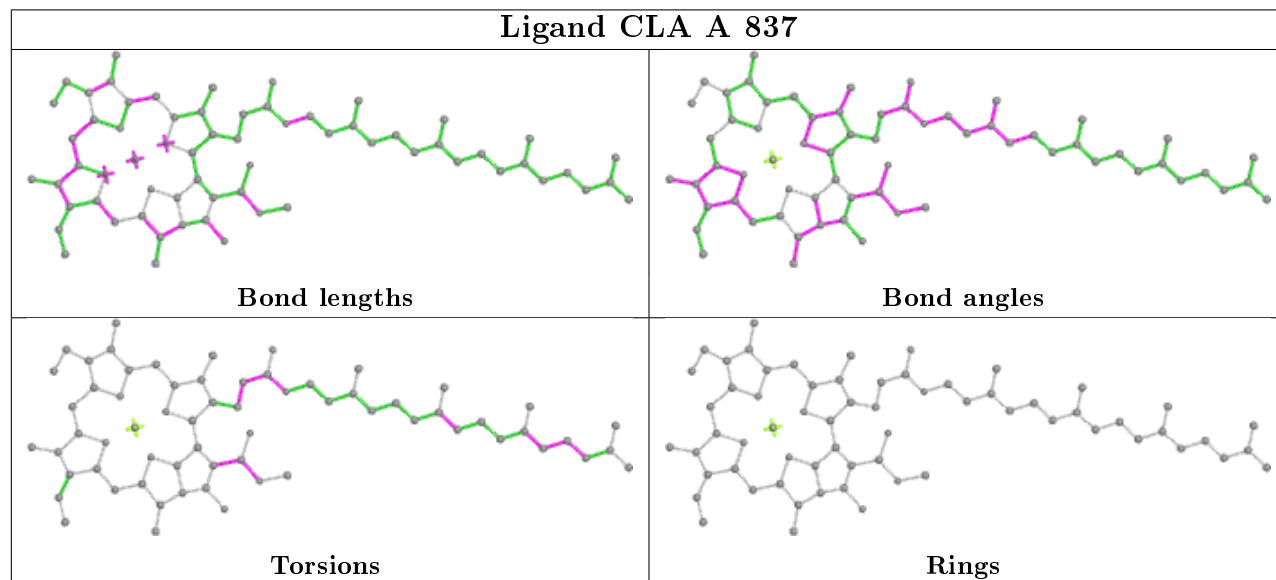
## Ligand CLA H 814



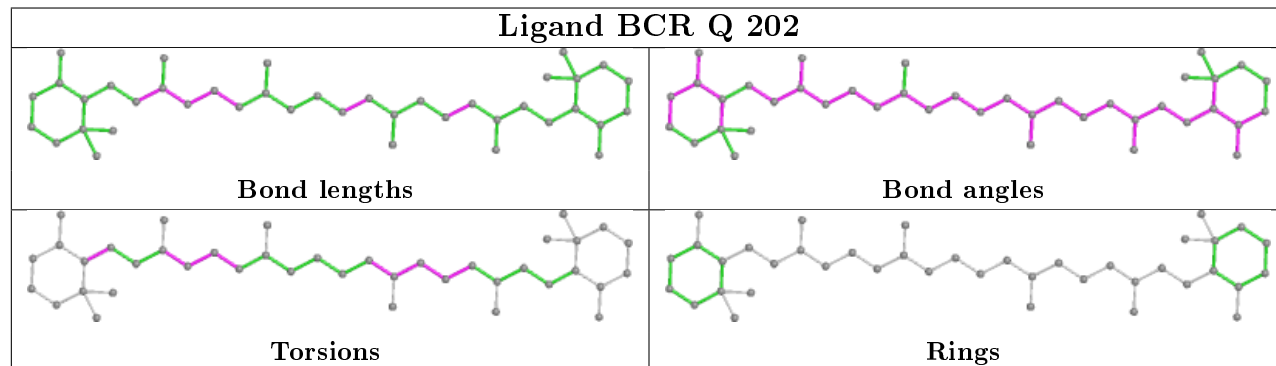
## Ligand CLA Y 824



## Ligand CLA A 837

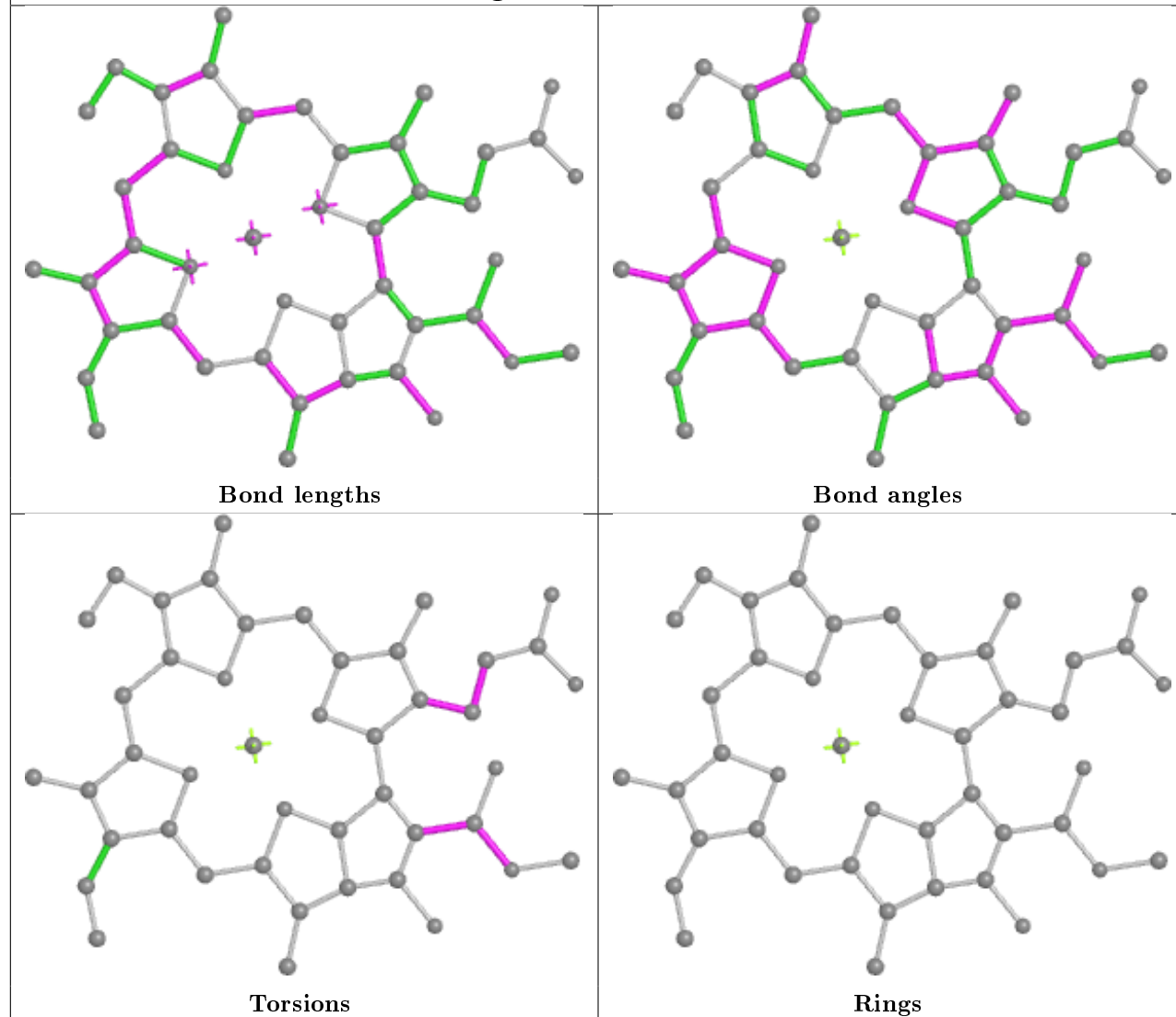


## Ligand BCR Q 202

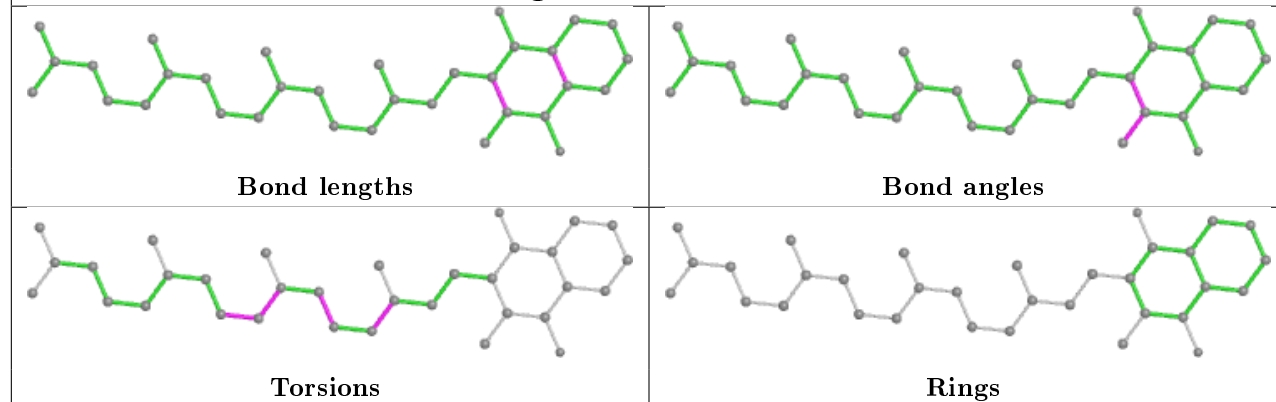




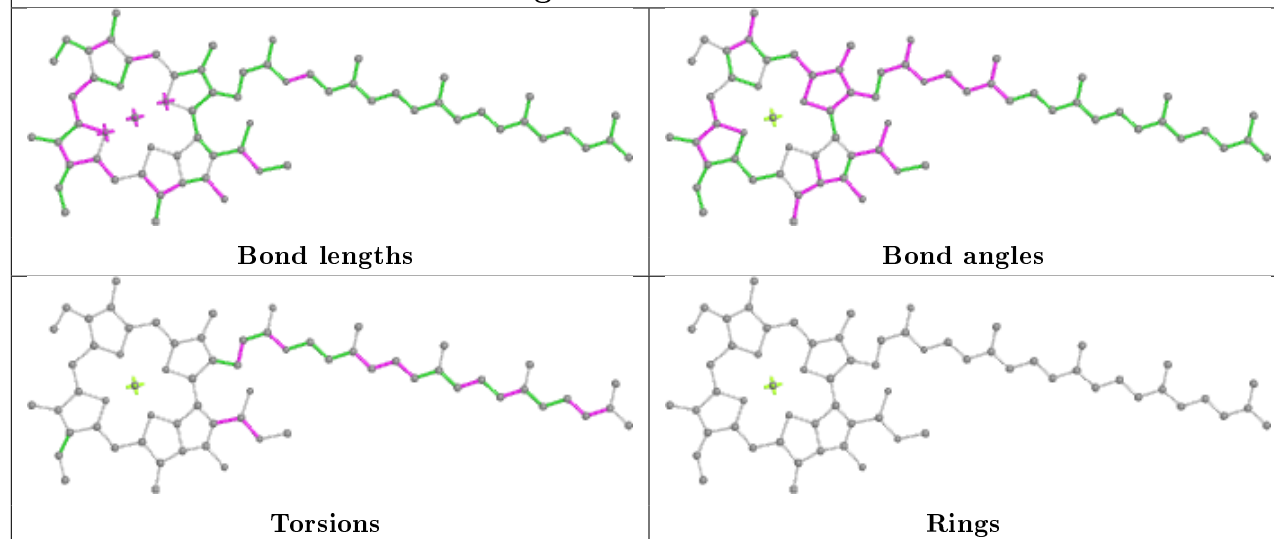
## Ligand CLA H 819



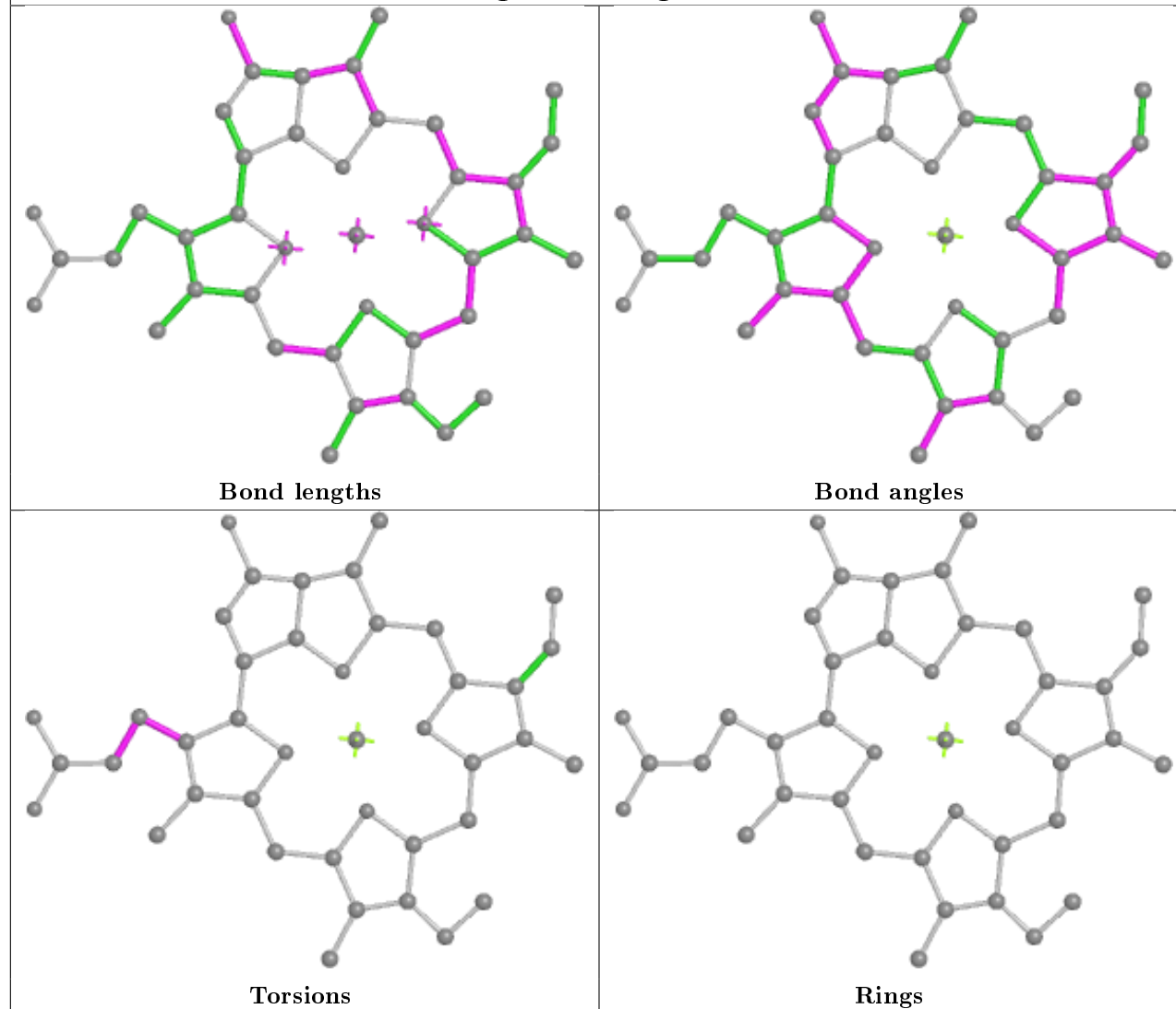
## Ligand PQN Y 844



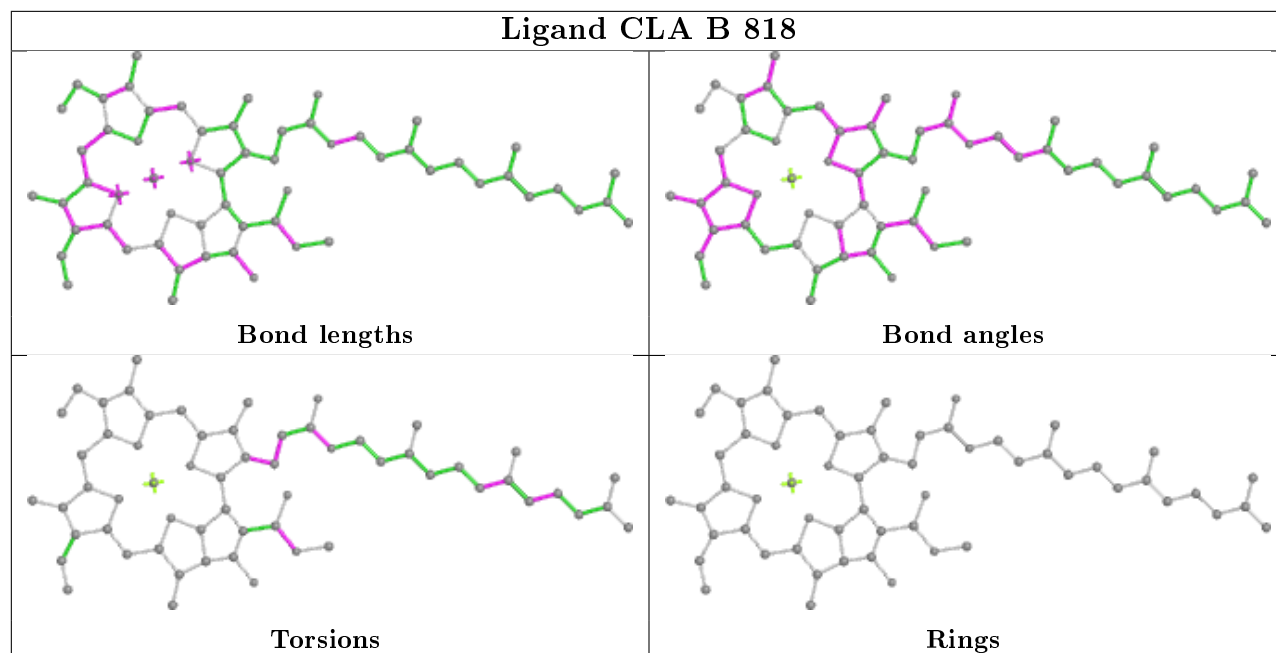
## Ligand CLA Z 823



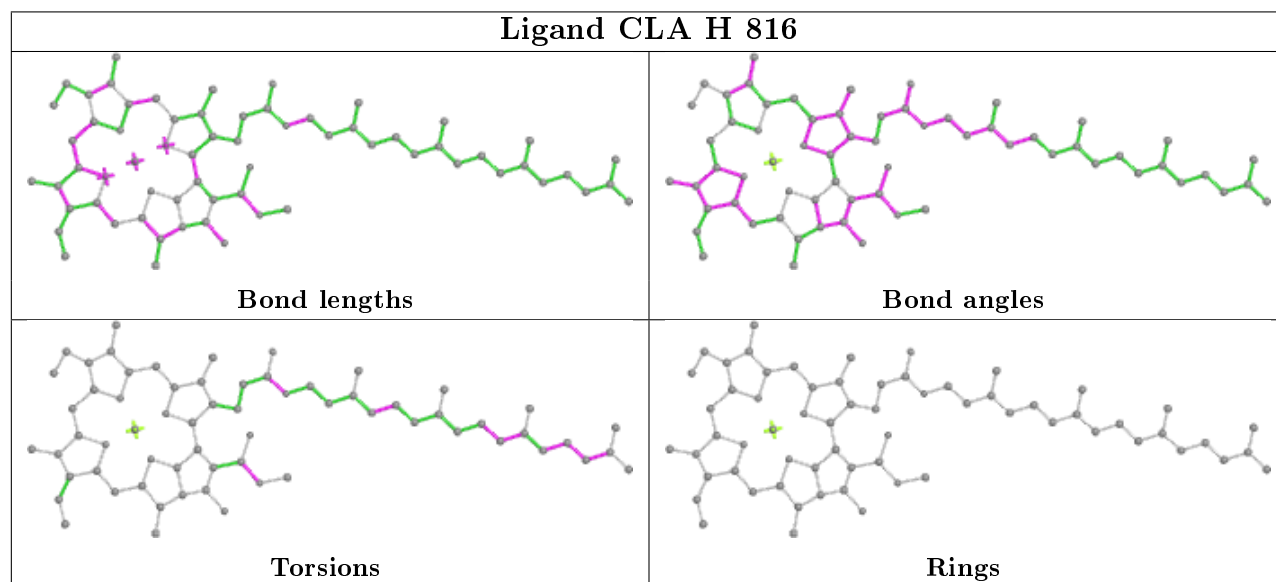
## Ligand CLA g 101



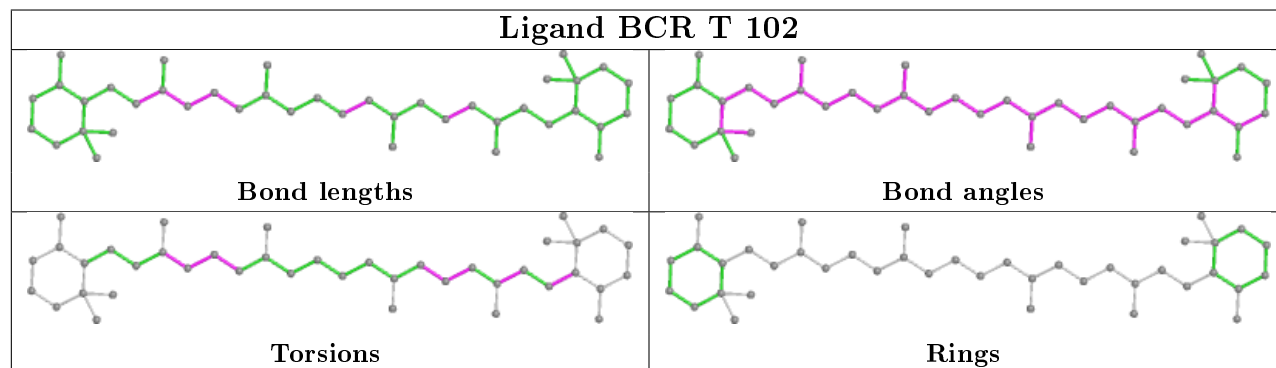
## Ligand CLA B 818

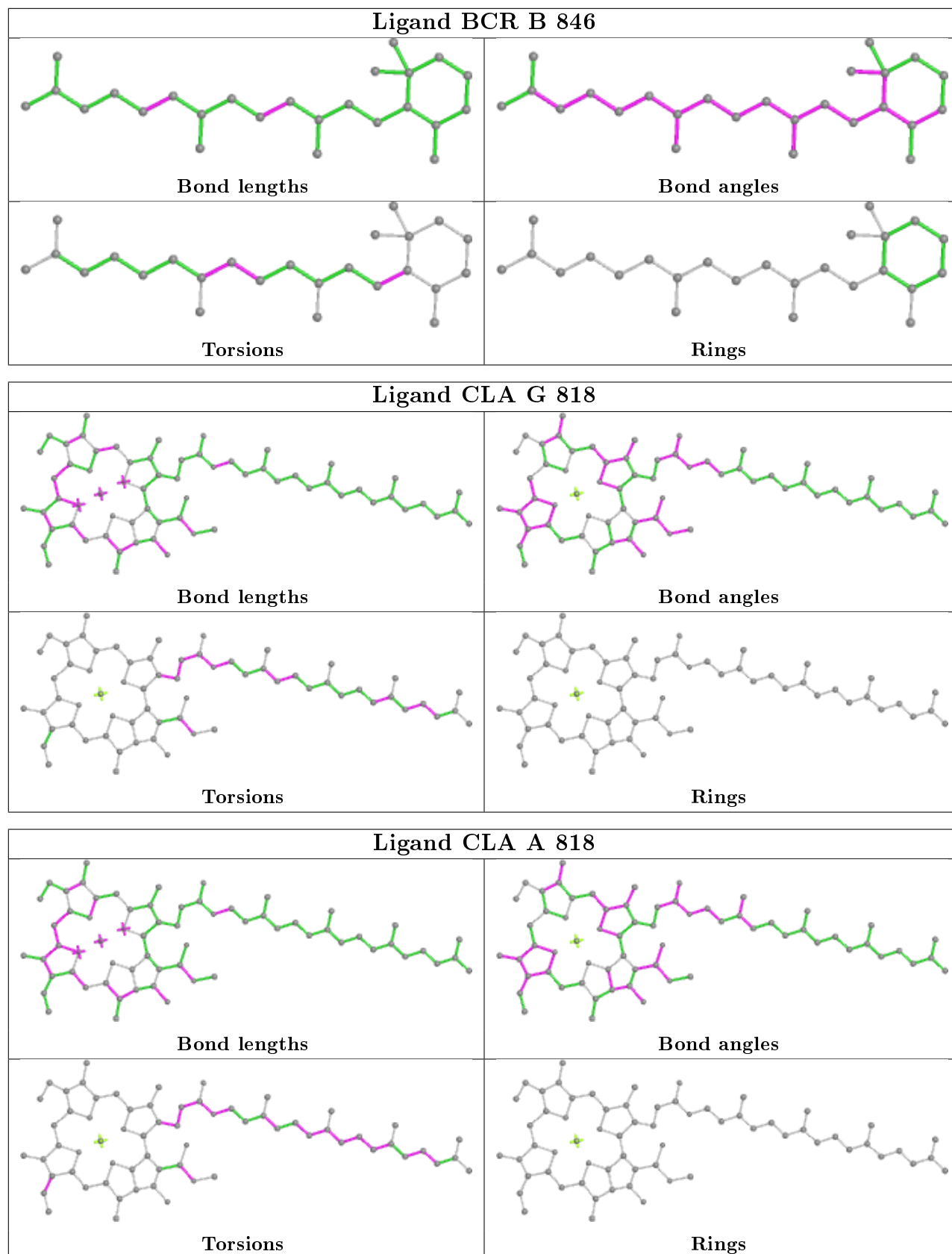


## Ligand CLA H 816

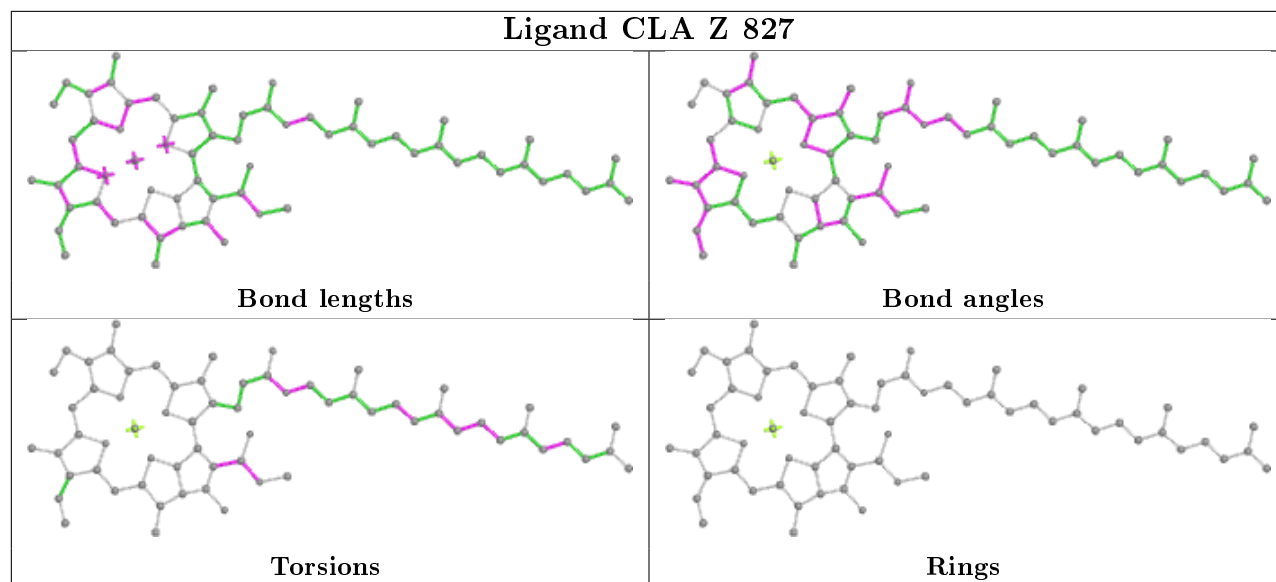


## Ligand BCR T 102

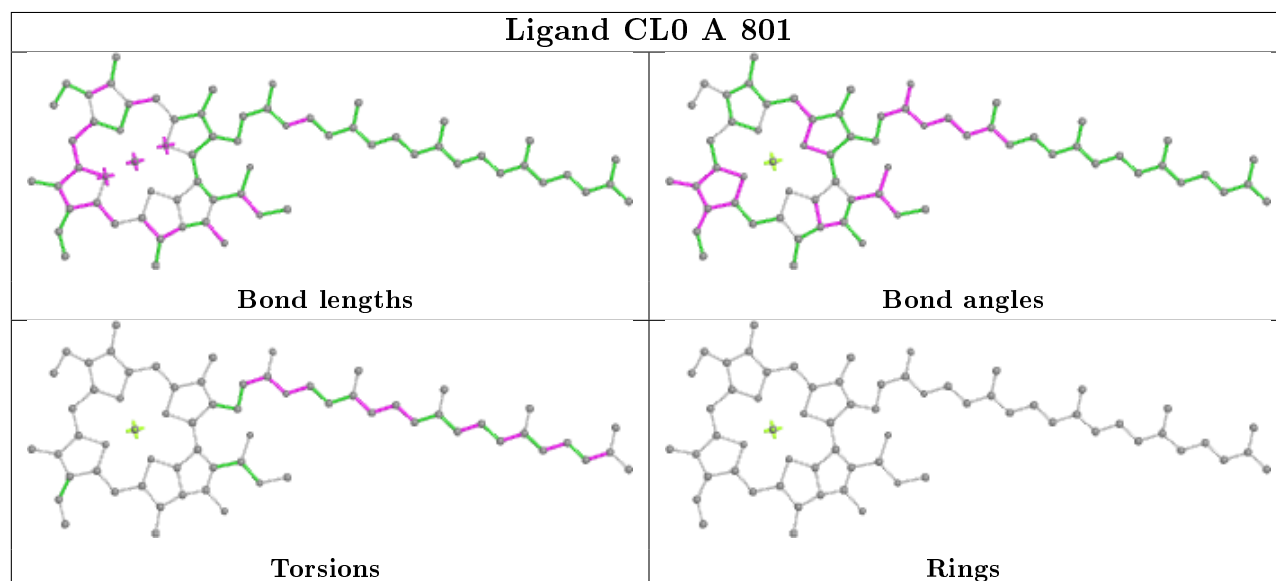




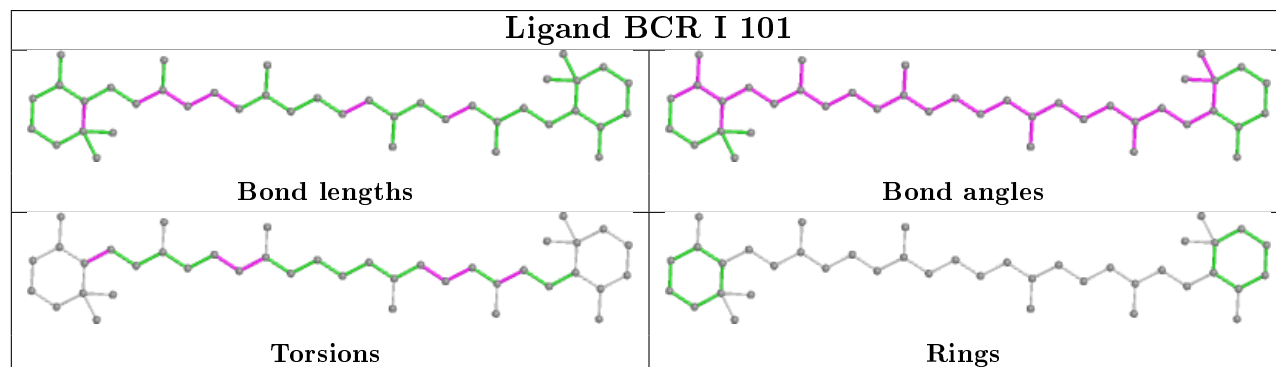
## Ligand CLA Z 827



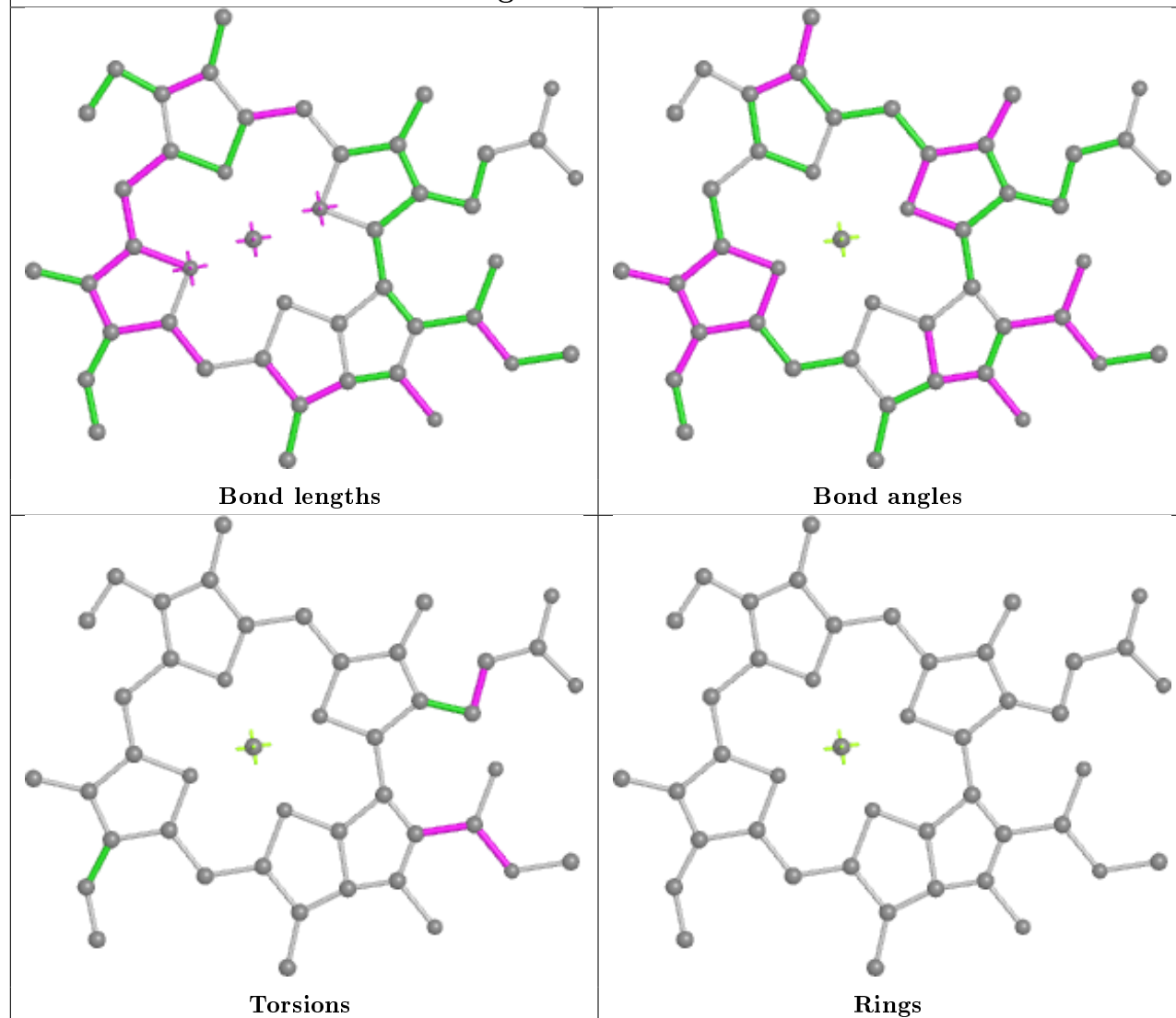
## Ligand CL0 A 801



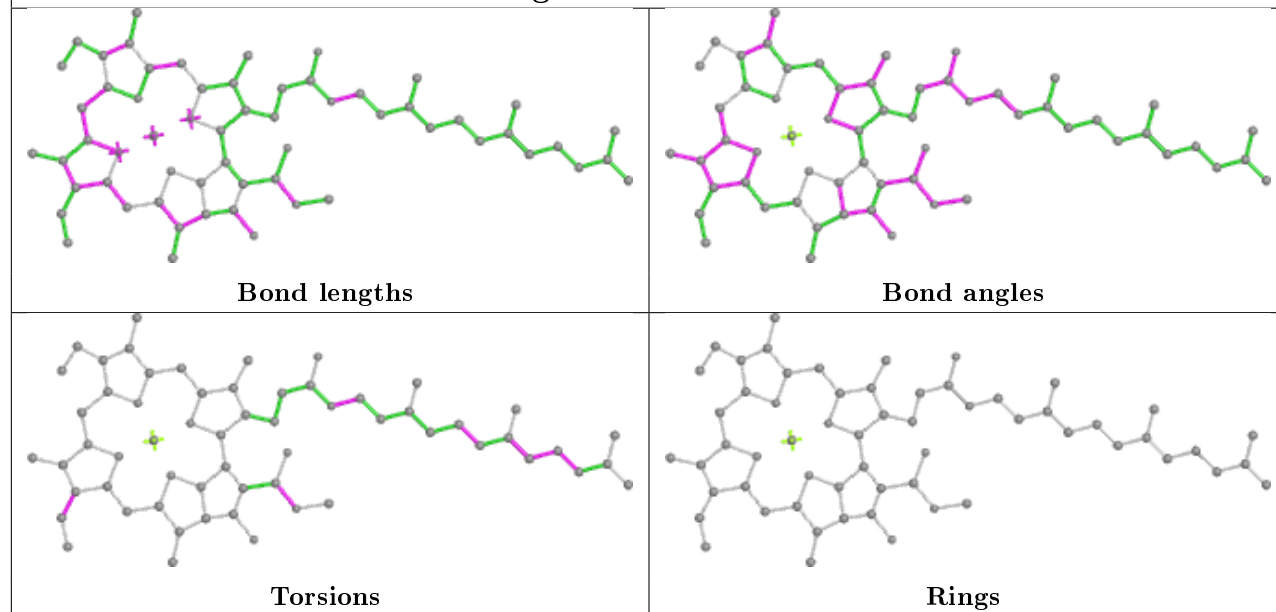
## Ligand BCR I 101



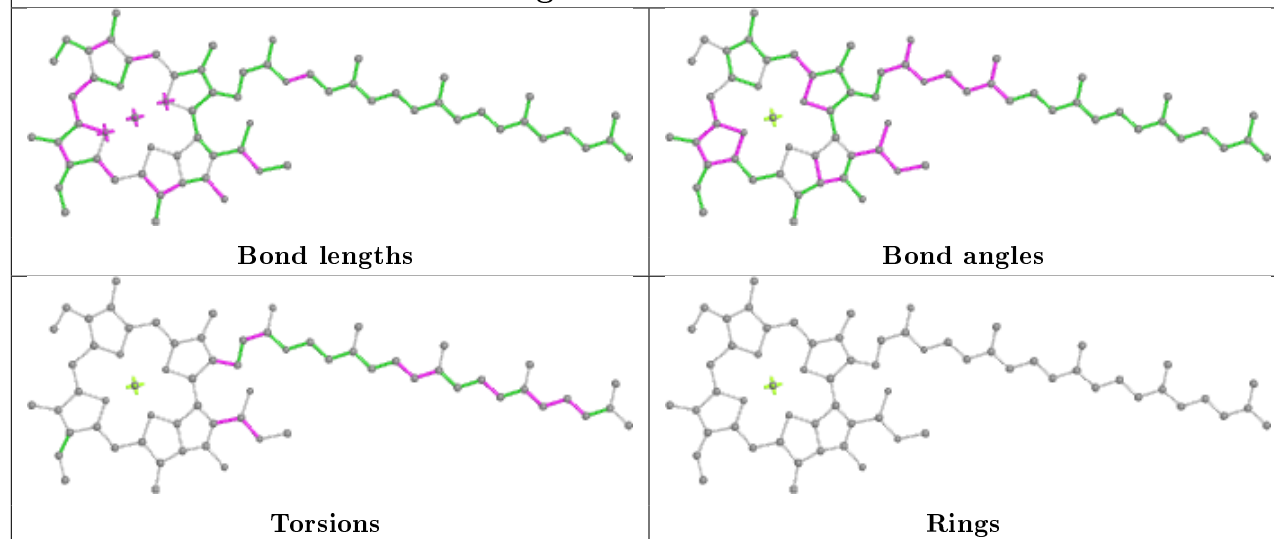
## Ligand CLA f 101



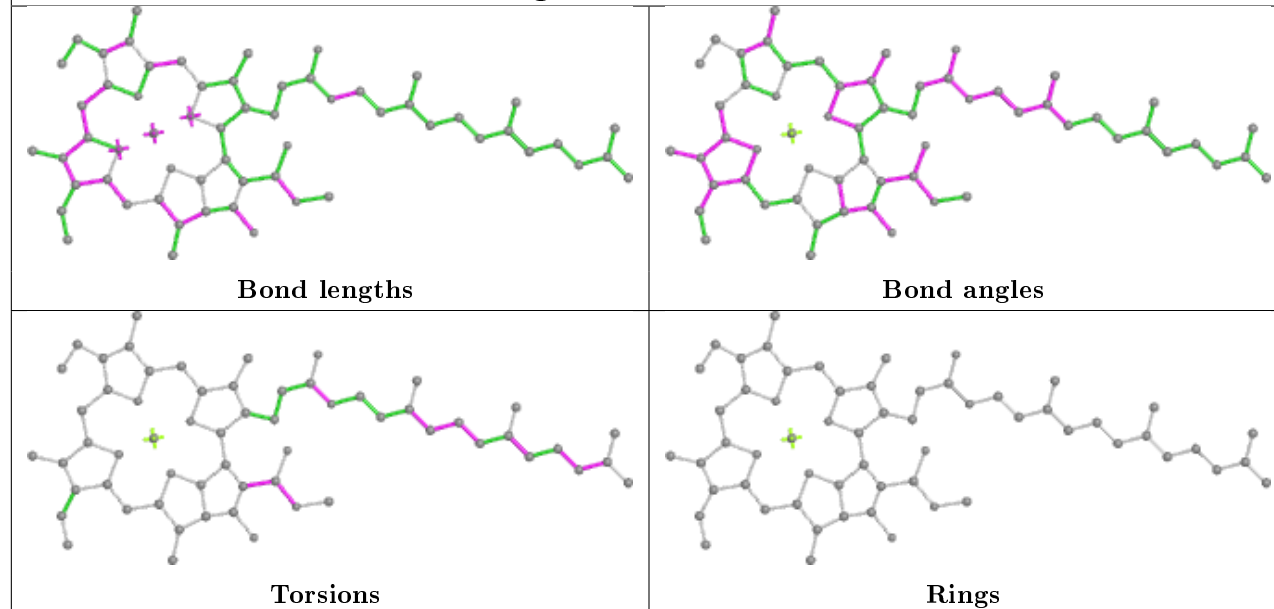
## Ligand CLA Y 817



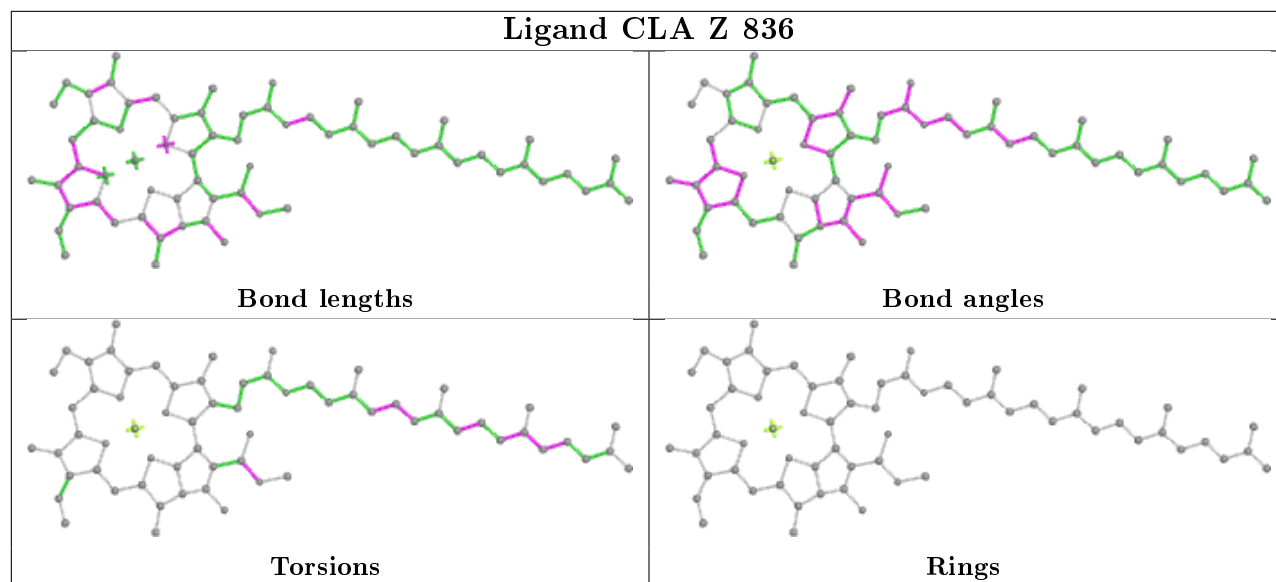
## Ligand CL0 Y 801



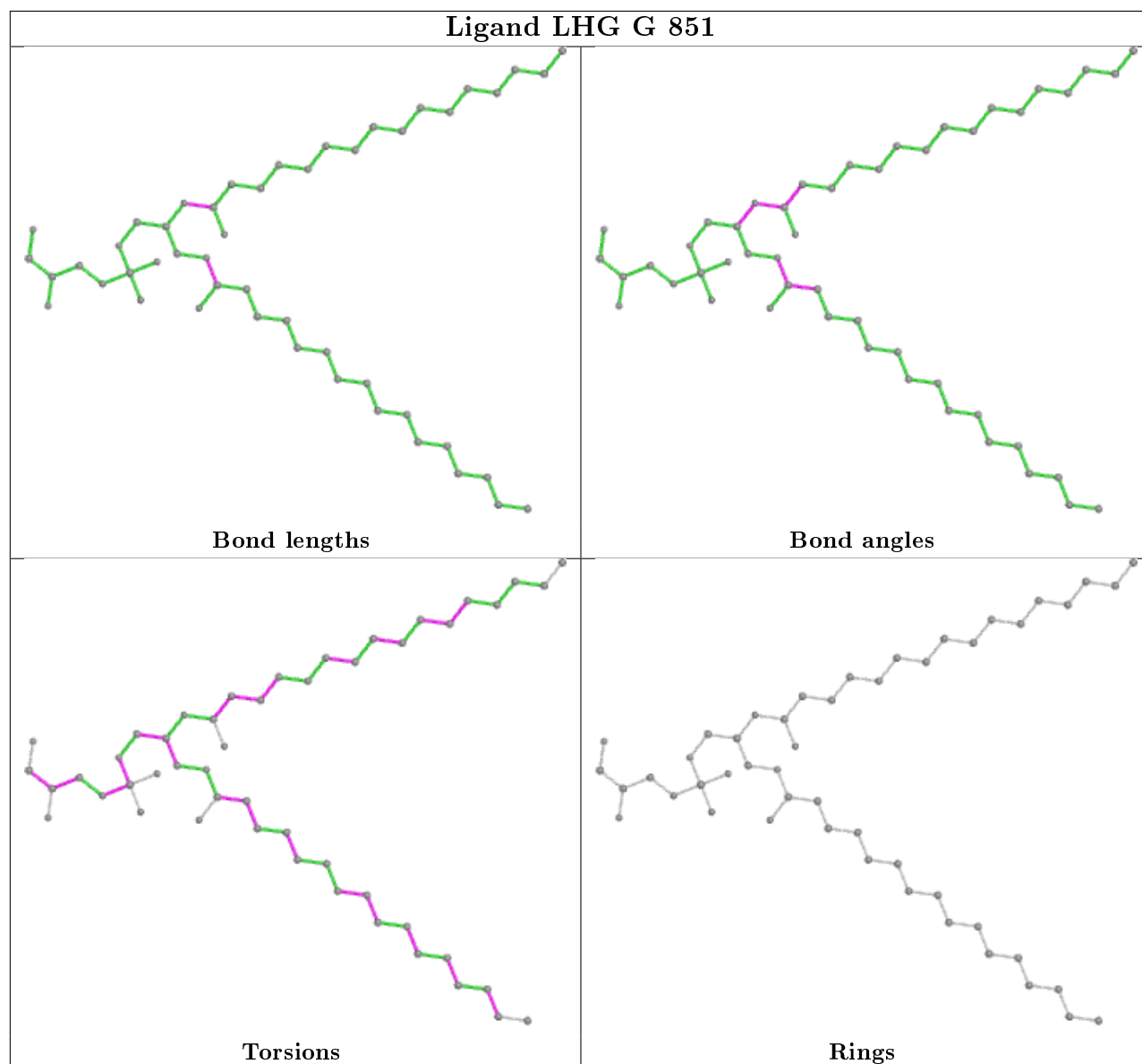
## Ligand CLA A 817



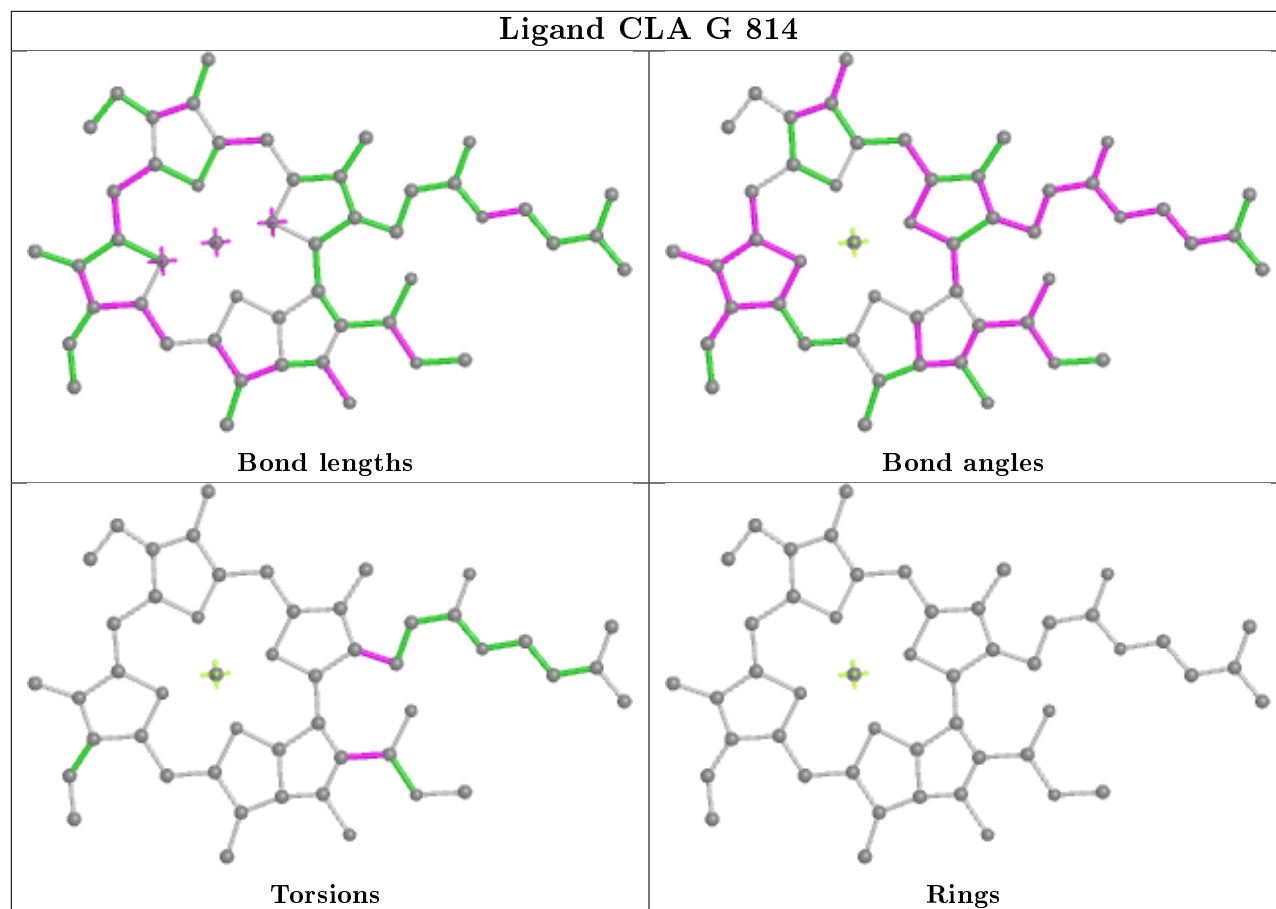
## Ligand CLA Z 836



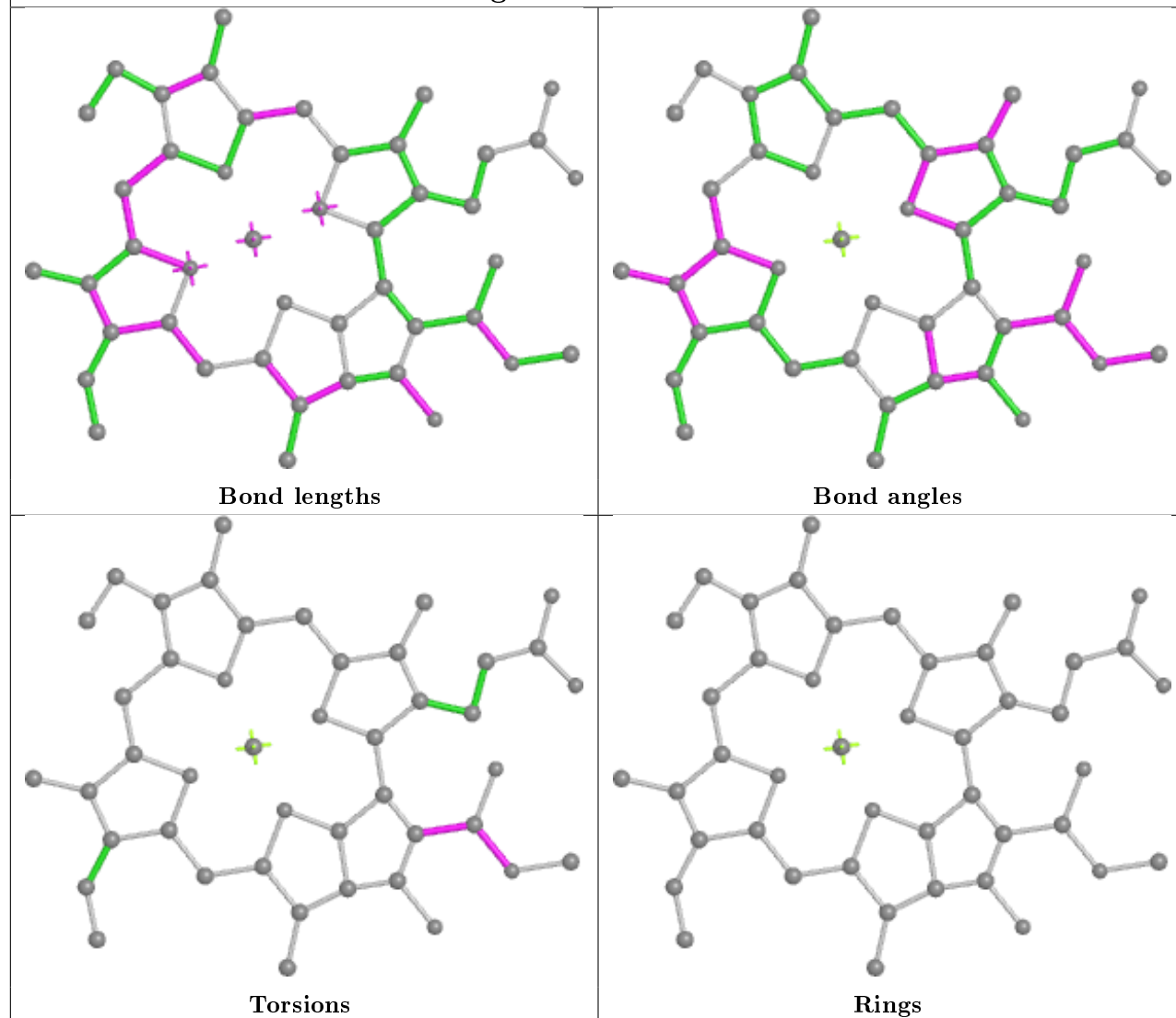
## Ligand LHG G 851



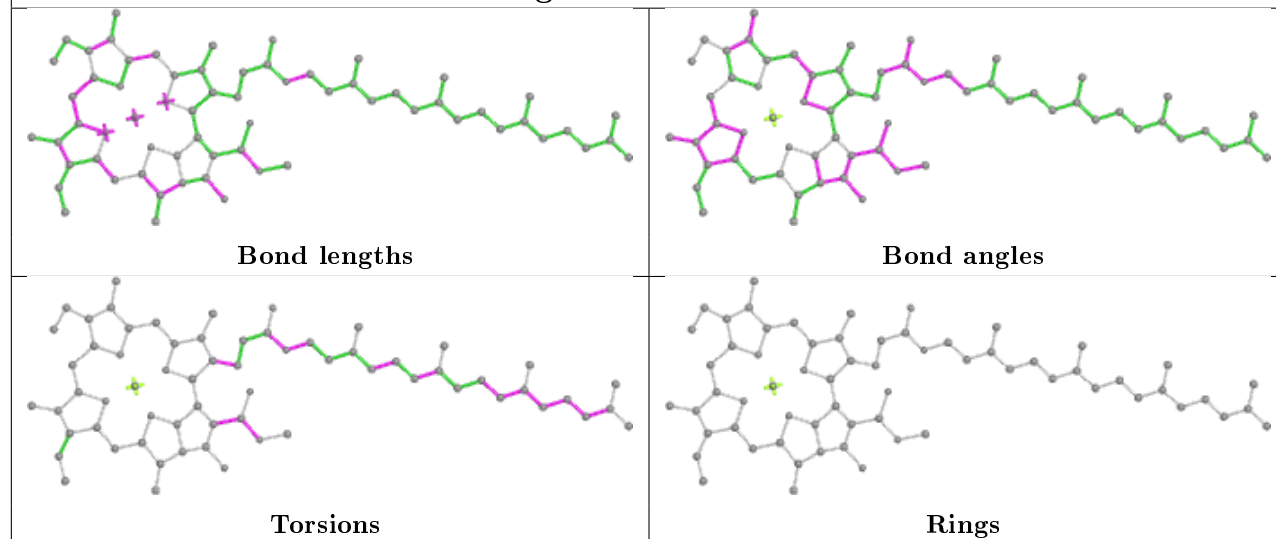




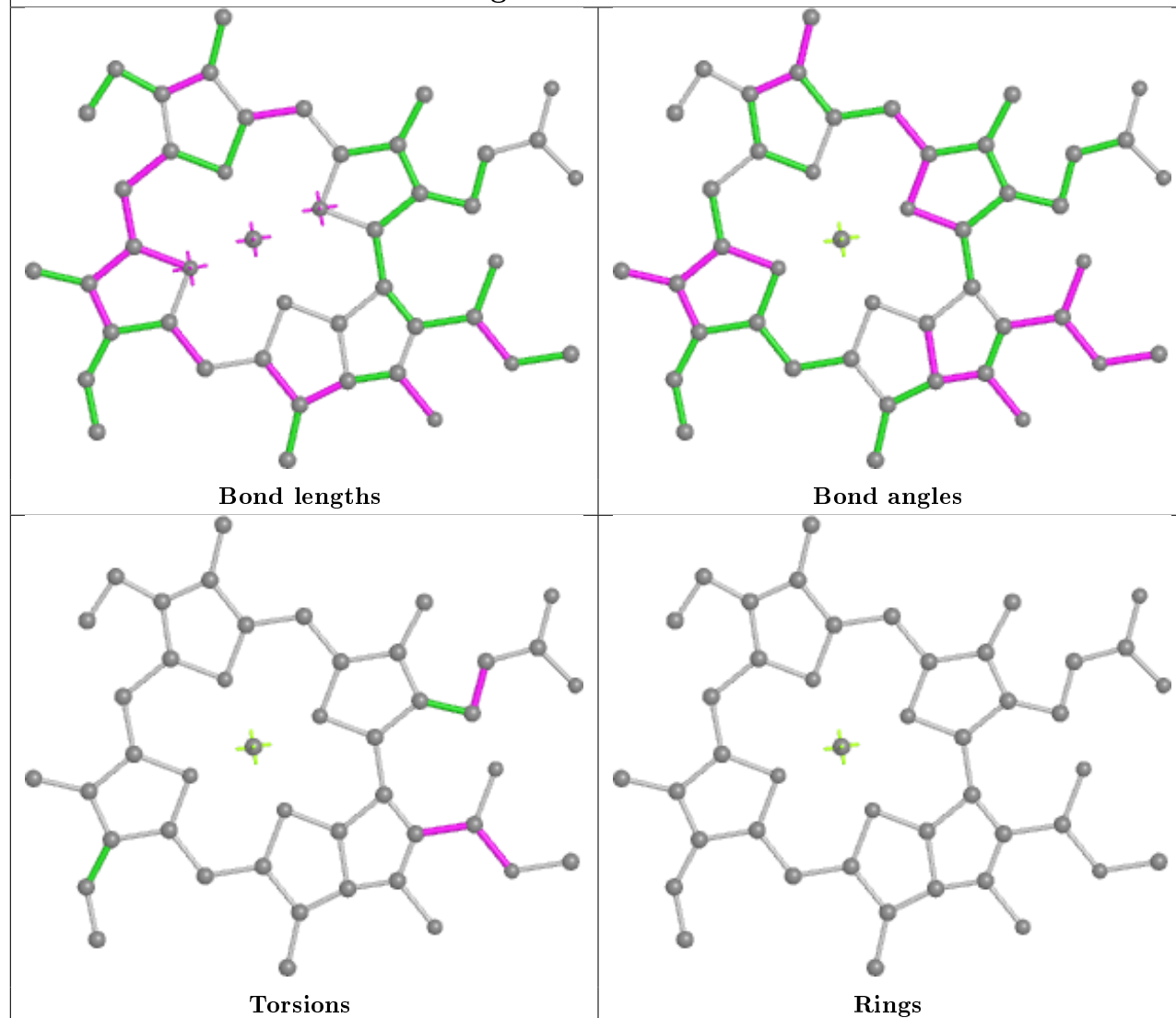
## Ligand CLA A 810



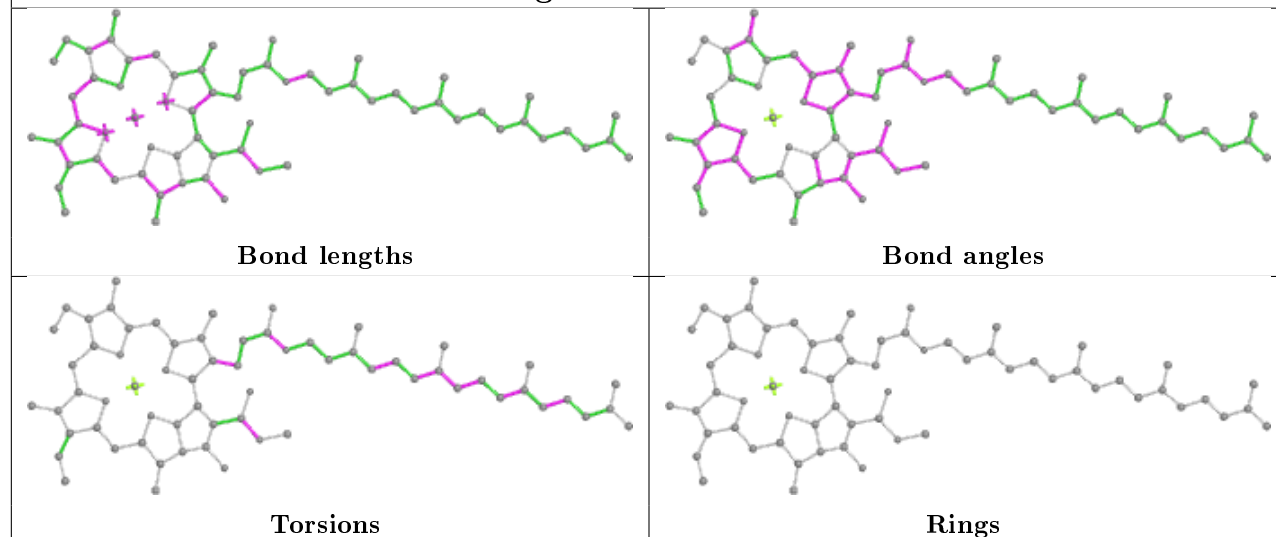
## Ligand CLA h 205



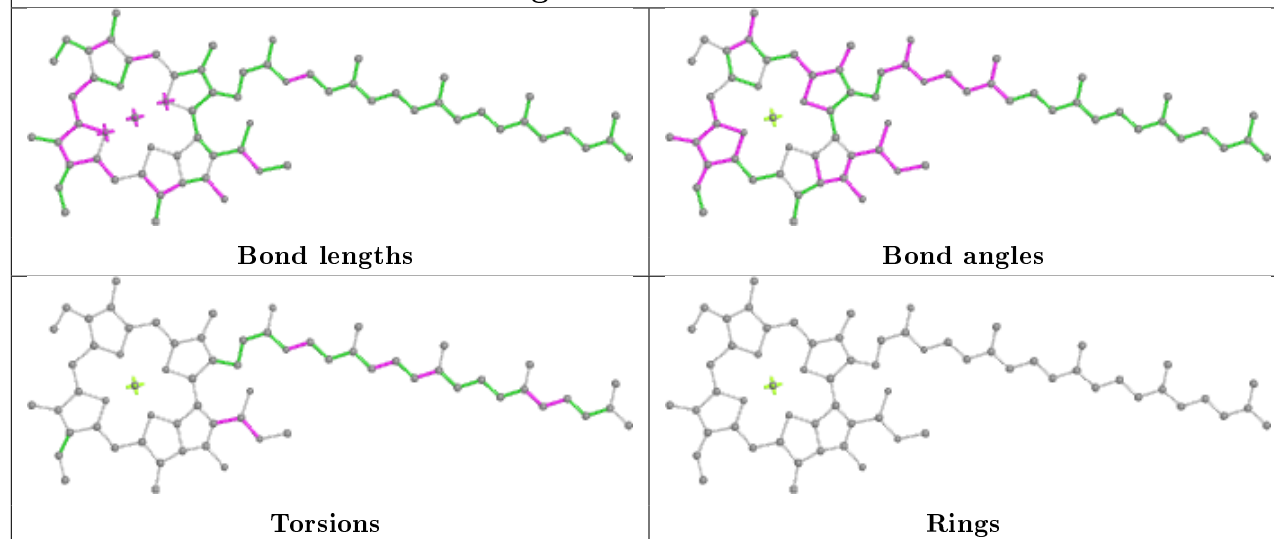
## Ligand CLA Y 836



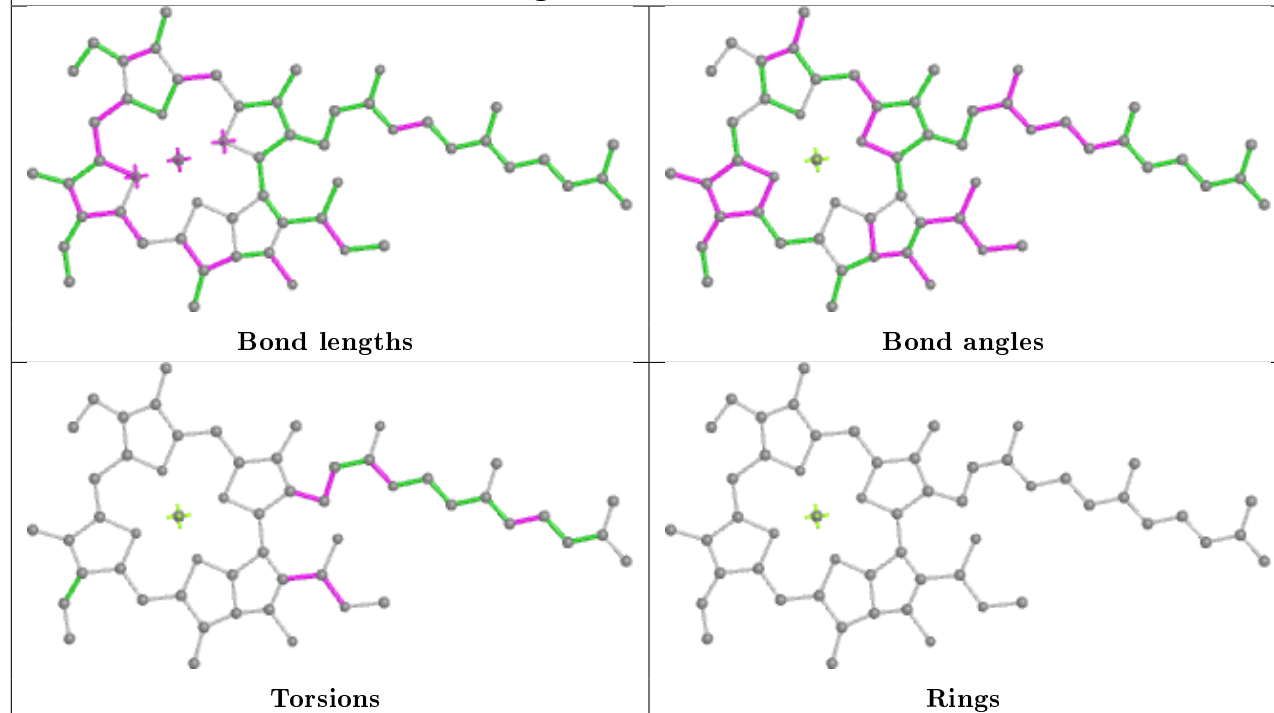
## Ligand CLA h 206



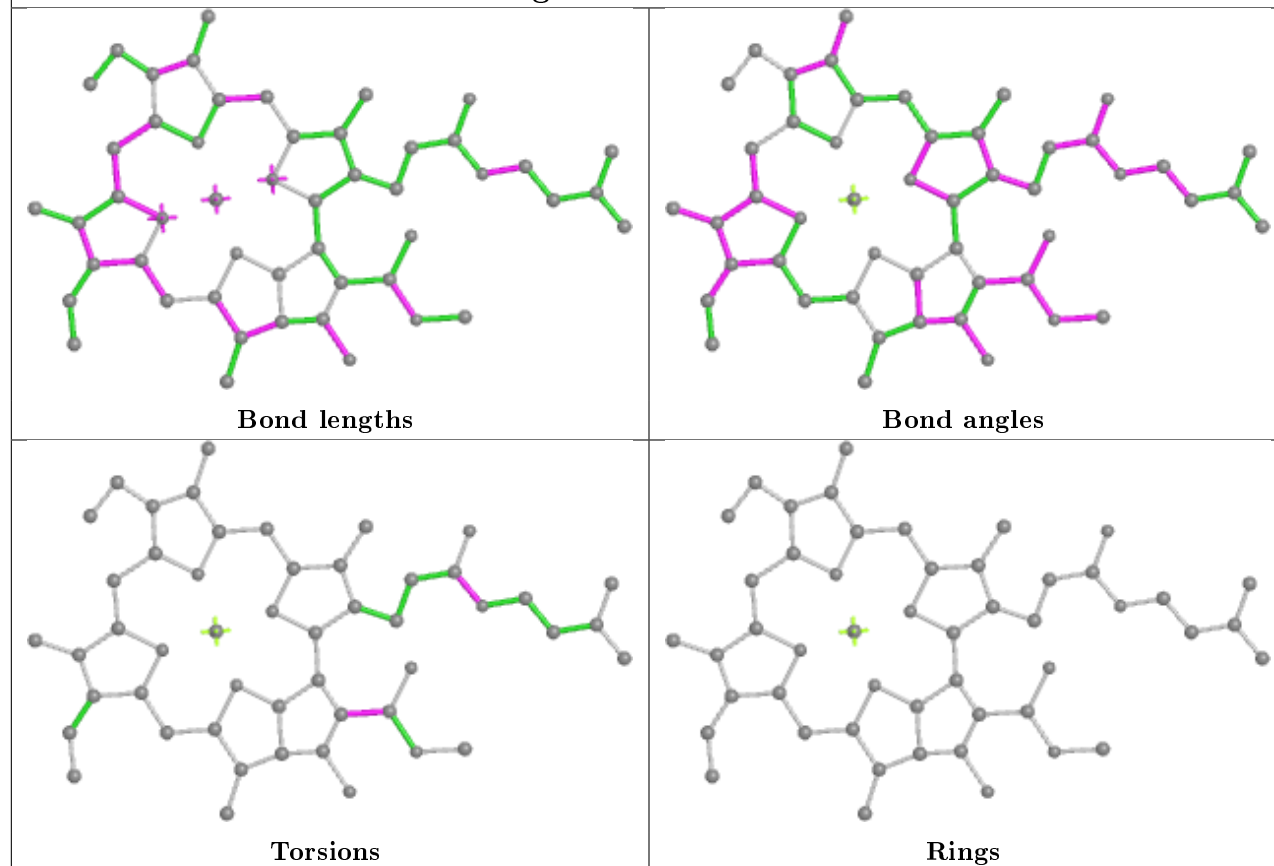
## Ligand CLA H 825



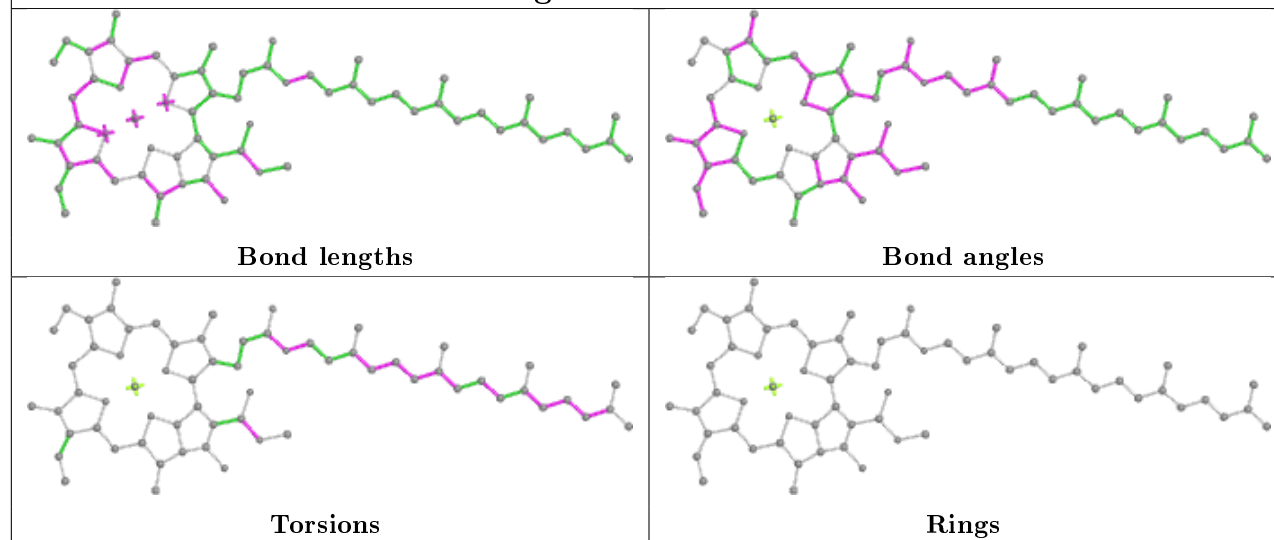
## Ligand CLA A 834

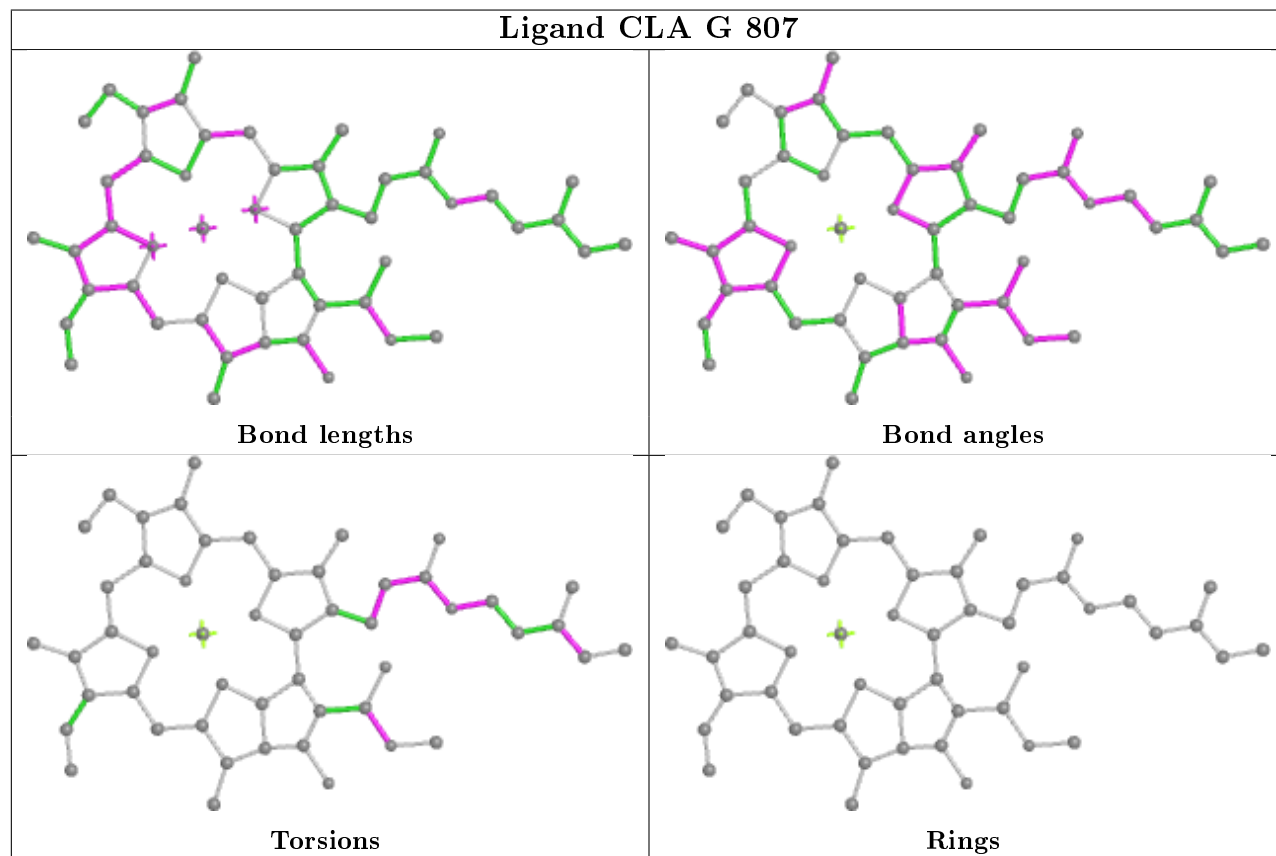
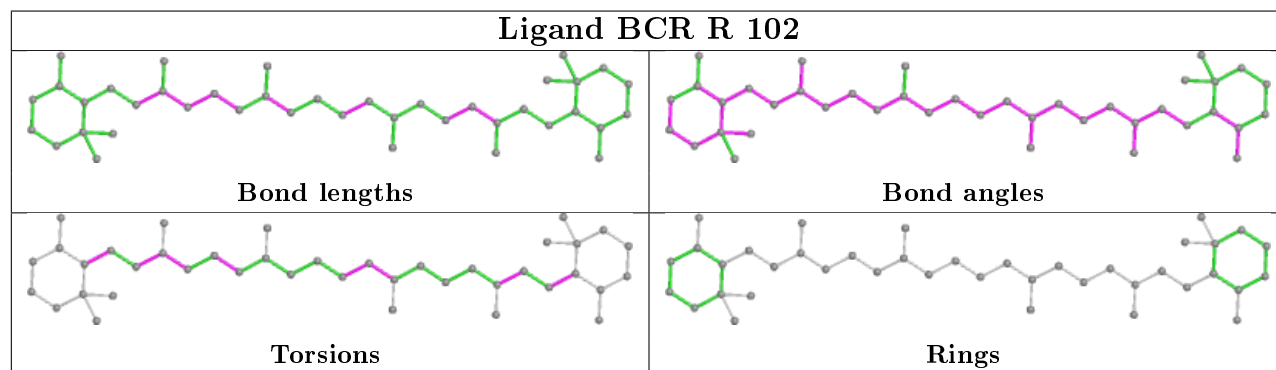
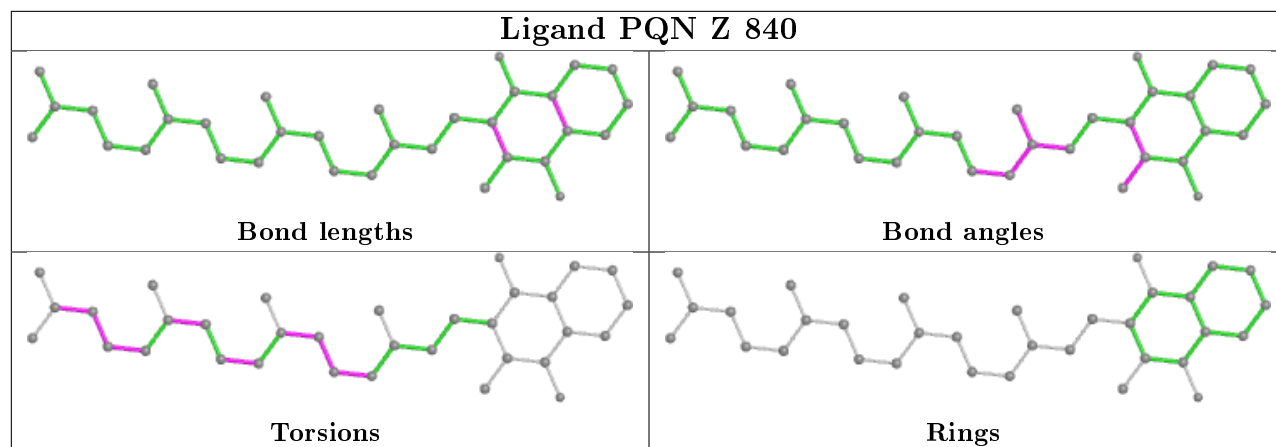


## Ligand CLA Y 831

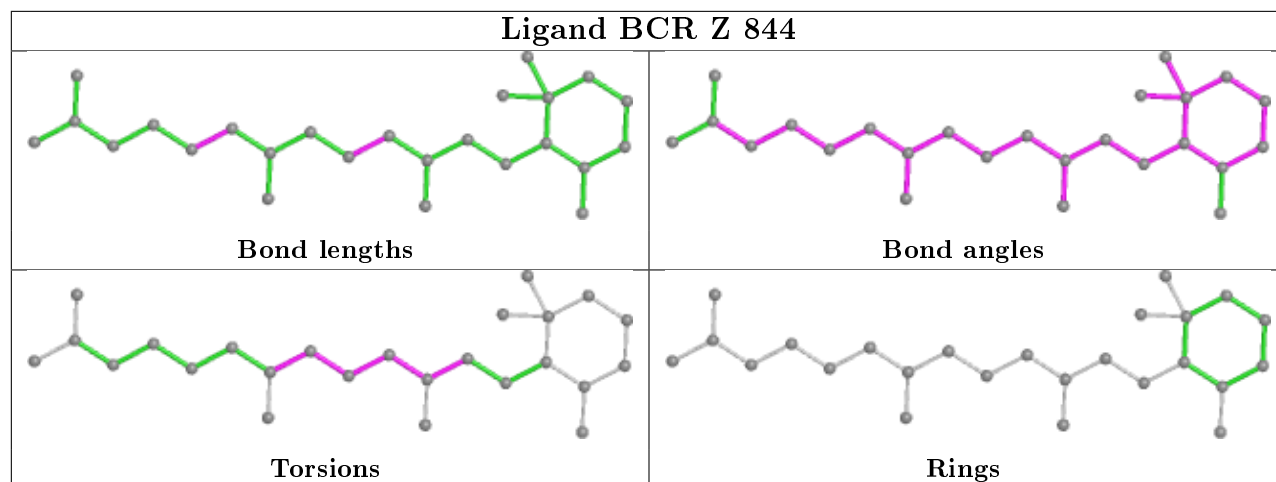


## Ligand CLA Z 805

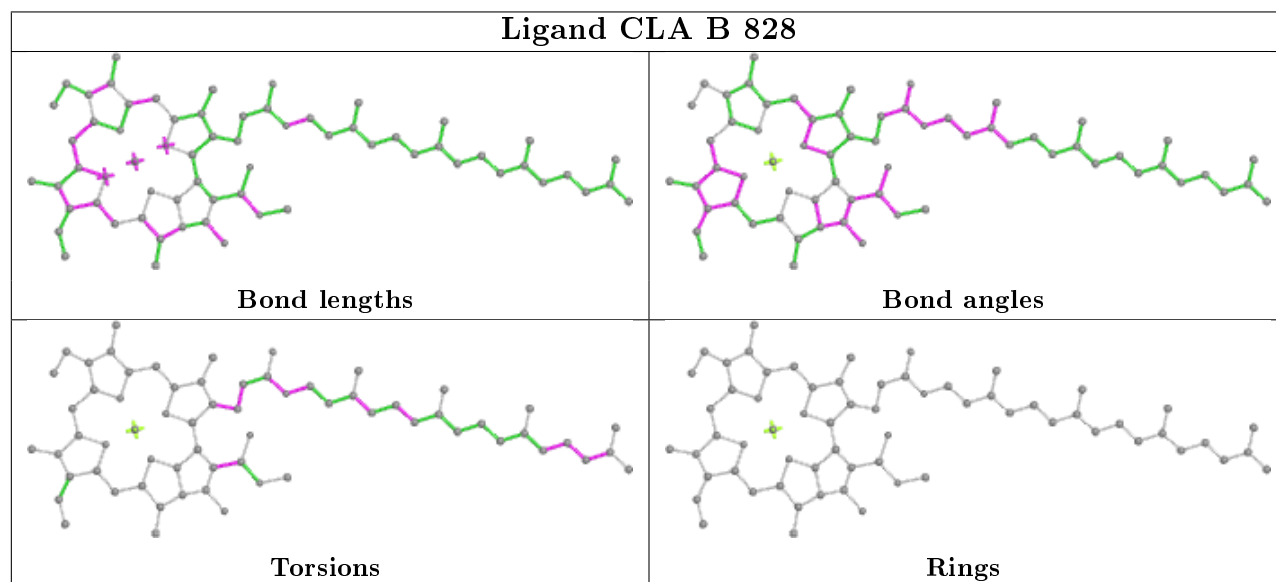




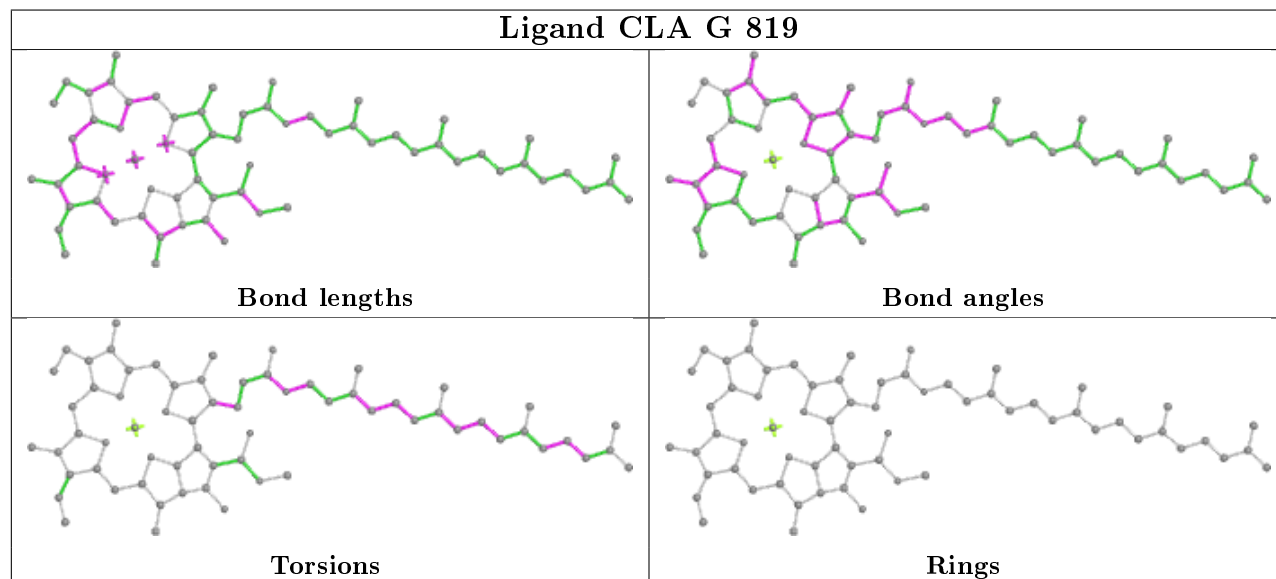
## Ligand BCR Z 844



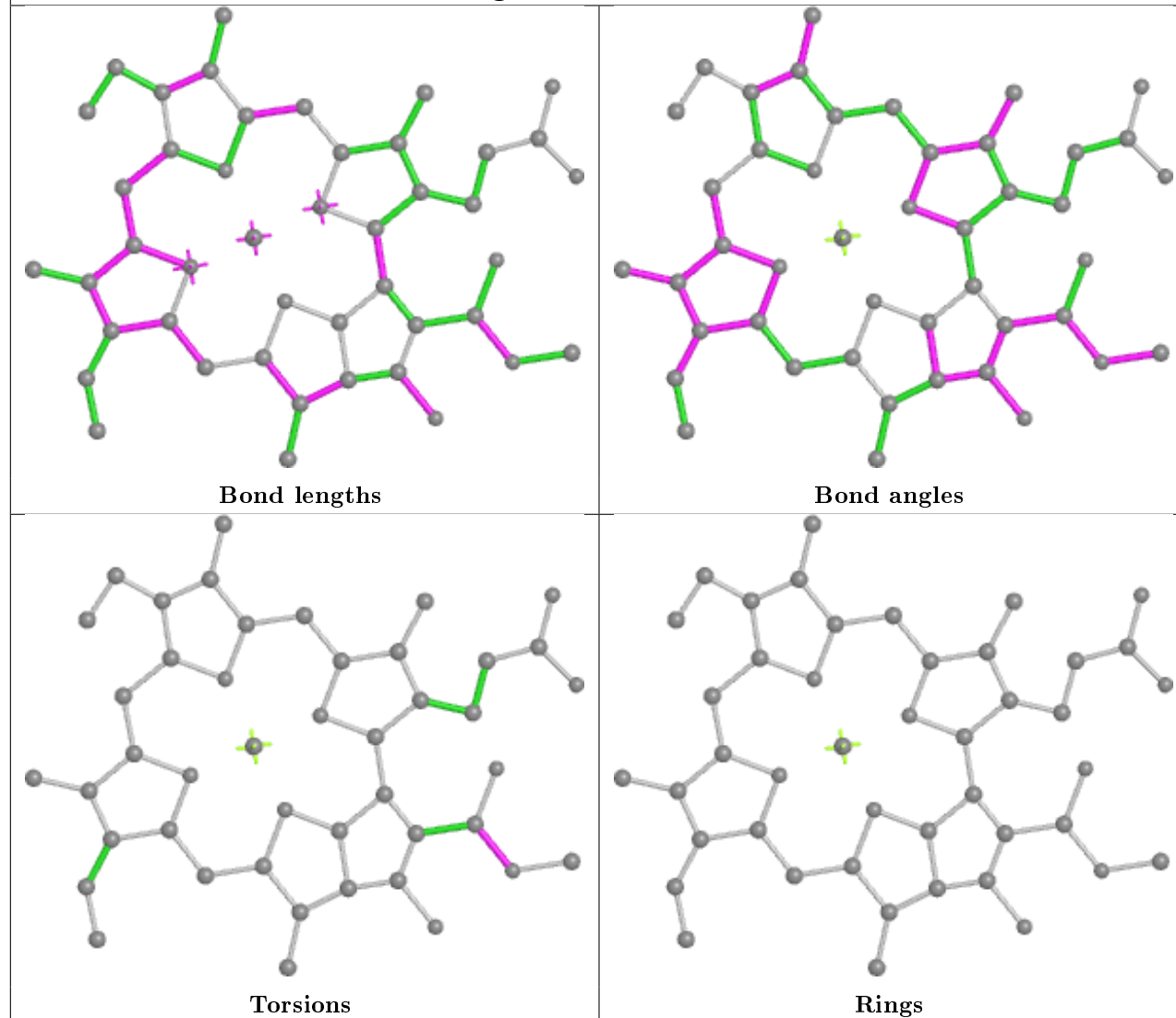
## Ligand CLA B 828



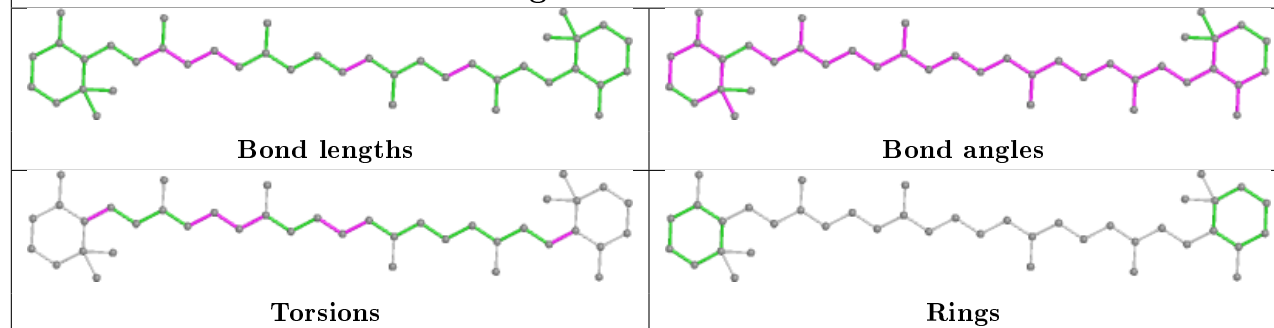
## Ligand CLA G 819



## Ligand CLA B 835

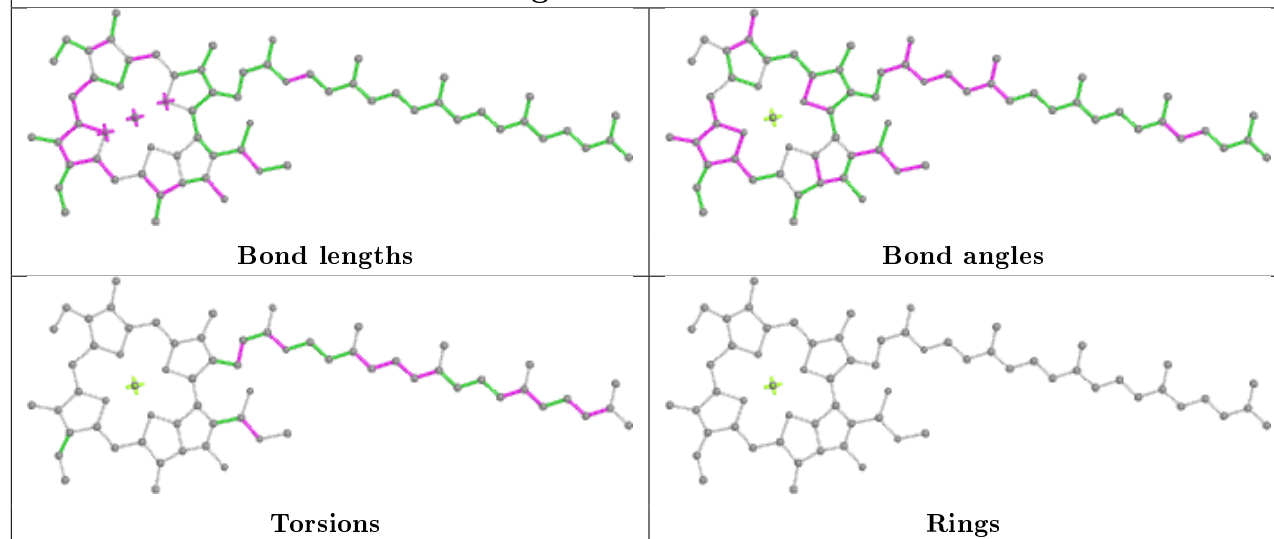


## Ligand BCR H 848

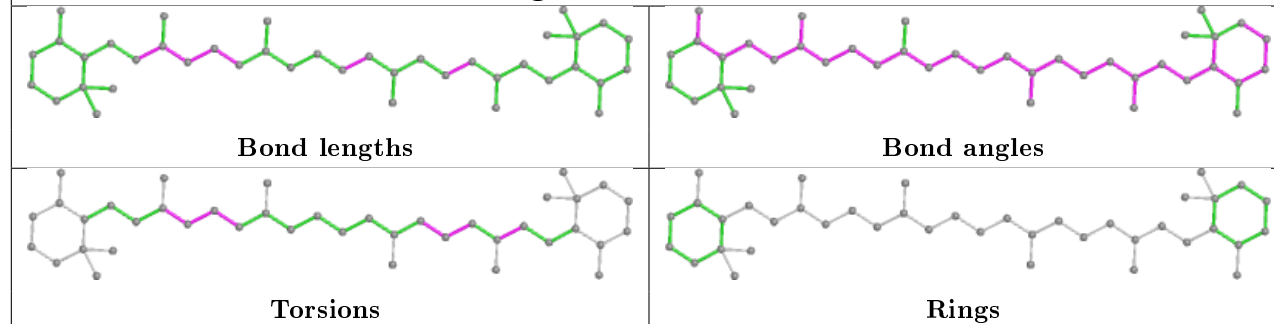




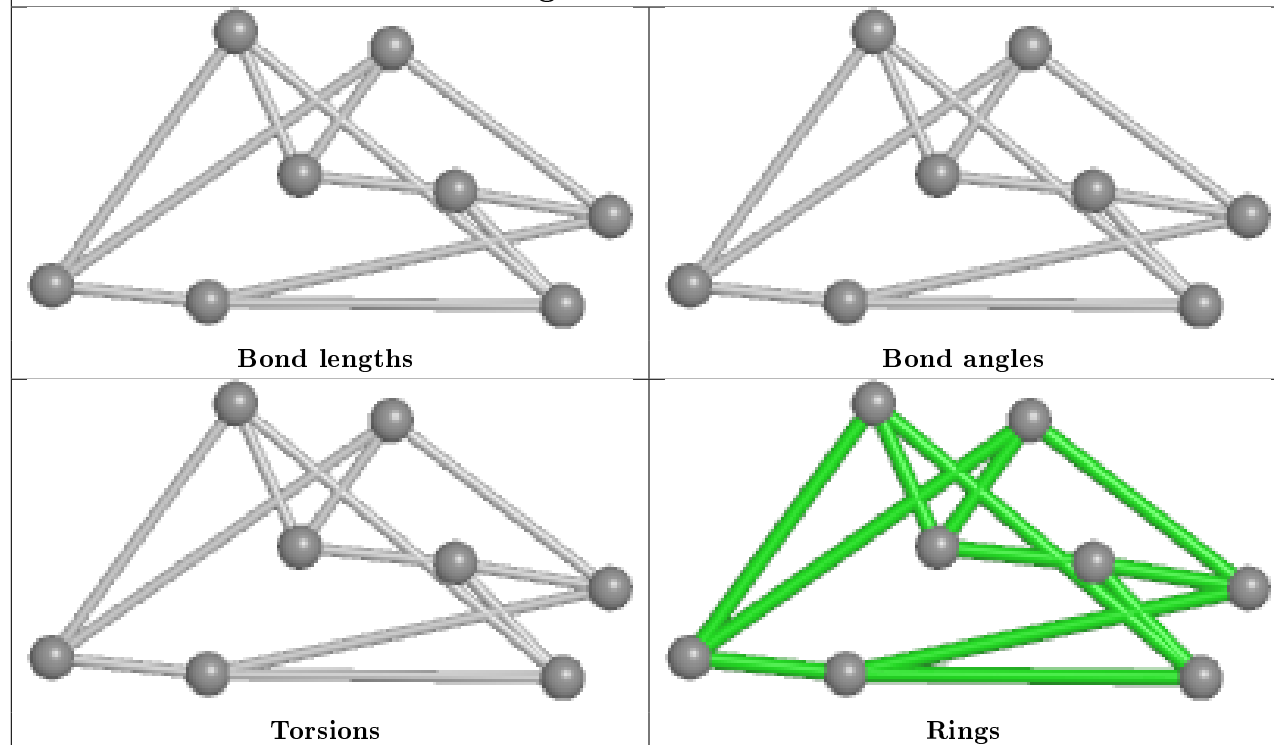
## Ligand CLA G 842



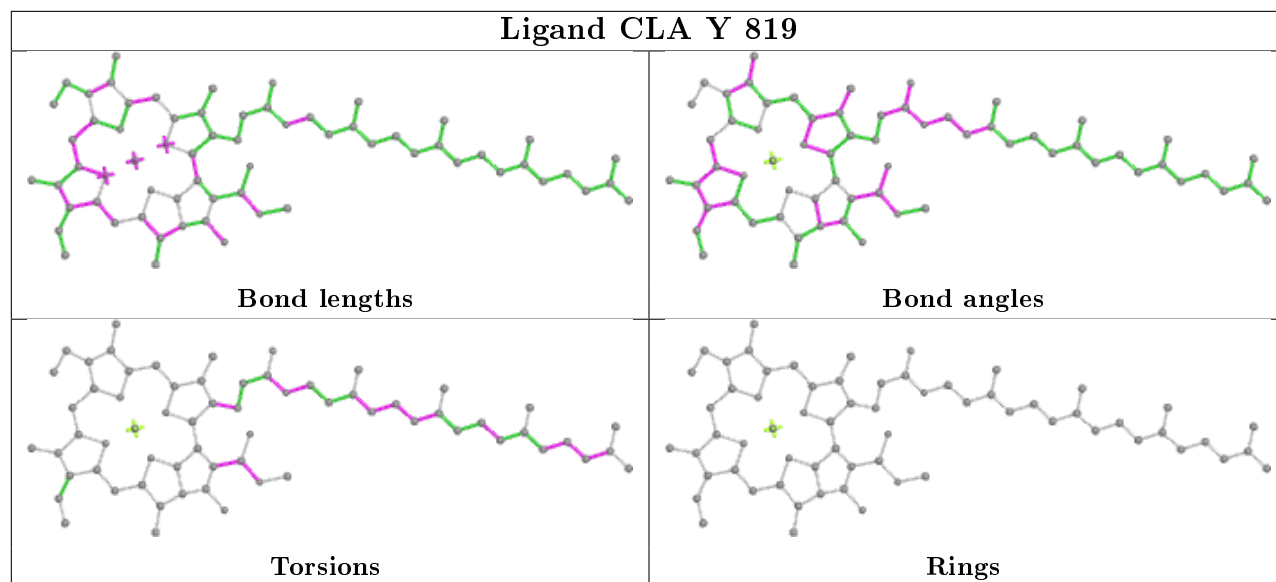
## Ligand BCR K 102



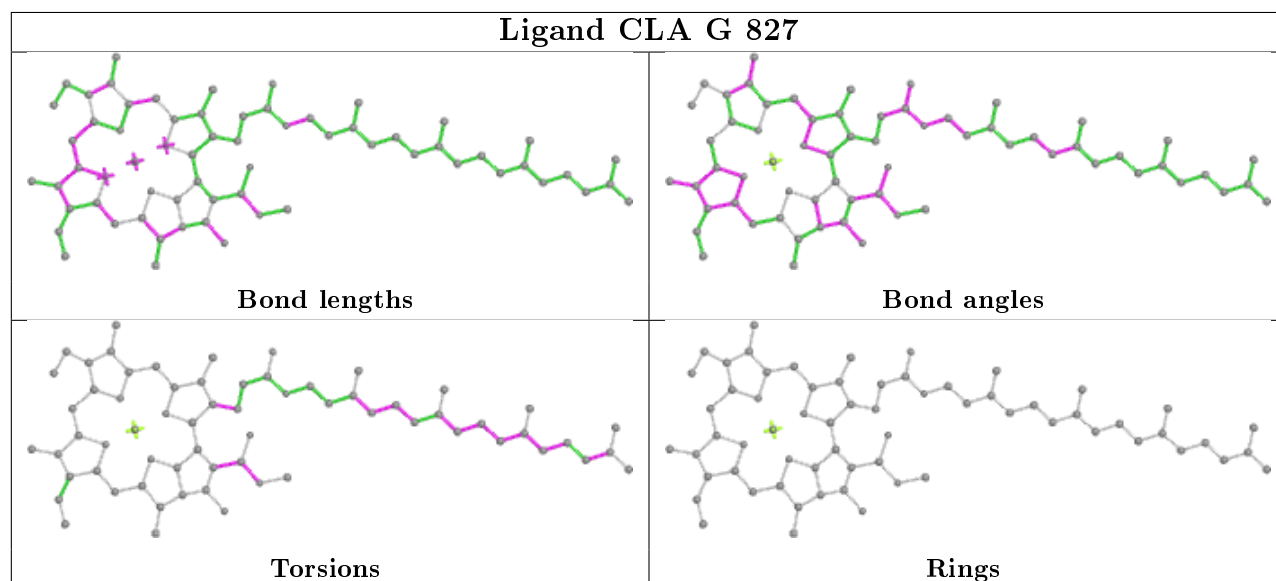
## Ligand SF4 G 845



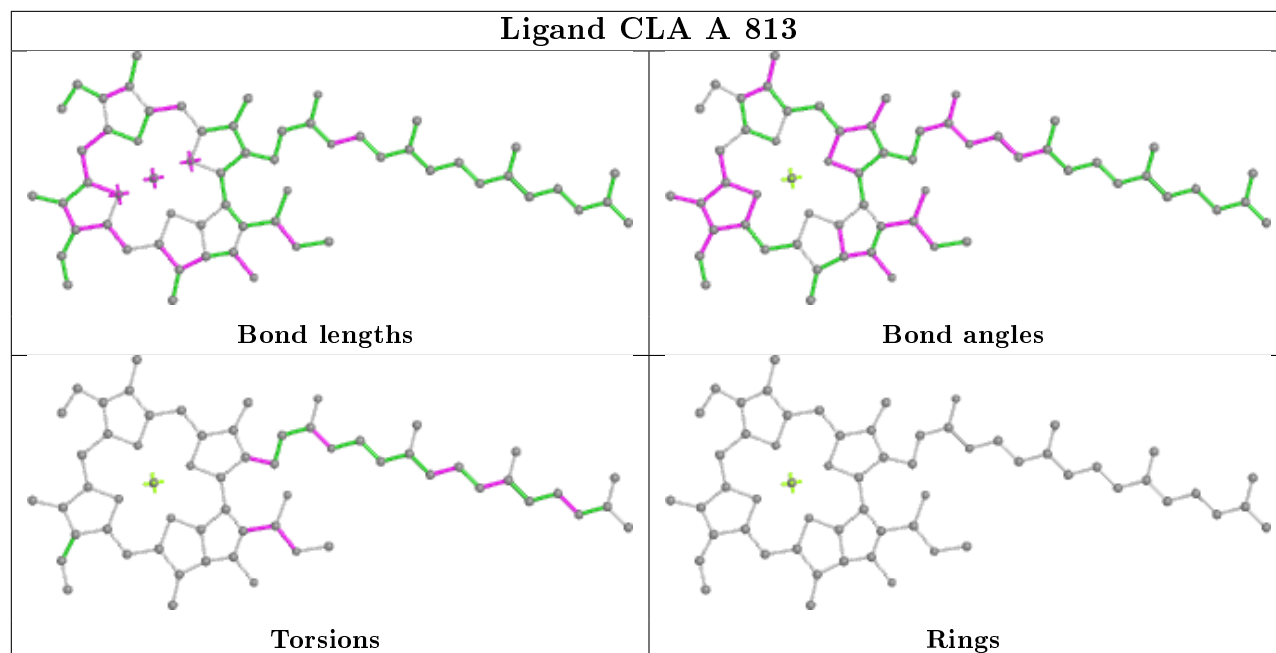
## Ligand CLA Y 819



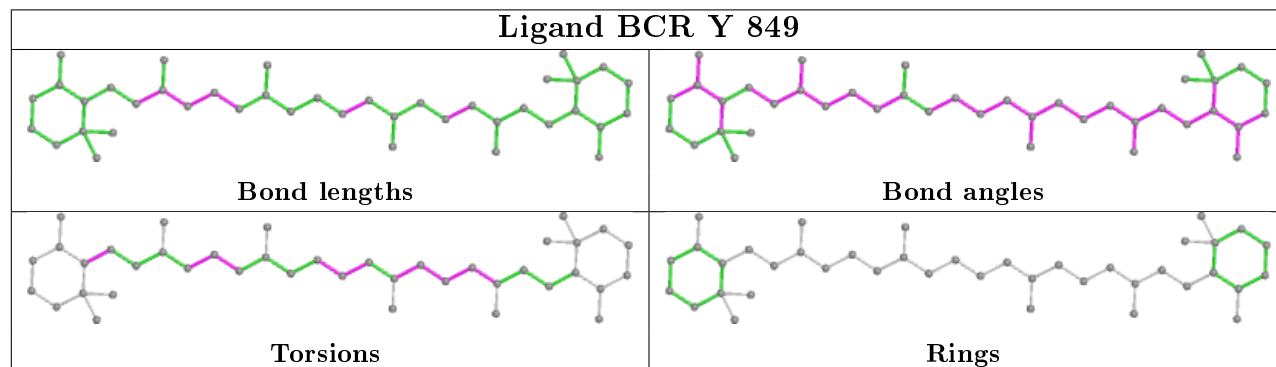
## Ligand CLA G 827

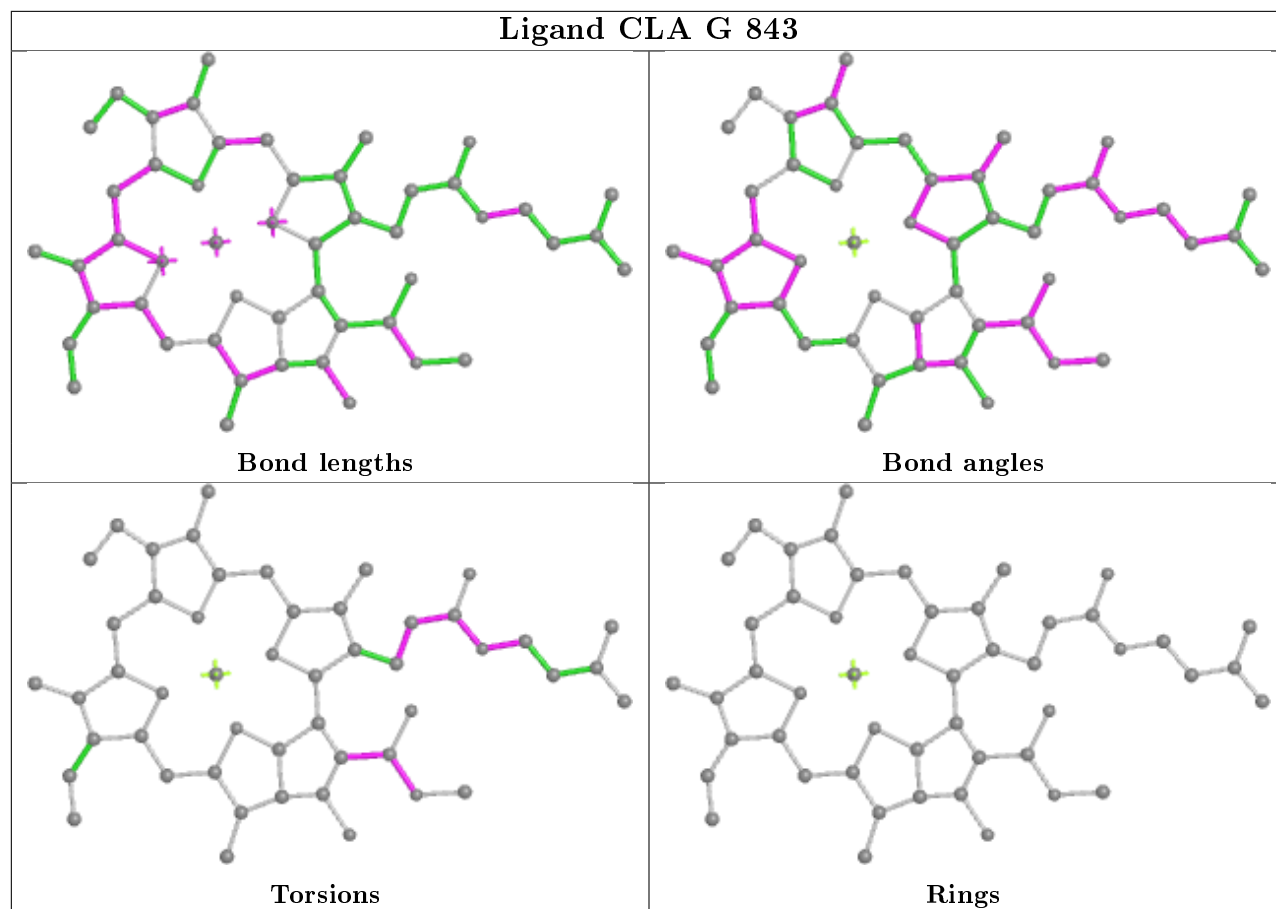


## Ligand CLA A 813



## Ligand BCR Y 849





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

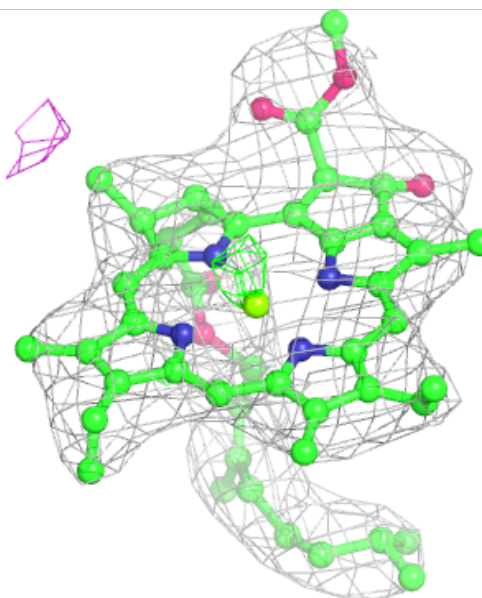
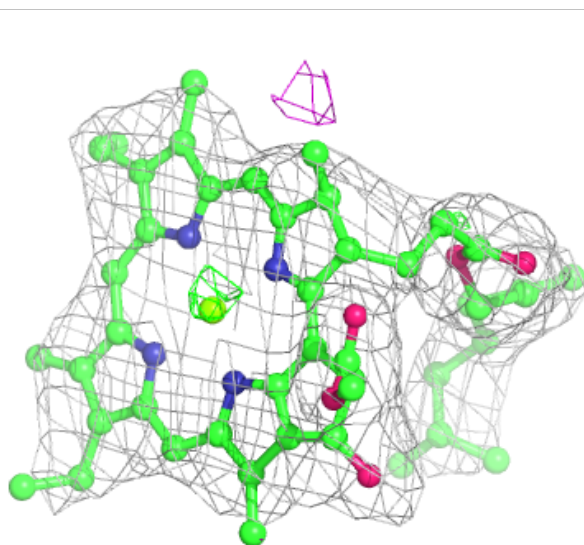
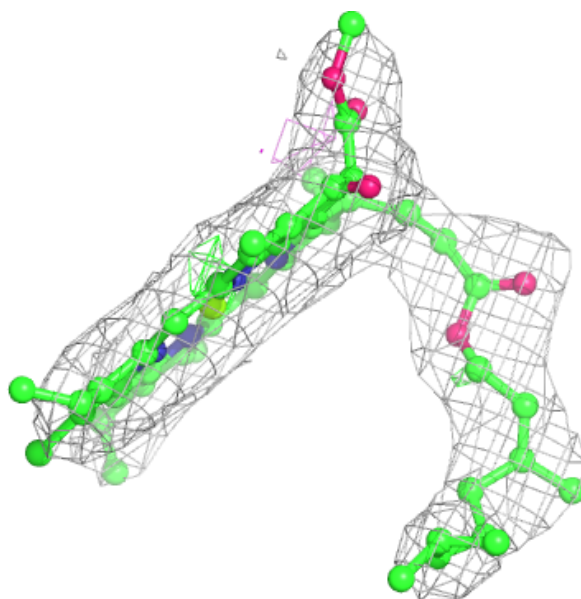
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

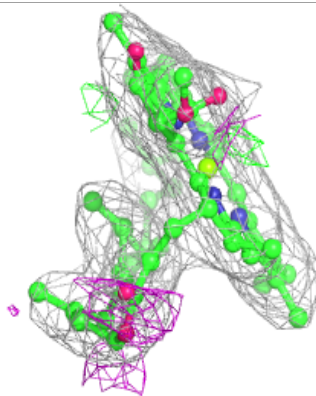
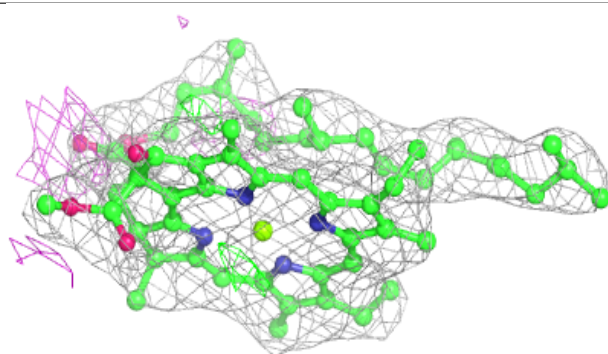
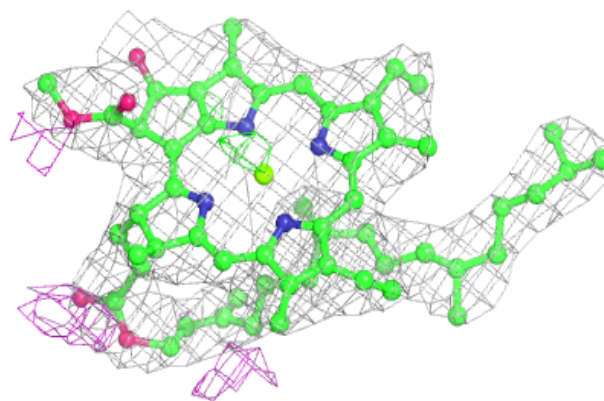
**Electron density around CLA B 811:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

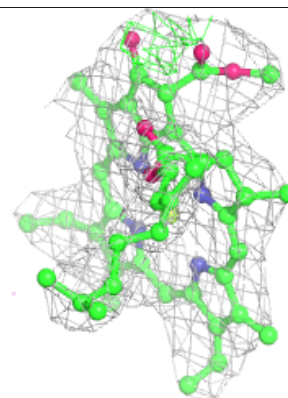
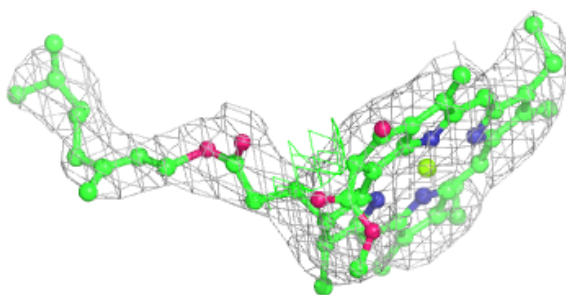
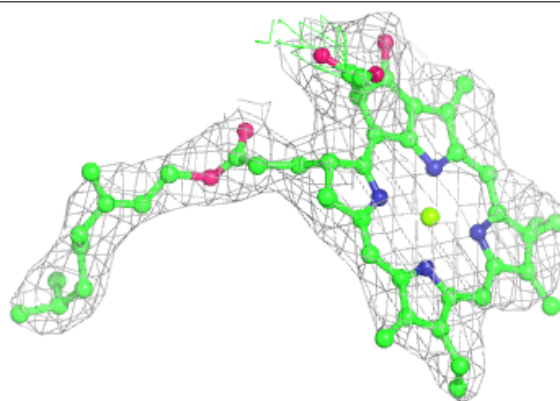


**Electron density around CLA B 817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

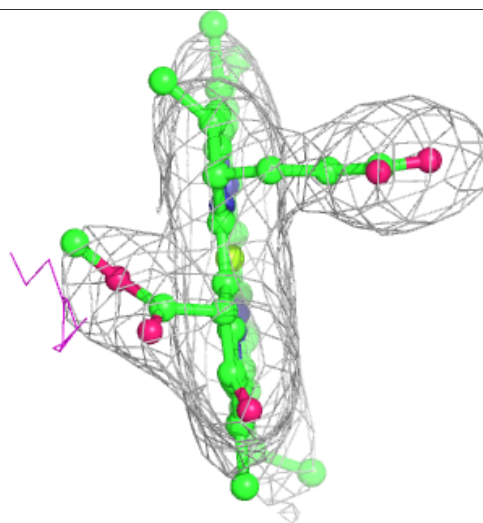
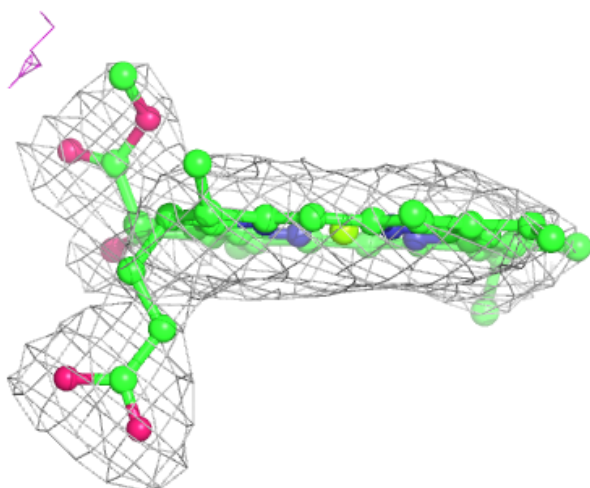
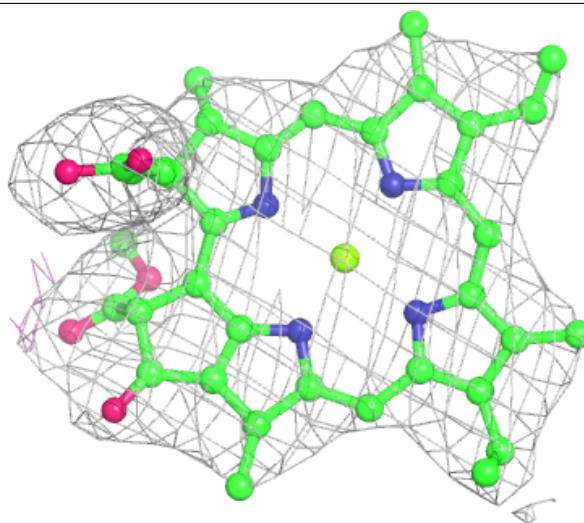
**Electron density around CLA B 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA H 820:**

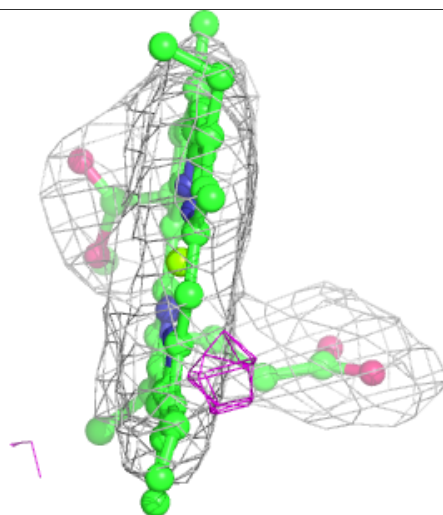
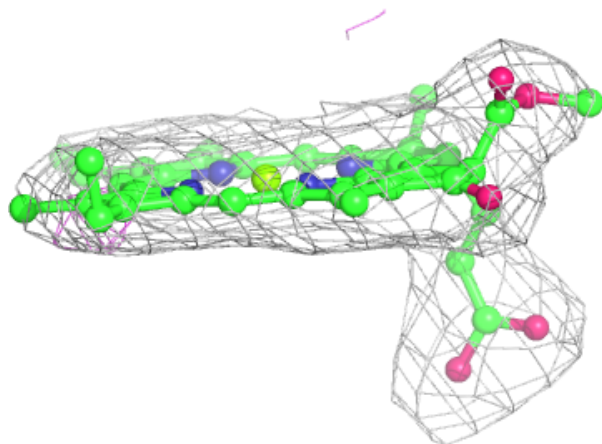
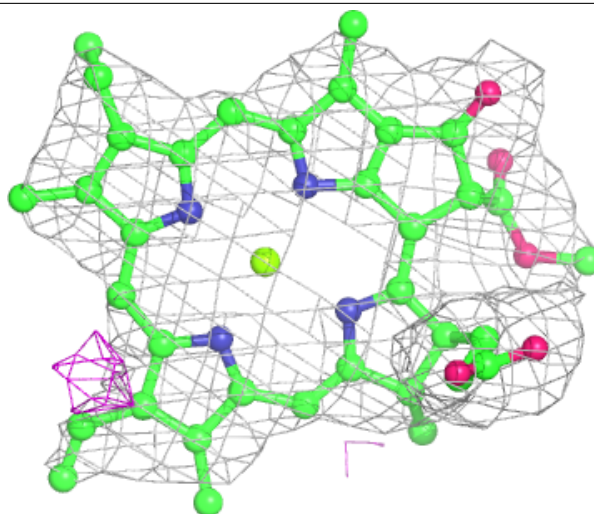
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





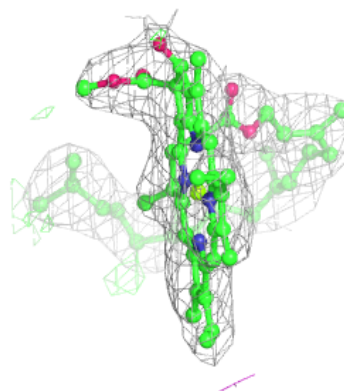
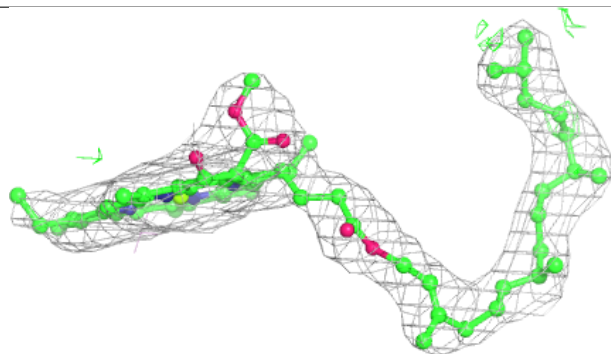
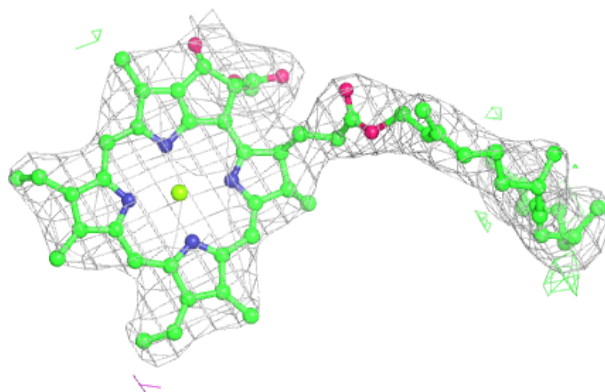
**Electron density around CLA Y 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

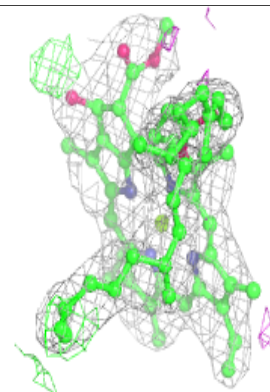
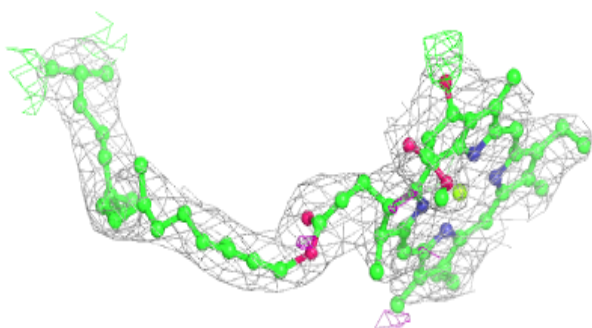
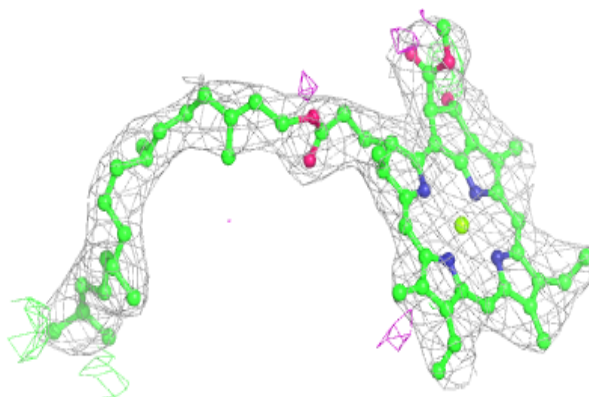


**Electron density around CLA Y 827:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

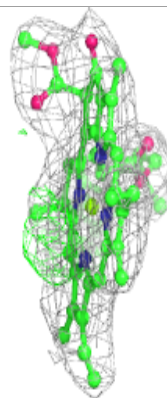
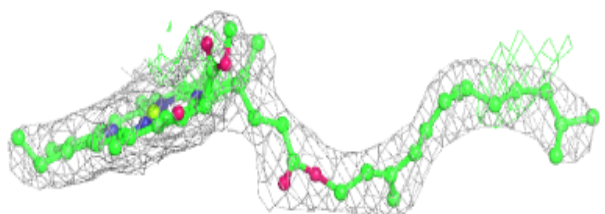
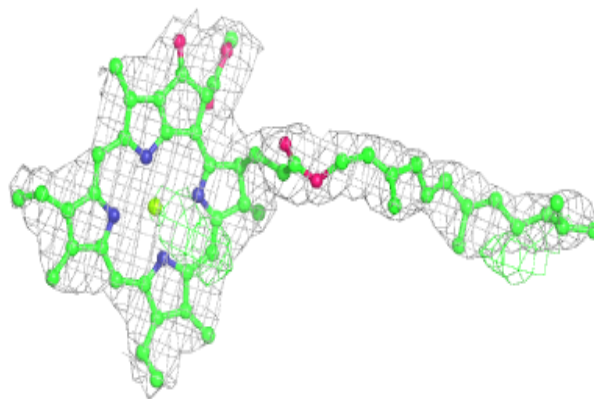
**Electron density around CLA A 852:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

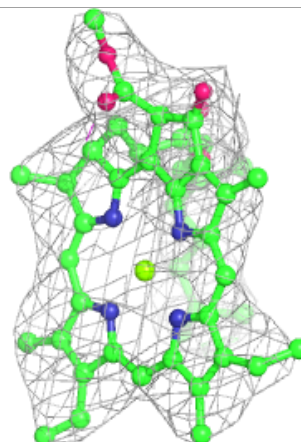
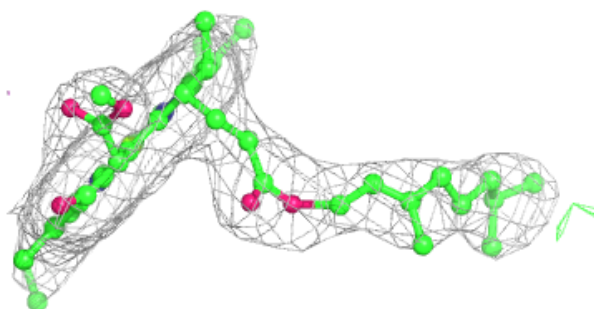
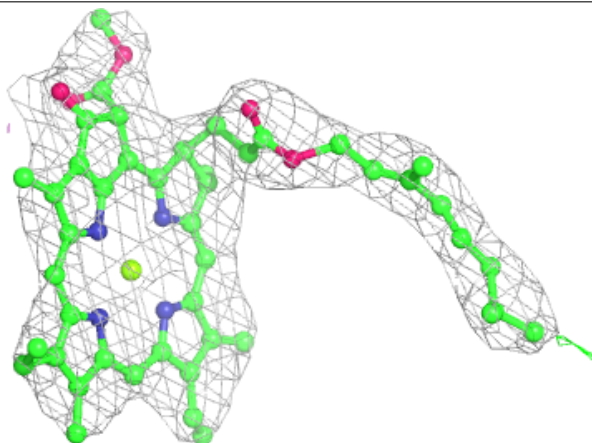


**Electron density around CLA A 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

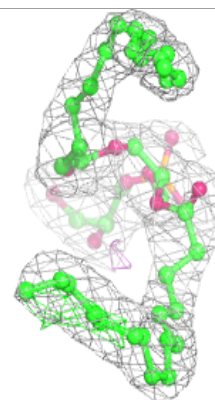
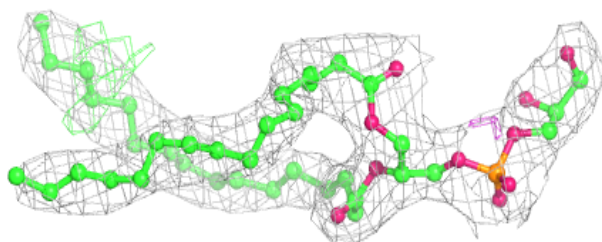
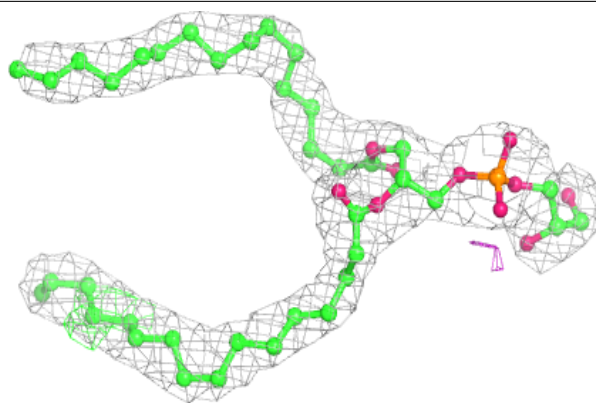
**Electron density around CLA Y 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

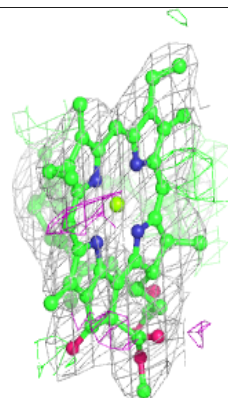
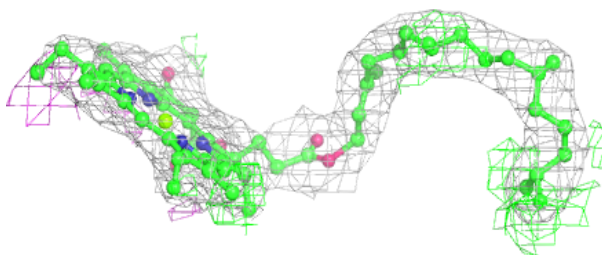
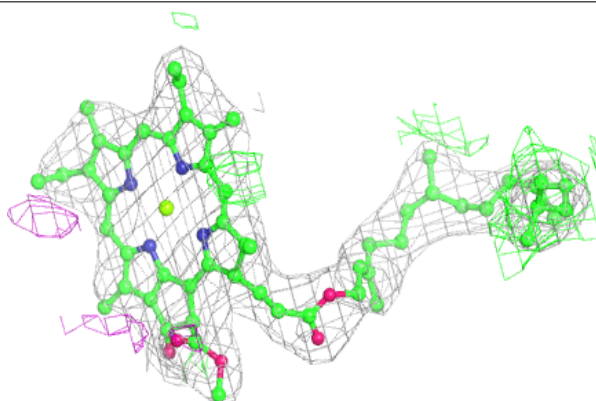


**Electron density around LHG Y 852:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Z 808:**

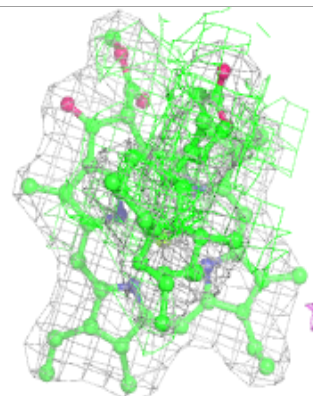
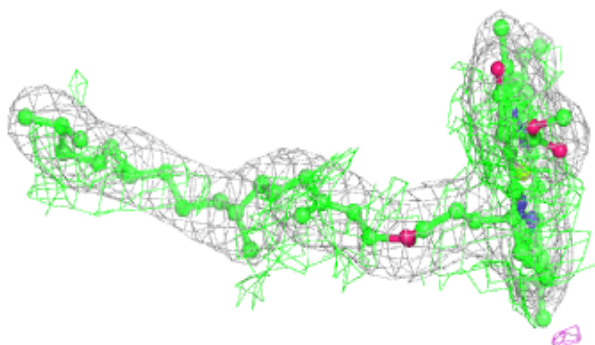
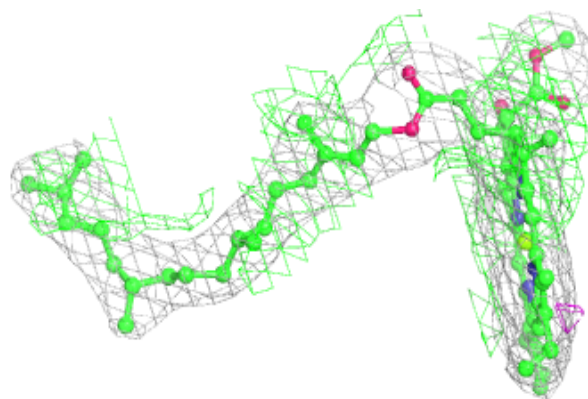
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



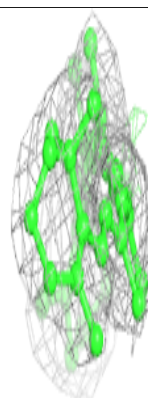
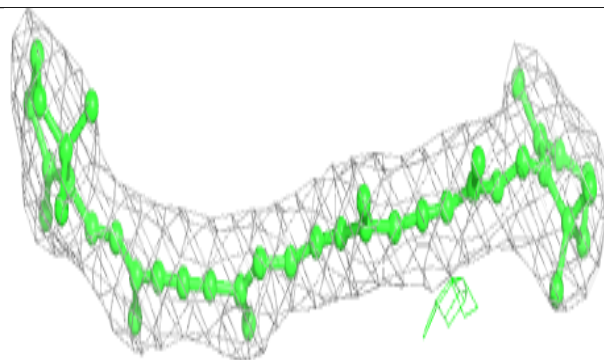
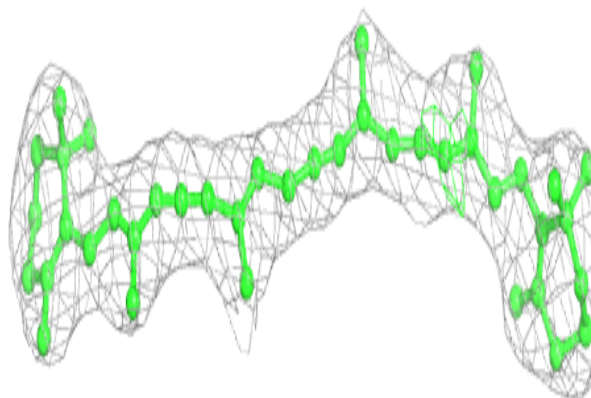


**Electron density around CLA B 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

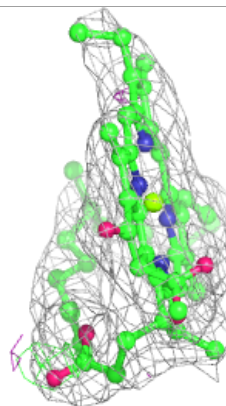
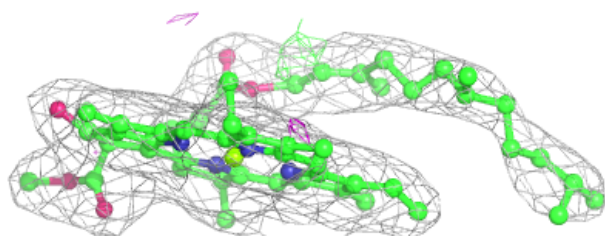
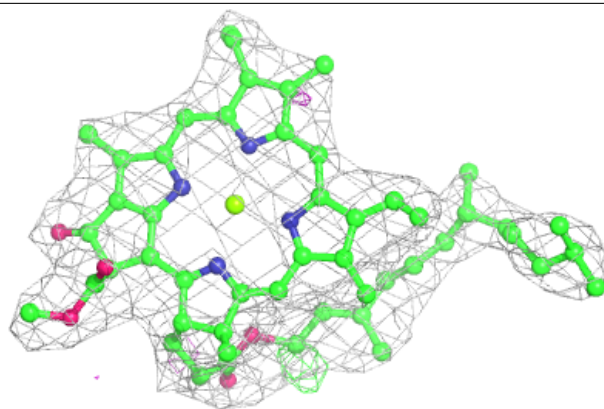
**Electron density around BCR M 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



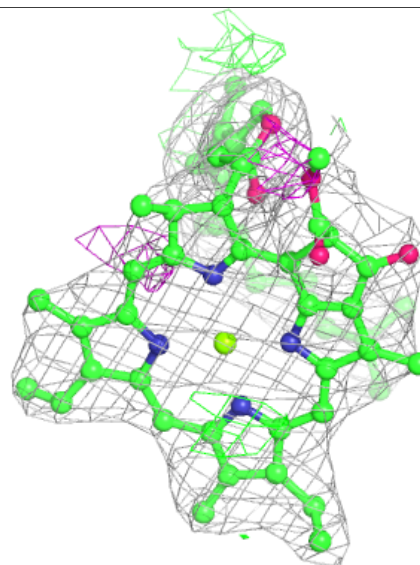
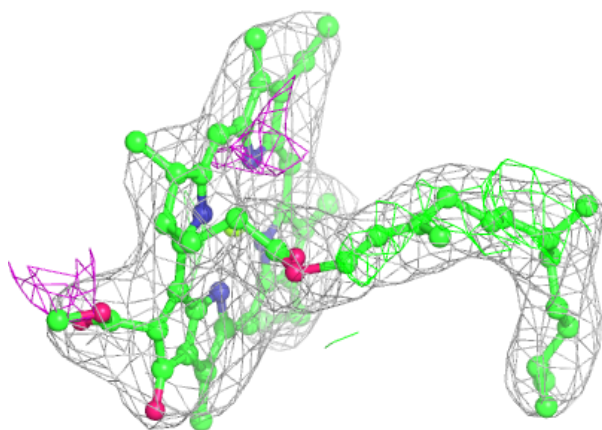
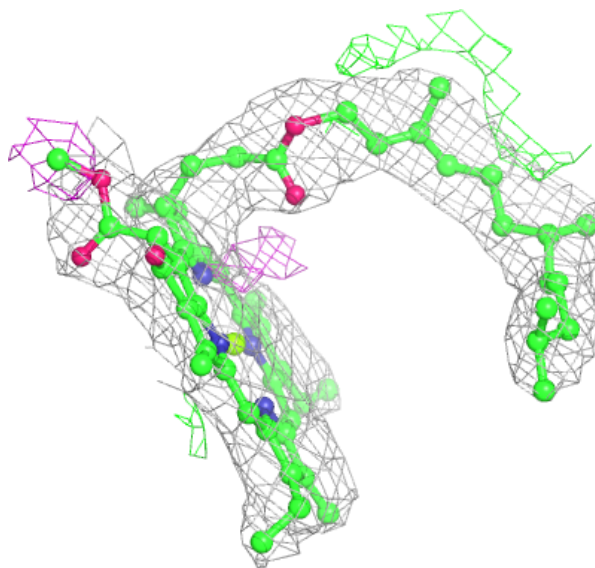
**Electron density around CLA H 817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



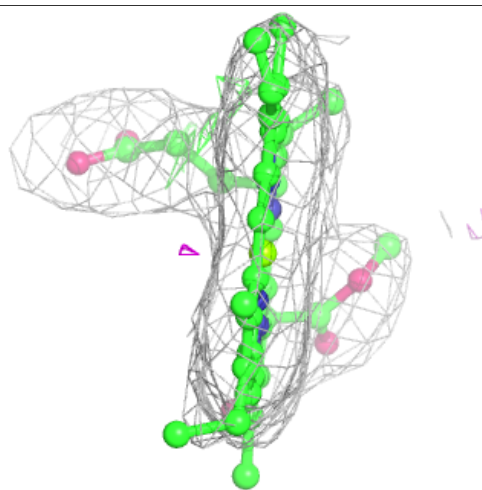
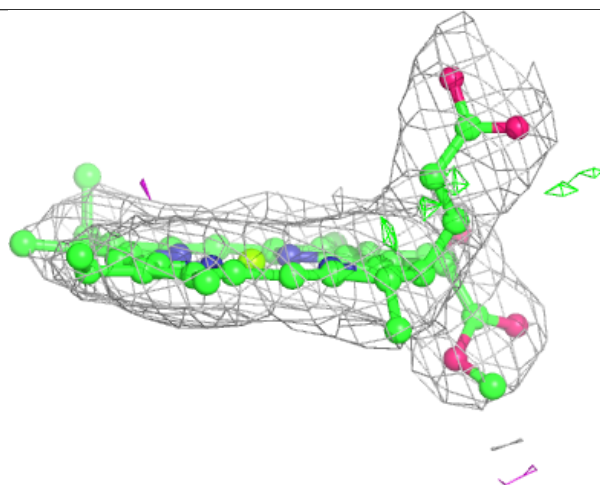
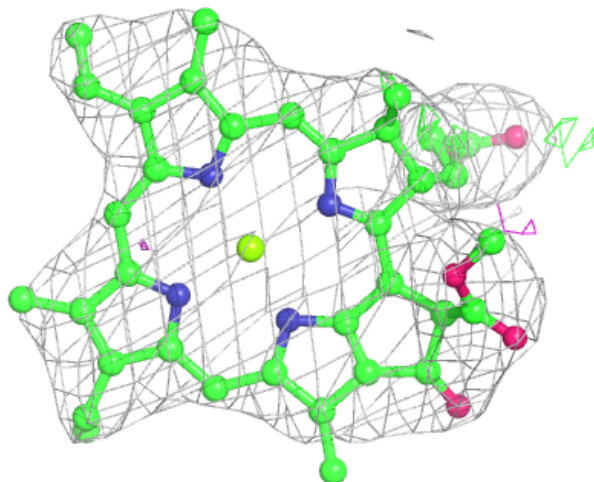
**Electron density around CLA H 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA H 831:**

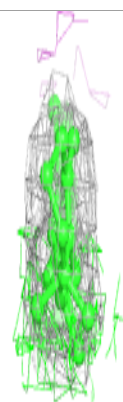
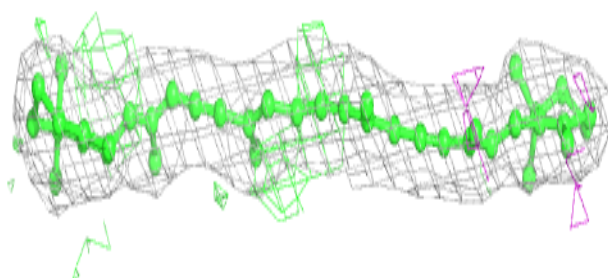
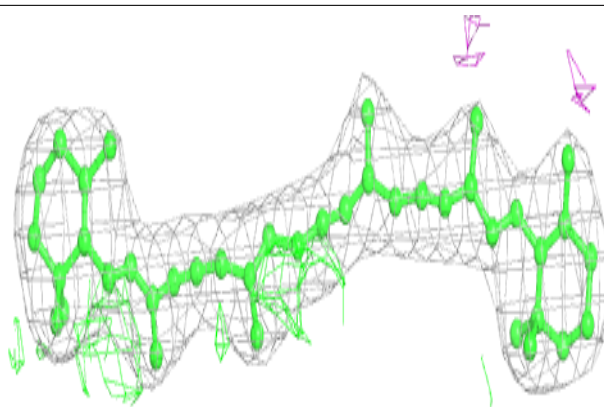
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



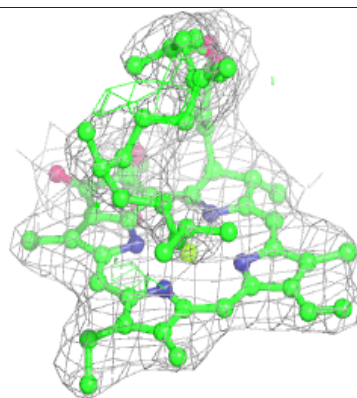
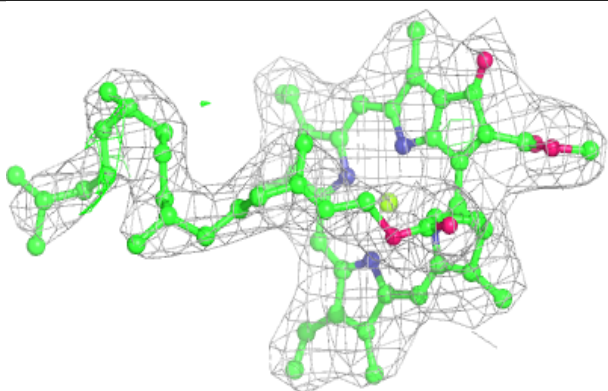
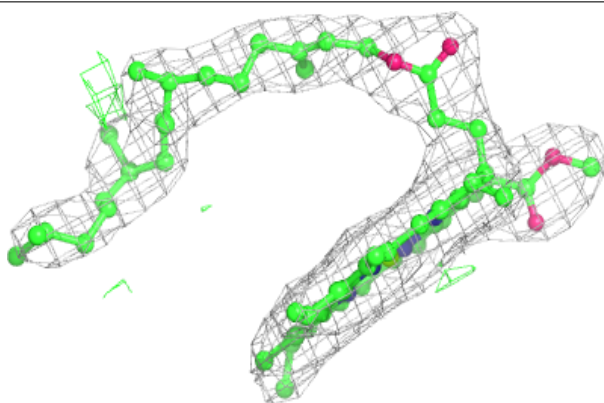


**Electron density around BCR U 1005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

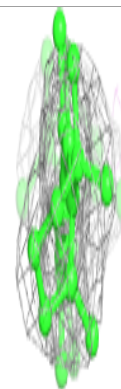
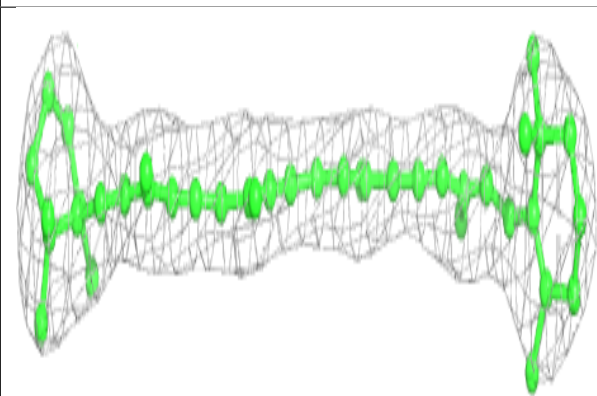
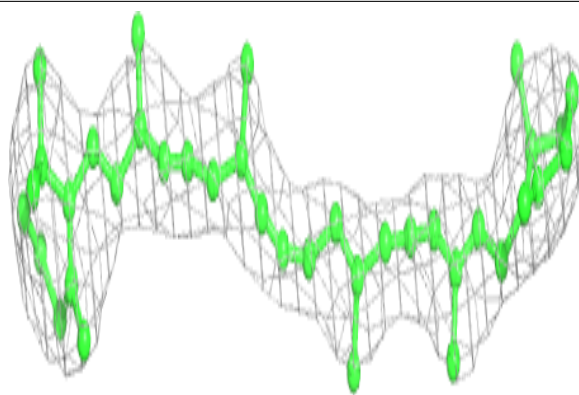
**Electron density around CLA A 832:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



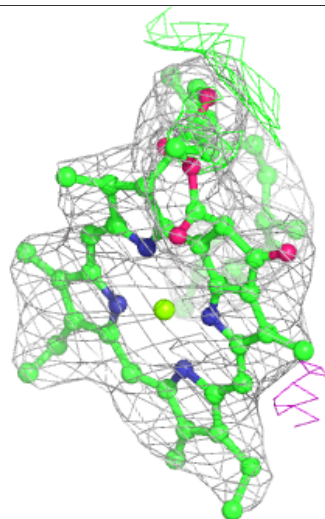
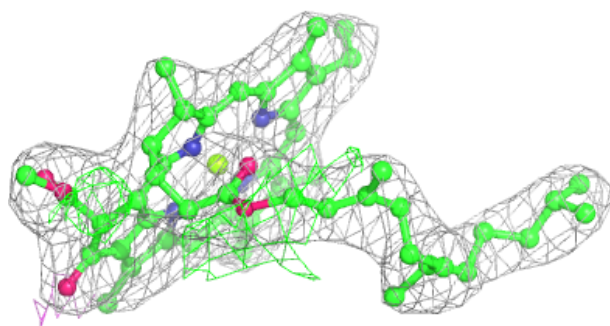
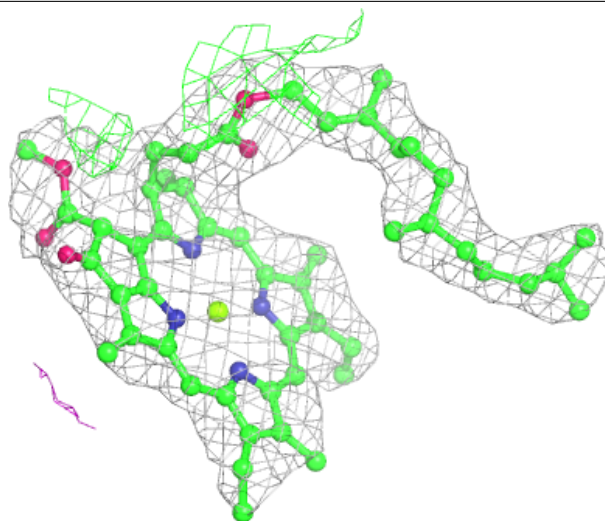
**Electron density around BCR G 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



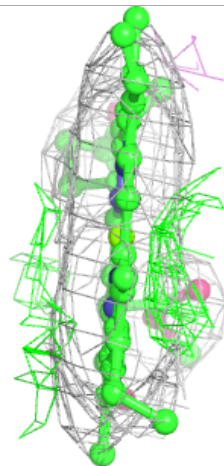
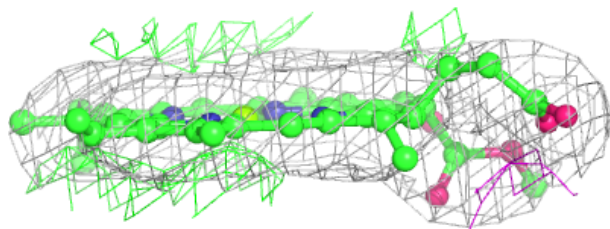
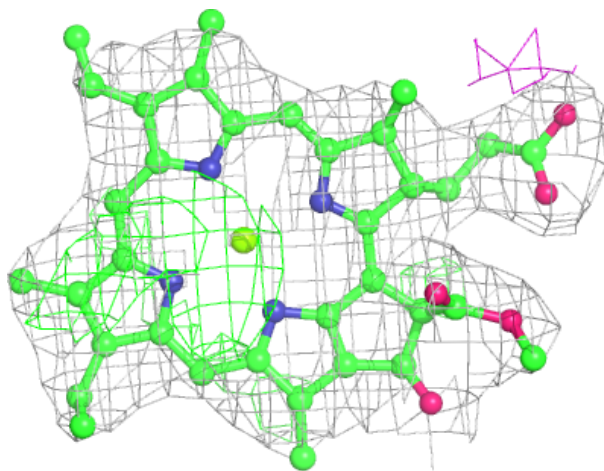
**Electron density around CLA G 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



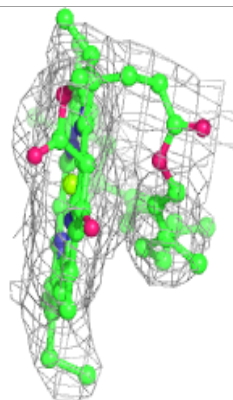
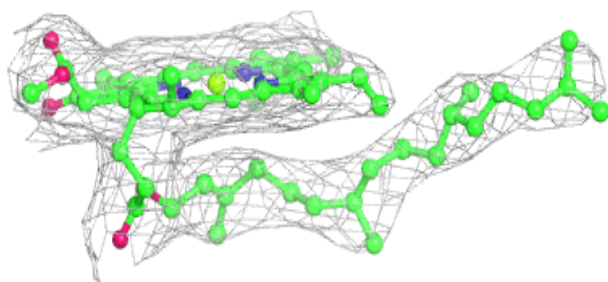
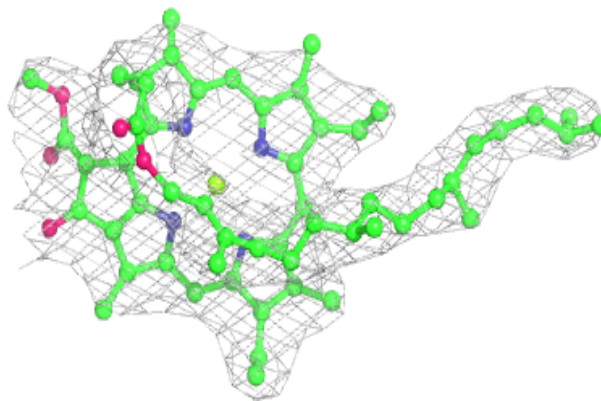
**Electron density around CLA d 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

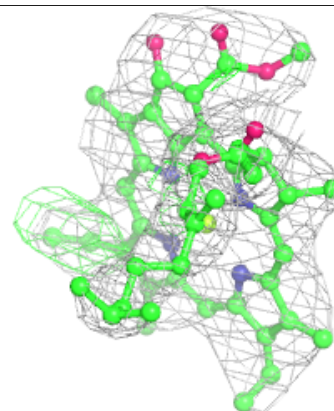
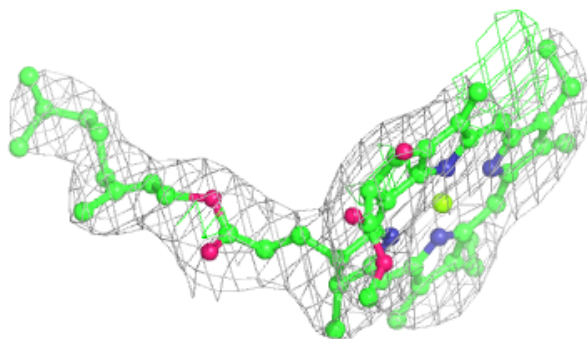
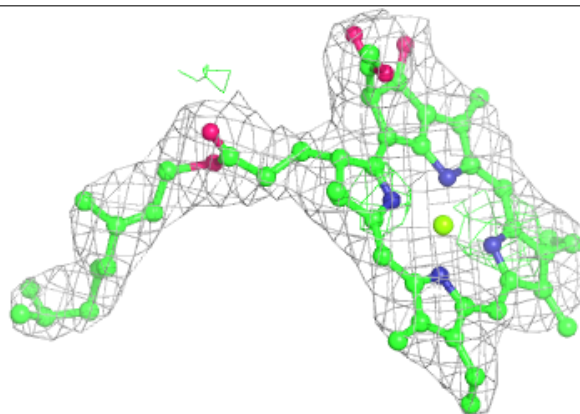


**Electron density around CLA B 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Z 831:**

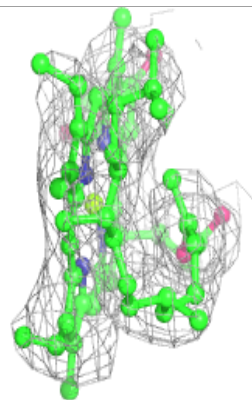
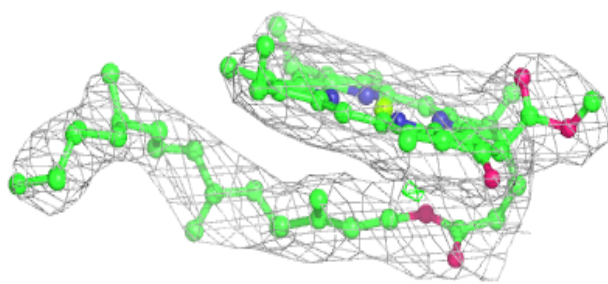
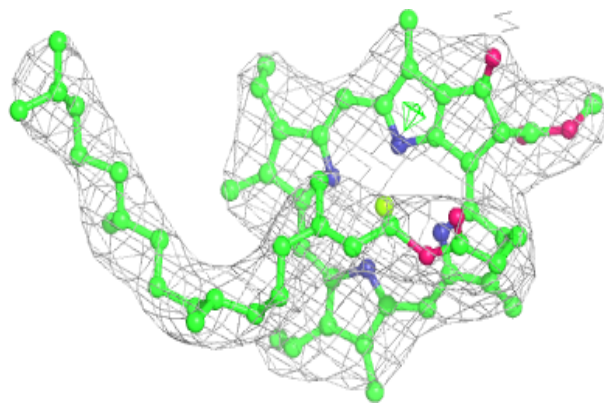
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



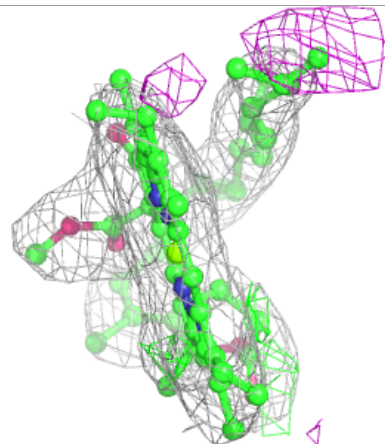
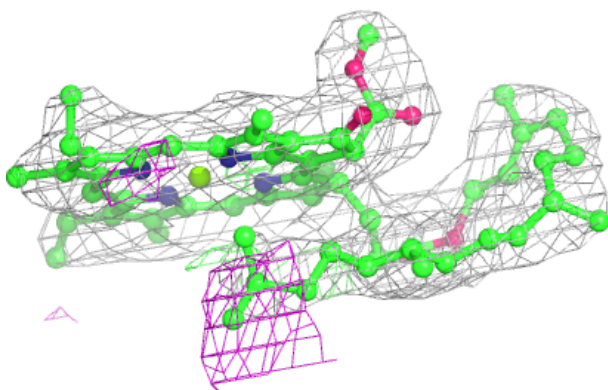
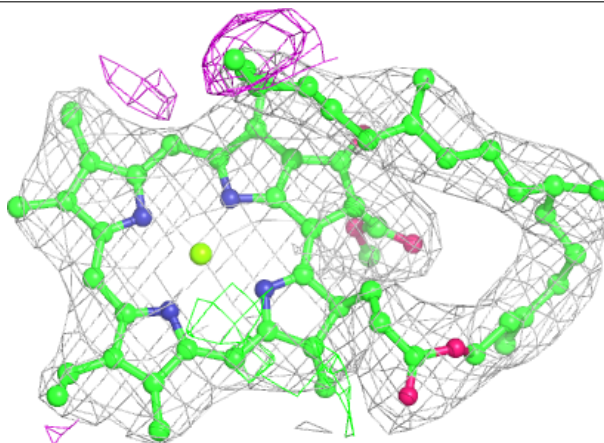


**Electron density around CLA B 838:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

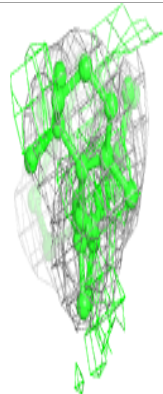
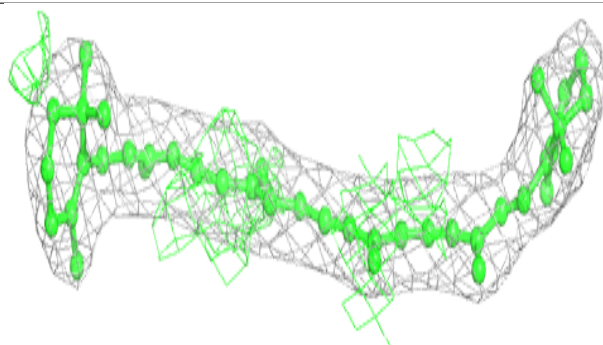
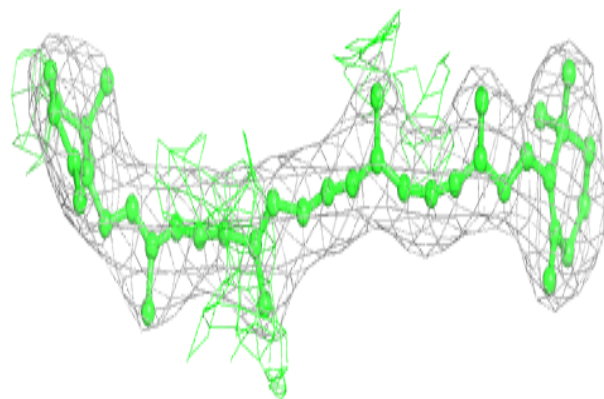
**Electron density around CLA H 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

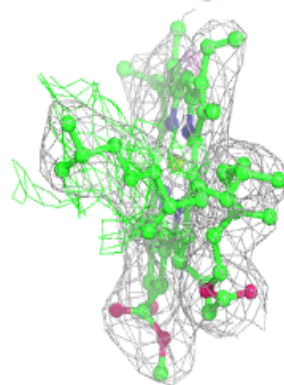
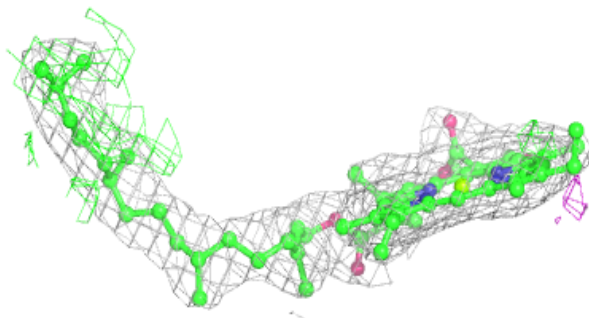
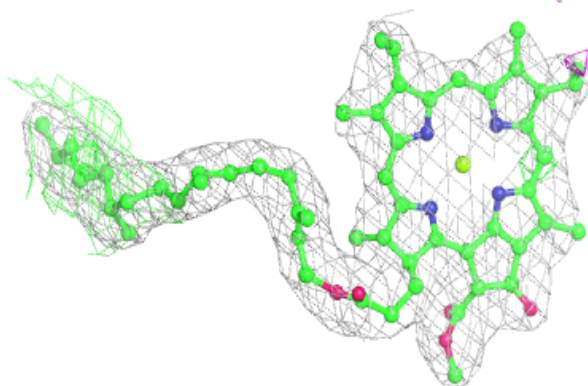


**Electron density around BCR e 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

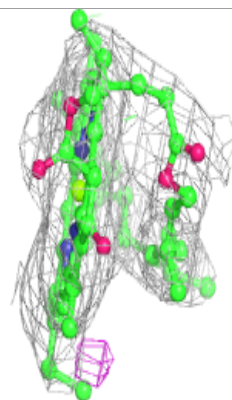
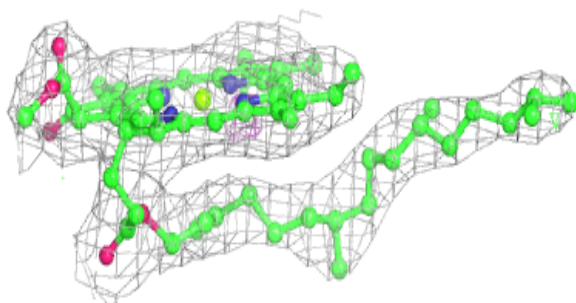
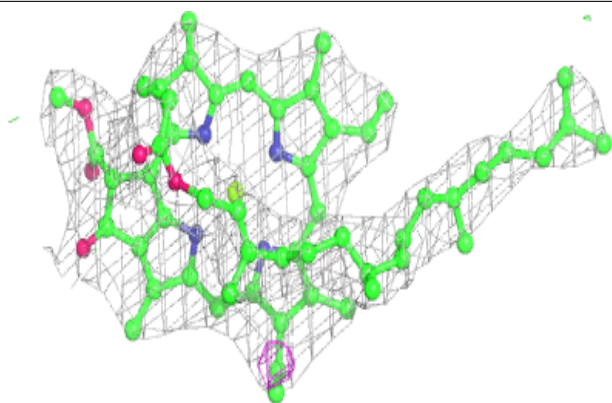
**Electron density around CLA Y 855:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

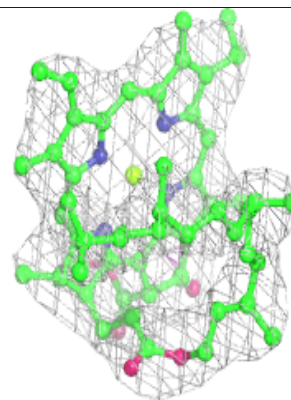
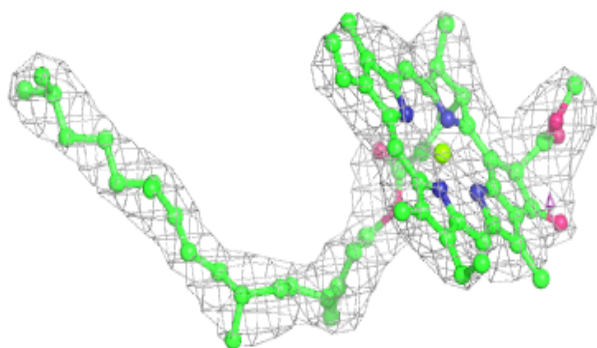
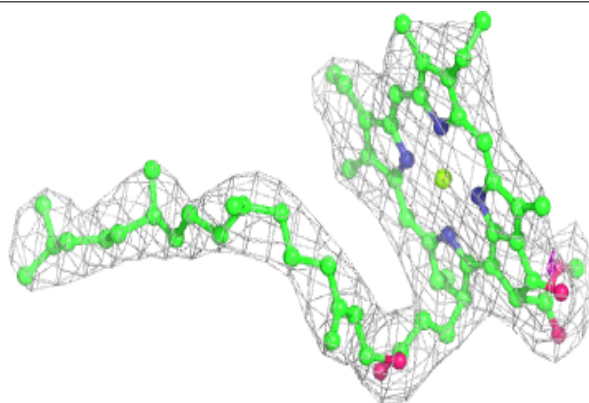


**Electron density around CLA G 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA H 813:**

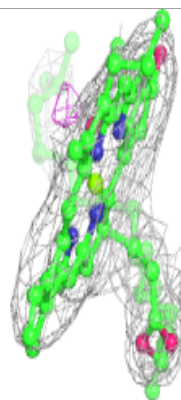
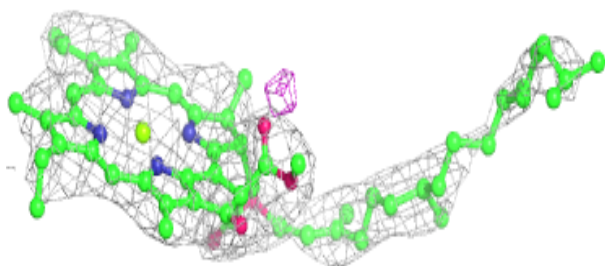
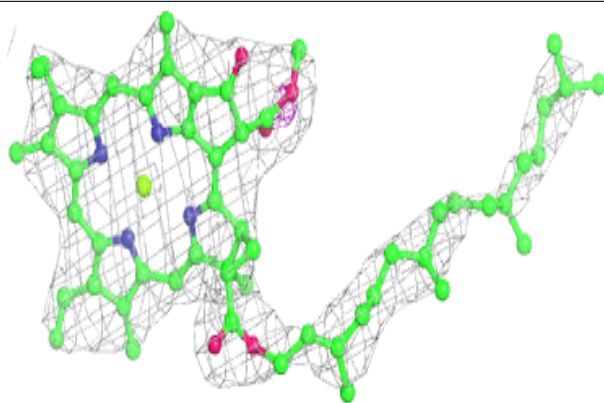
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



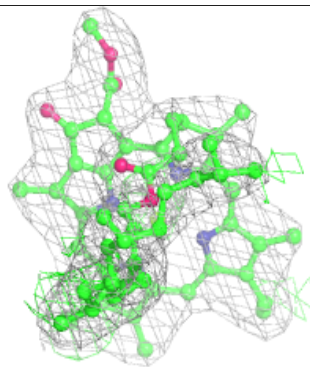
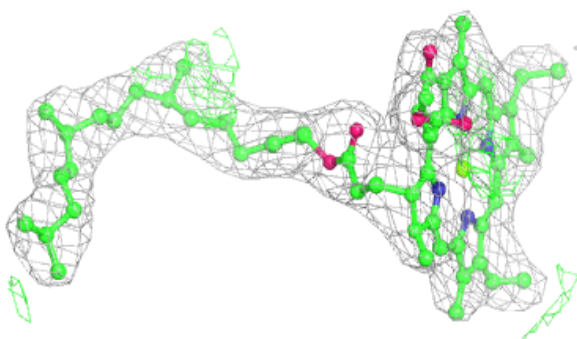
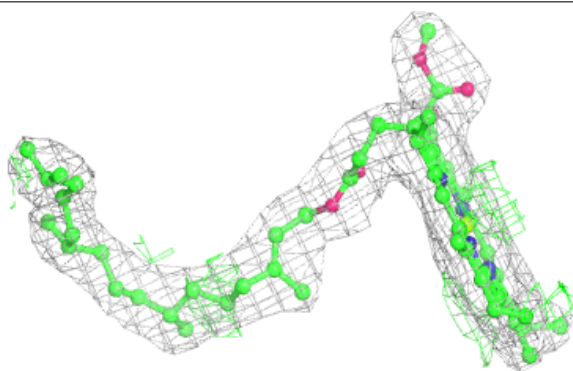


**Electron density around CLA A 822:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

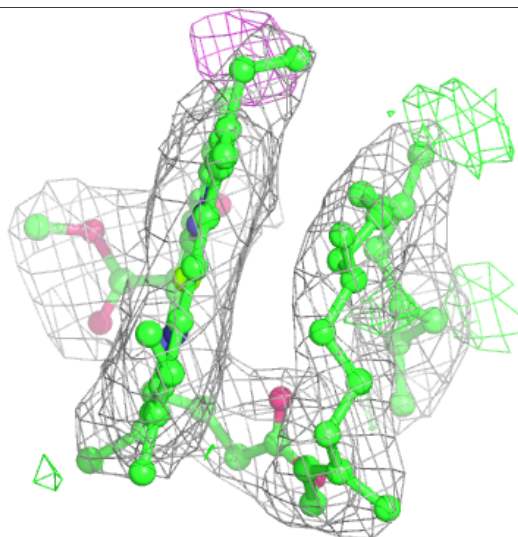
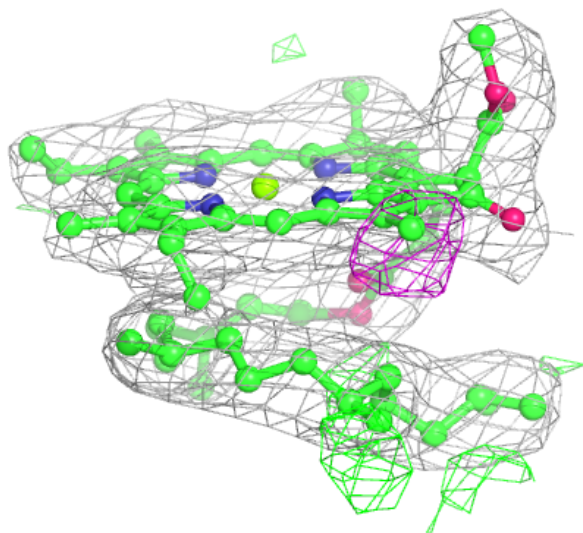
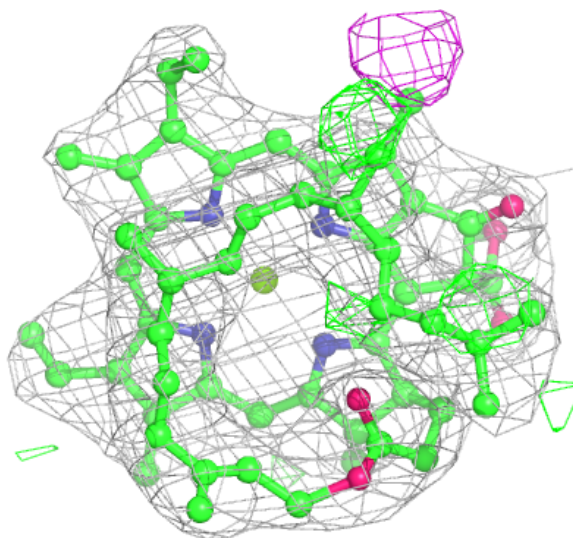
**Electron density around CLA H 837:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



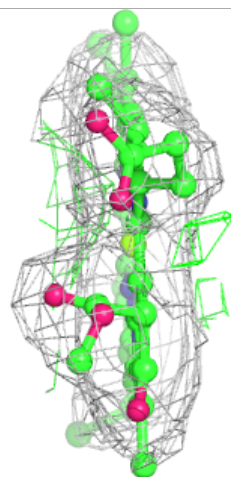
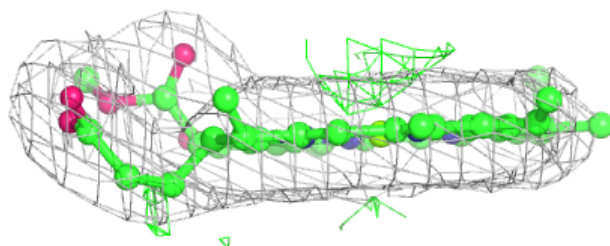
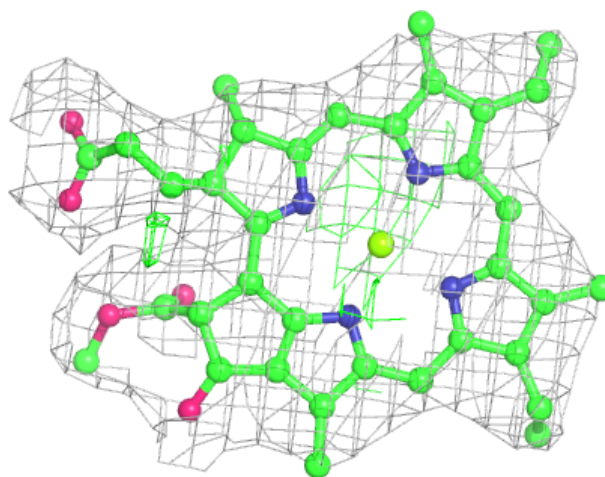
**Electron density around CLA L 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



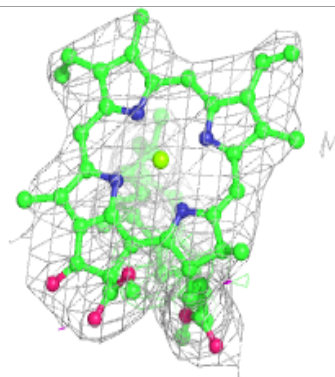
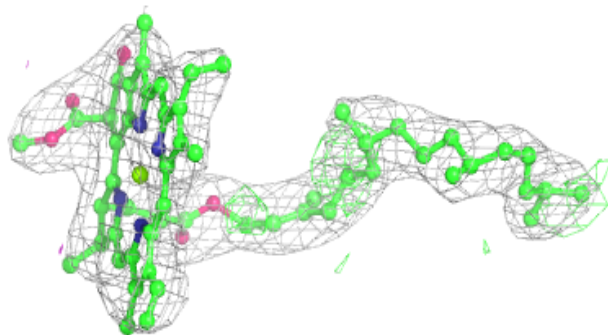
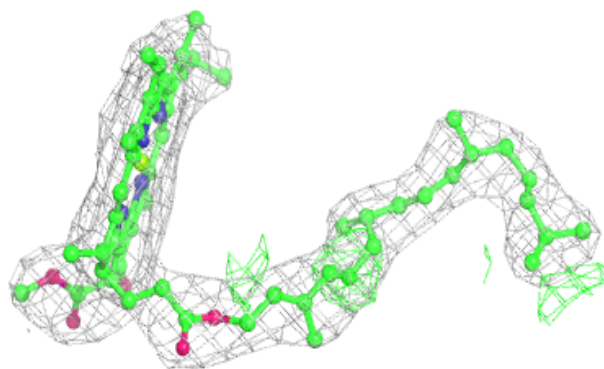
**Electron density around CLA F 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



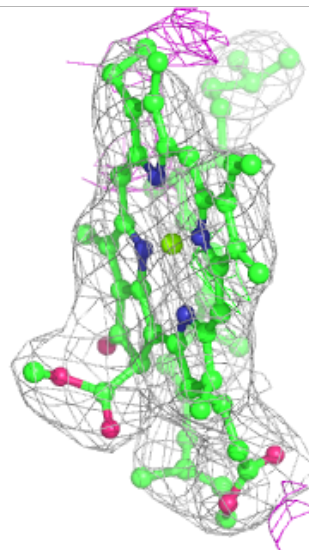
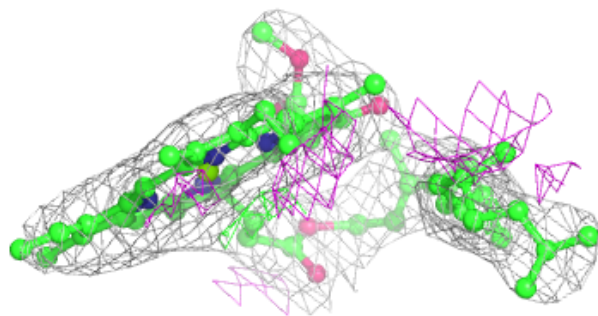
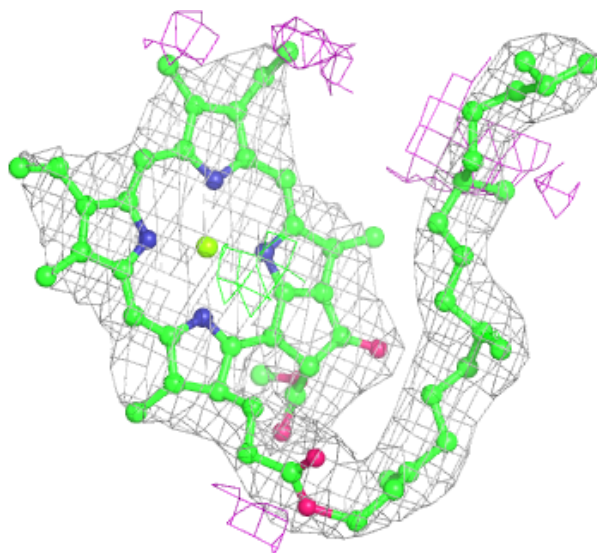
**Electron density around CLA Y 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



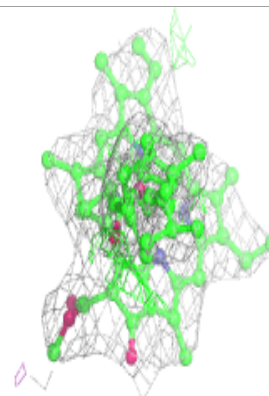
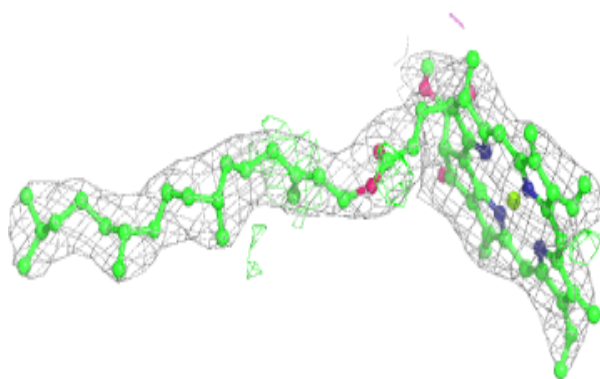
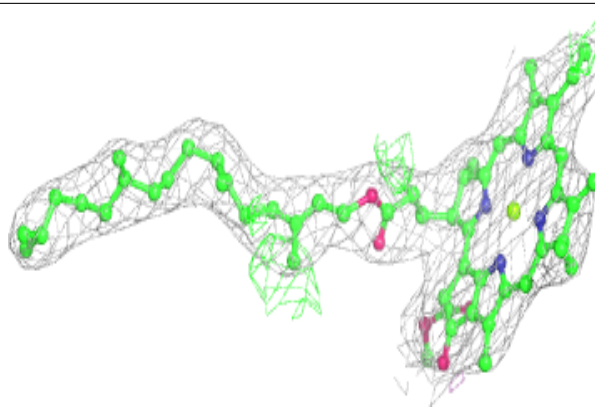
**Electron density around CLA Y 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 809:**

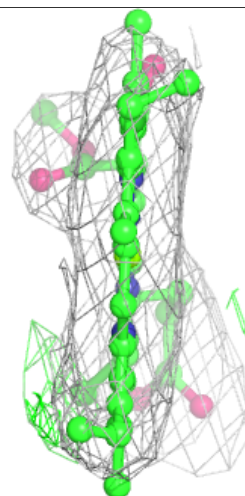
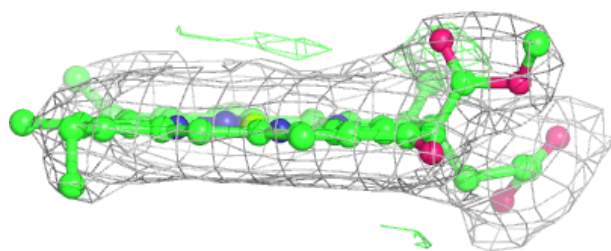
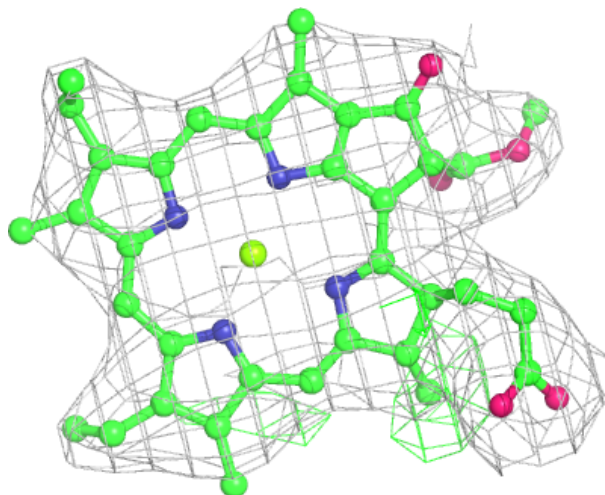
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





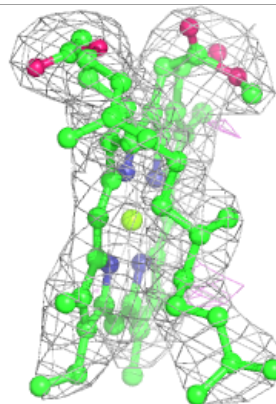
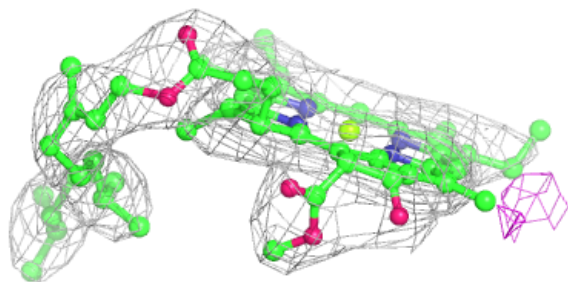
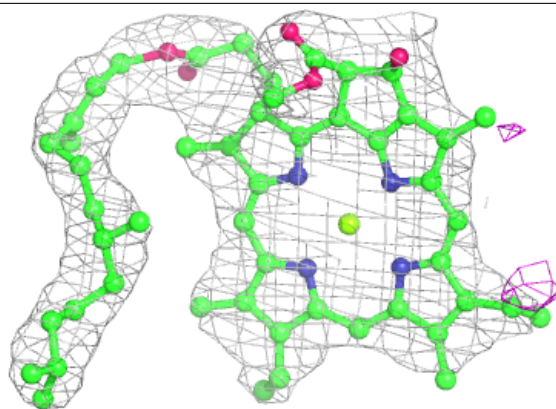
**Electron density around CLA W 1701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

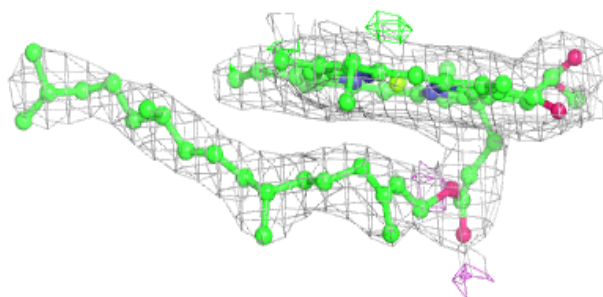
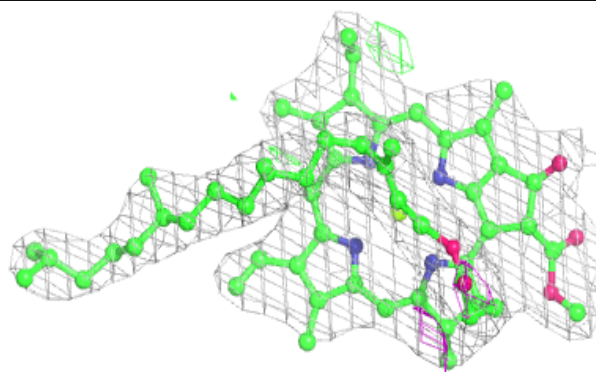


**Electron density around CLA G 813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Y 840:**

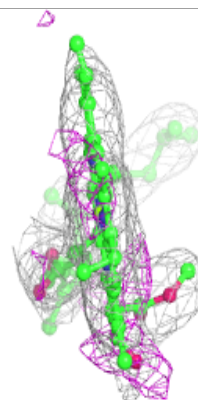
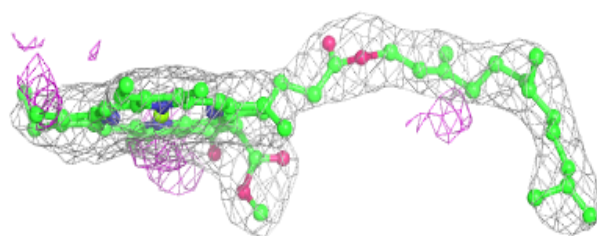
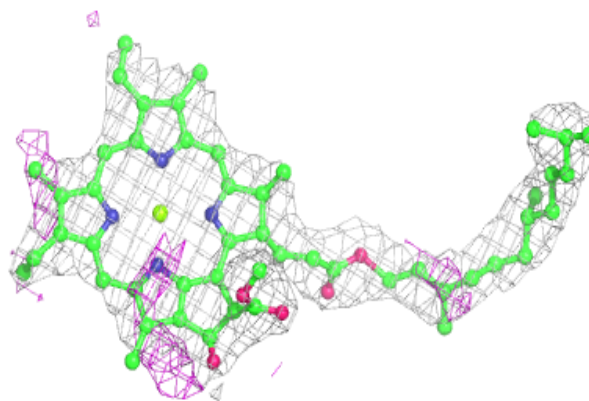
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



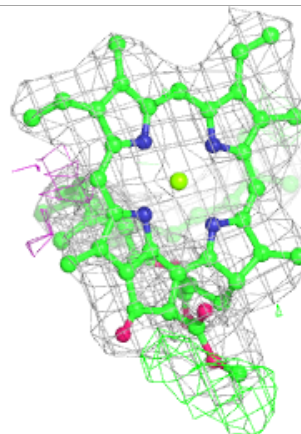
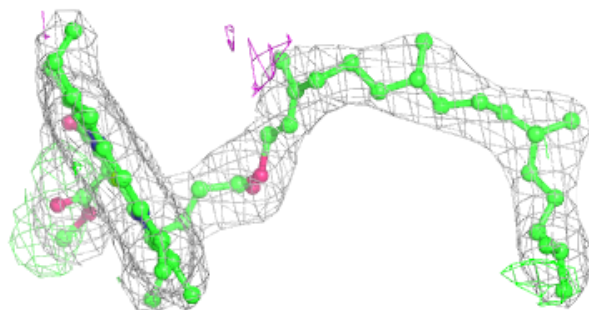
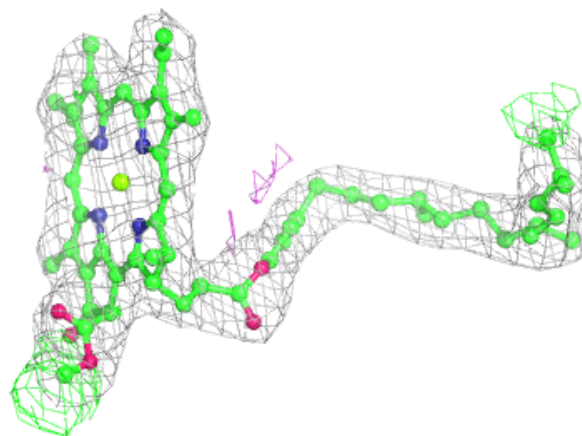


**Electron density around CLA B 837:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

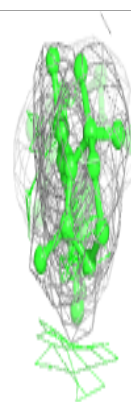
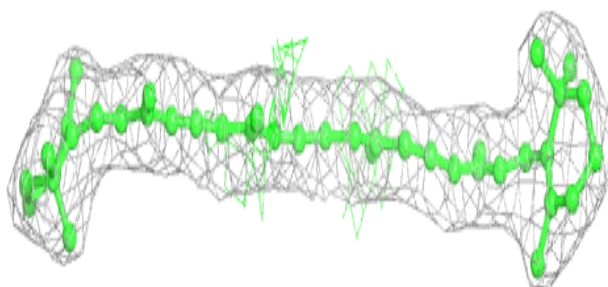
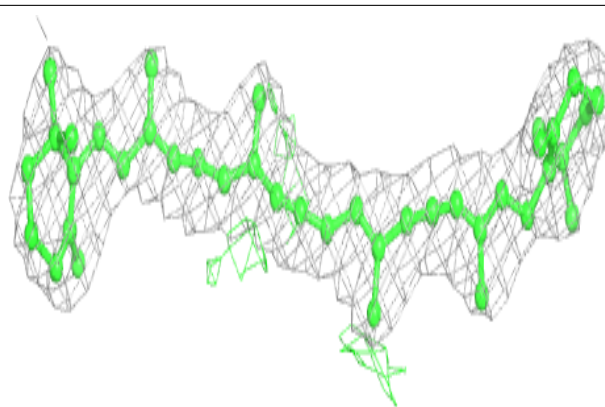
**Electron density around CLA U 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



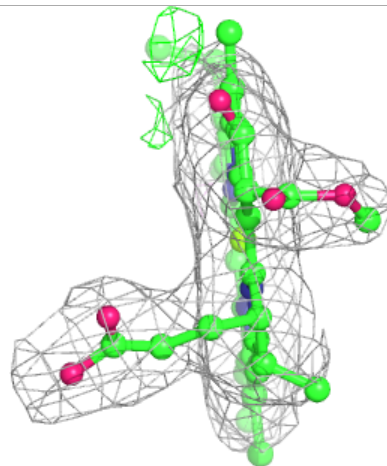
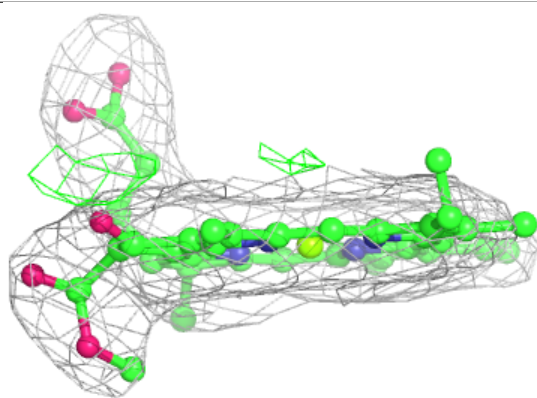
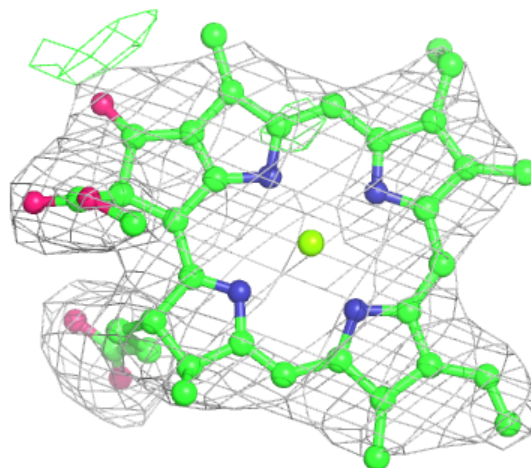
**Electron density around BCR H 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



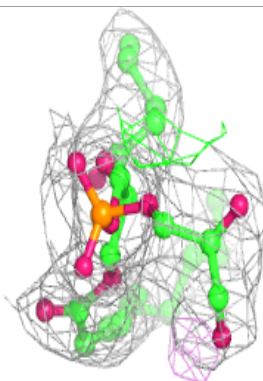
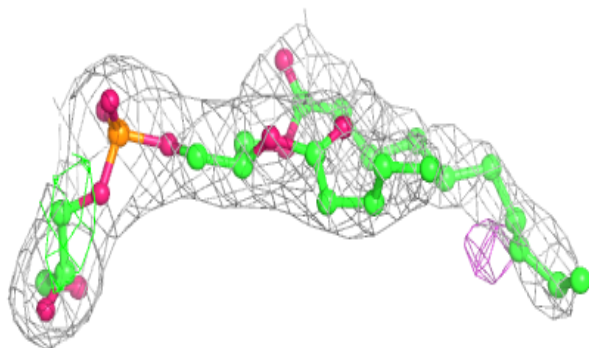
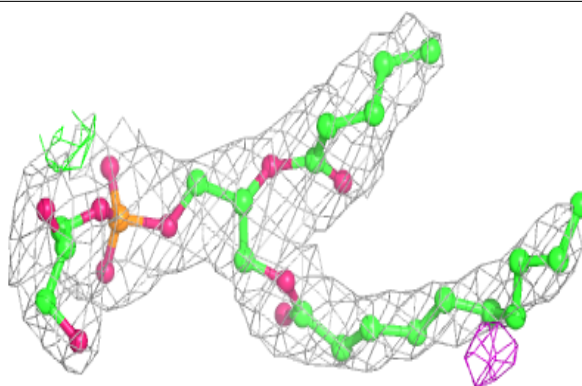
**Electron density around CLA B 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

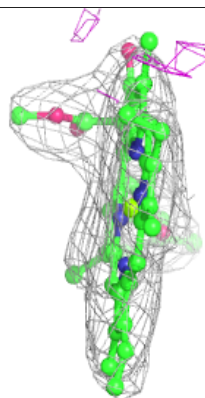
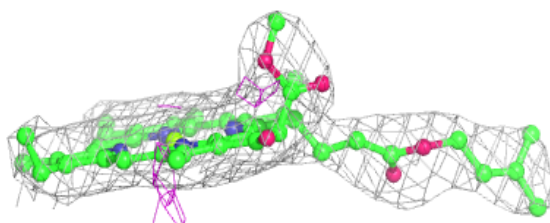
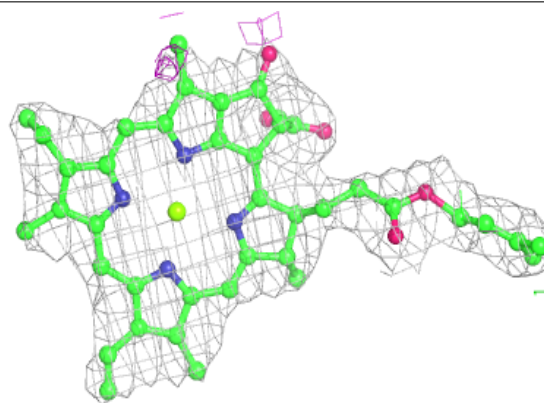


**Electron density around LHG G 852:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

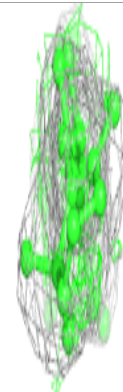
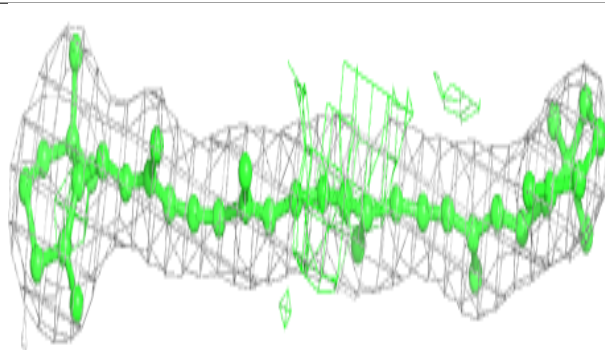
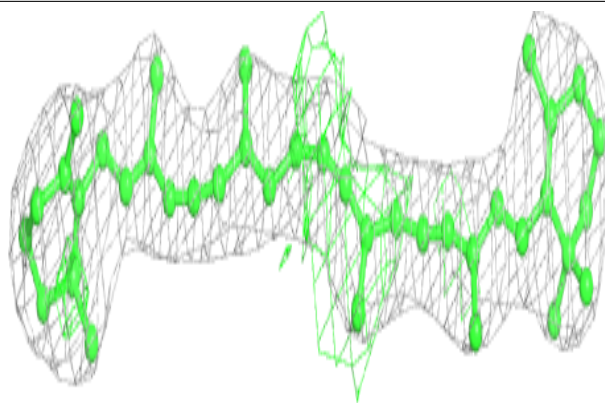
**Electron density around CLA A 836:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR J 103:**

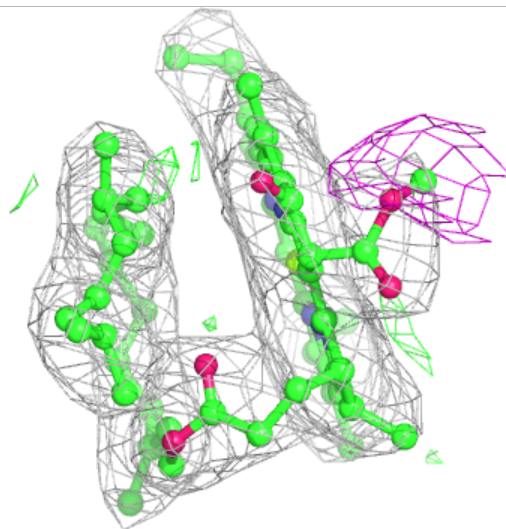
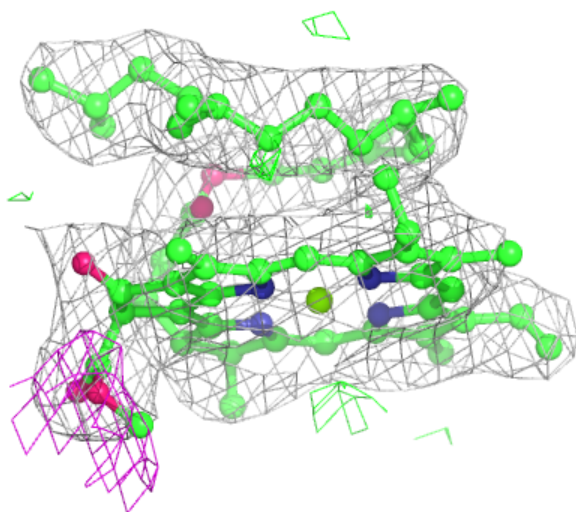
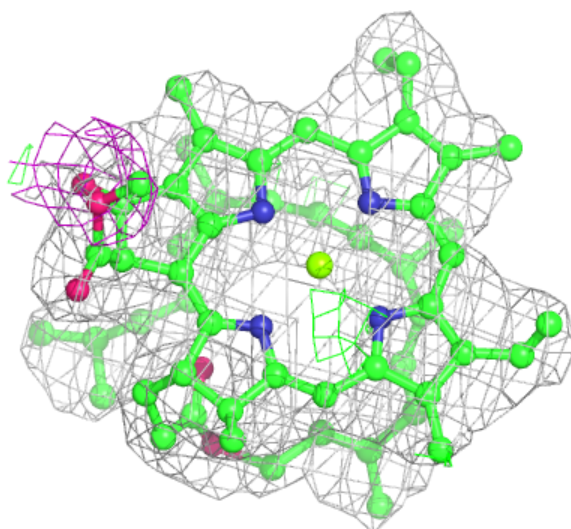
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





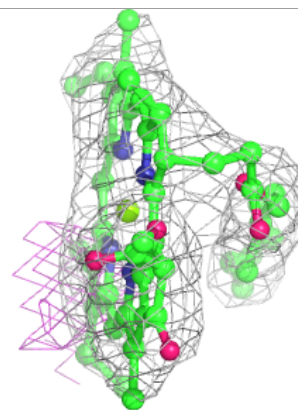
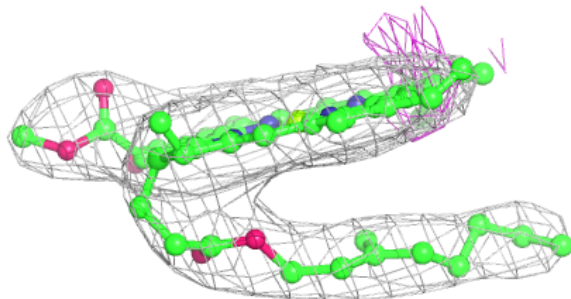
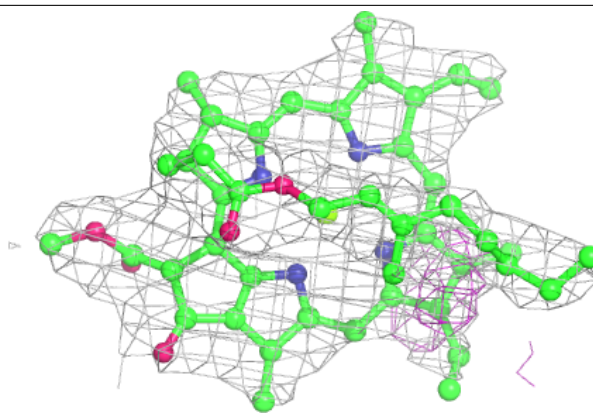
**Electron density around CLA U 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

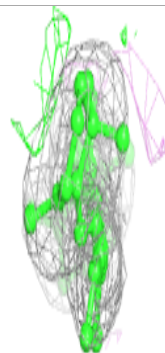
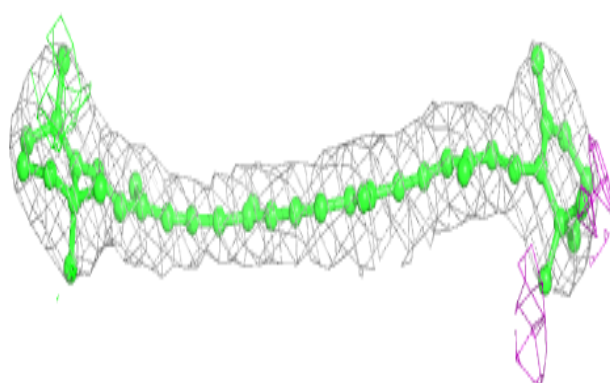
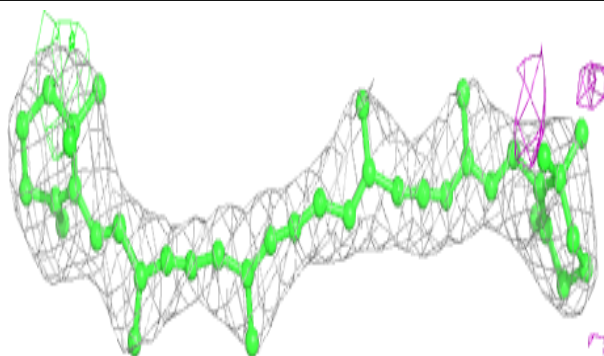


**Electron density around CLA A 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

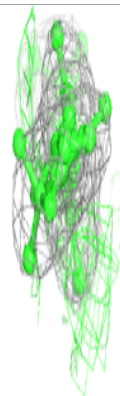
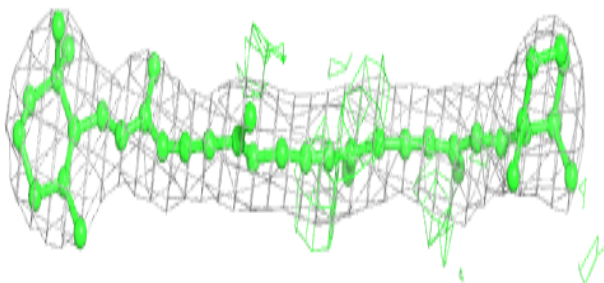
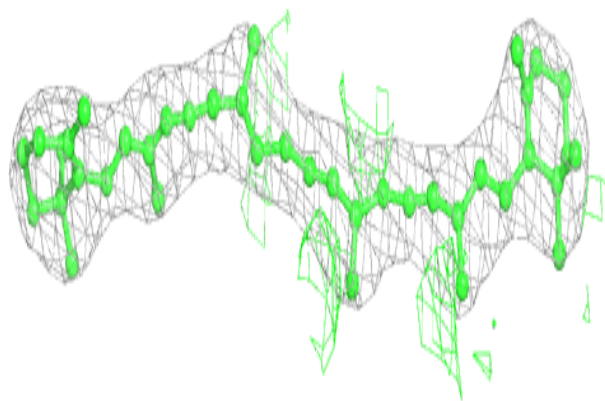
**Electron density around BCR A 847:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR G 854:**

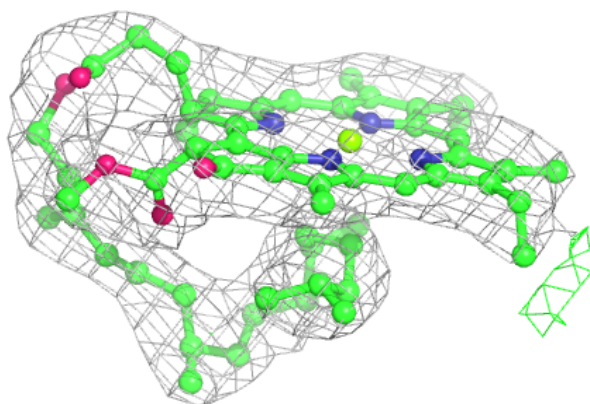
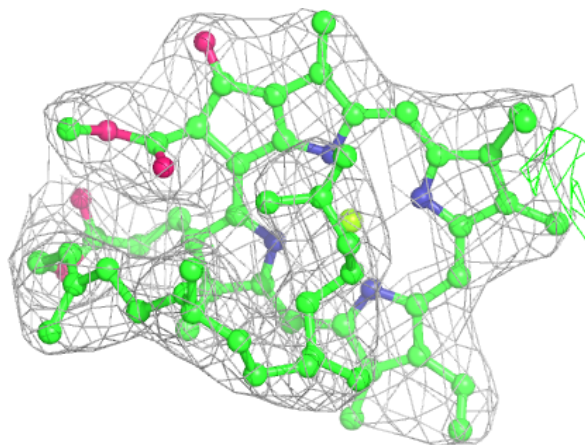
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





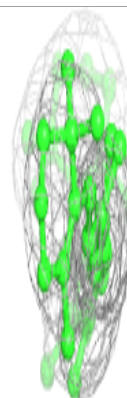
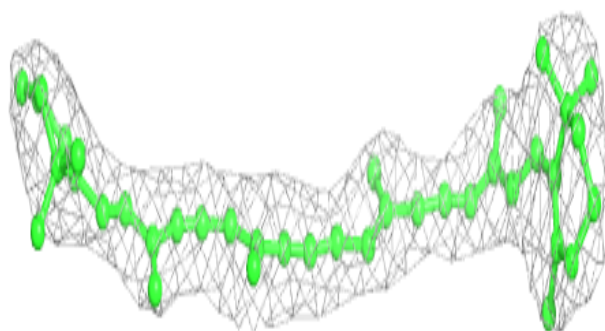
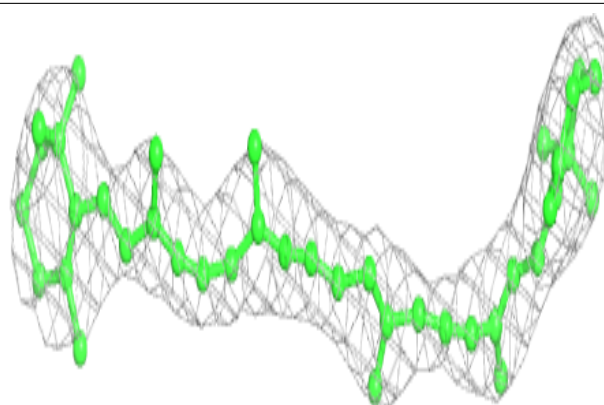
**Electron density around CLA H 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

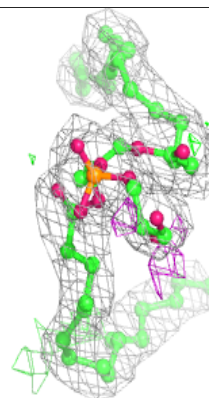
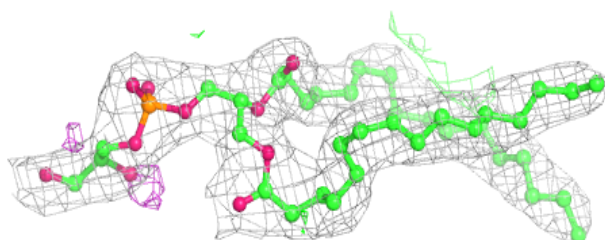
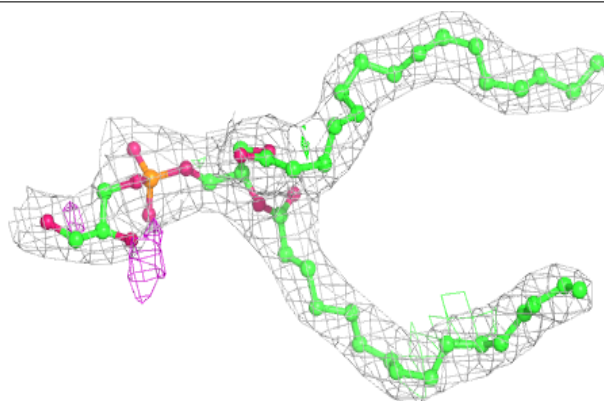


**Electron density around BCR Y 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

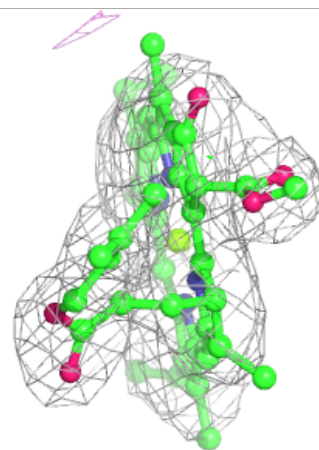
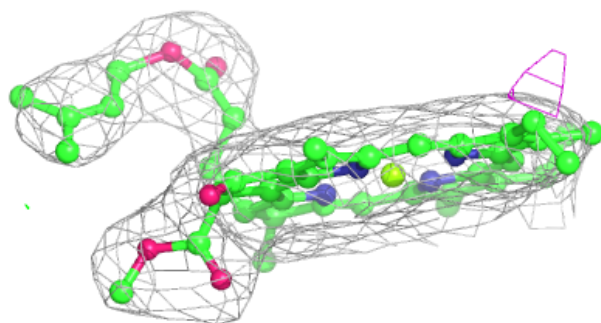
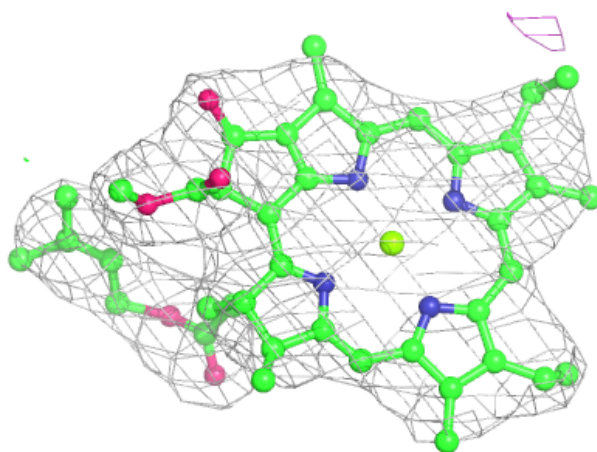
**Electron density around LHG A 850:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



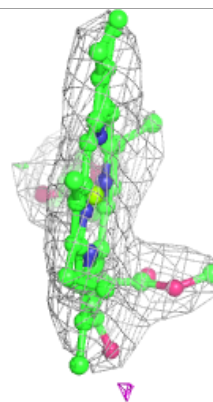
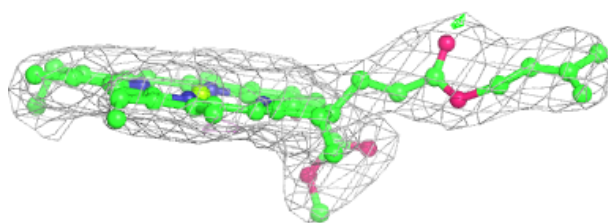
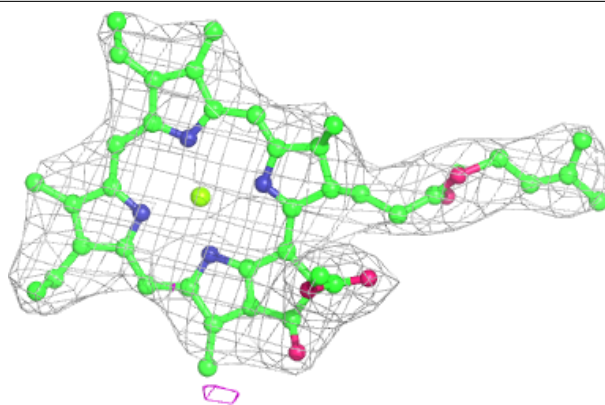
**Electron density around CLA G 816:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



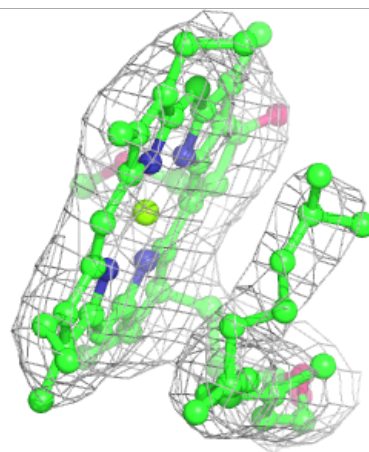
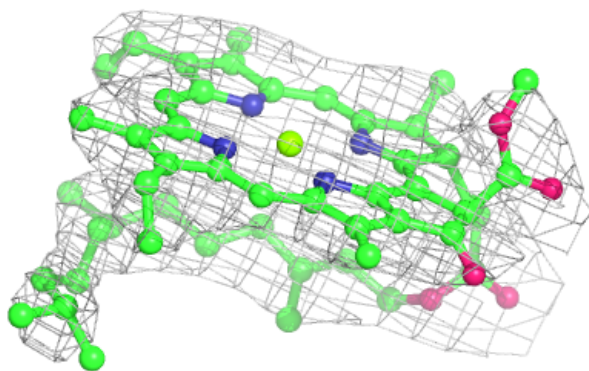
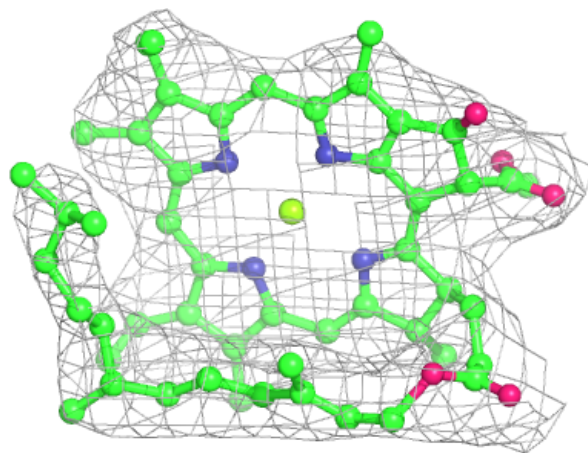
**Electron density around CLA G 836:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 820:**

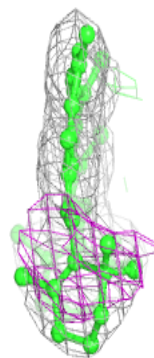
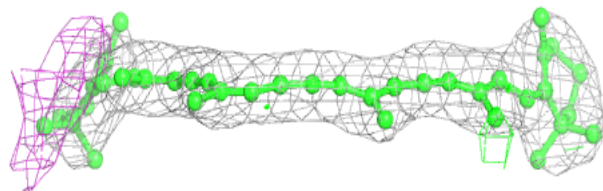
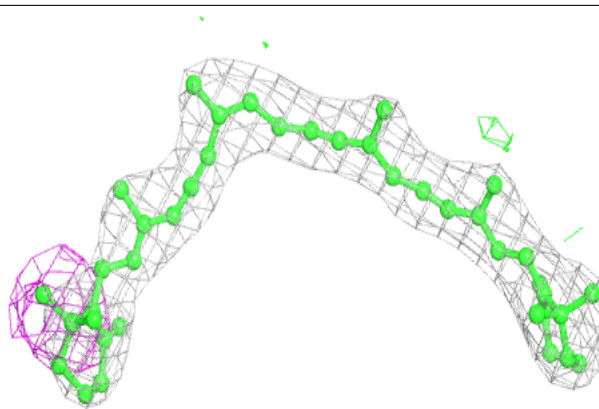
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



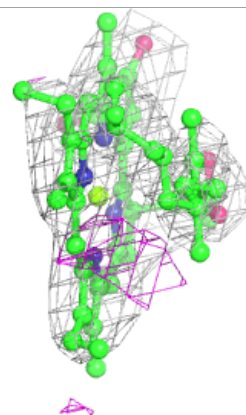
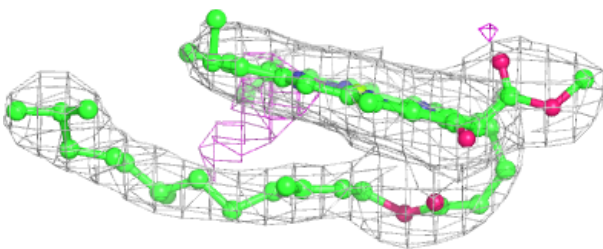
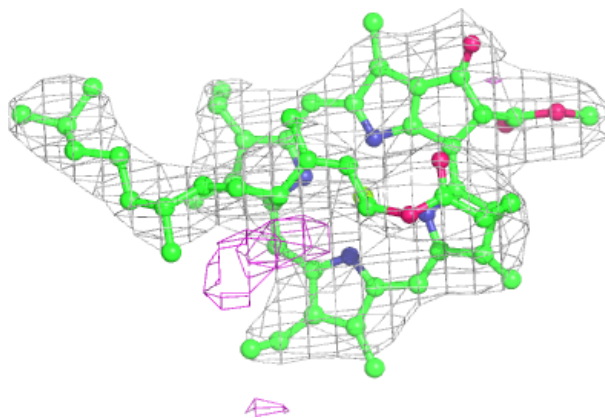


**Electron density around BCR d 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

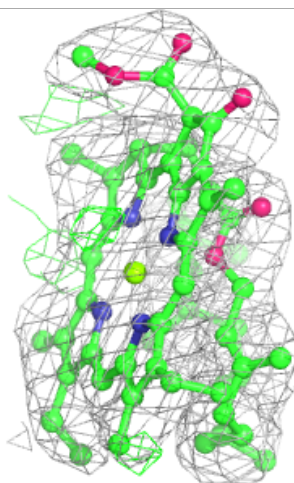
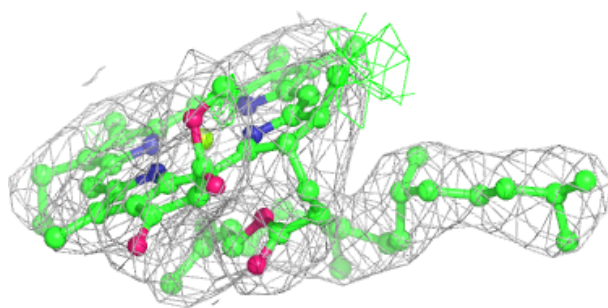
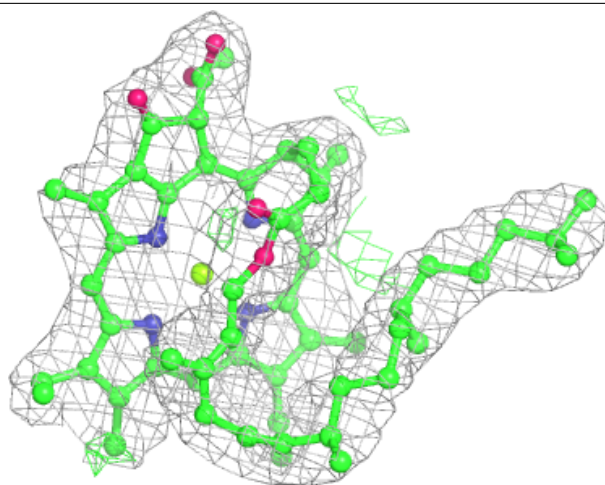
**Electron density around CLA G 817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



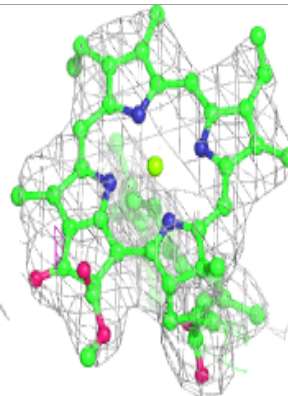
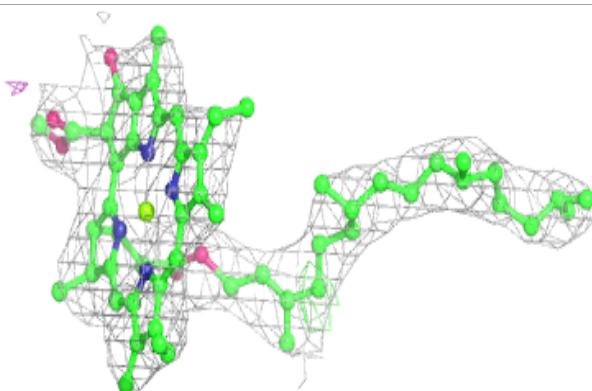
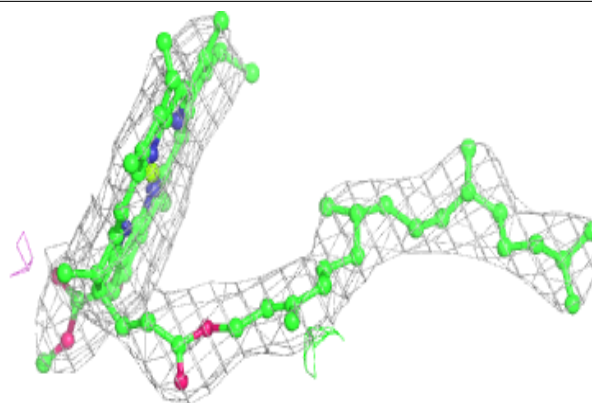
**Electron density around CLA H 807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

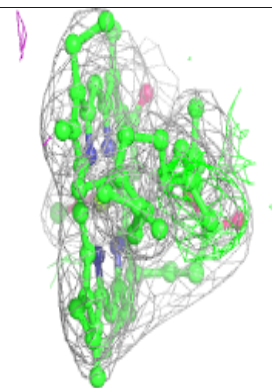
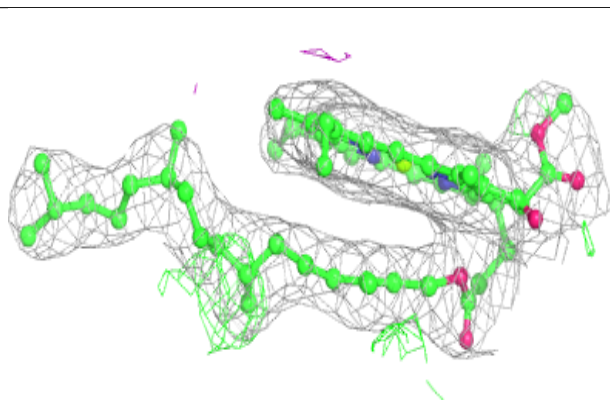
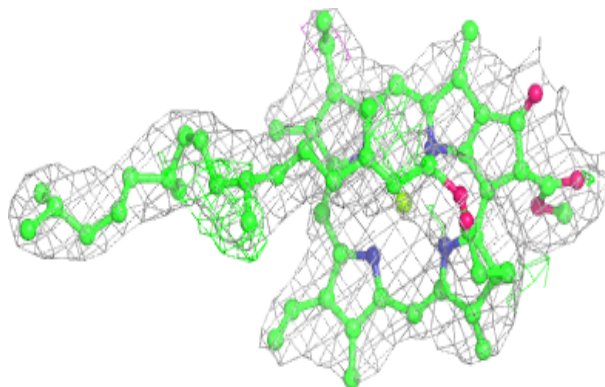


**Electron density around CLA Y 811:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Y 838:**

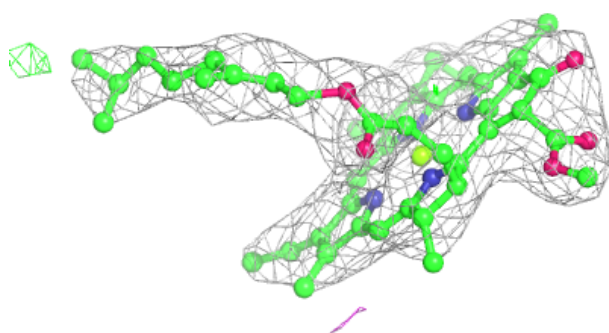
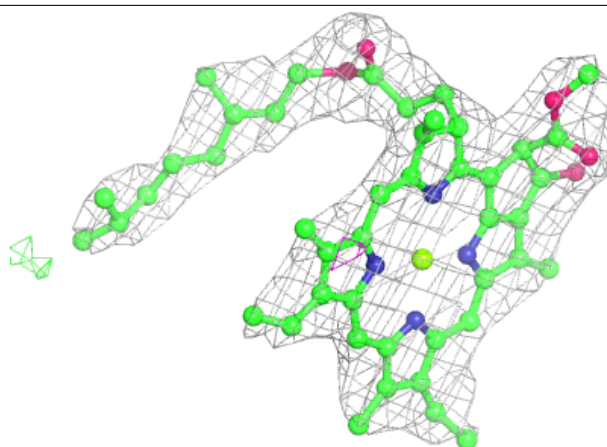
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



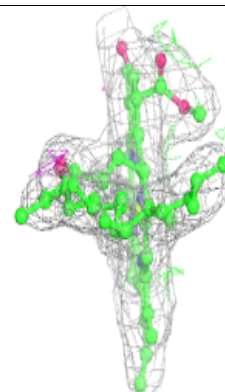
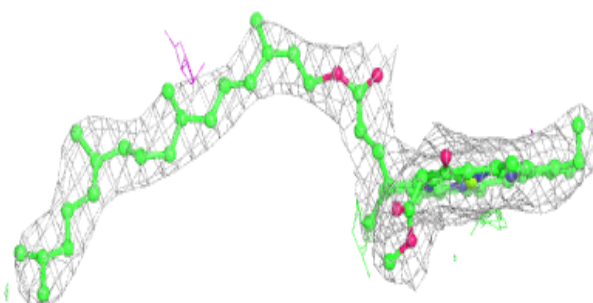
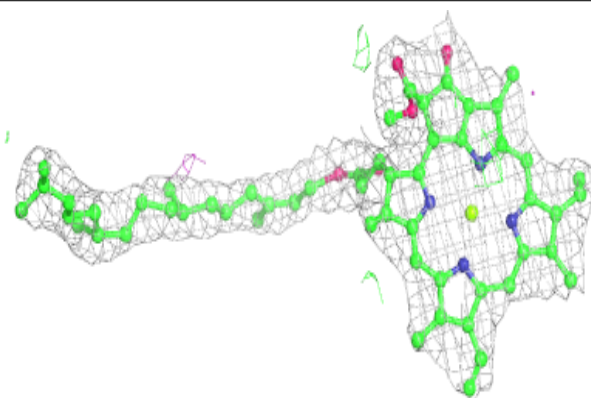


**Electron density around CLA H 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

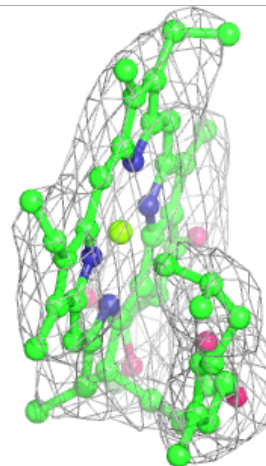
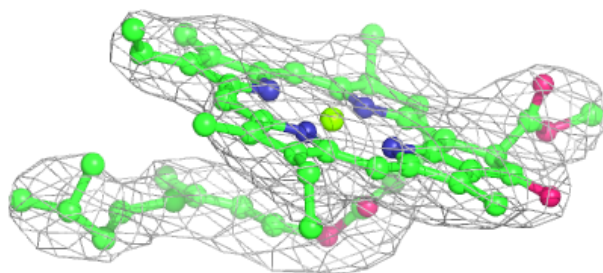
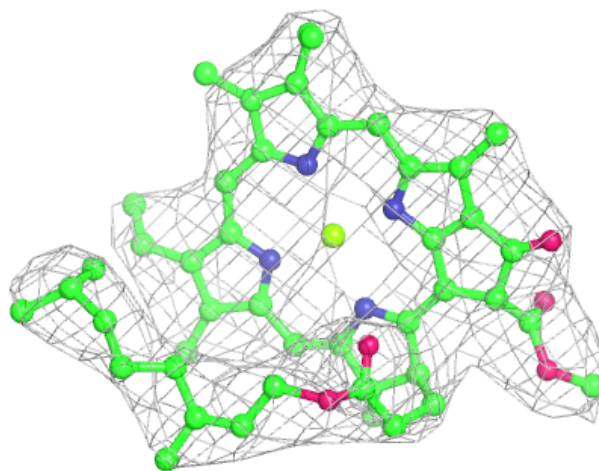
**Electron density around CLA B 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



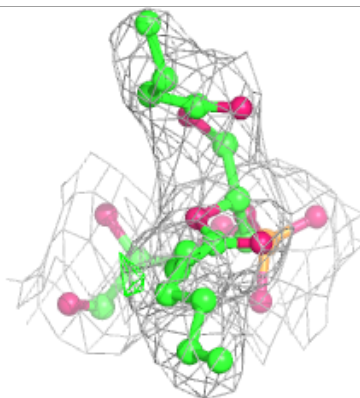
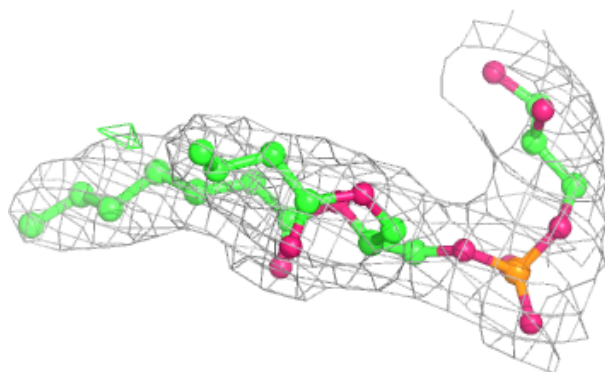
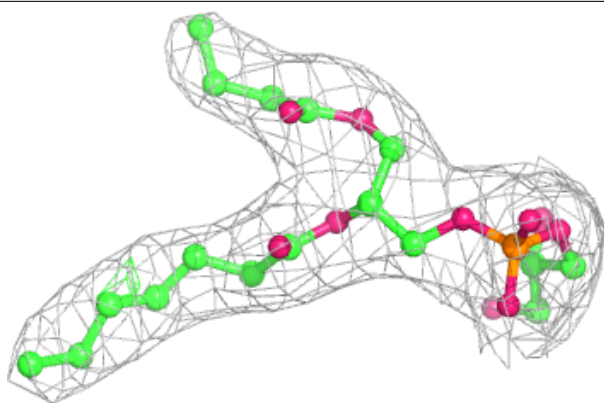
**Electron density around CLA Y 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



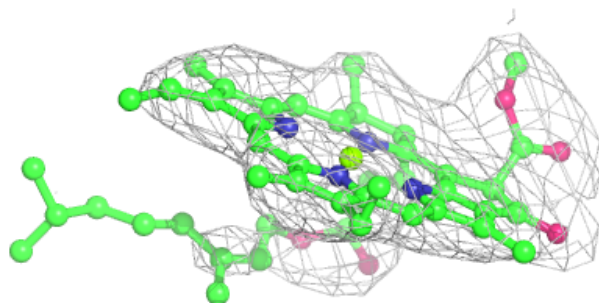
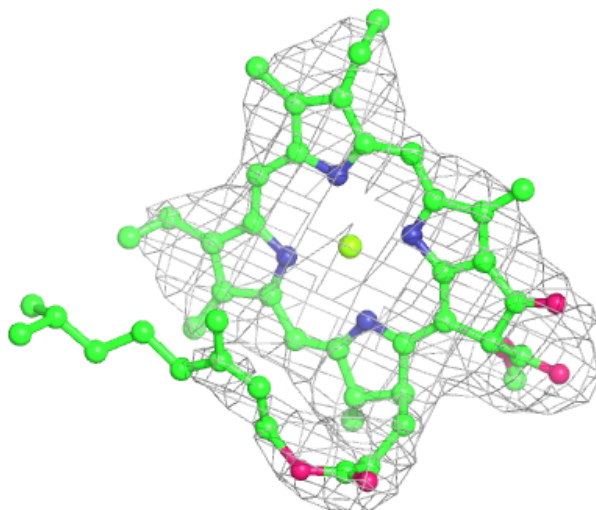
**Electron density around LHG j 101:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



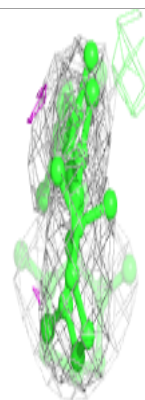
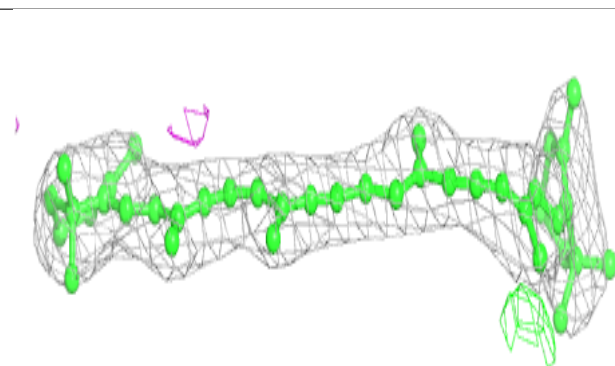
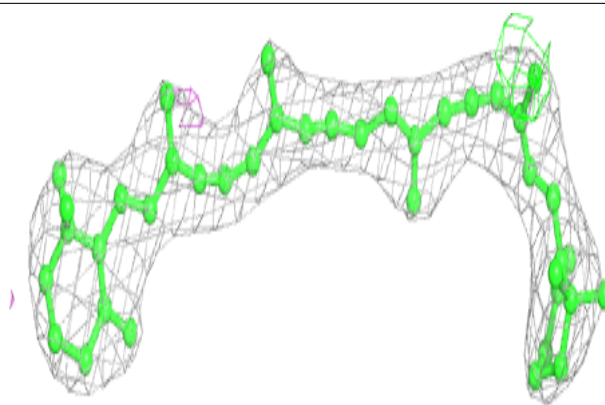
**Electron density around CLA J 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



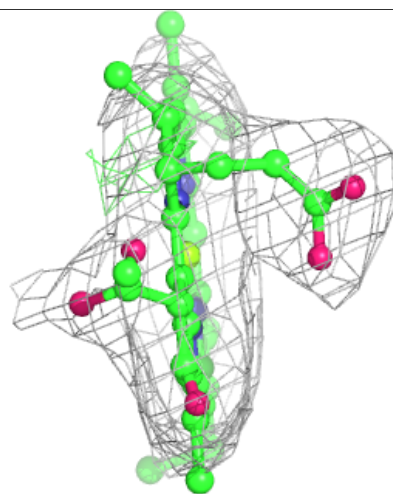
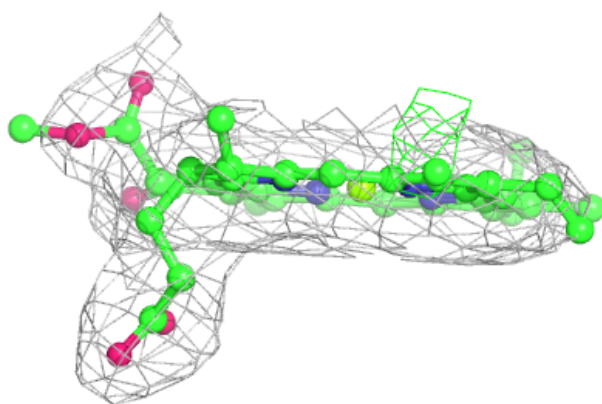
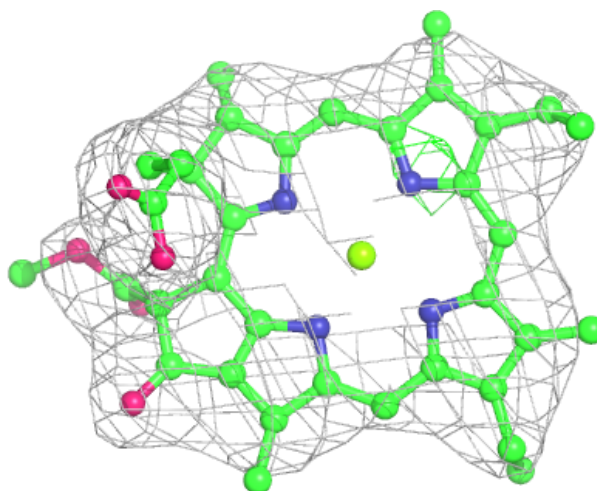
**Electron density around BCR B 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA S 1102:**

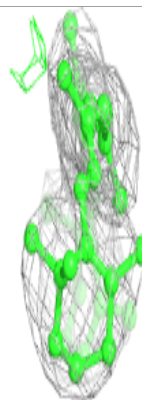
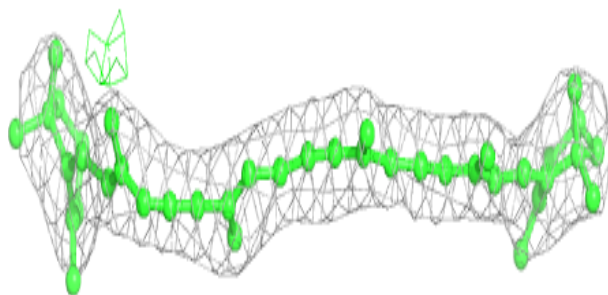
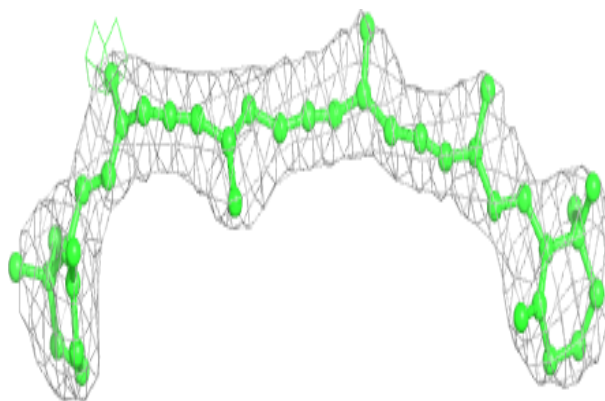
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



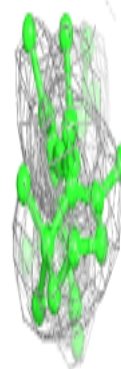
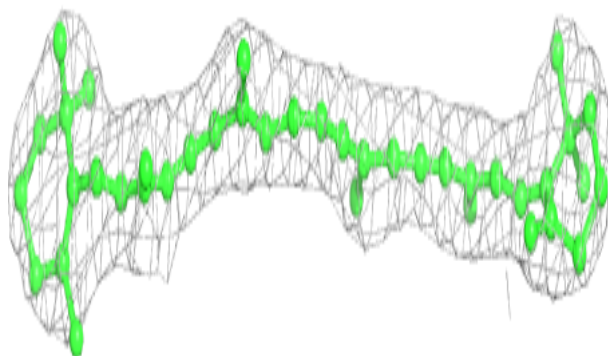
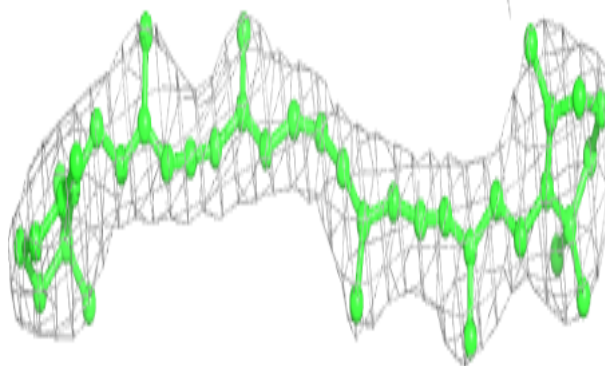


**Electron density around BCR H 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

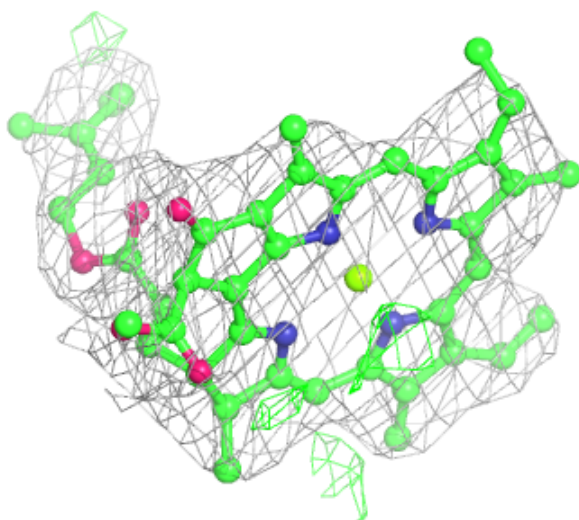
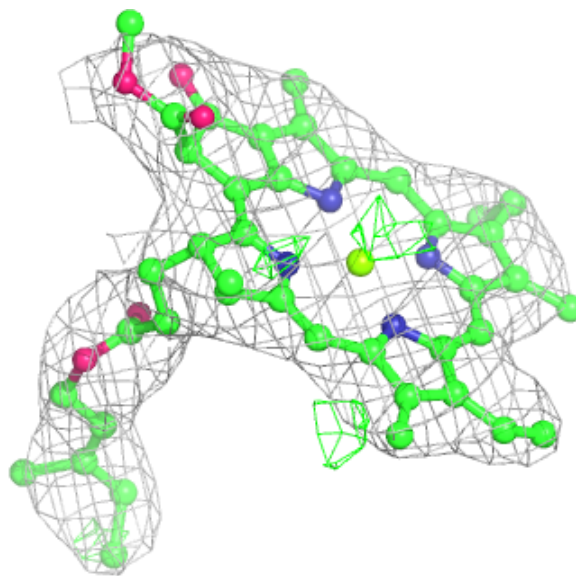
**Electron density around BCR A 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 807:**

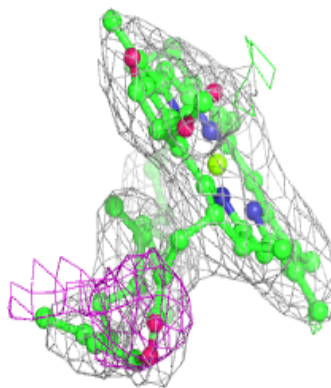
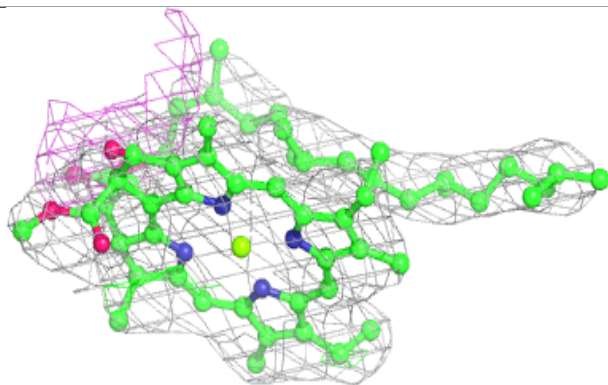
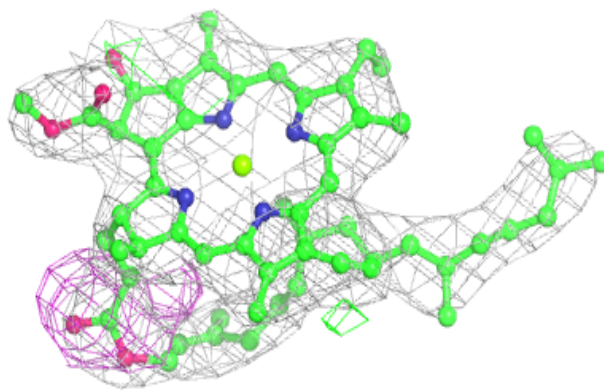
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





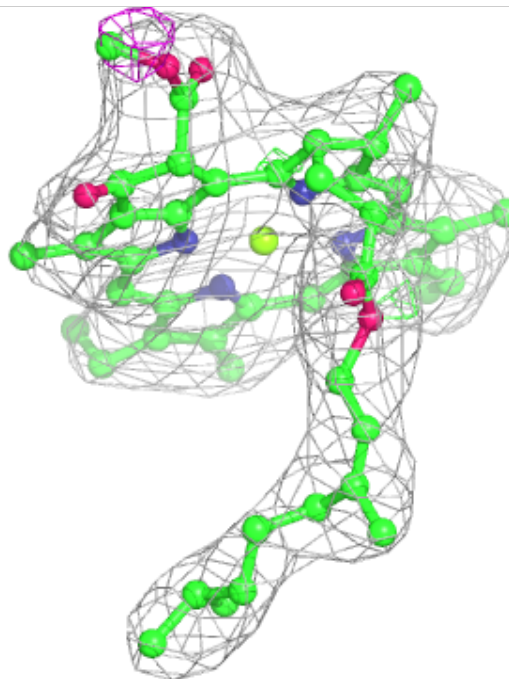
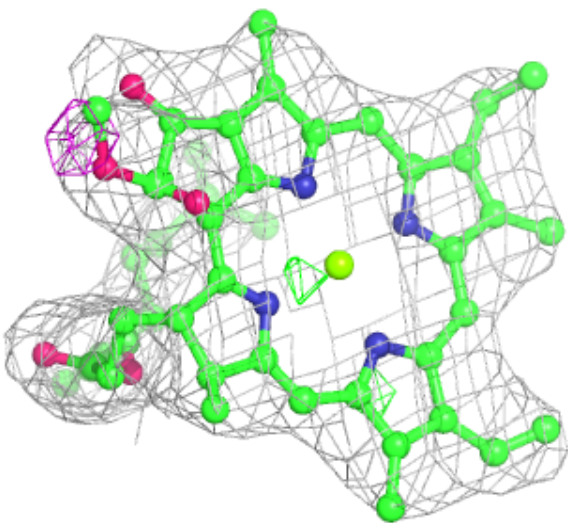
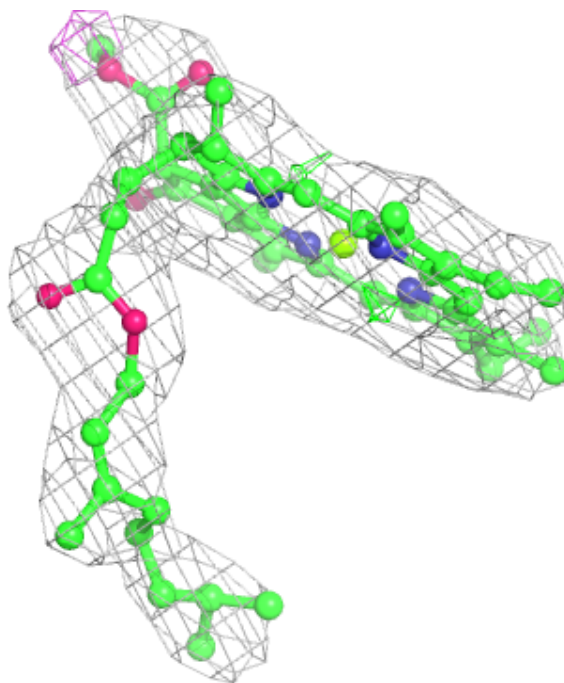
**Electron density around CLA Z 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



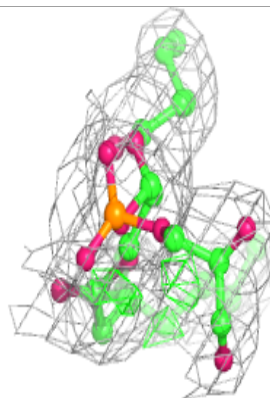
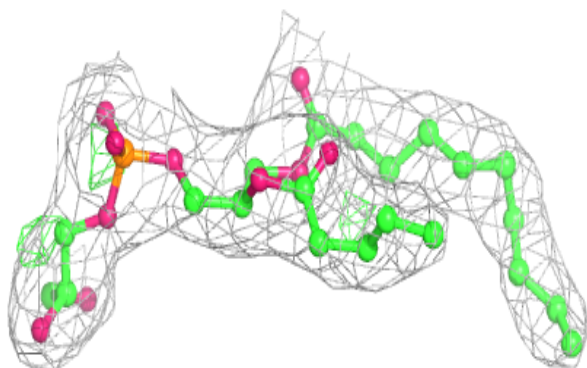
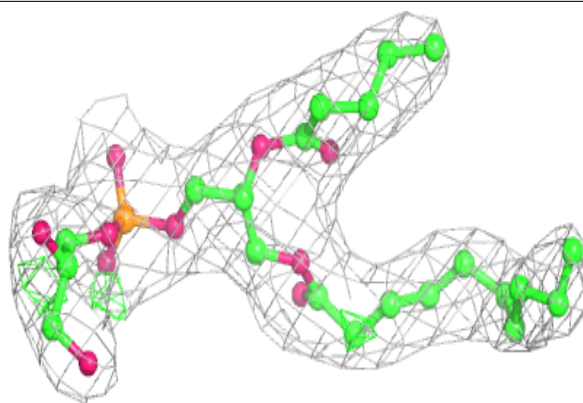
**Electron density around CLA H 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

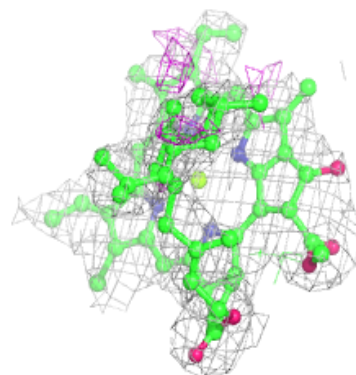
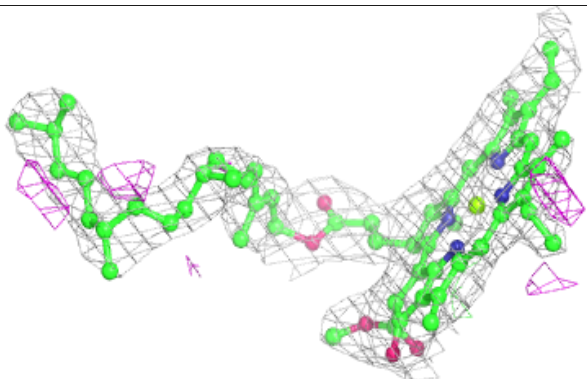
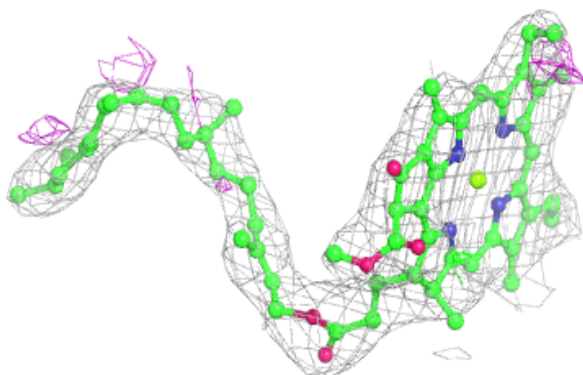


**Electron density around LHG A 851:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

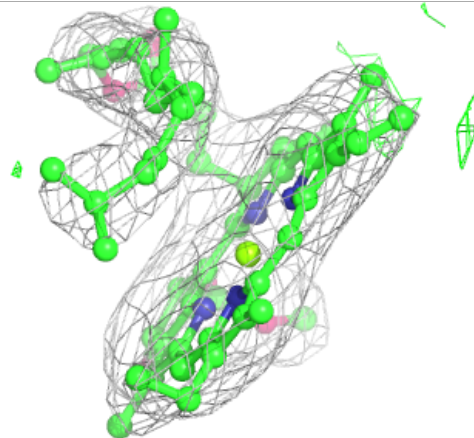
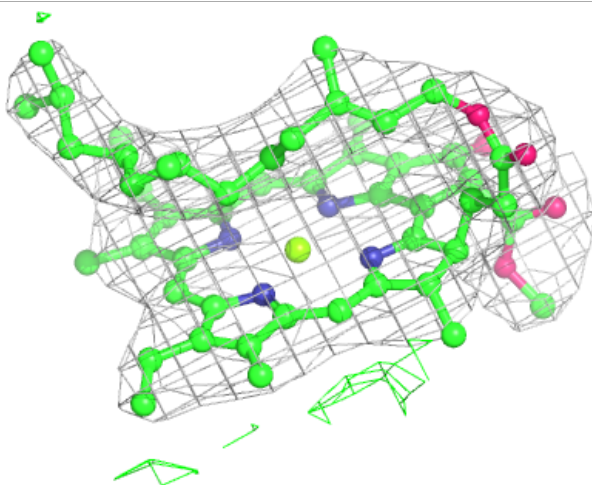
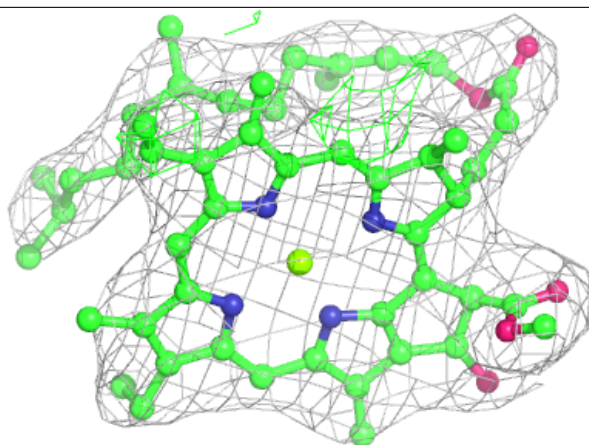
**Electron density around CLA H 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



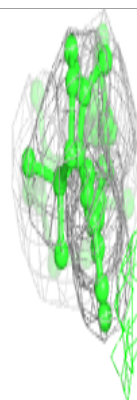
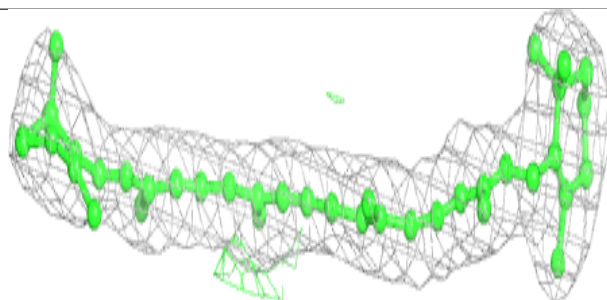
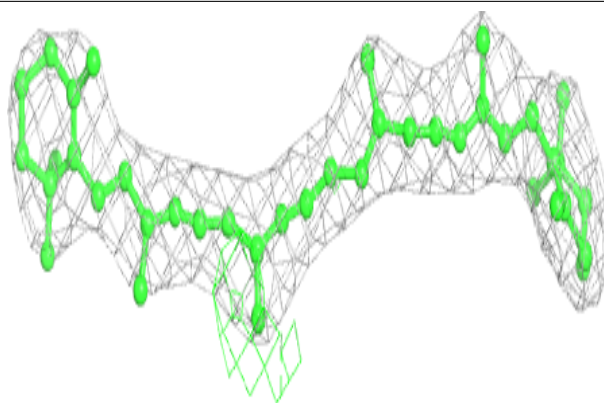
**Electron density around CLA Y 820:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

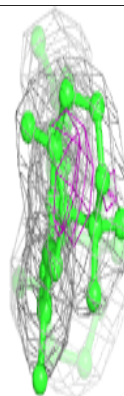
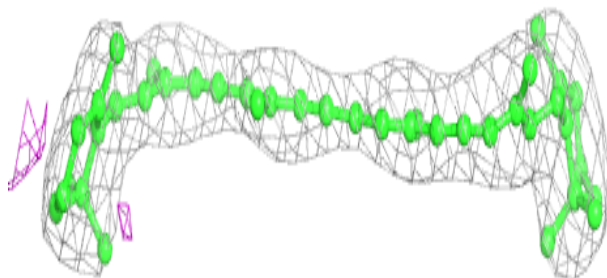
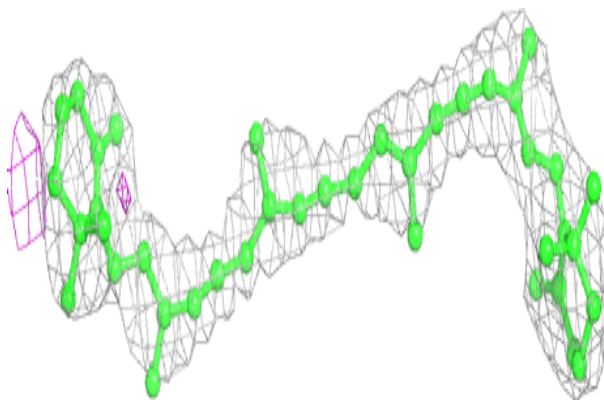


**Electron density around BCR G 849:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR H 842:**

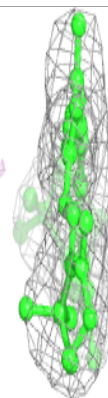
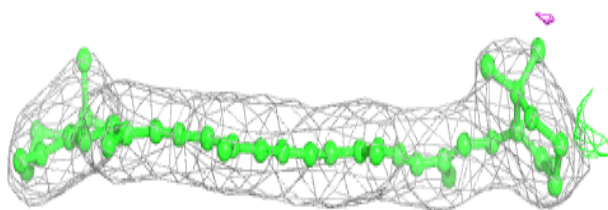
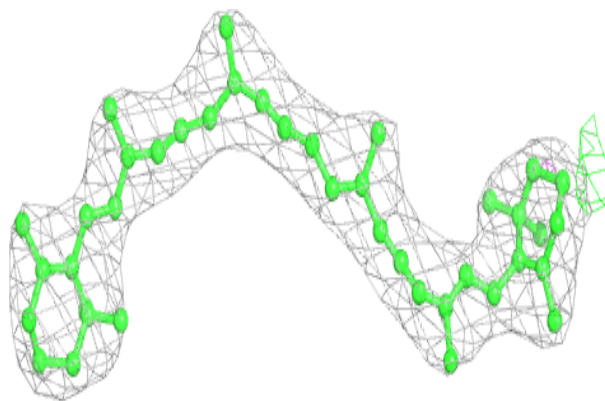
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





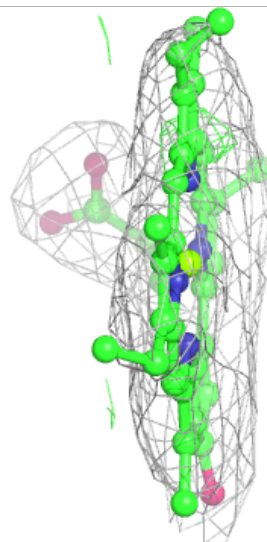
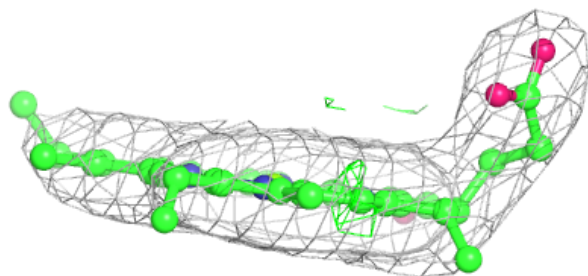
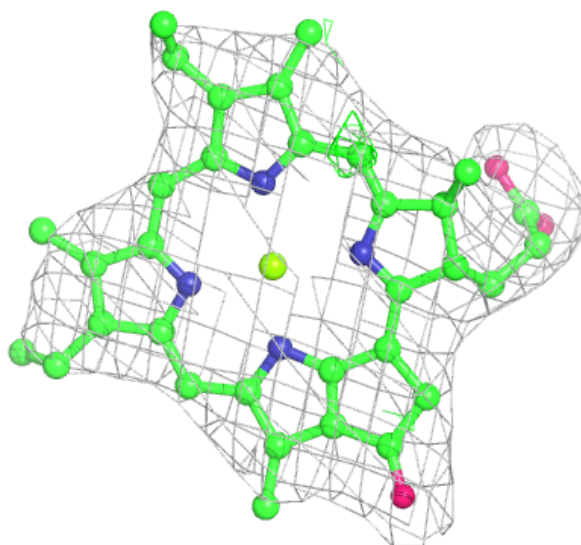
**Electron density around BCR Y 851:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



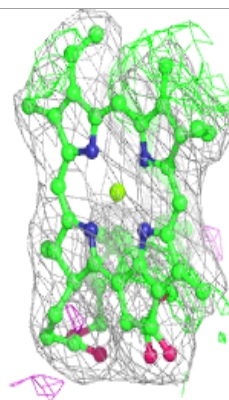
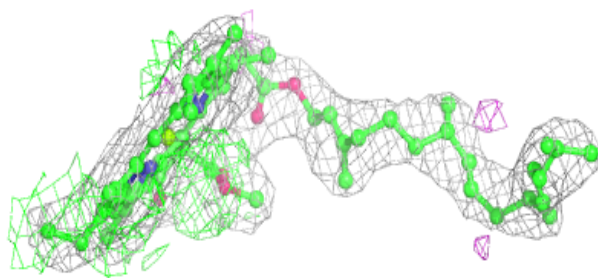
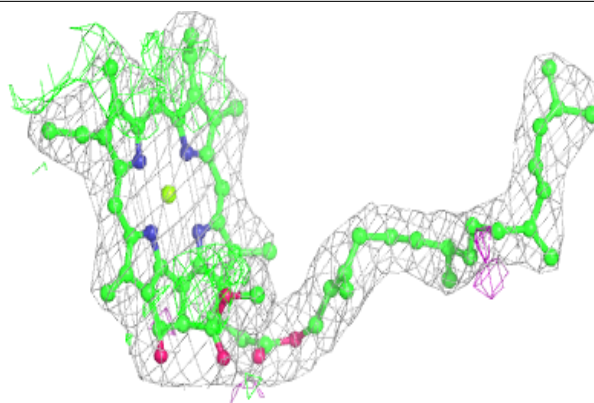
**Electron density around CLA T 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

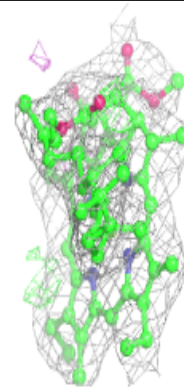
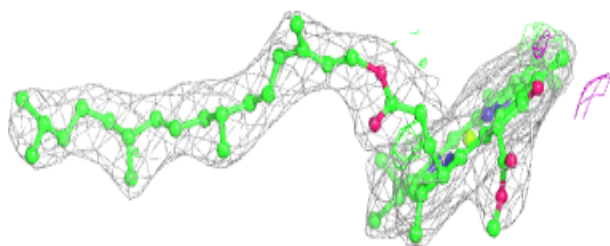
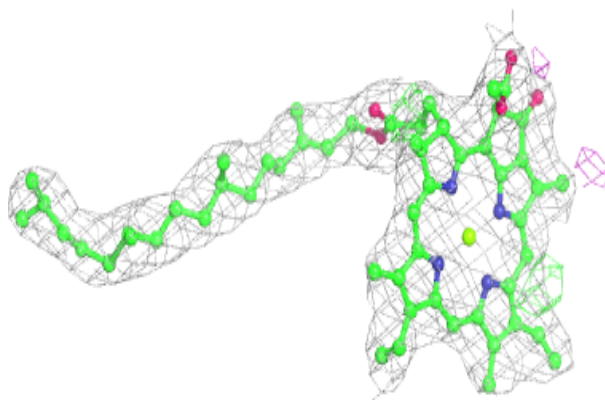


**Electron density around CLA U 1006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Y 834:**

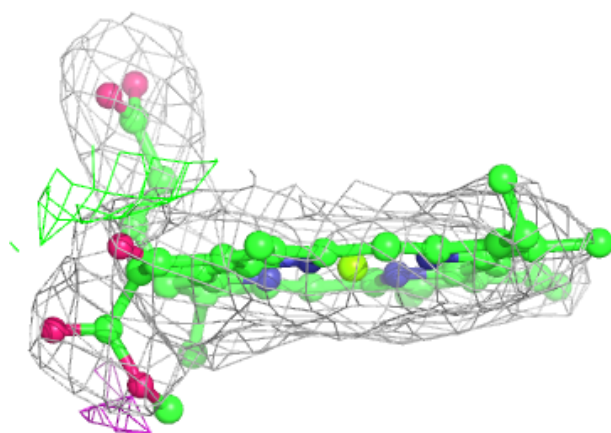
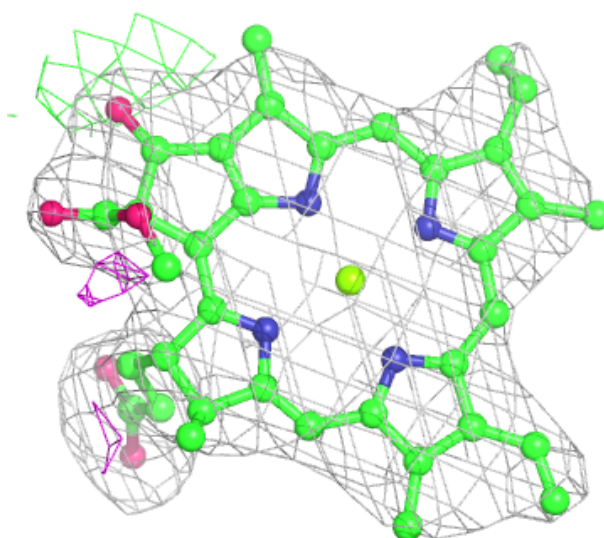
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





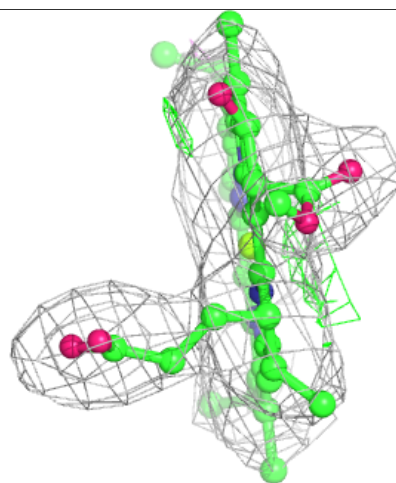
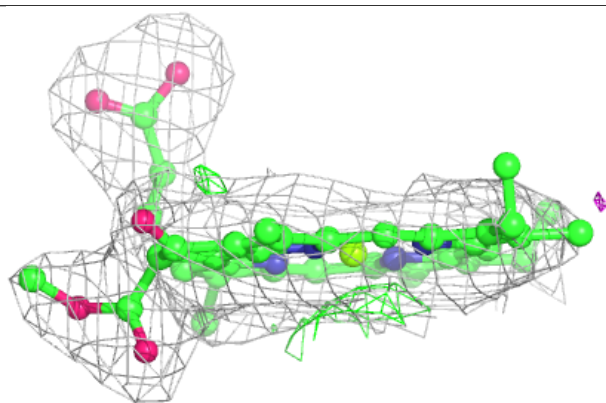
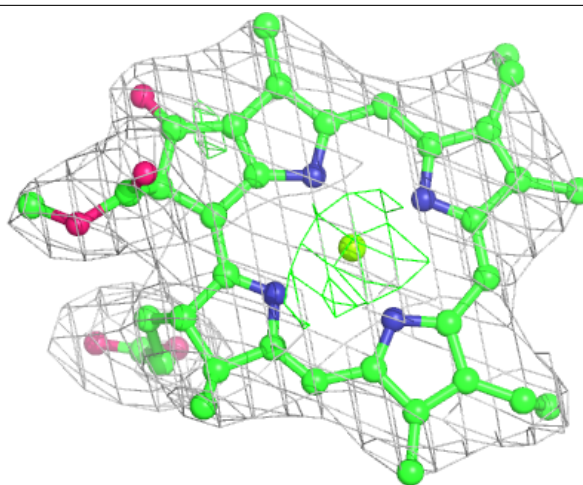
**Electron density around CLA Z 832:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



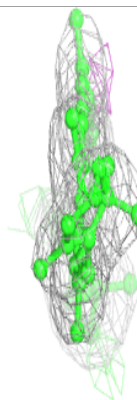
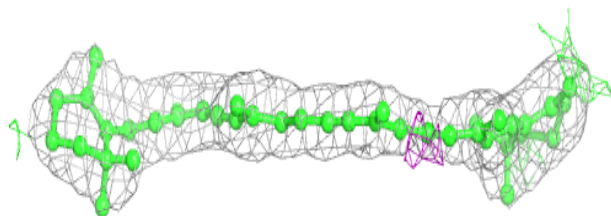
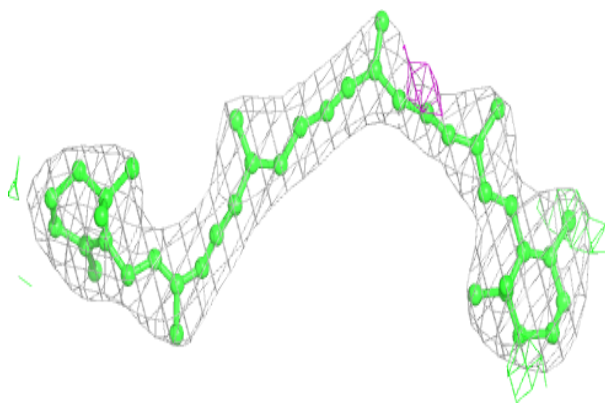
**Electron density around CLA Z 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



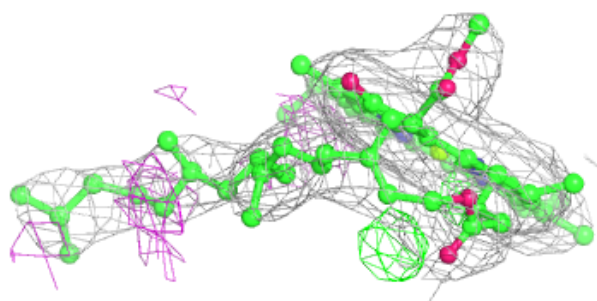
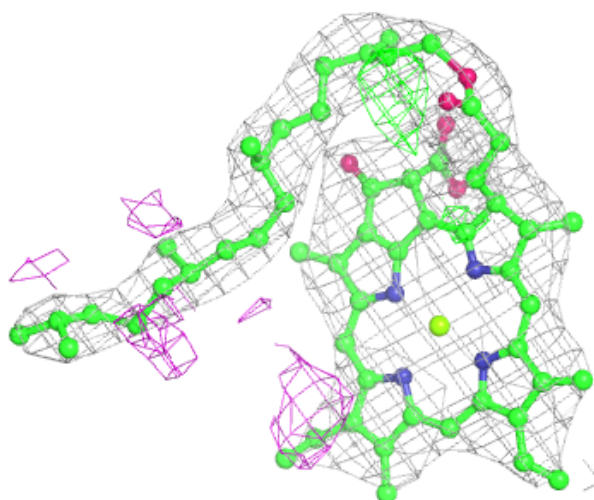
**Electron density around BCR A 849:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



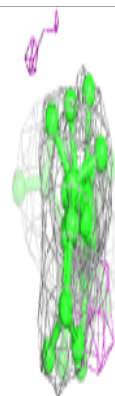
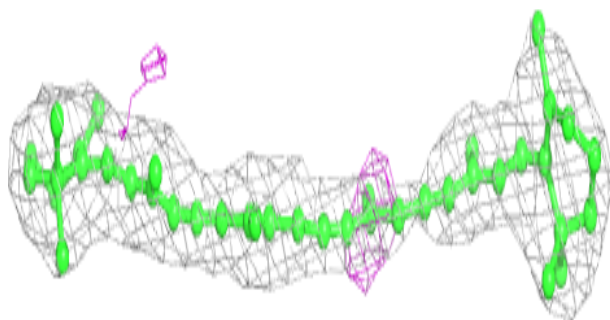
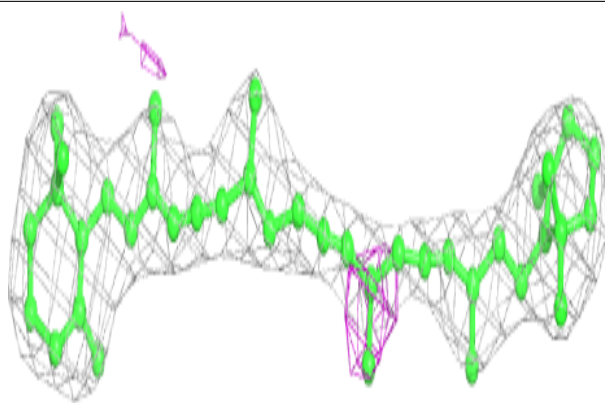
**Electron density around CLA A 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

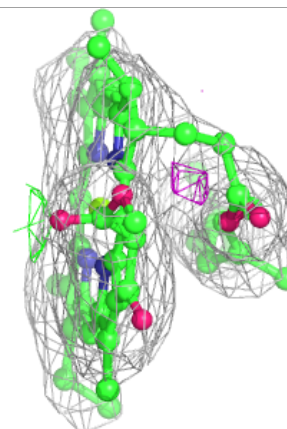
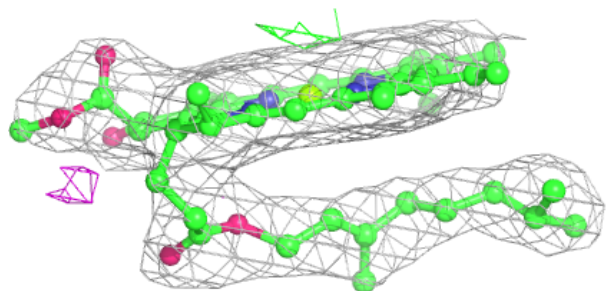
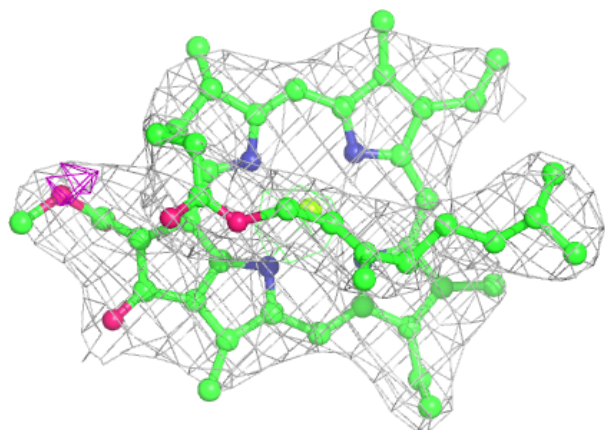


**Electron density around BCR B 851:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

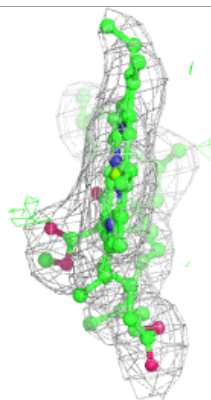
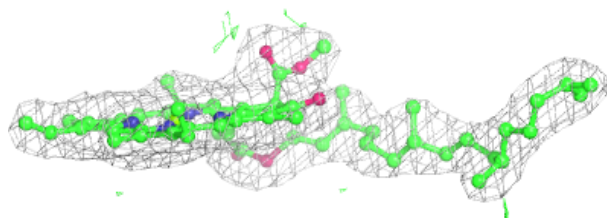
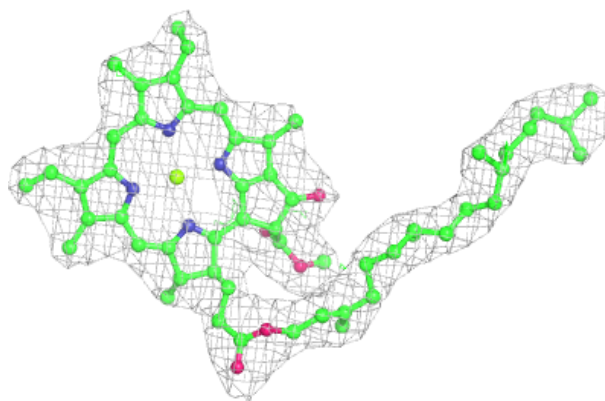
**Electron density around CLA H 821:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA L 207:**

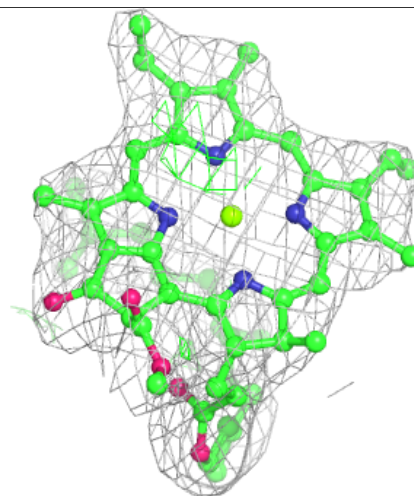
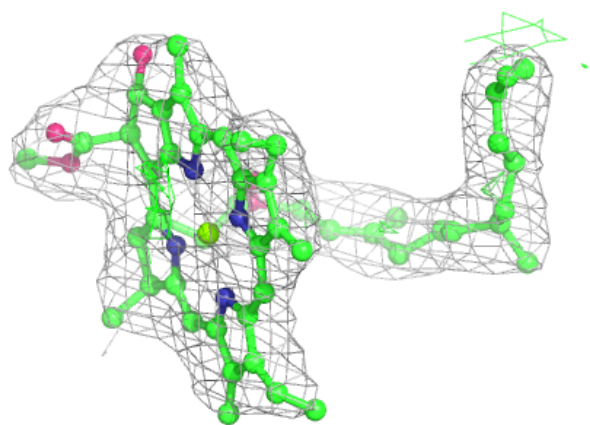
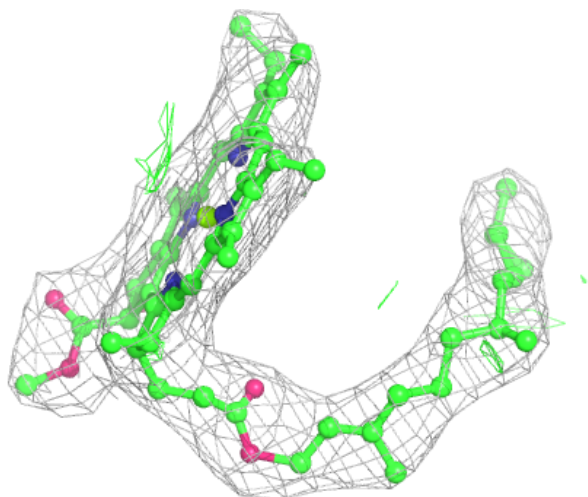
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





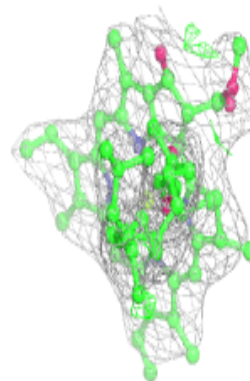
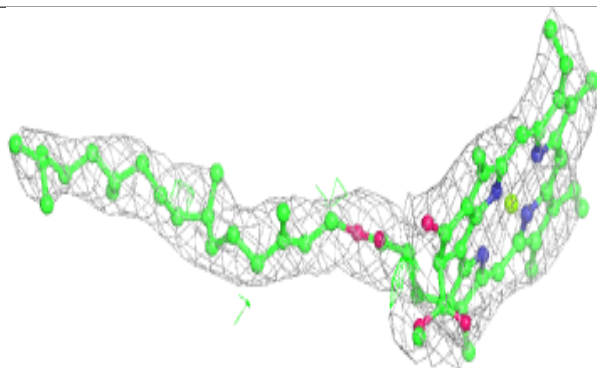
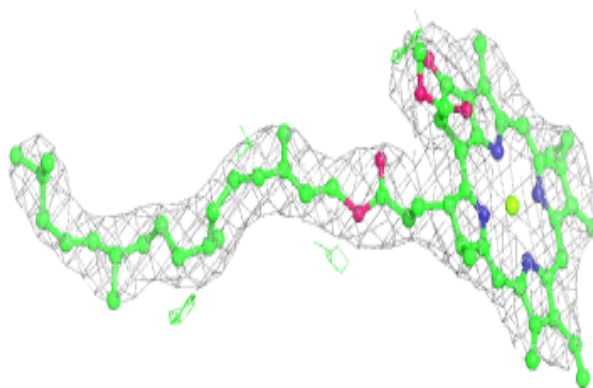
**Electron density around CLA B 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

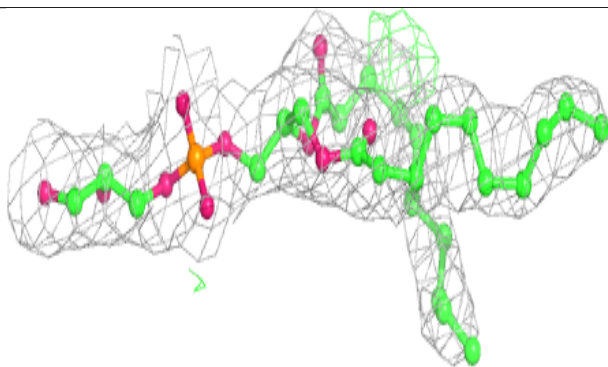
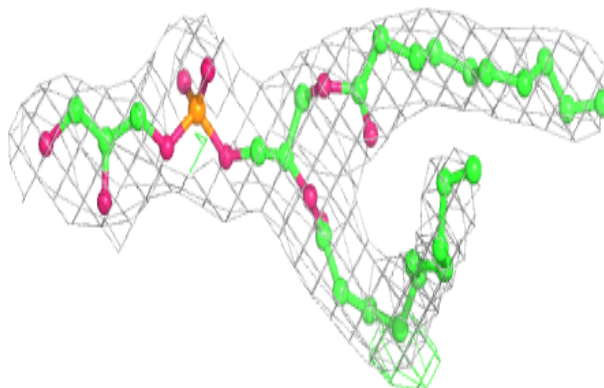


**Electron density around CLA G 809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LHG H 847:**

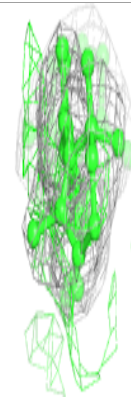
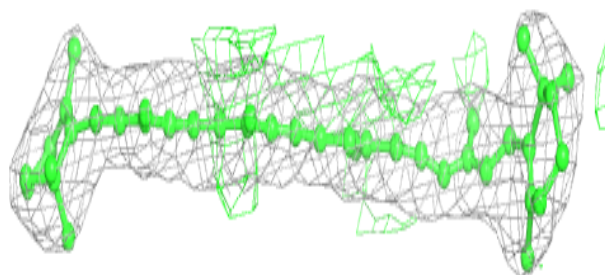
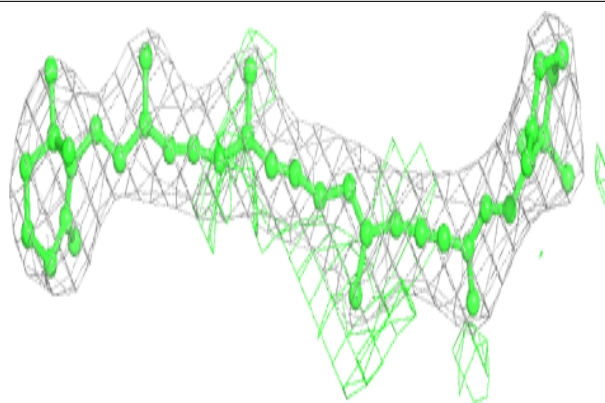
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





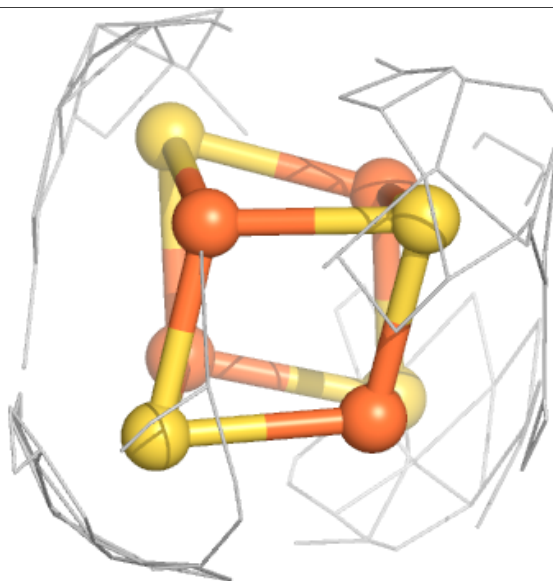
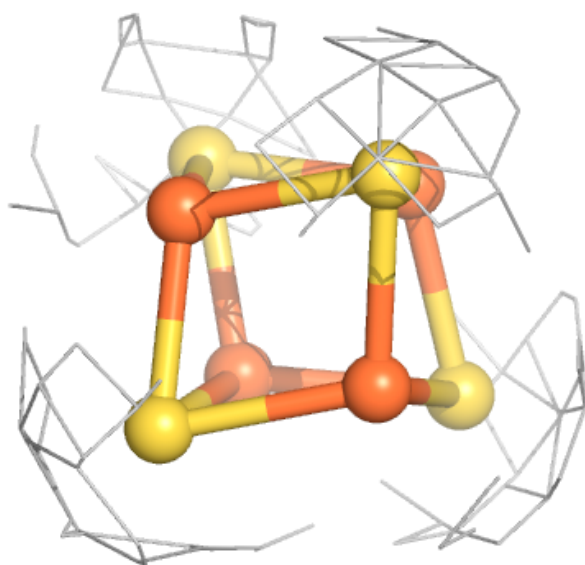
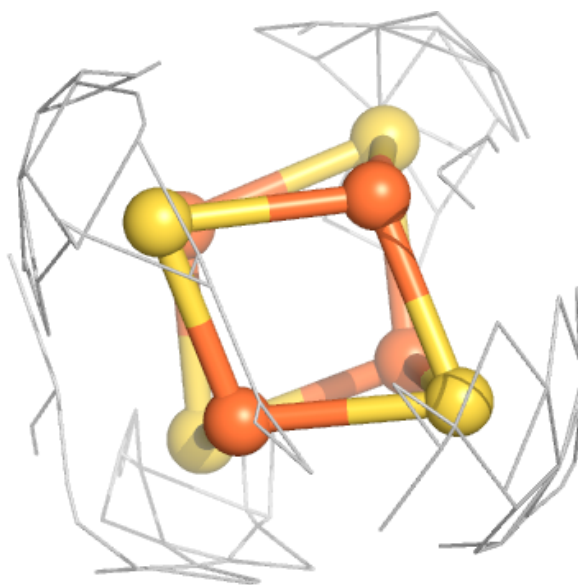
**Electron density around BCR B 848:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



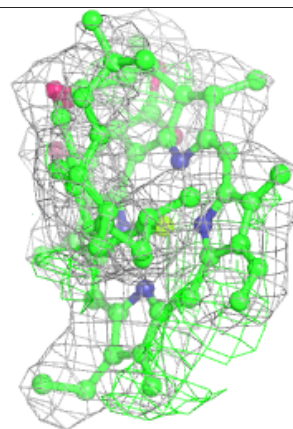
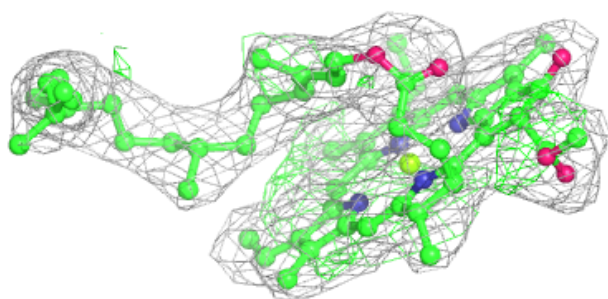
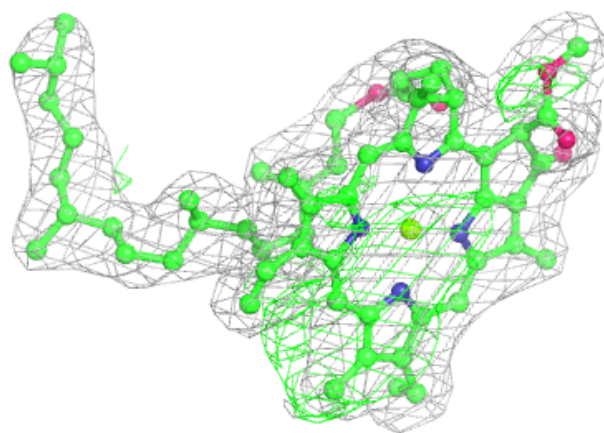
**Electron density around SF4 a 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



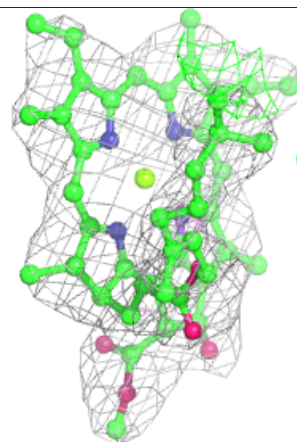
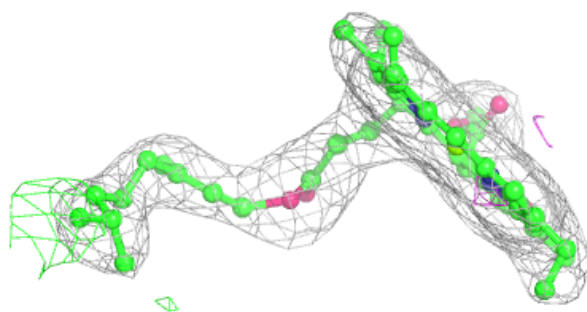
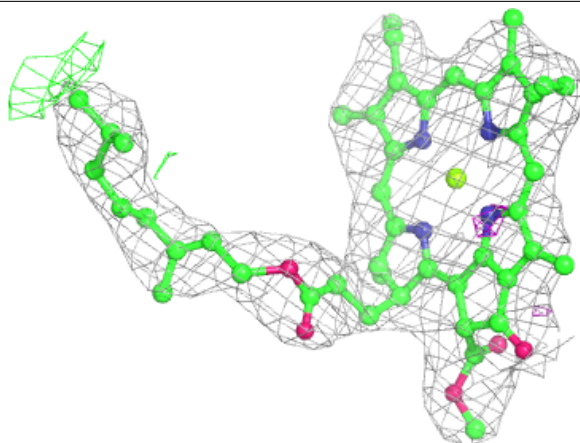
**Electron density around CLA A 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

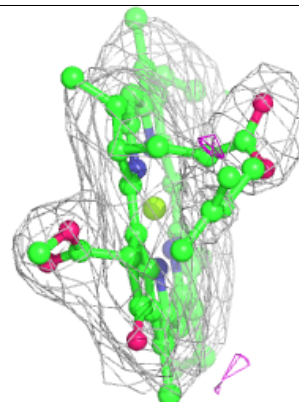
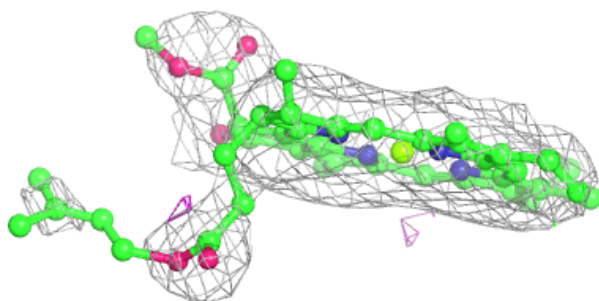
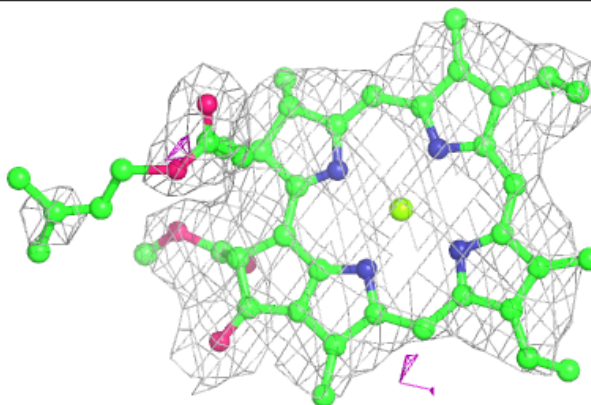


**Electron density around CLA G 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

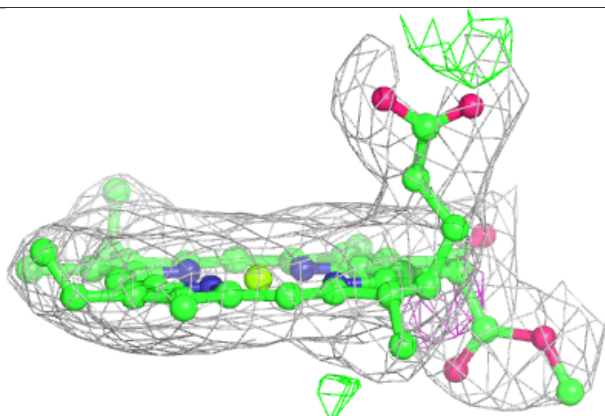
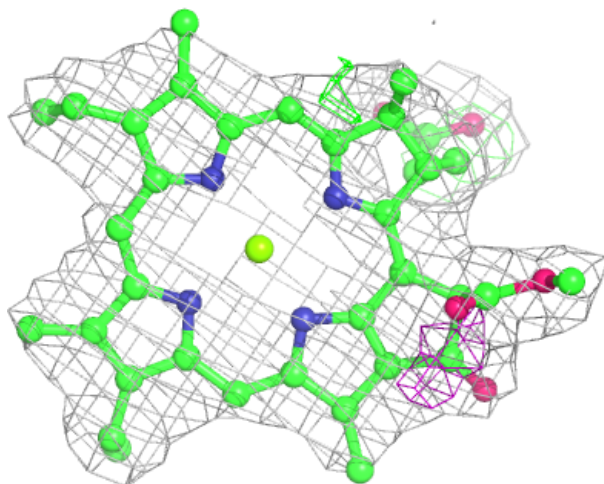
**Electron density around CLA A 816:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Z 837:**

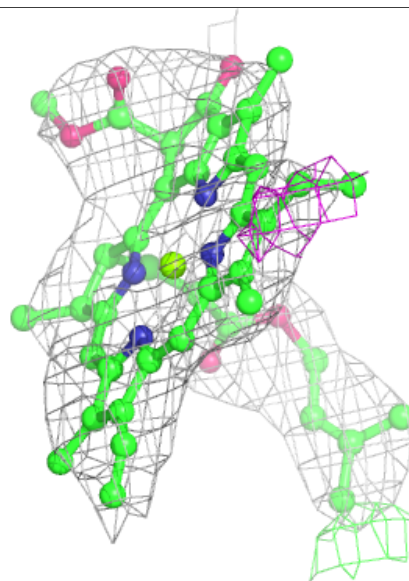
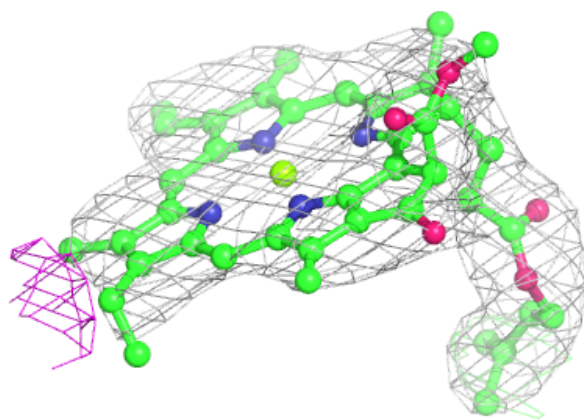
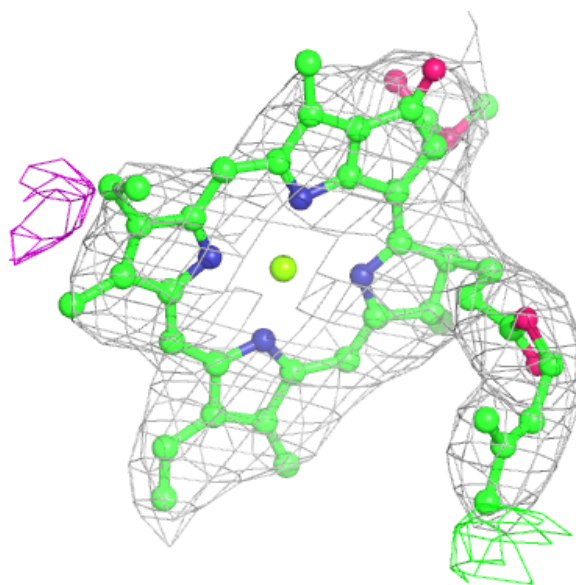
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





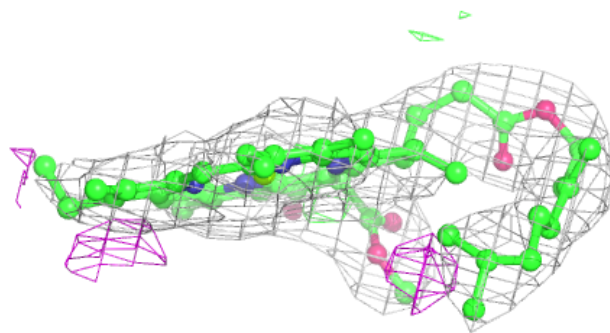
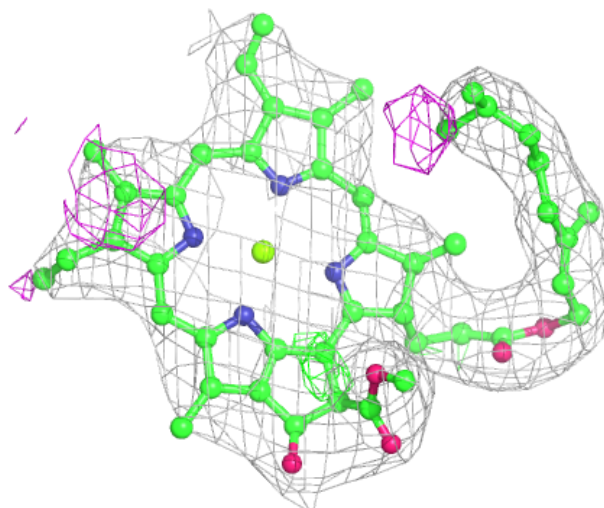
**Electron density around CLA A 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



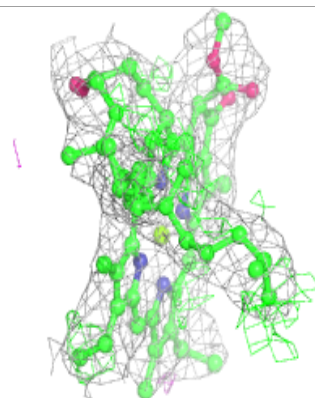
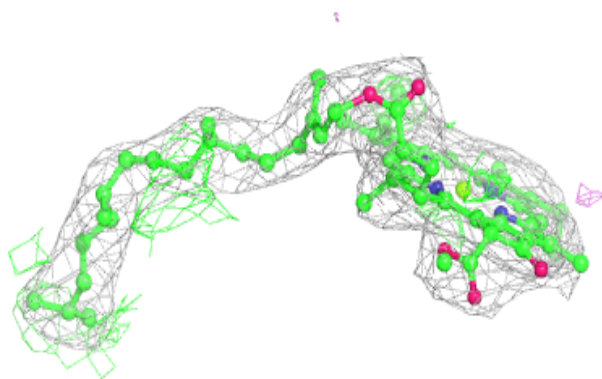
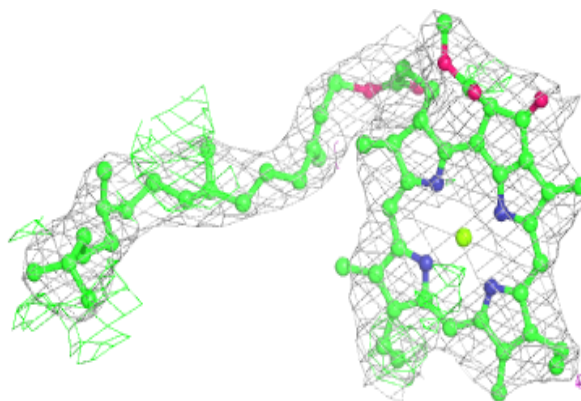
**Electron density around CLA H 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

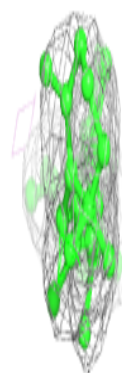
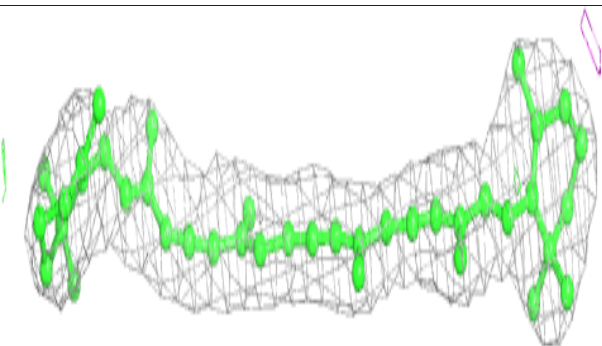
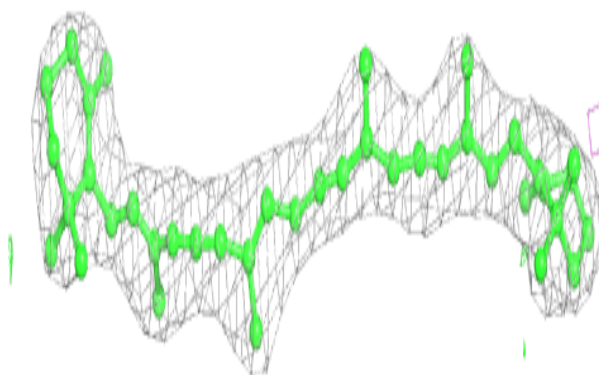


**Electron density around CLA B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR h 202:**

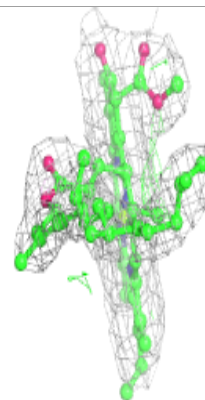
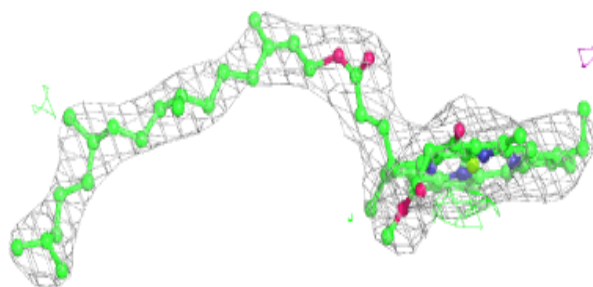
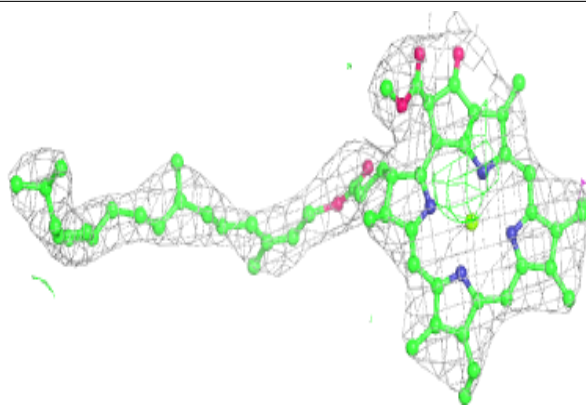
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



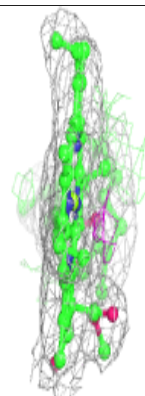
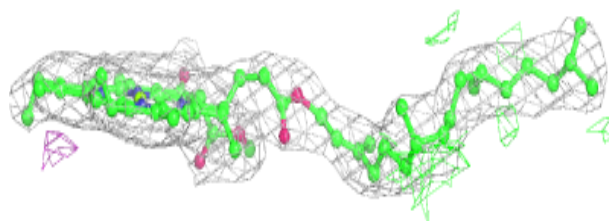
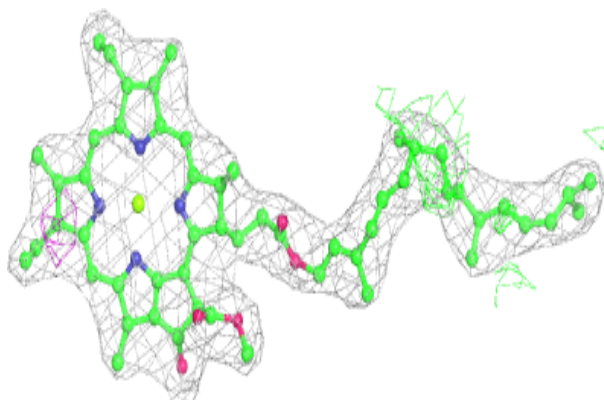


**Electron density around CLA H 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

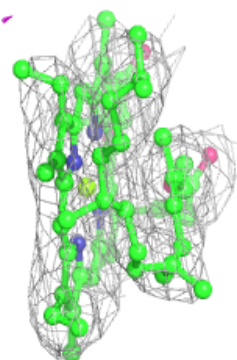
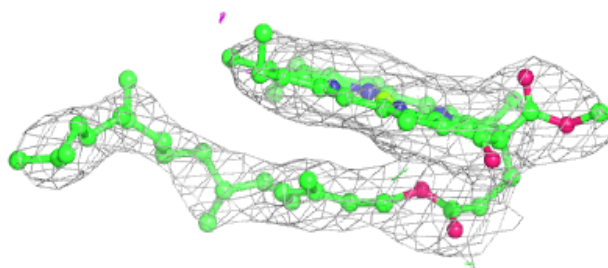
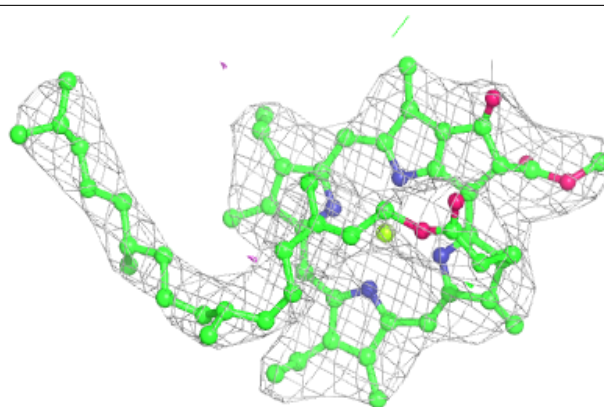
**Electron density around CLA Y 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

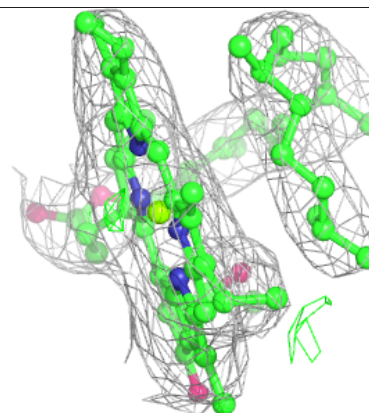
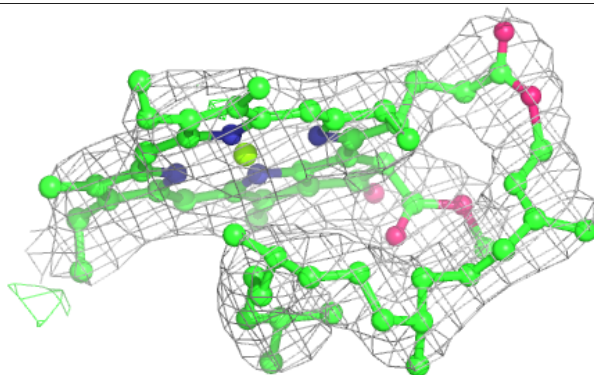
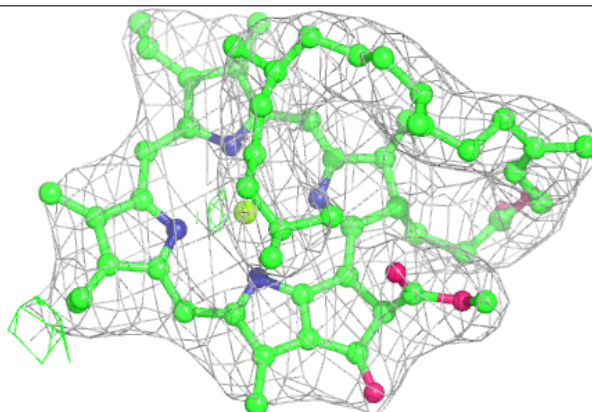


**Electron density around CLA H 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

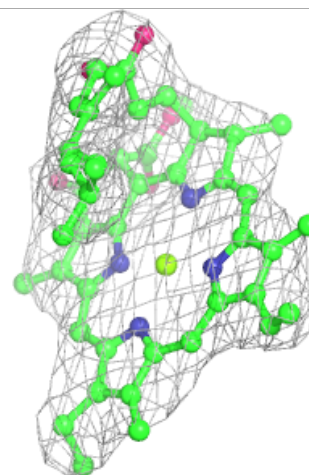
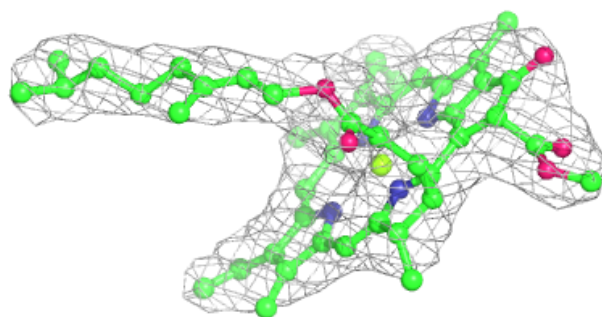
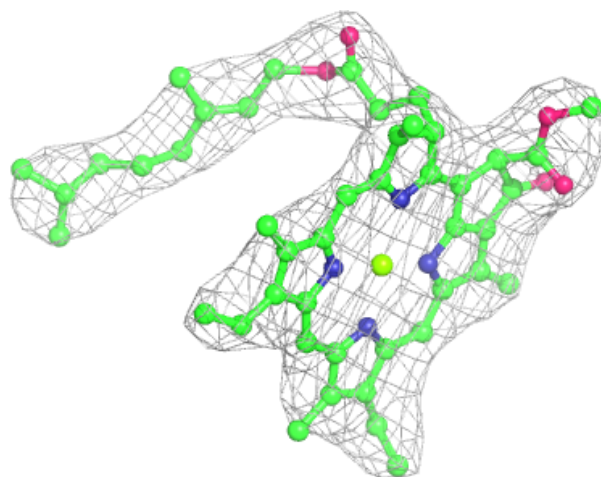
**Electron density around CLA G 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



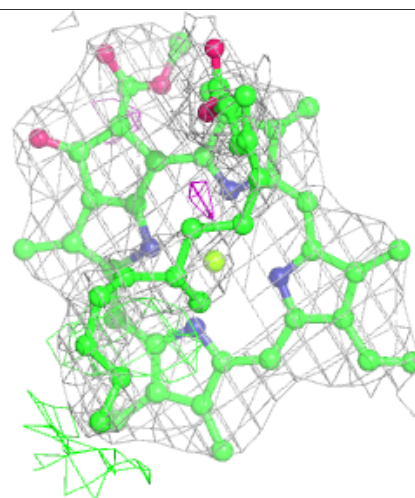
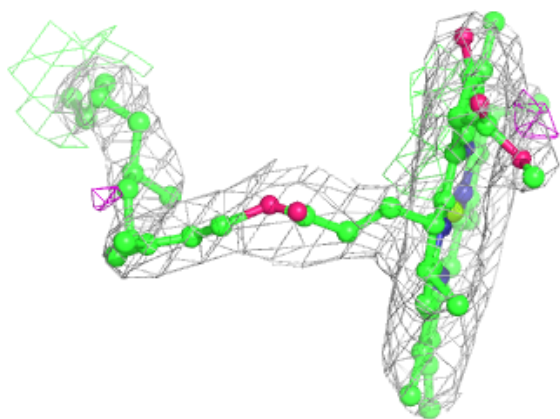
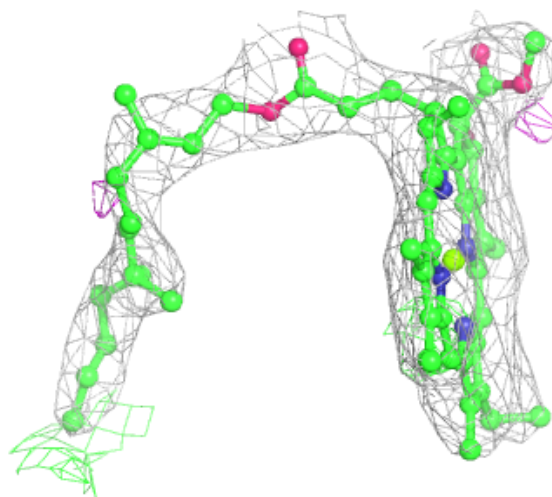
**Electron density around CLA Z 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



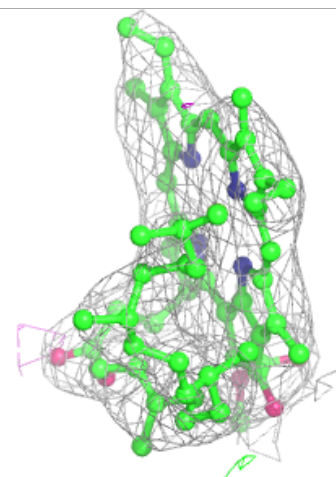
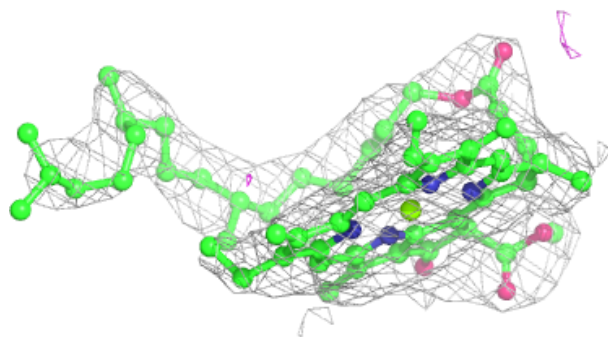
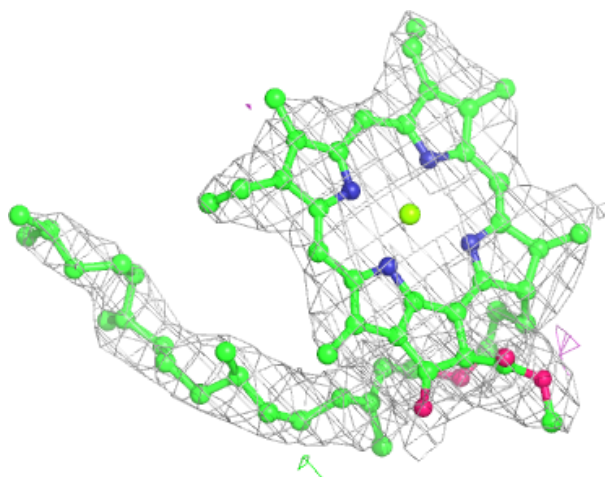
**Electron density around CLA A 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 829:**

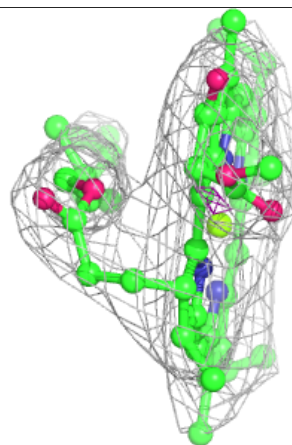
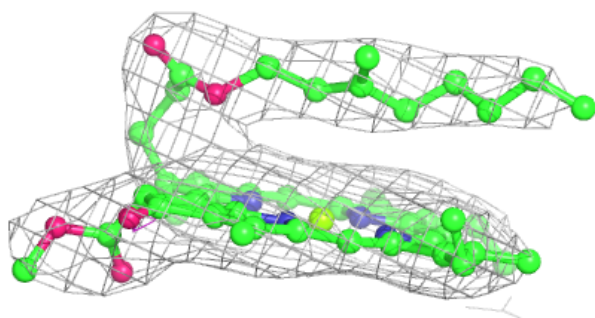
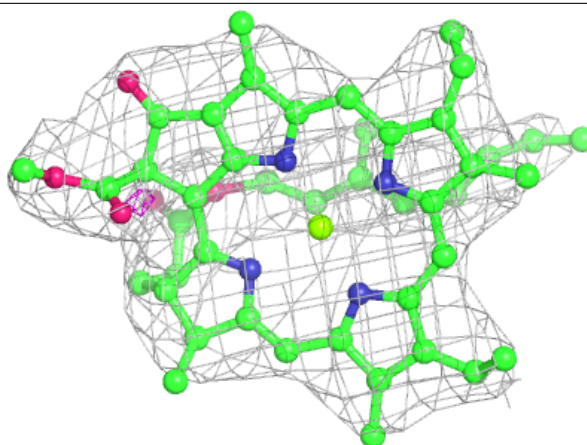
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



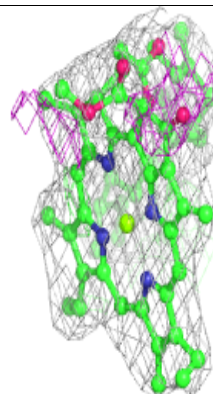
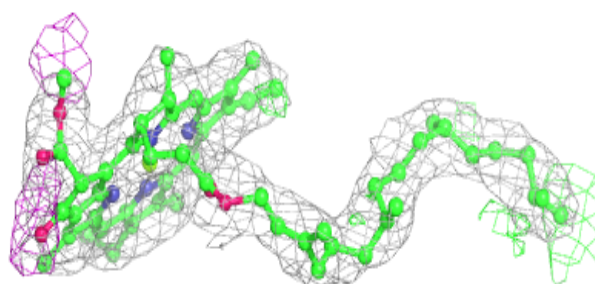
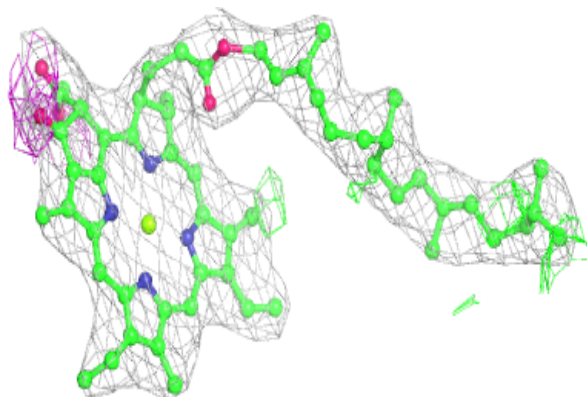


**Electron density around CLA G 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

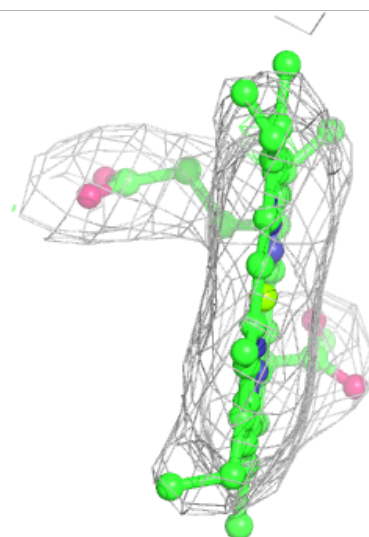
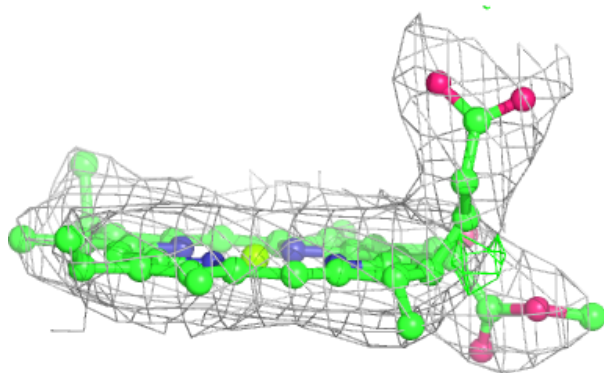
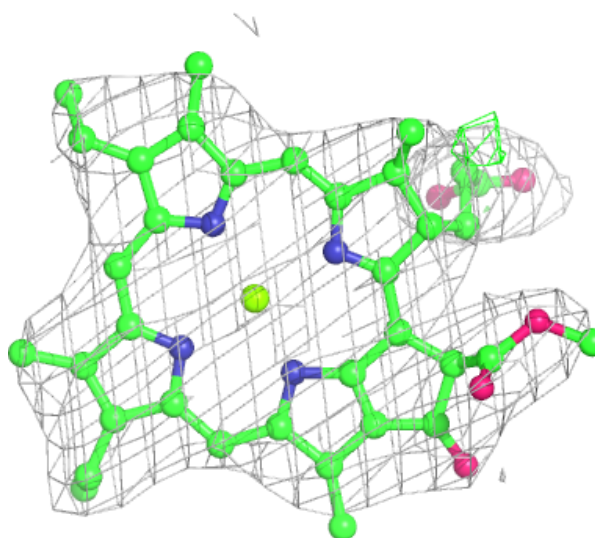
**Electron density around CLA Y 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



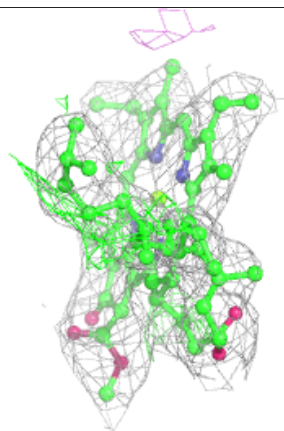
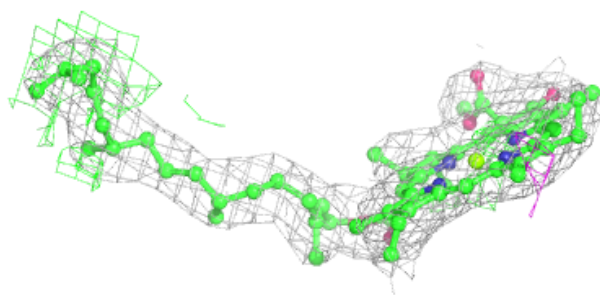
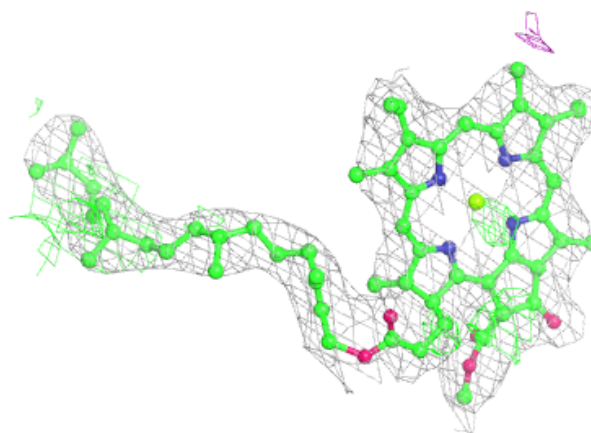
**Electron density around CLA H 832:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Z 801:**

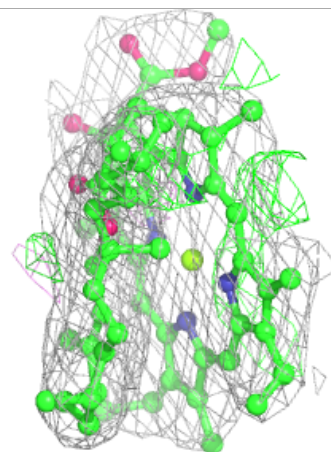
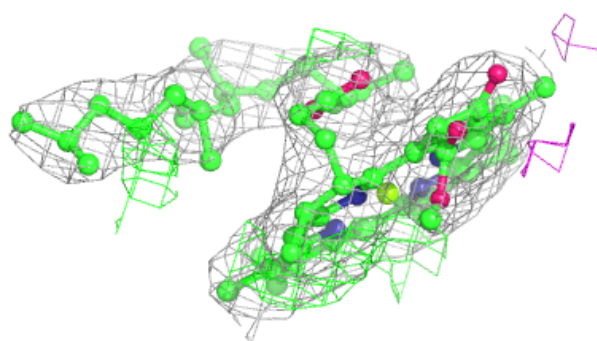
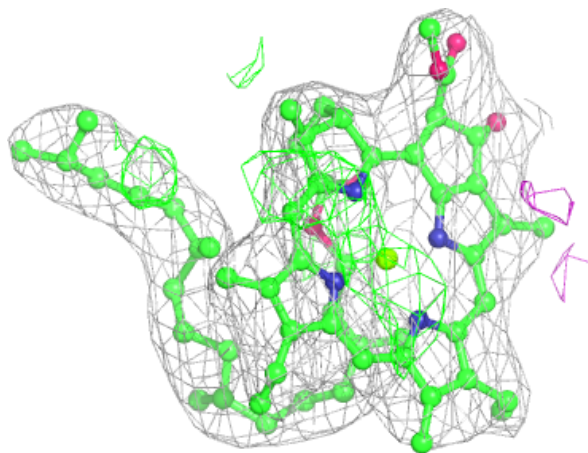
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





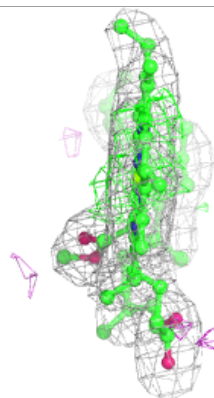
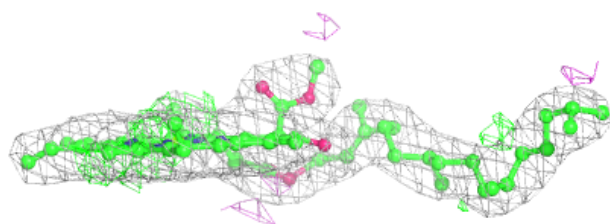
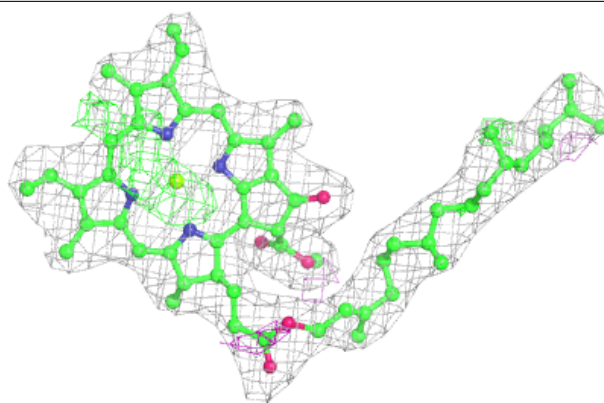
**Electron density around CLA Z 807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

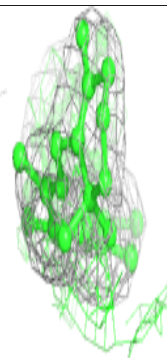
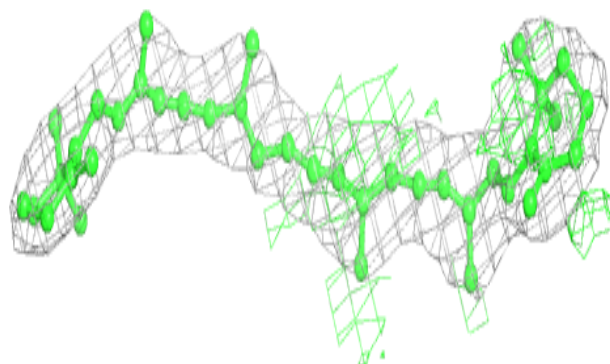
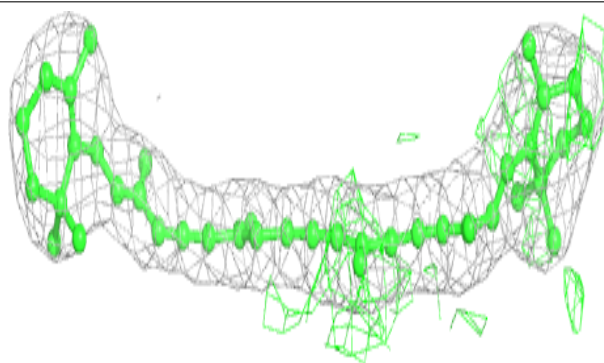


**Electron density around CLA U 1004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

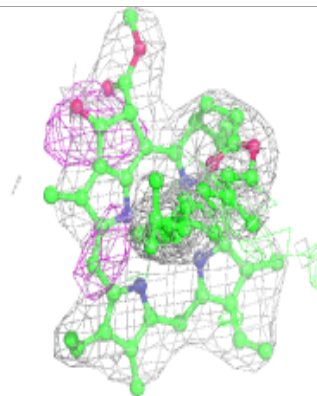
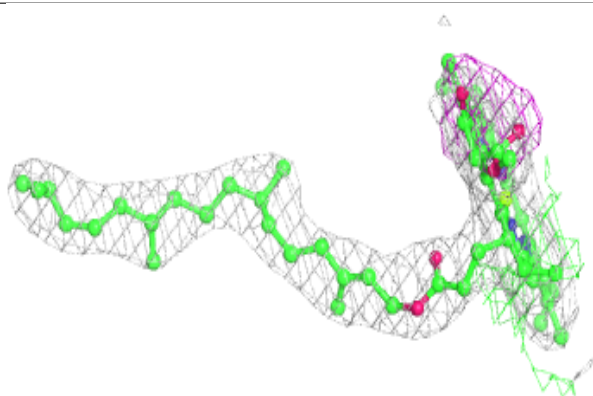
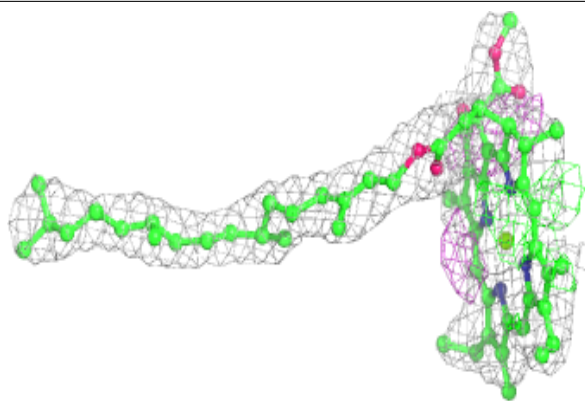
**Electron density around BCR J 104:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

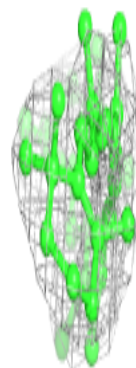
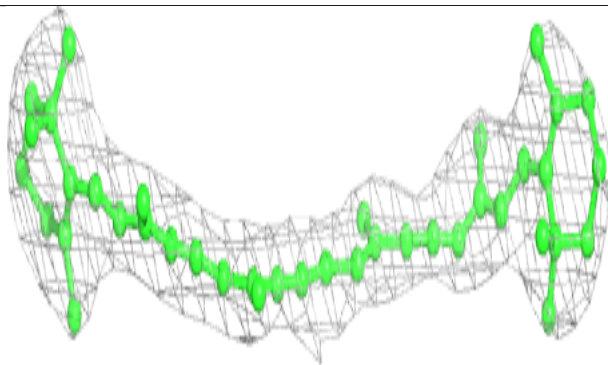
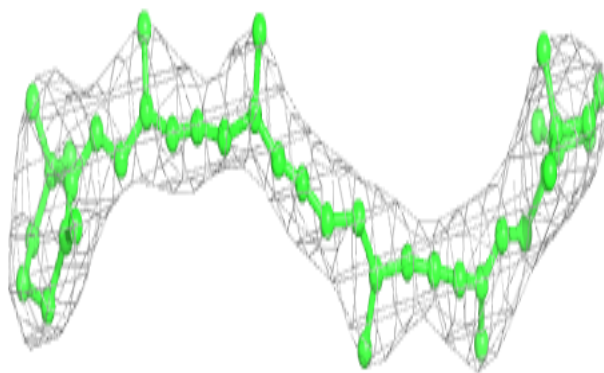


**Electron density around CLA H 827:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

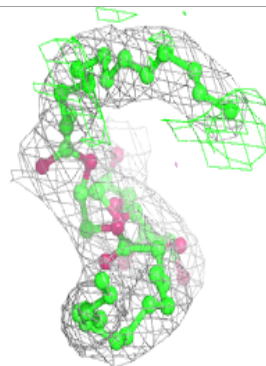
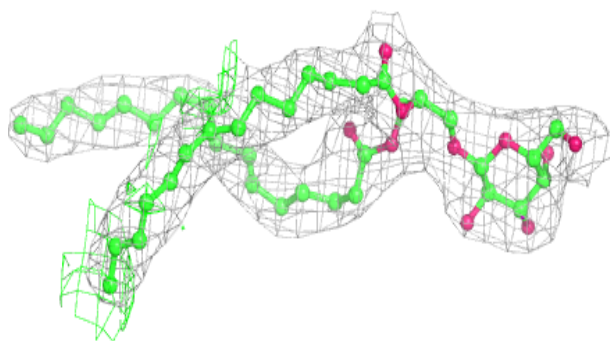
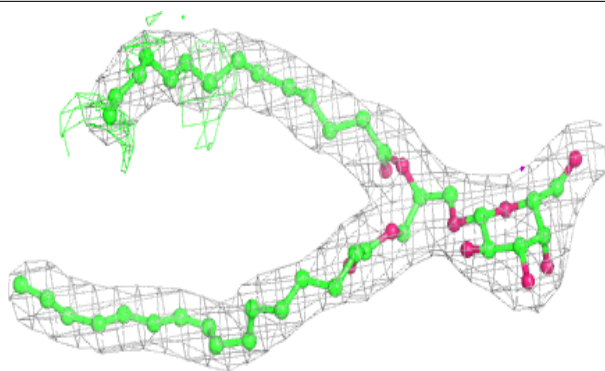
**Electron density around BCR Y 848:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

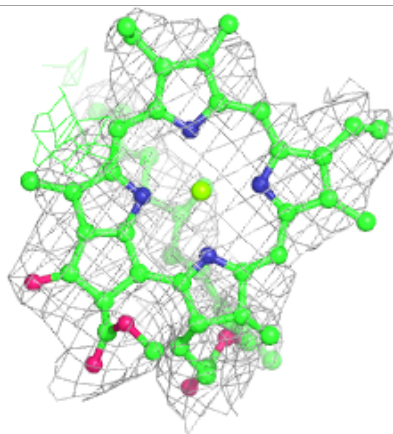
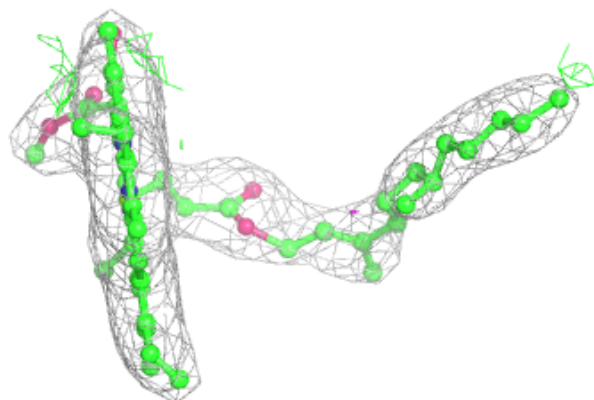
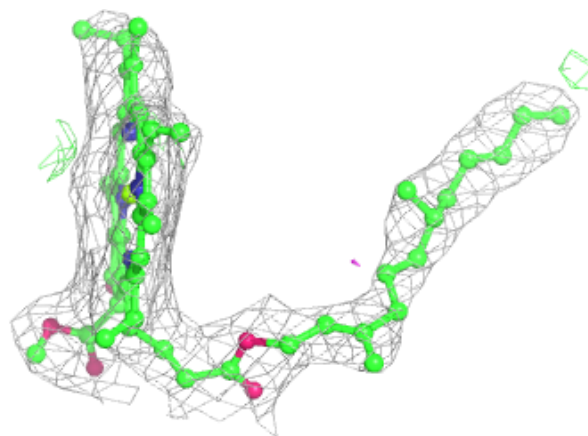


**Electron density around LMG Z 847:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 804:**

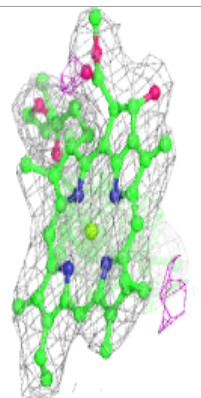
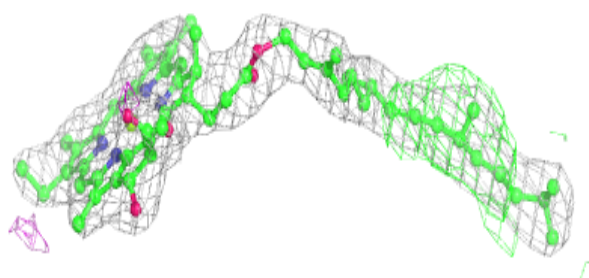
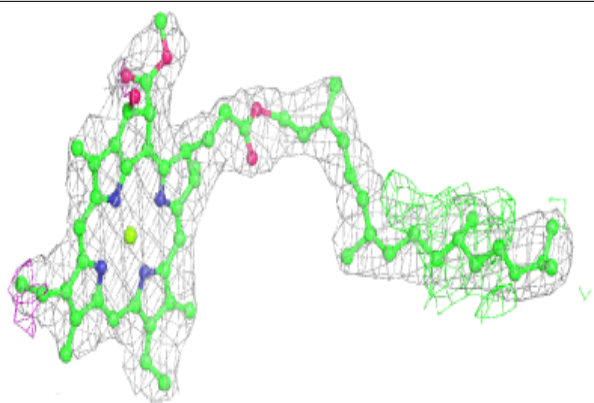
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



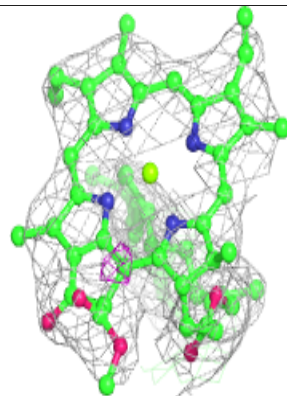
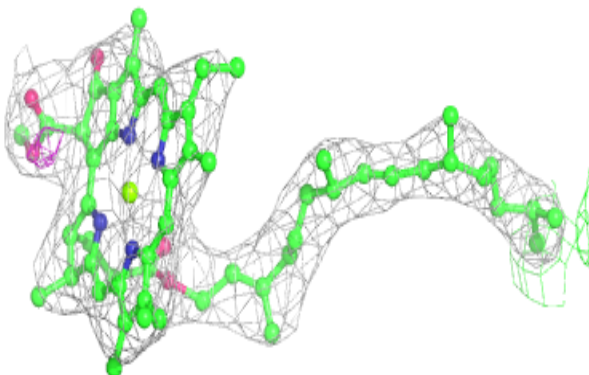
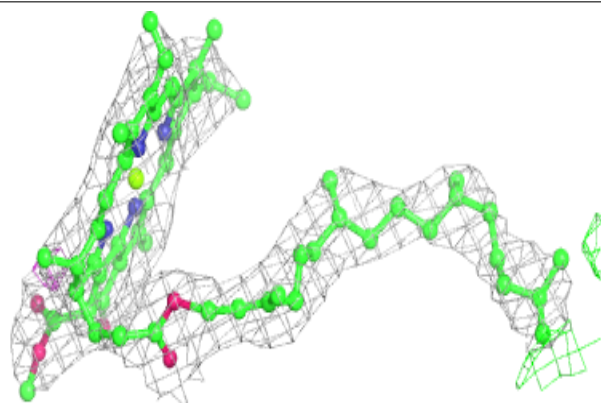


**Electron density around CLA Y 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

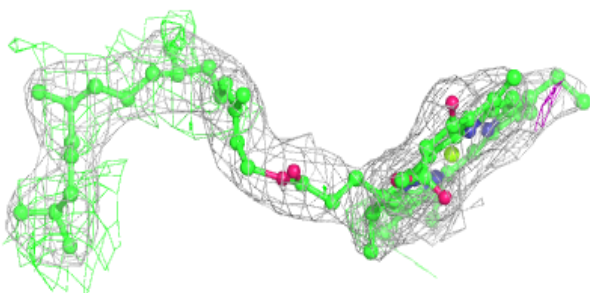
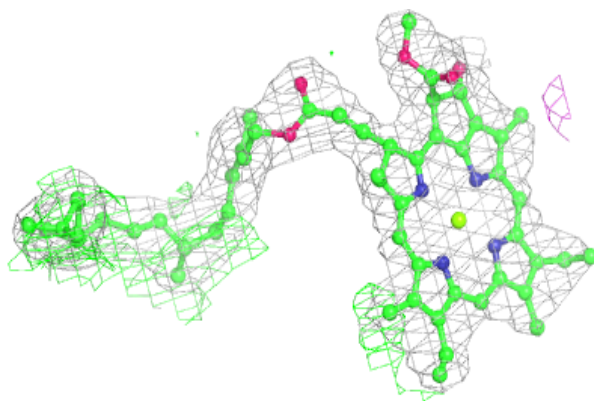
**Electron density around CLA G 811:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

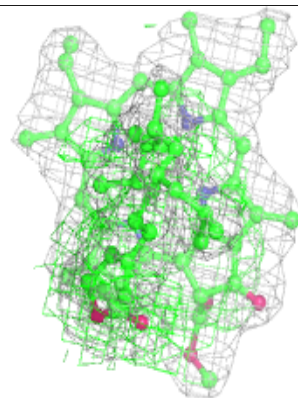
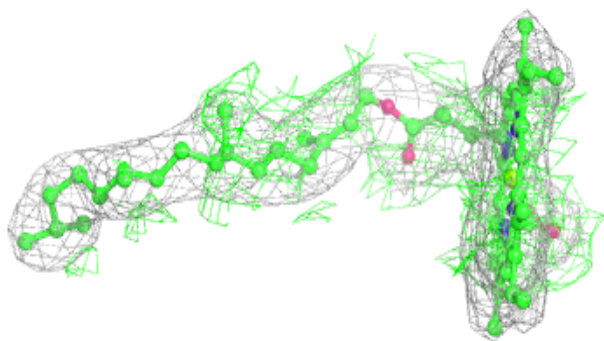
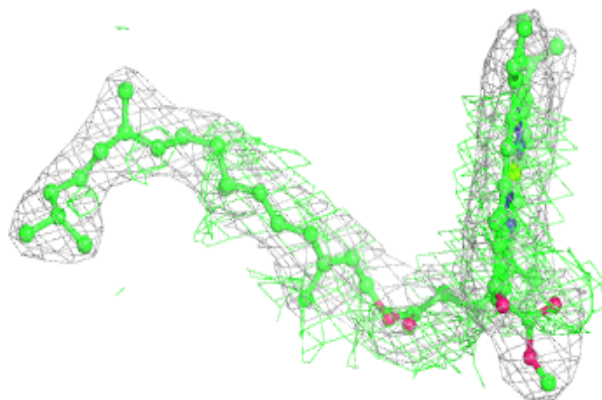


**Electron density around CLA H 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

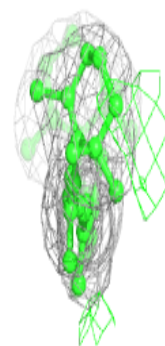
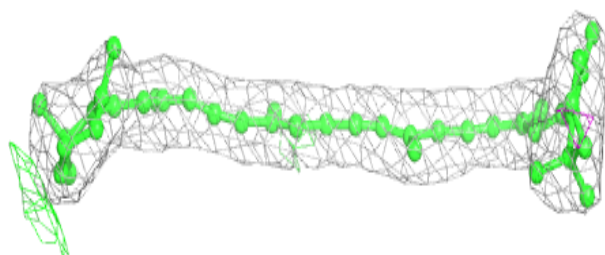
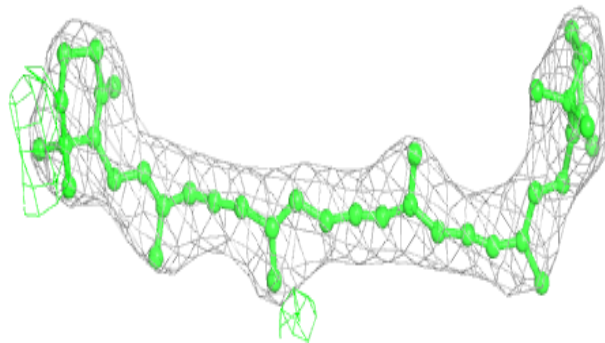
**Electron density around CLA H 838:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

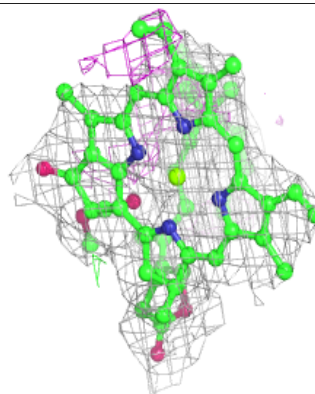
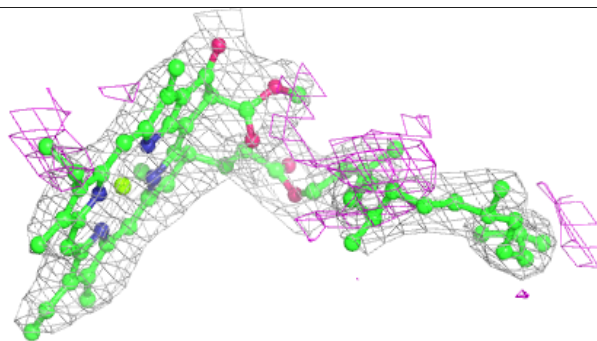
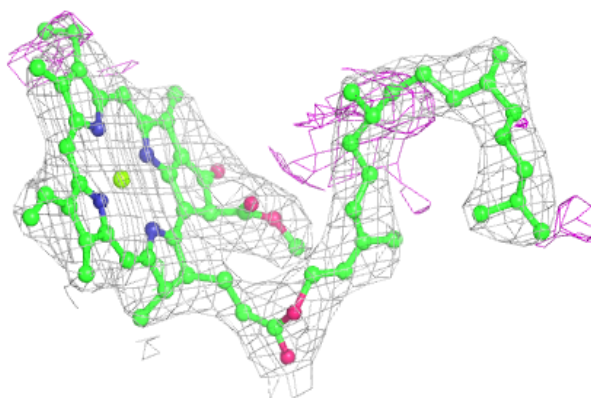


**Electron density around BCR L 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

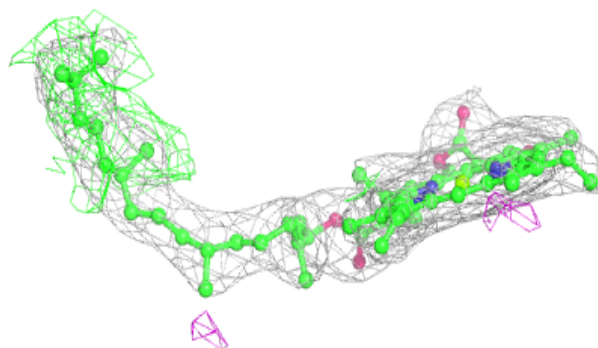
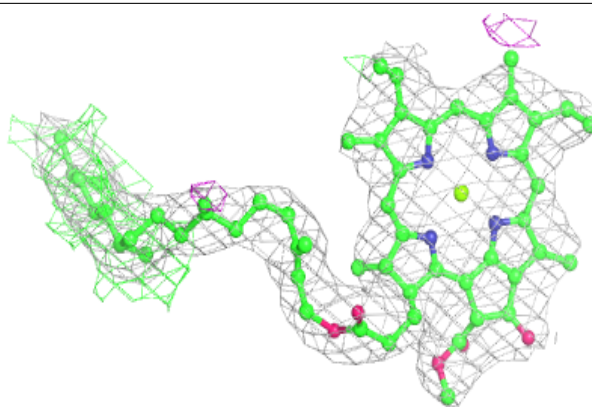
**Electron density around CL0 G 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

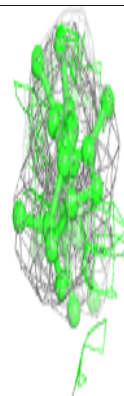
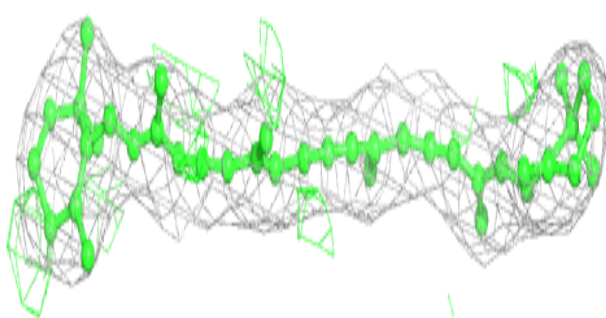
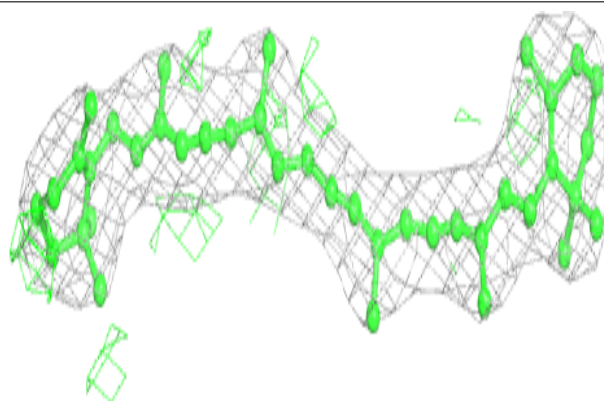


**Electron density around CLA B 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR f 103:**

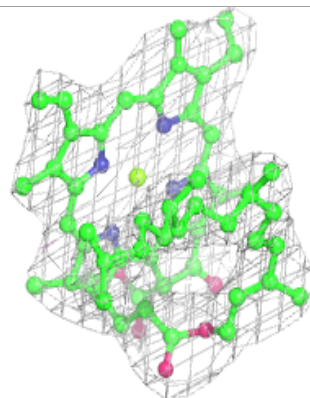
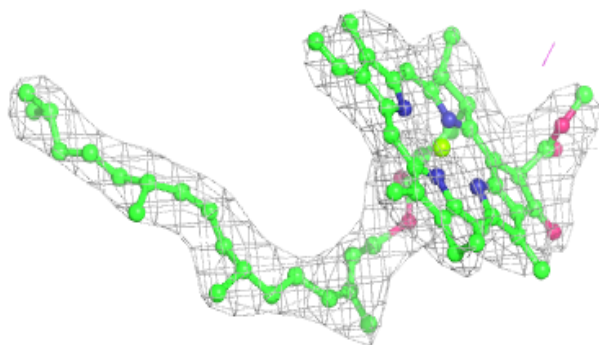
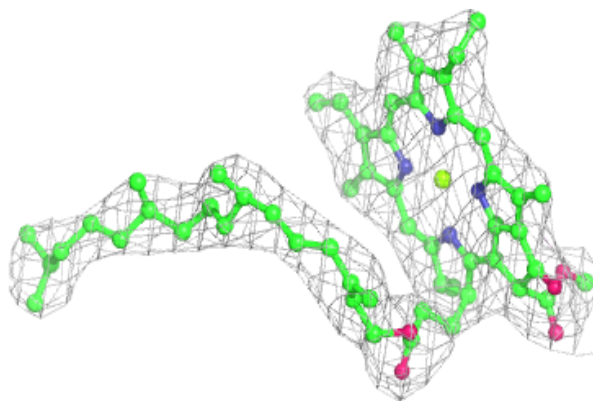
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





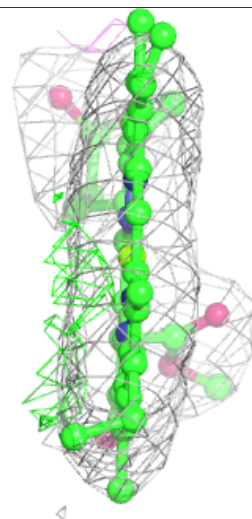
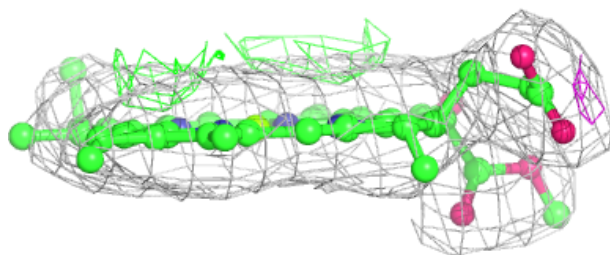
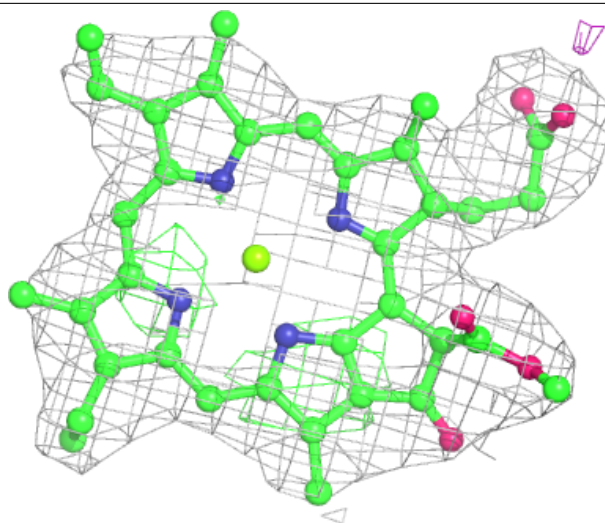
**Electron density around CLA Z 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



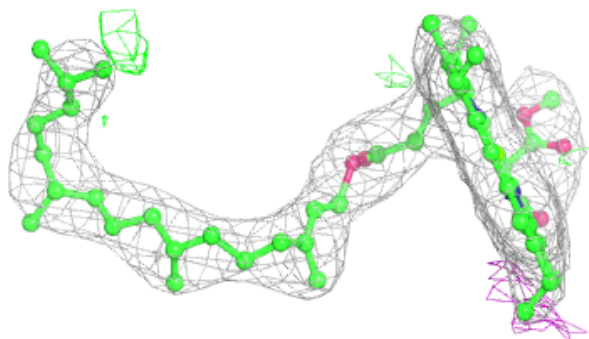
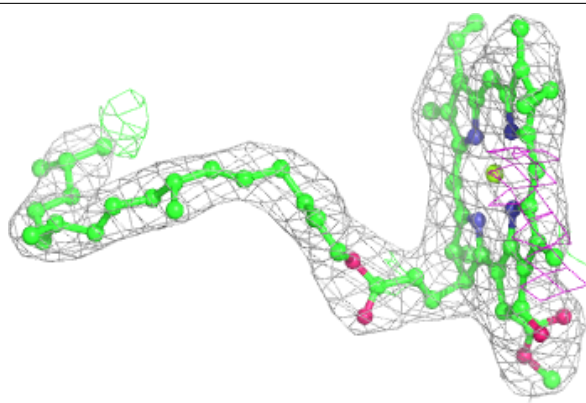
**Electron density around CLA j 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

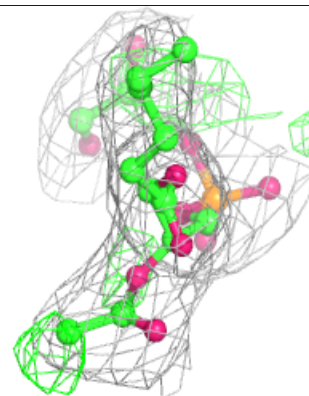
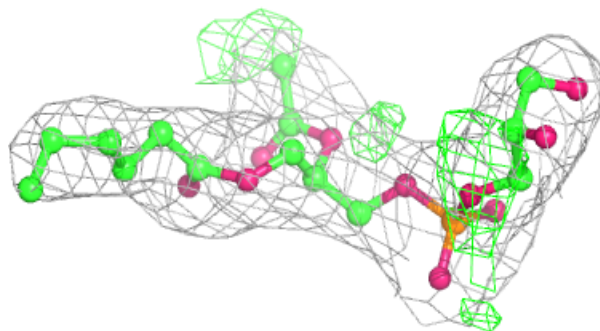
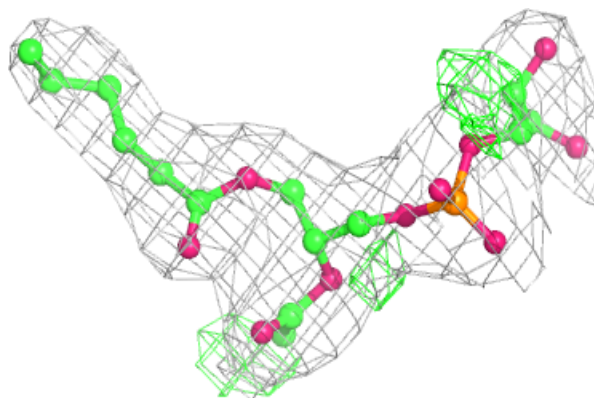


**Electron density around CLA L 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

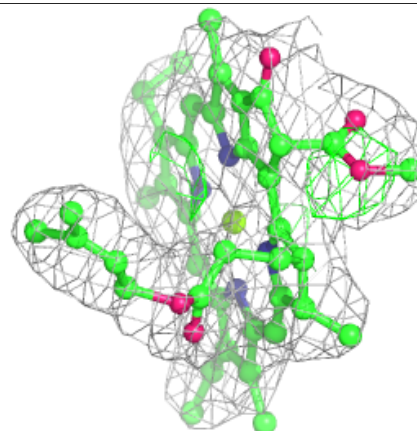
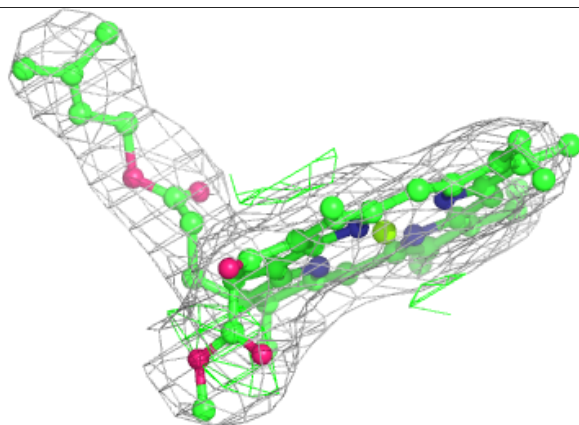
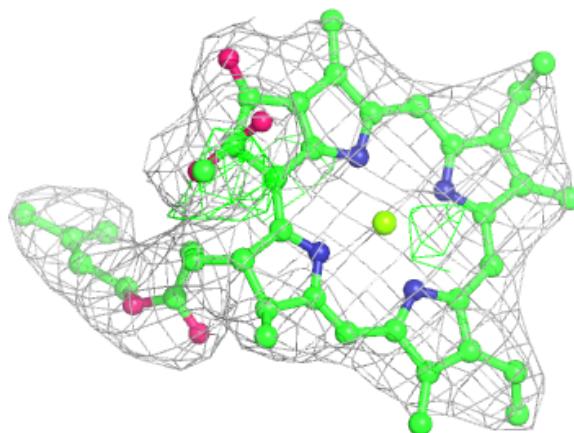
**Electron density around LHG Y 853:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



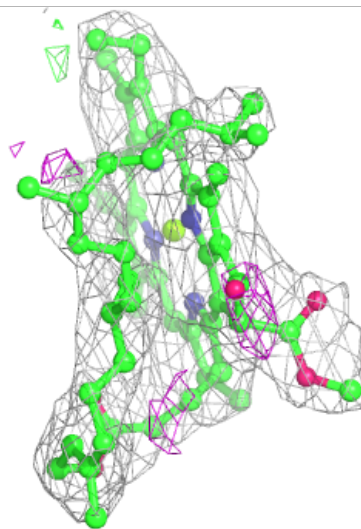
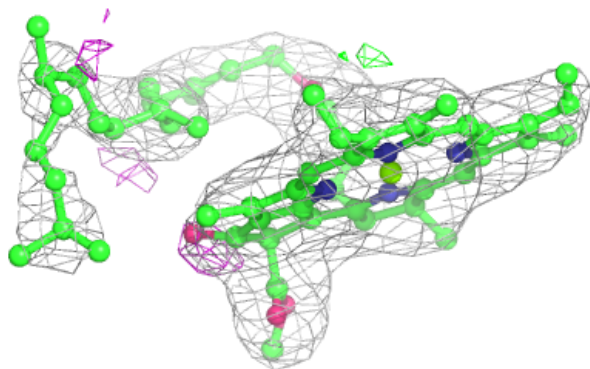
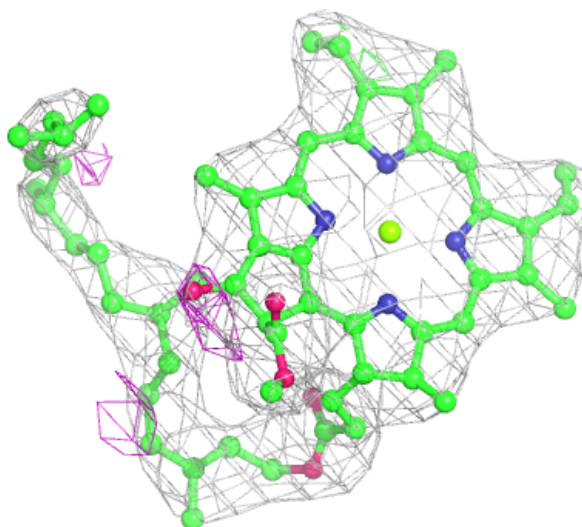
**Electron density around CLA A 838:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



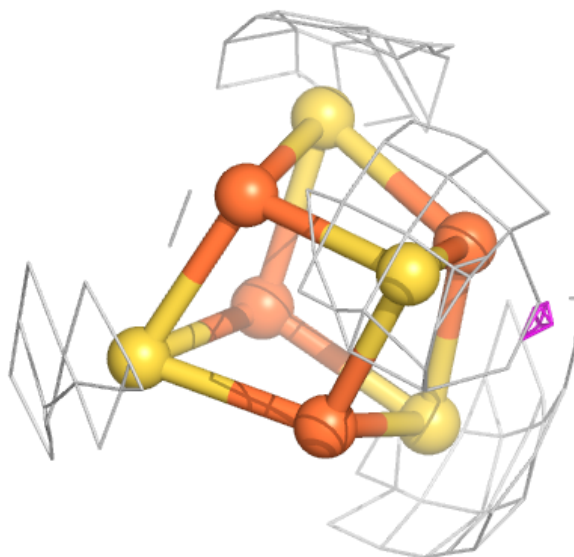
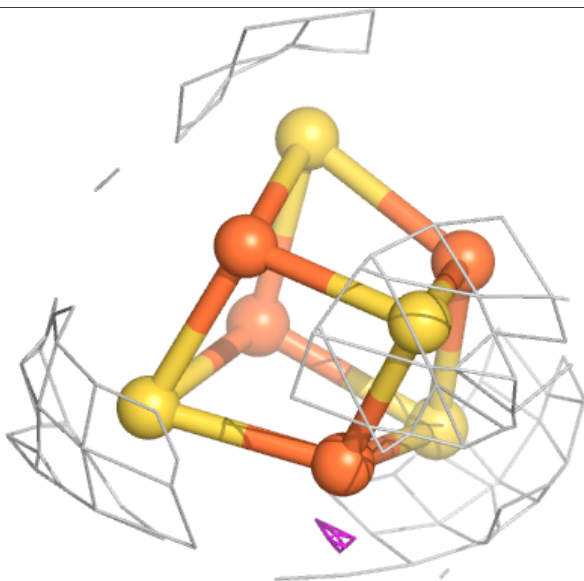
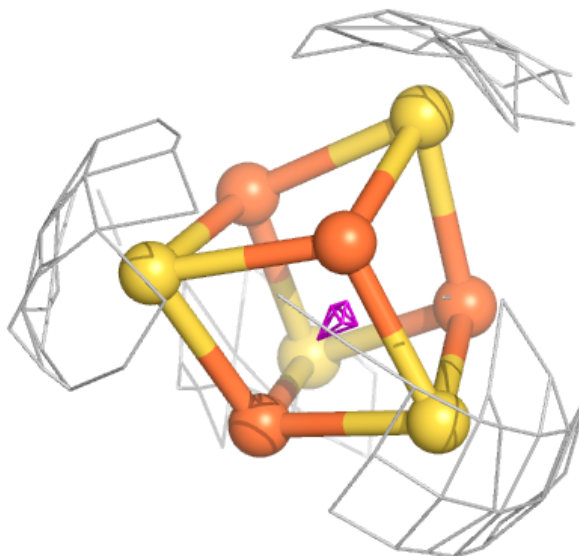
**Electron density around CLA Z 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SF4 N 102:**

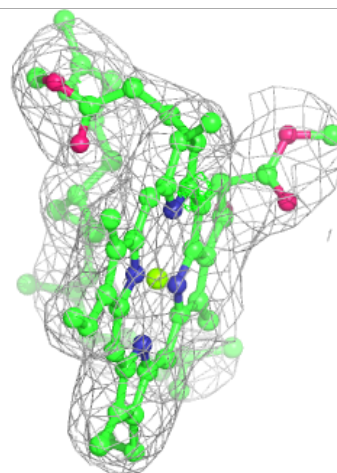
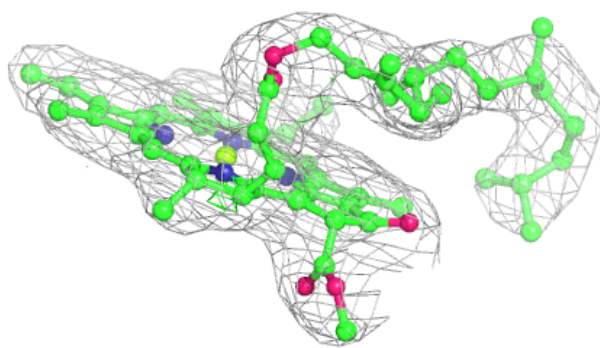
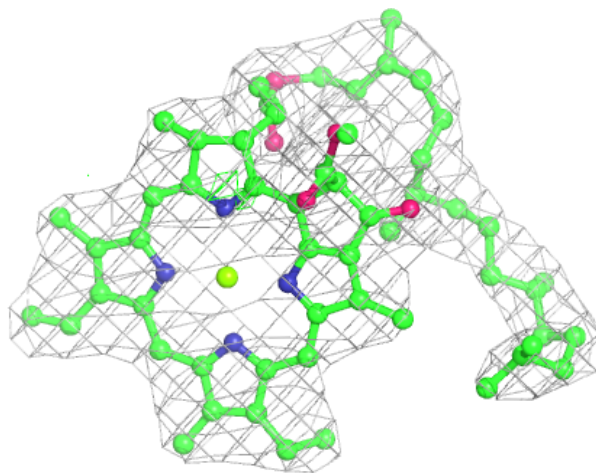
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





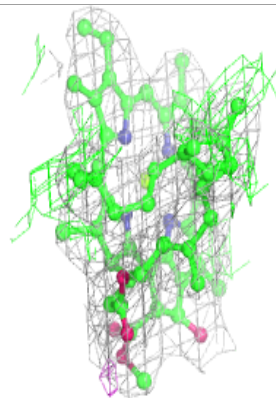
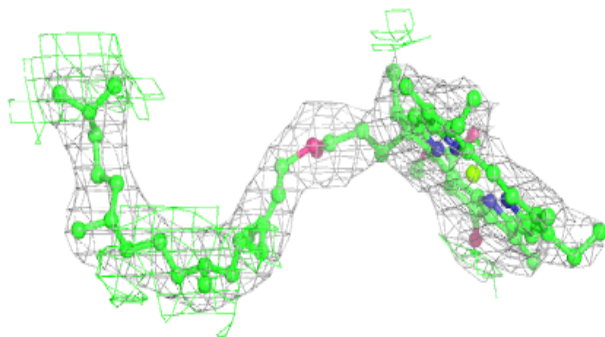
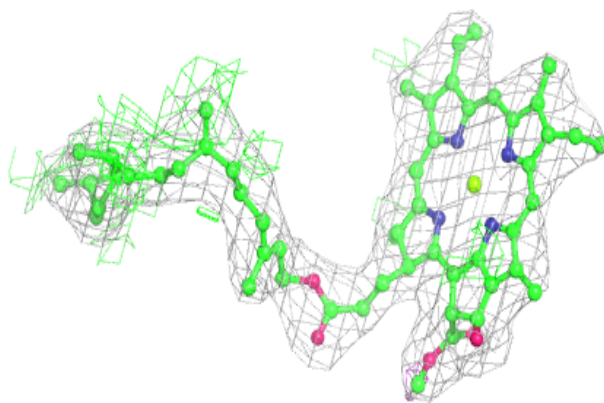
**Electron density around CLA B 832:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 810:**

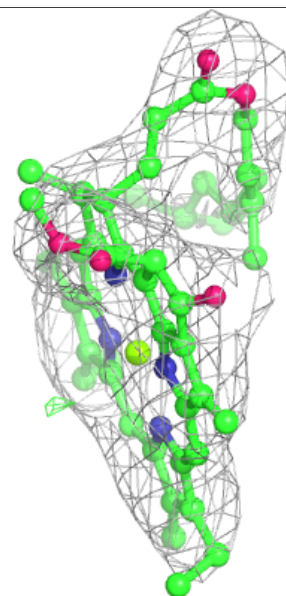
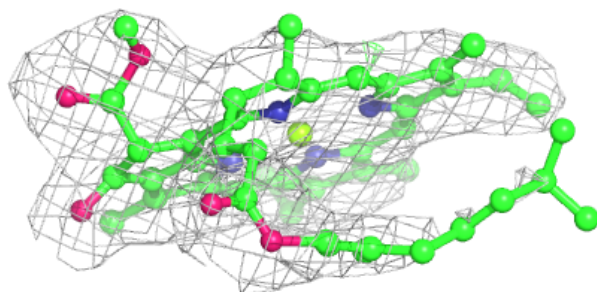
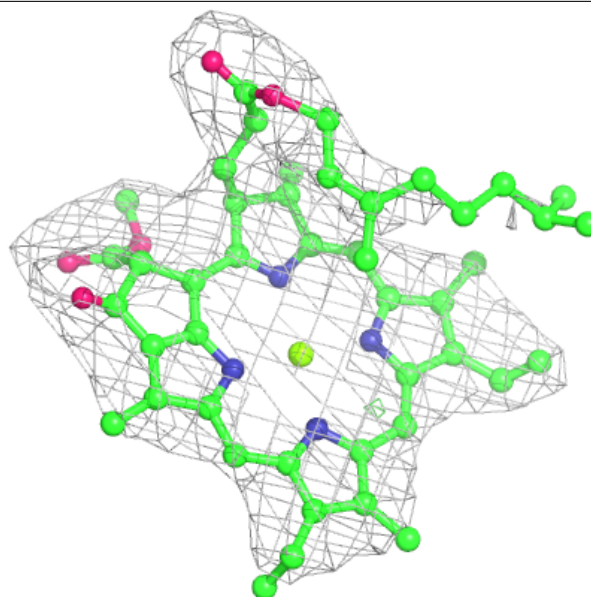
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





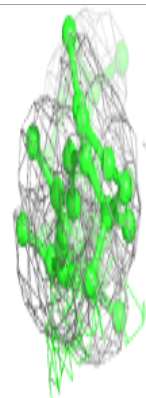
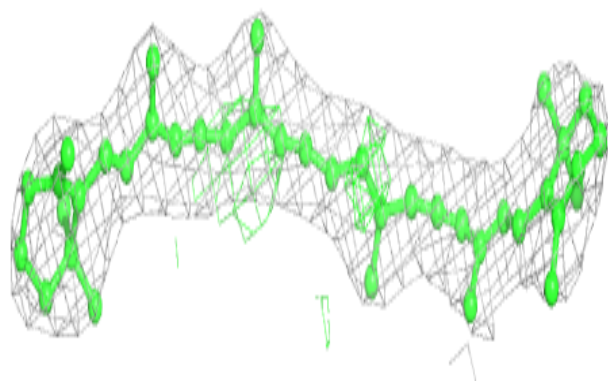
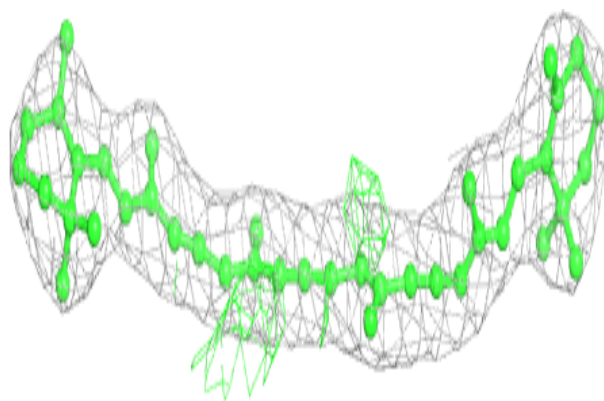
**Electron density around CLA S 1103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



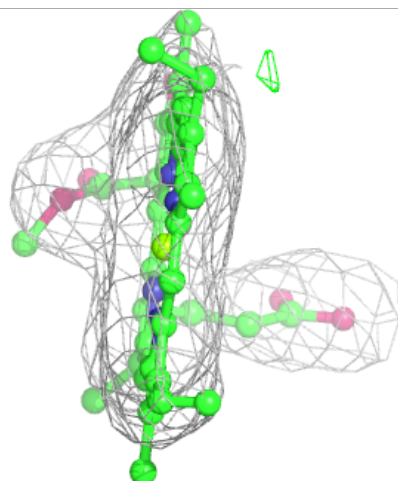
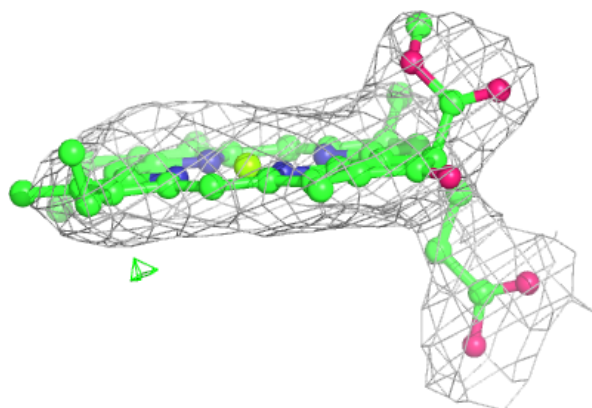
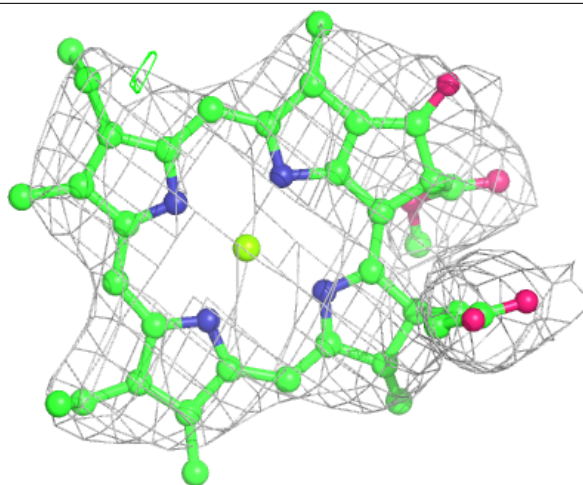
**Electron density around BCR f 104:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



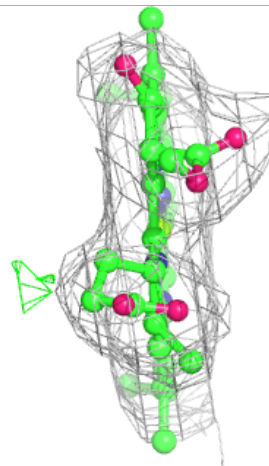
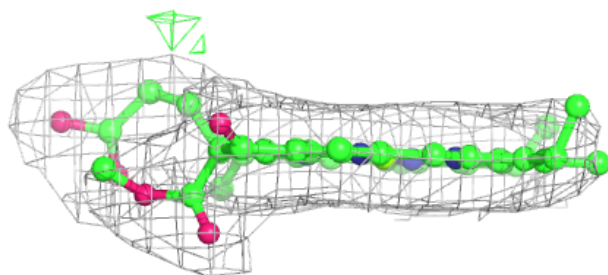
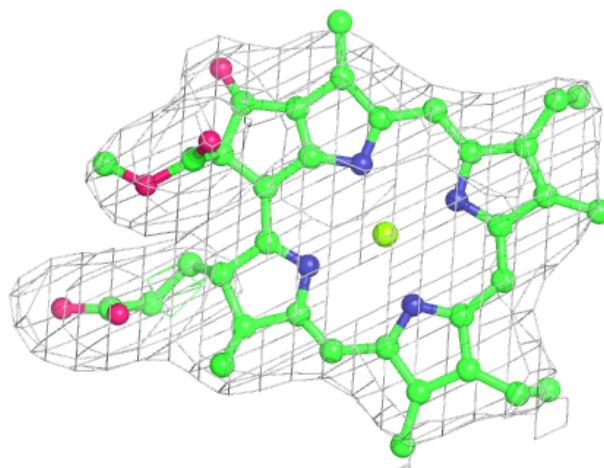
**Electron density around CLA T 103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



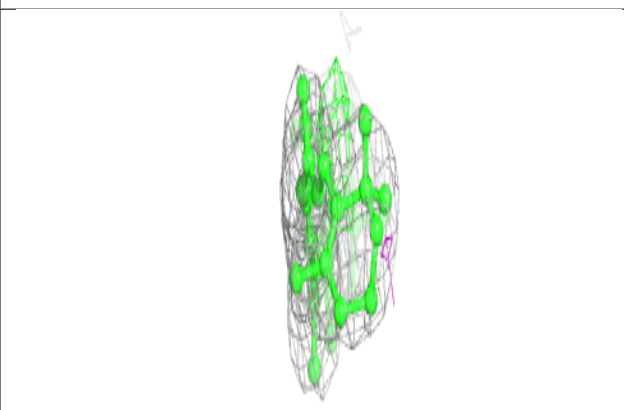
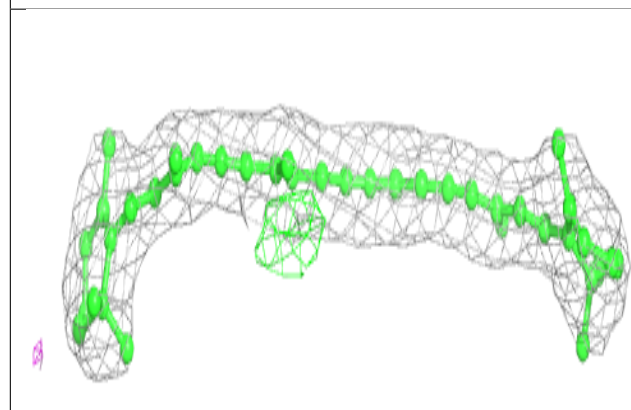
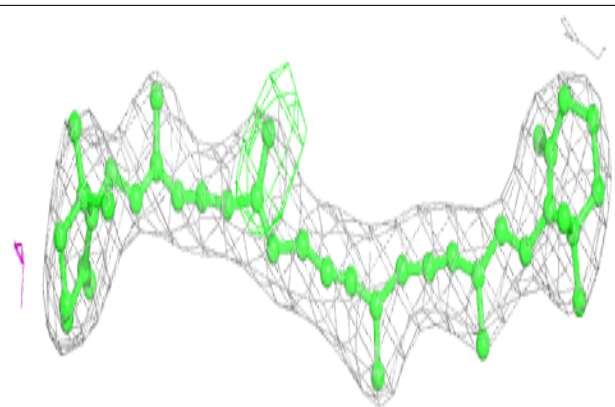
**Electron density around CLA H 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

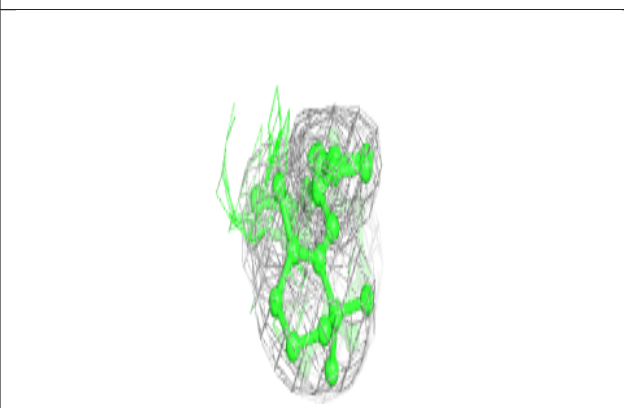
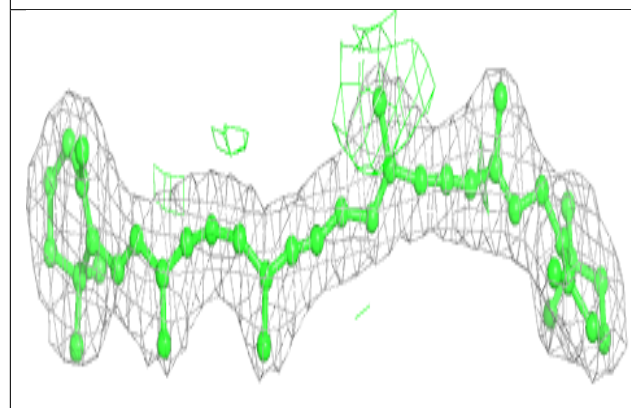
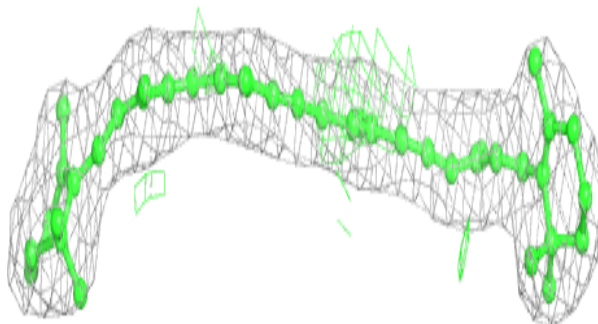


**Electron density around BCR Y 850:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

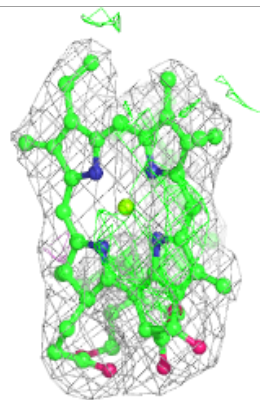
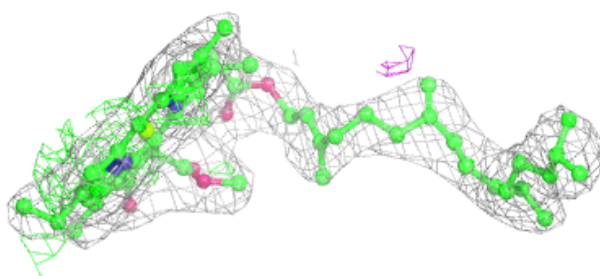
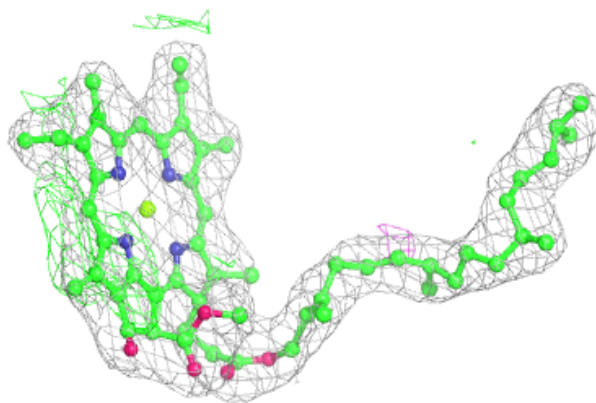
**Electron density around BCR R 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

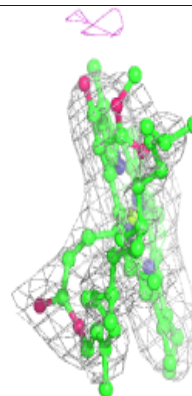
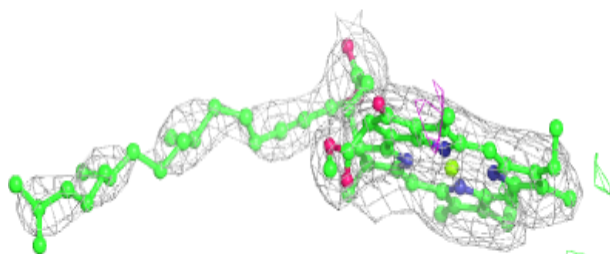
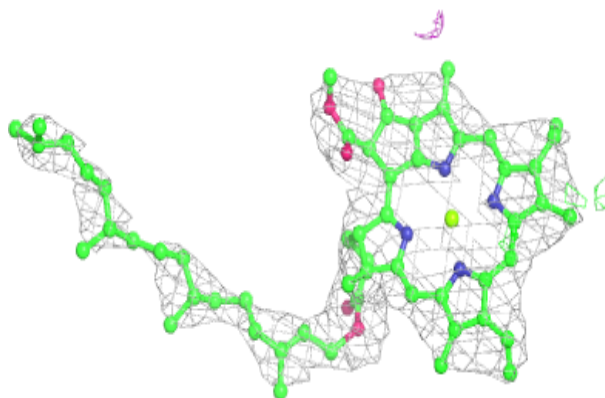


**Electron density around CLA H 809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Y 822:**

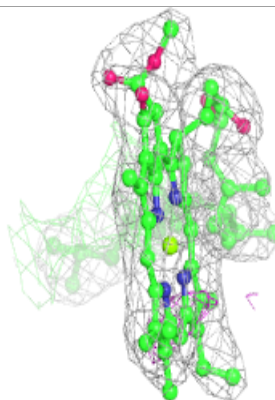
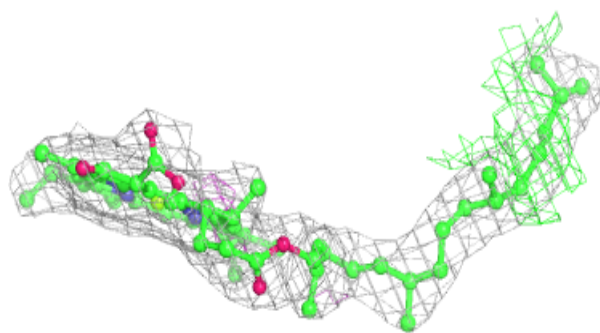
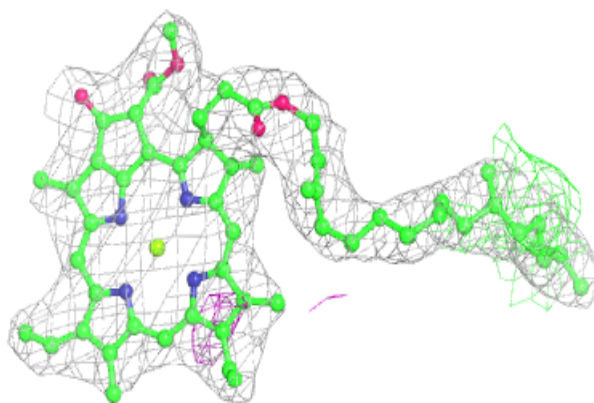
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



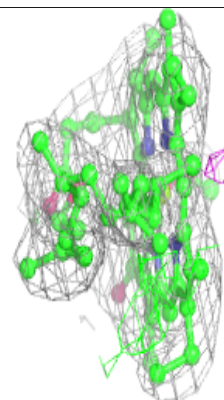
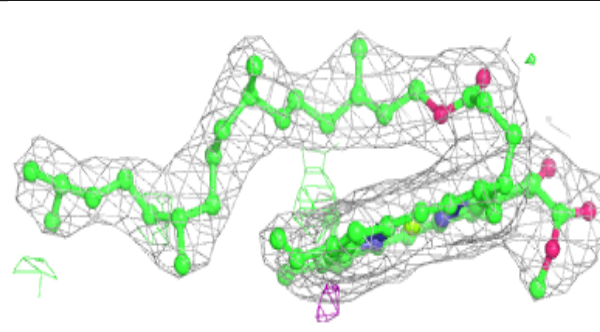
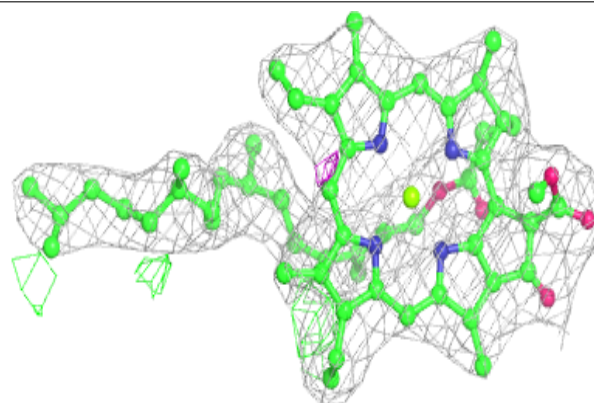


**Electron density around CLA H 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

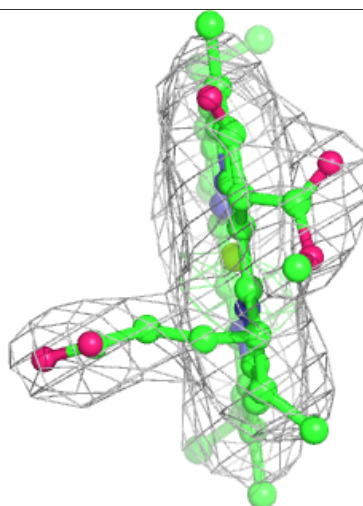
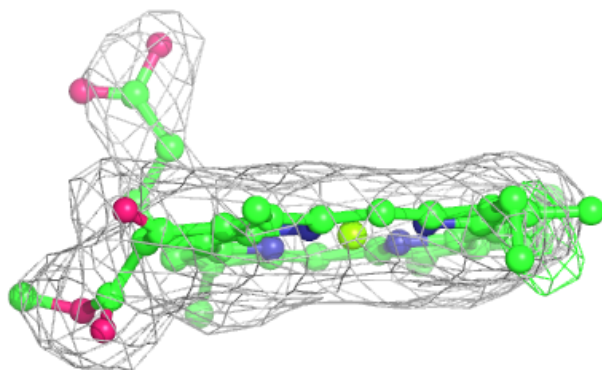
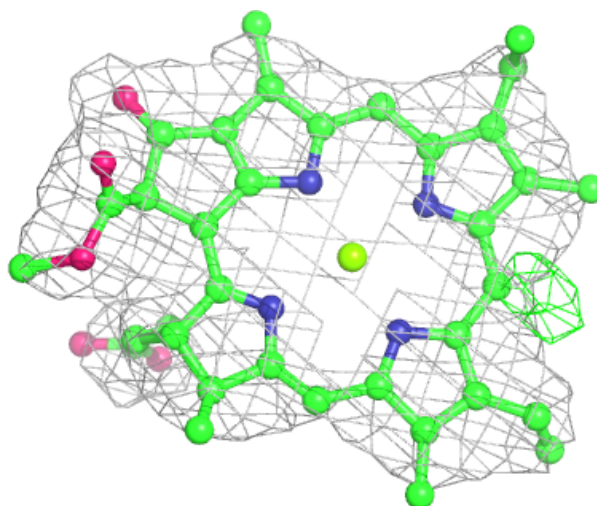
**Electron density around CLA G 837:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA J 101:**

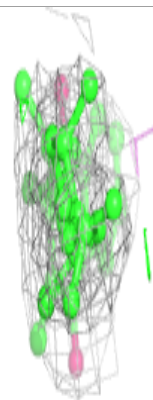
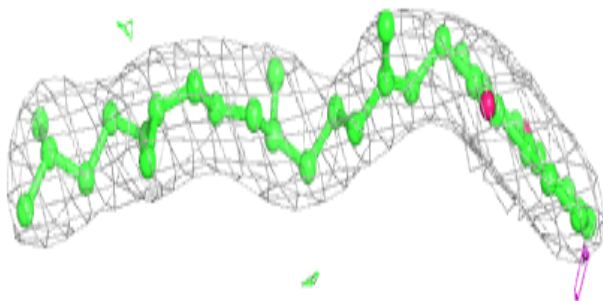
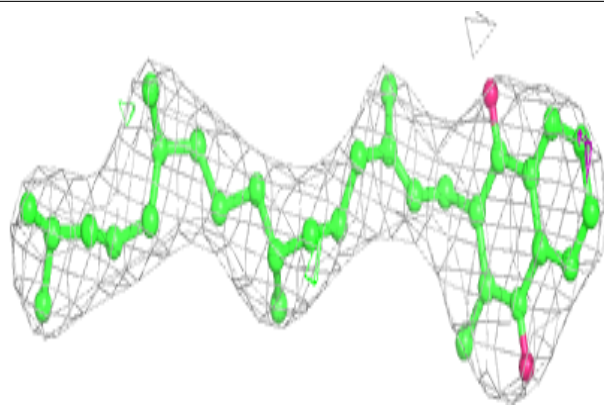
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



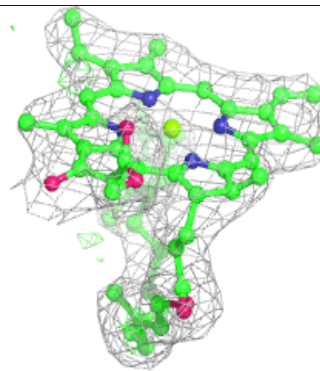
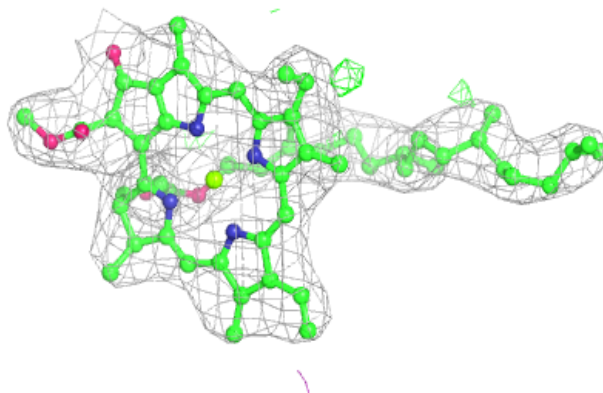
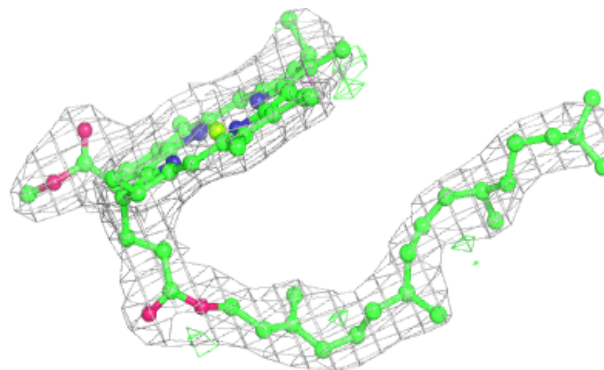


**Electron density around PQN G 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

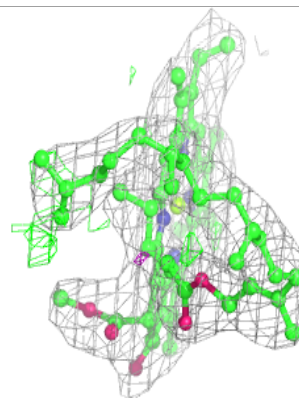
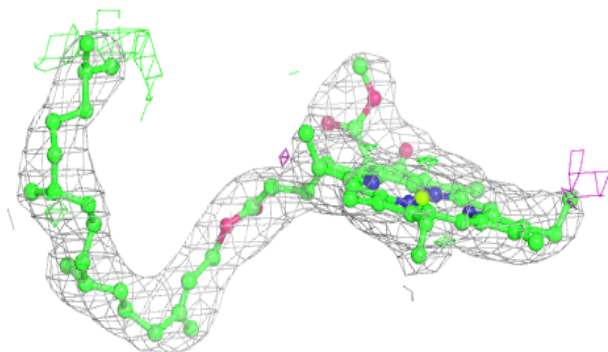
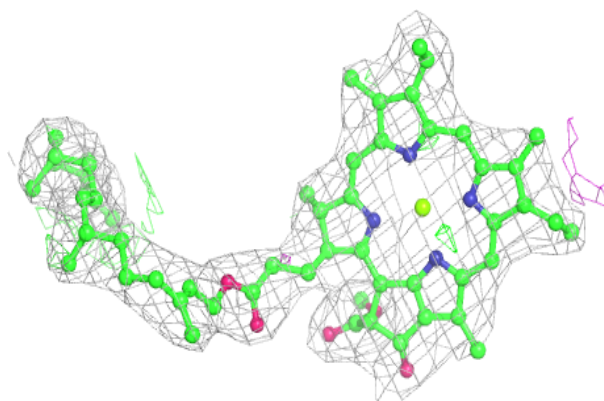
**Electron density around CLA Y 832:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

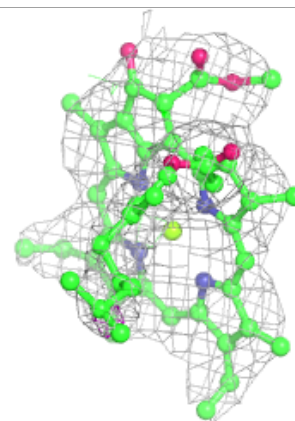
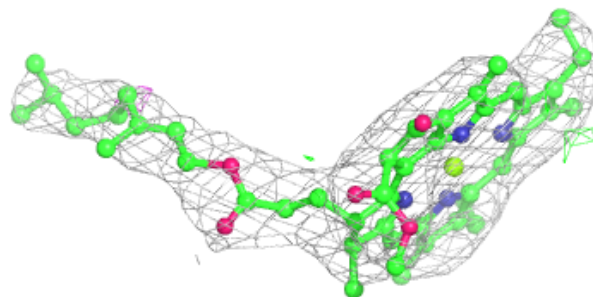
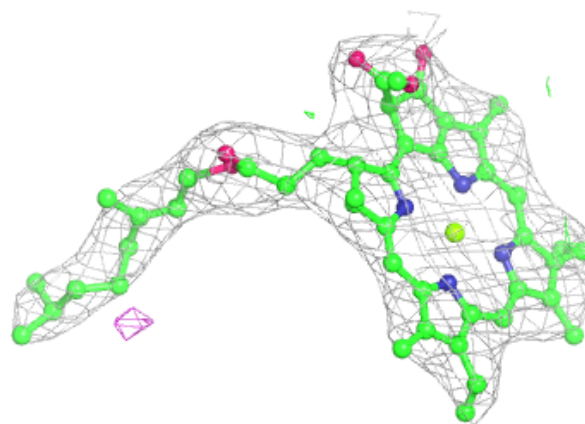


**Electron density around CLA A 827:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

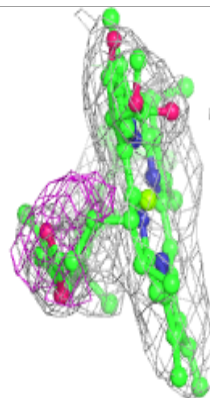
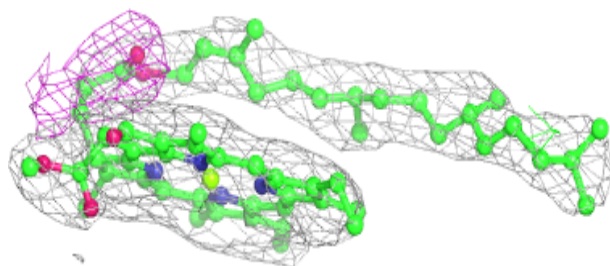
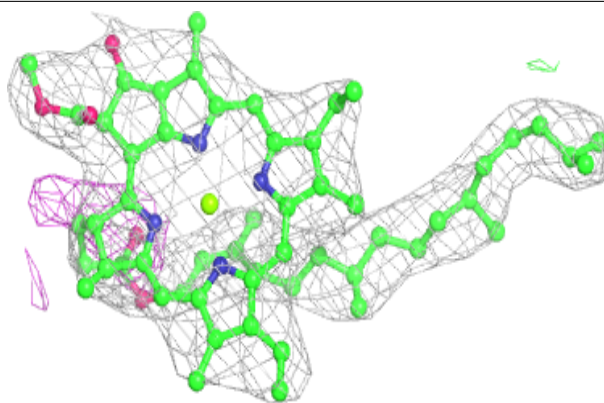
**Electron density around CLA H 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

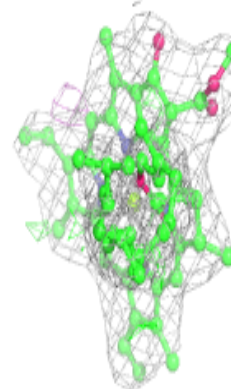
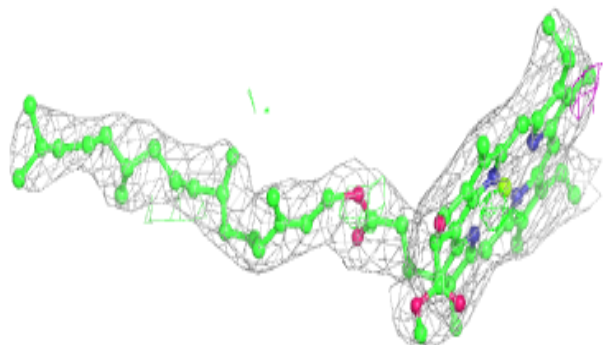
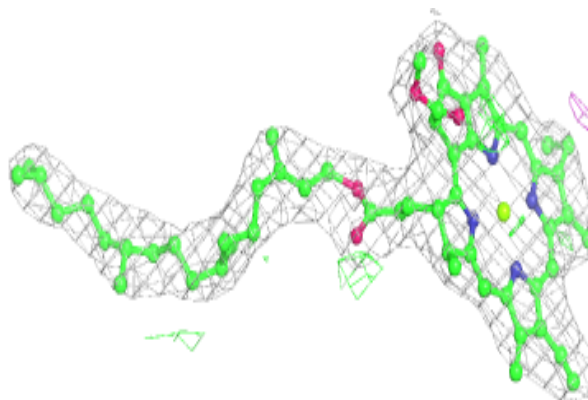


**Electron density around CLA Y 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

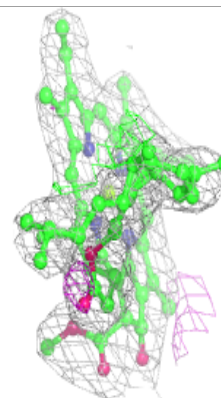
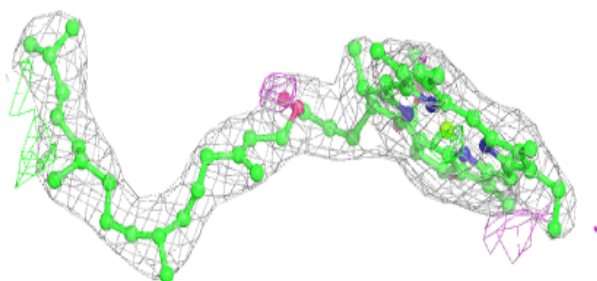
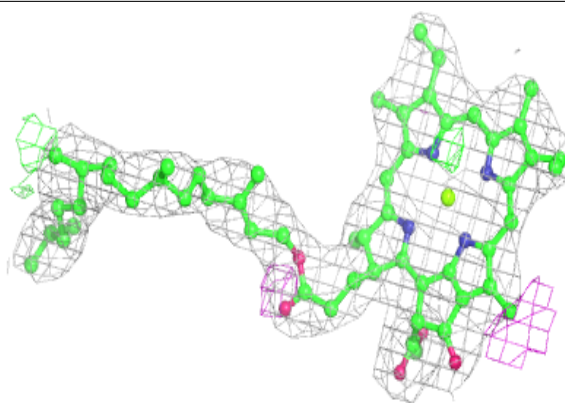
**Electron density around CLA A 809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

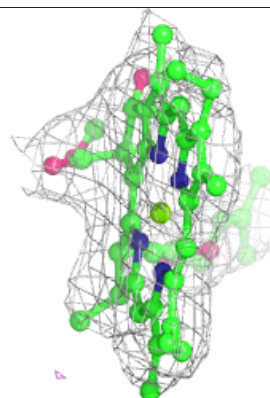
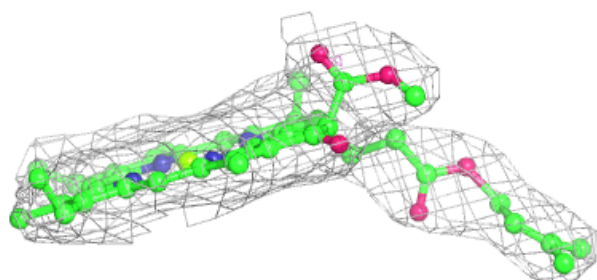
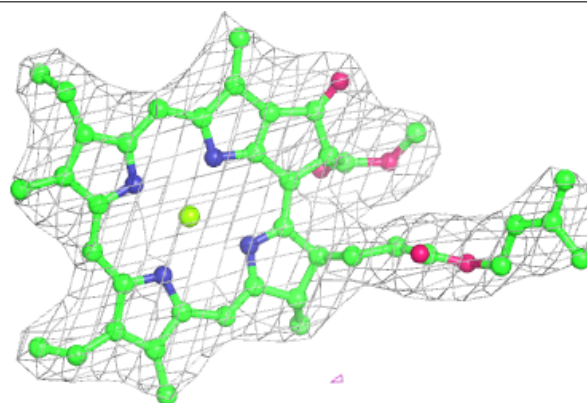


**Electron density around CLA B 813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 840:**

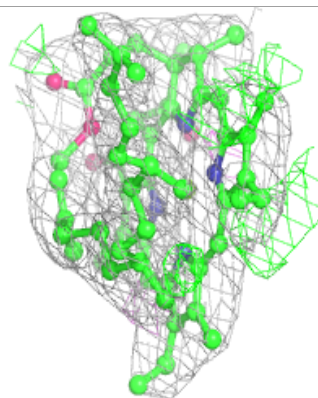
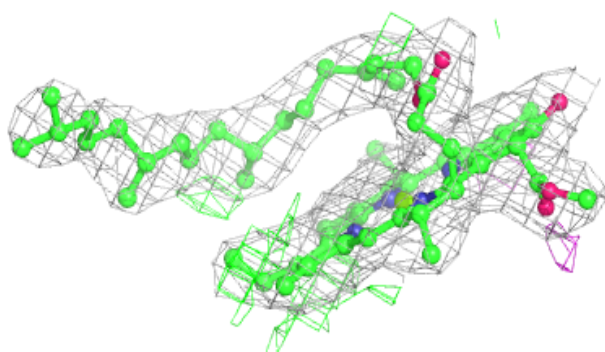
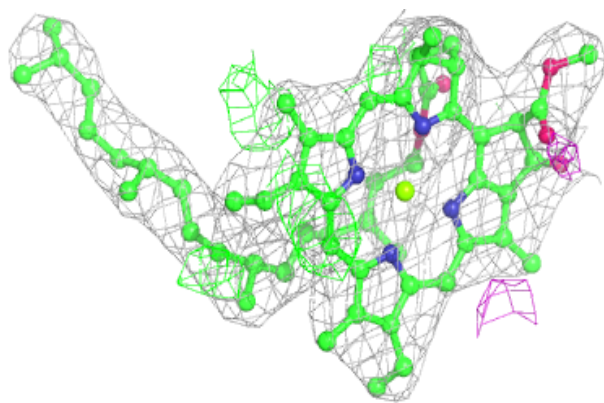
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





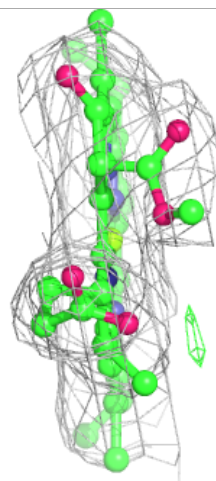
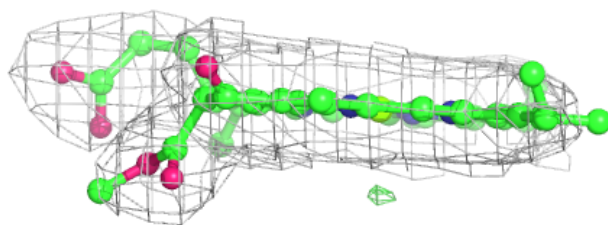
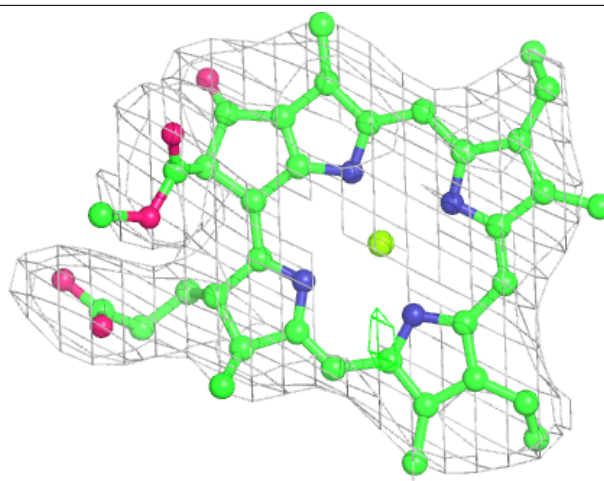
**Electron density around CLA Z 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



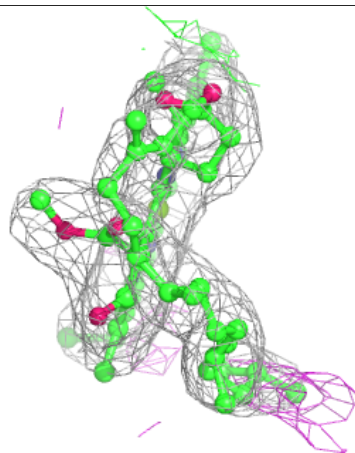
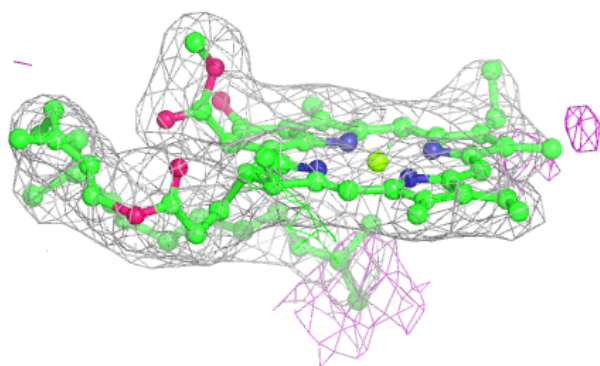
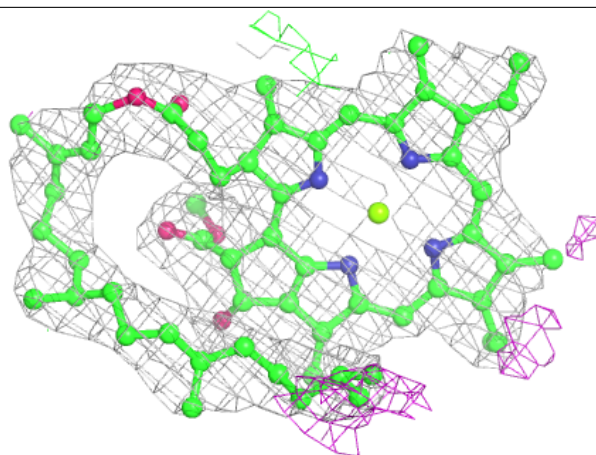
**Electron density around CLA Z 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



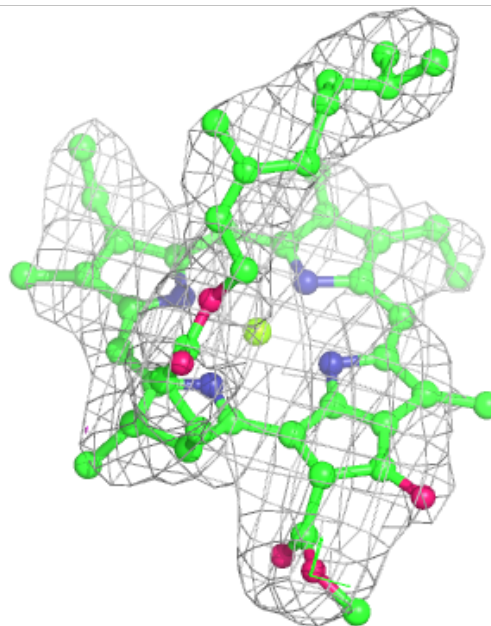
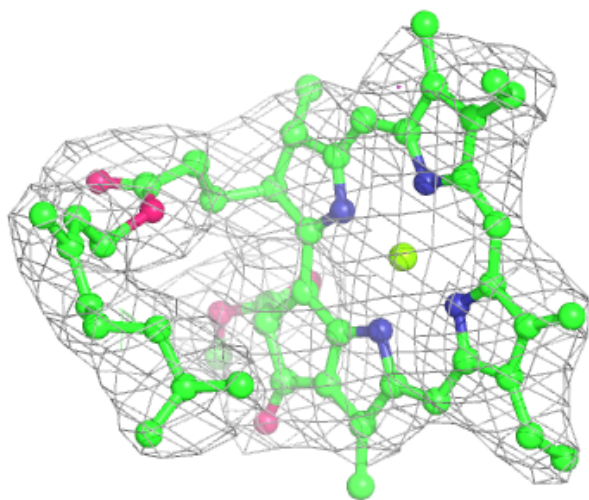
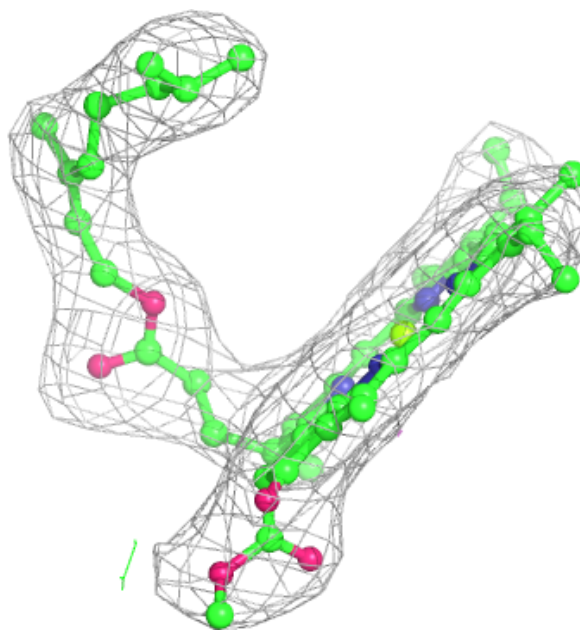
**Electron density around CLA B 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Z 809:**

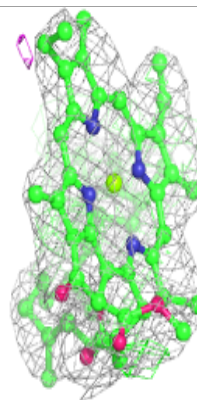
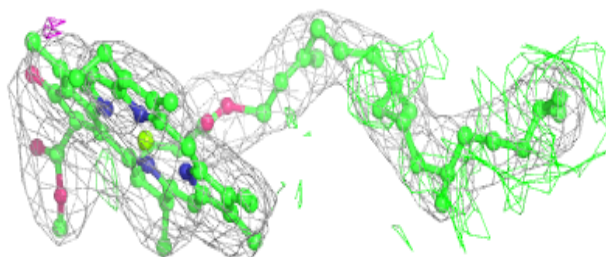
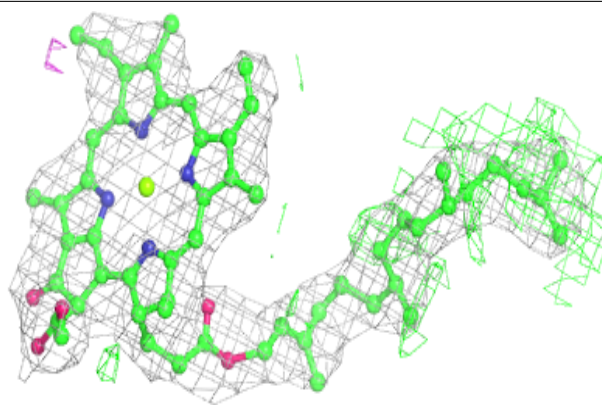
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



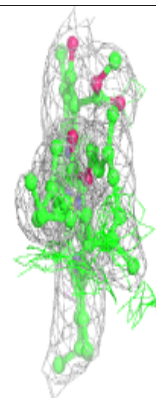
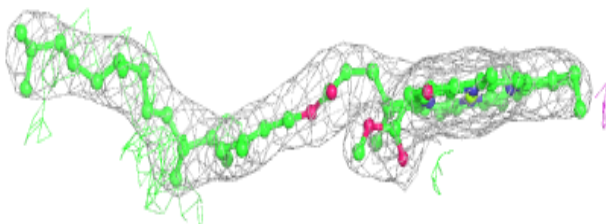
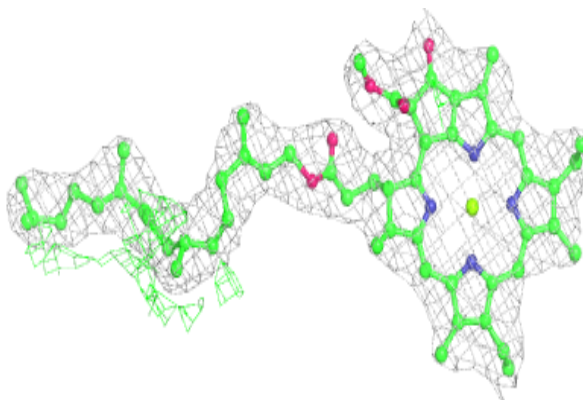


**Electron density around CLA G 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

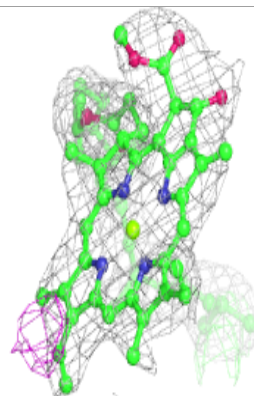
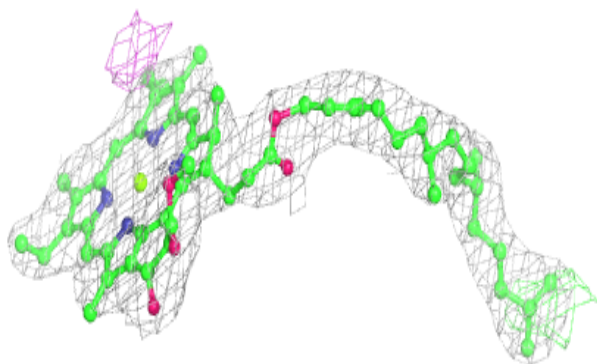
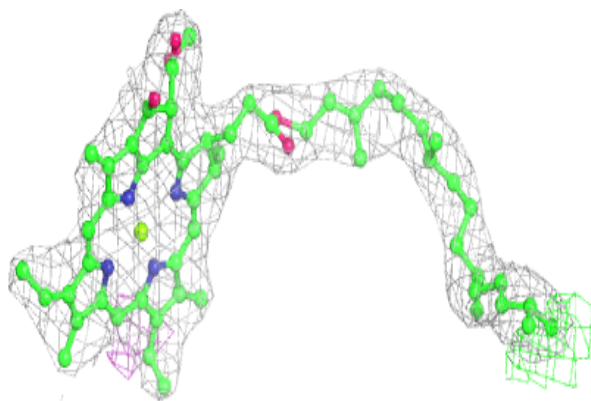
**Electron density around CLA G 832:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

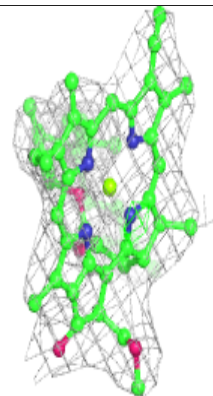
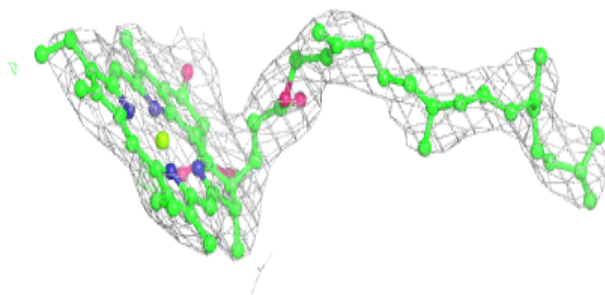
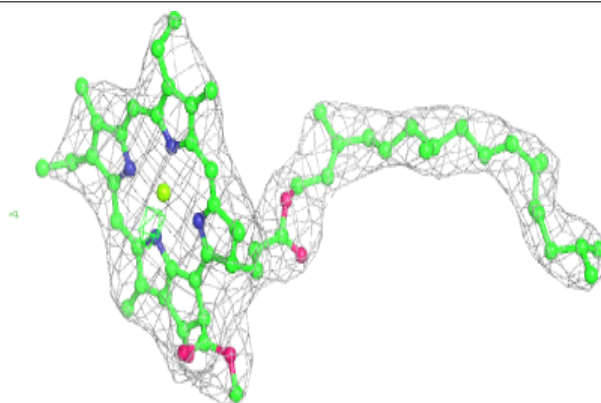


**Electron density around CLA H 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

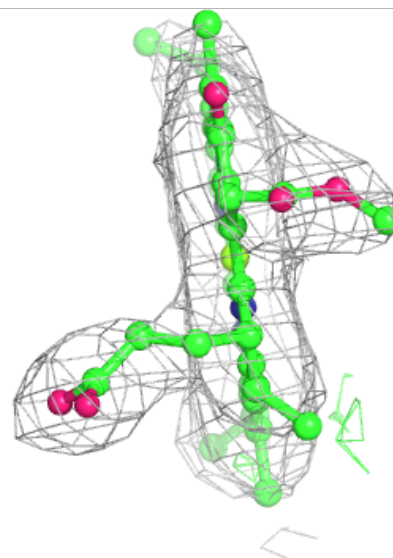
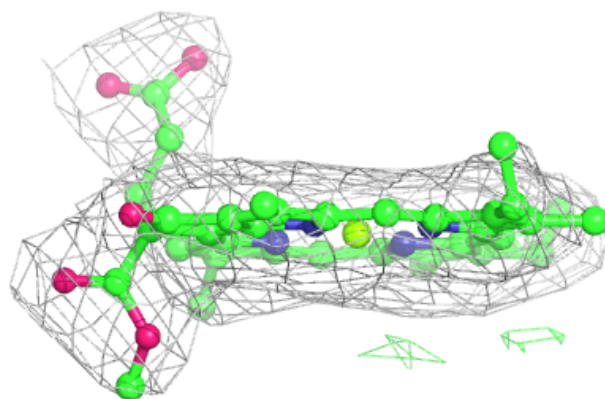
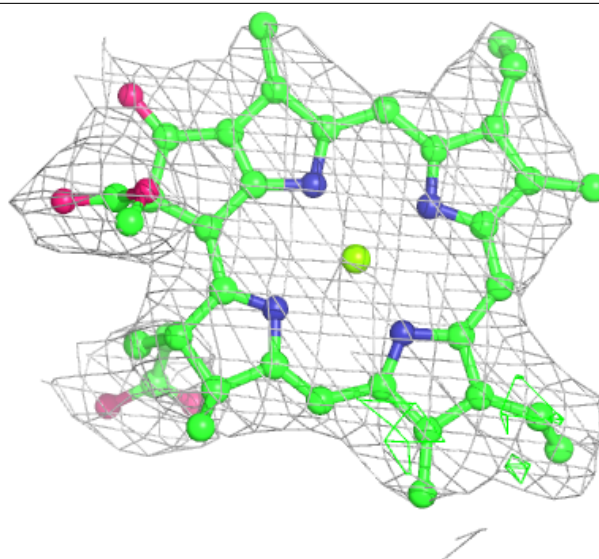
**Electron density around CLA Y 821:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



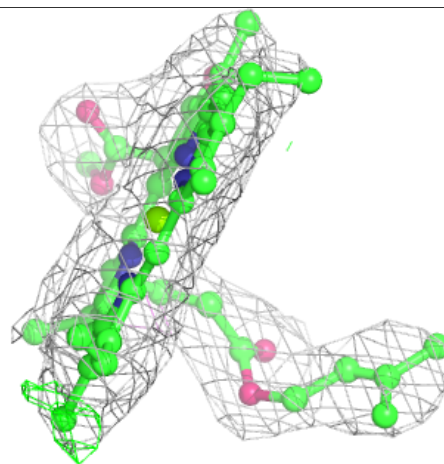
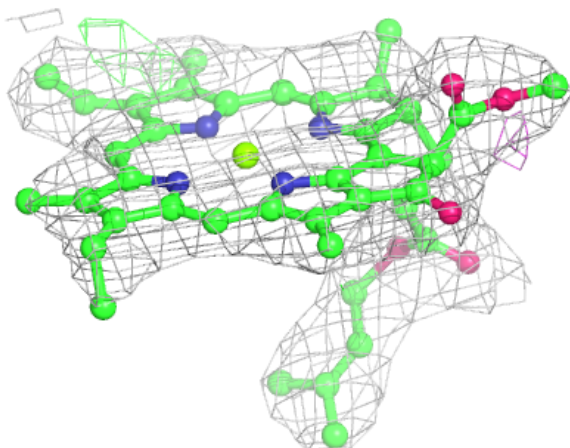
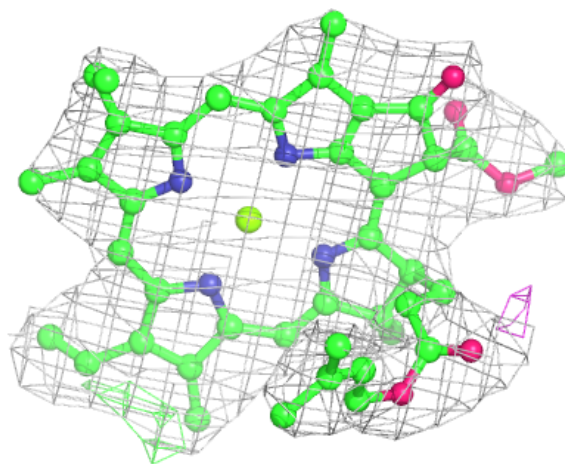
**Electron density around CLA Z 828:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



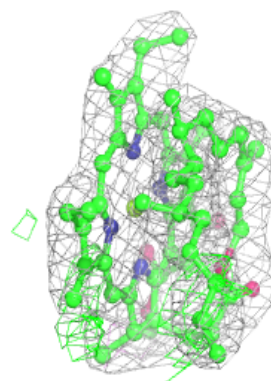
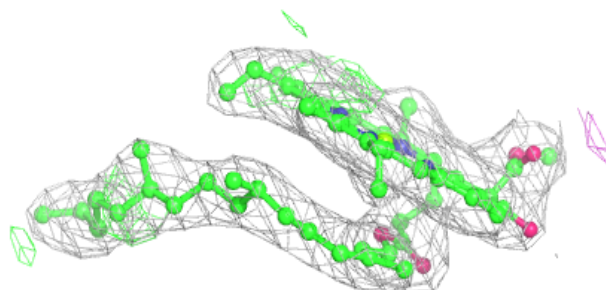
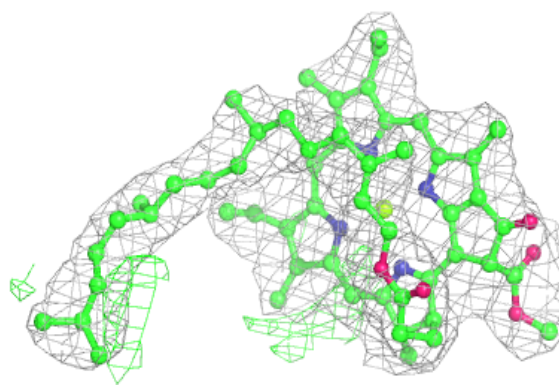
**Electron density around CLA B 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA H 806:**

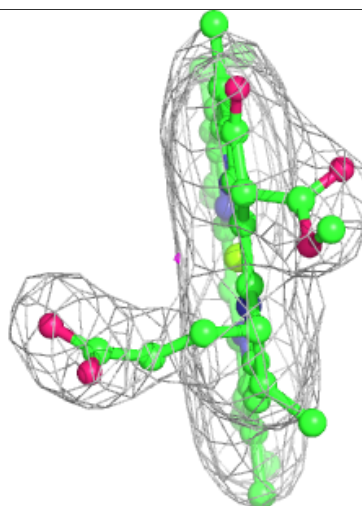
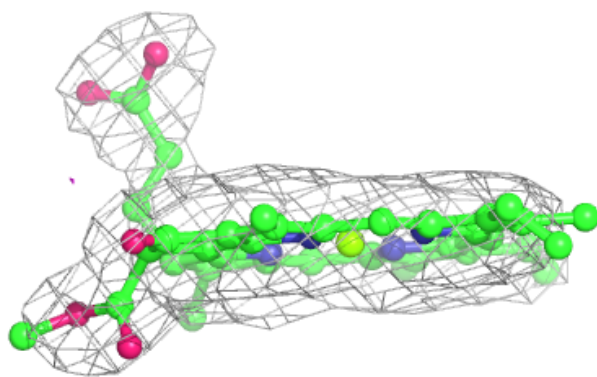
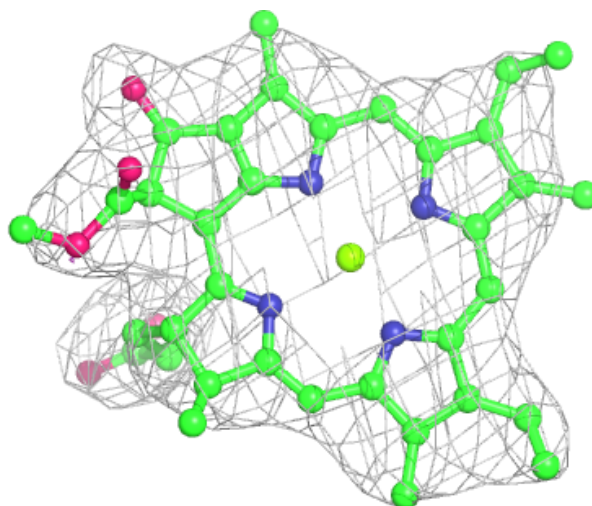
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





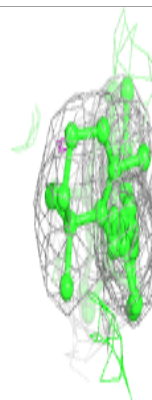
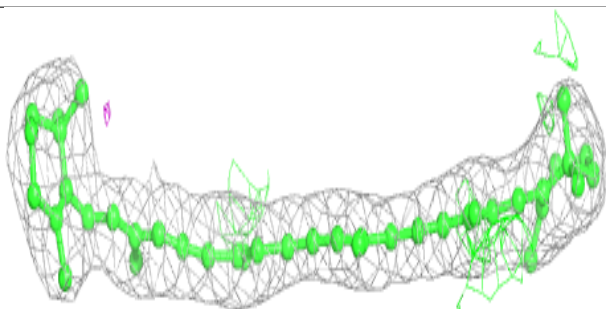
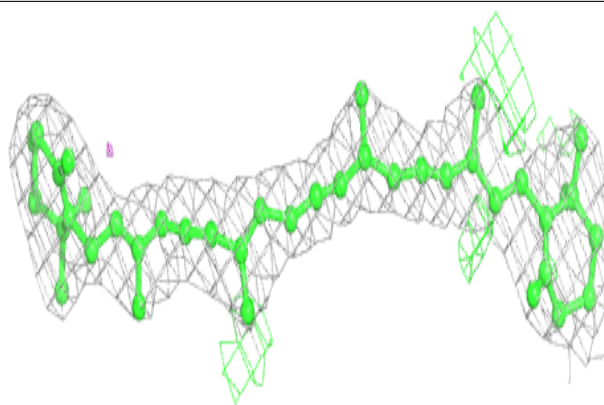
**Electron density around CLA G 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

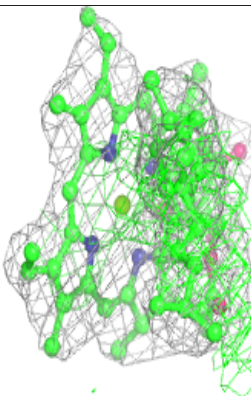
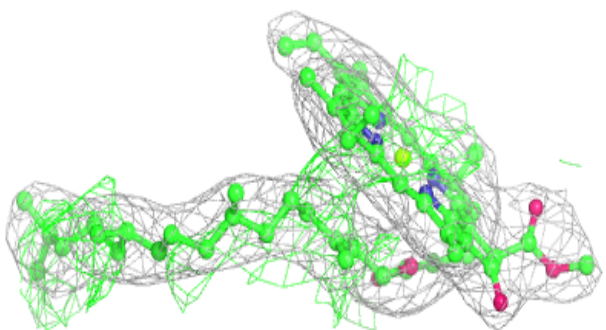
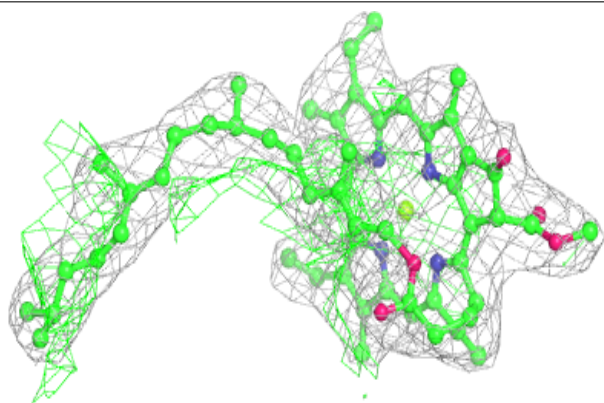


**Electron density around BCR A 848:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

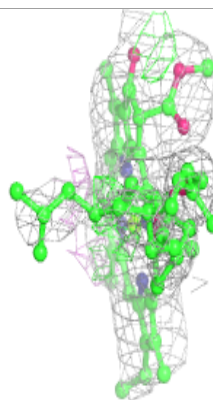
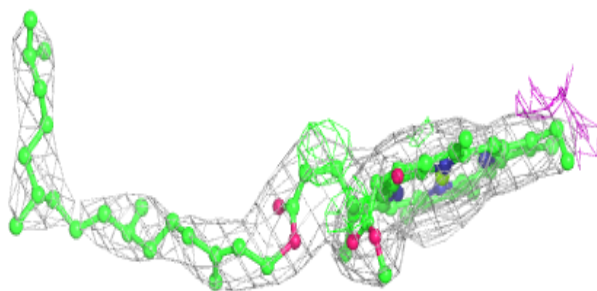
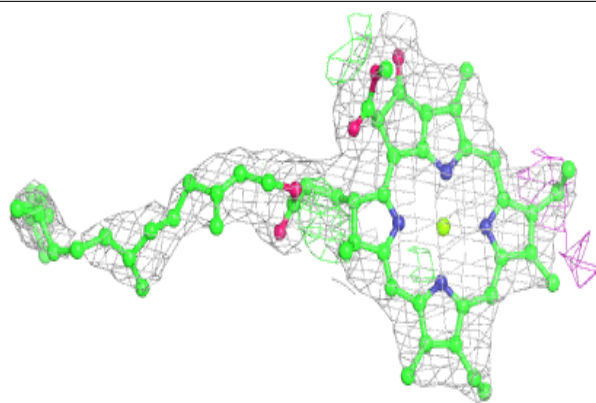
**Electron density around CLA G 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 805:**

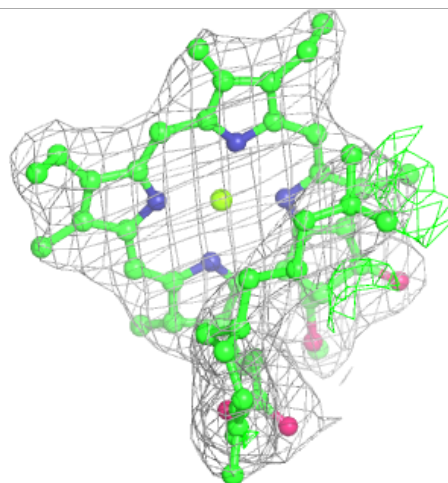
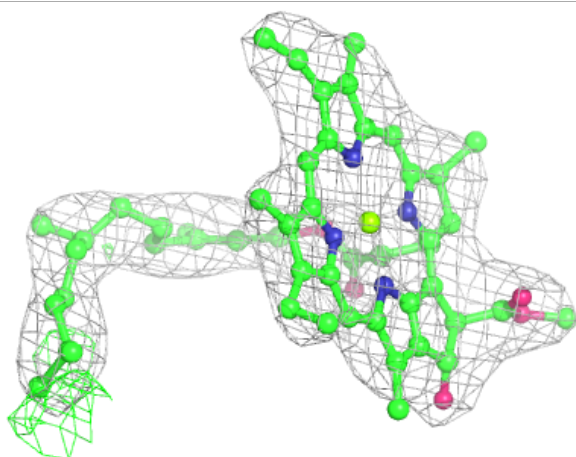
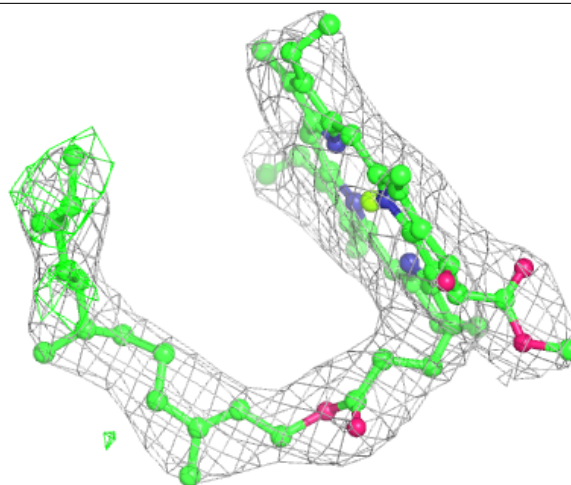
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





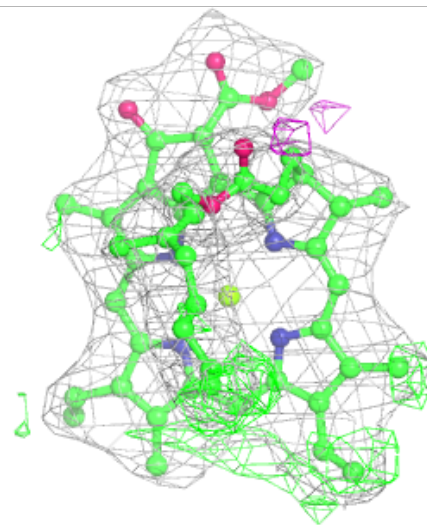
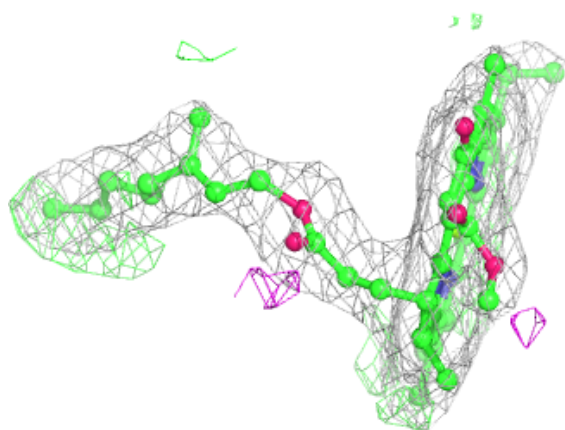
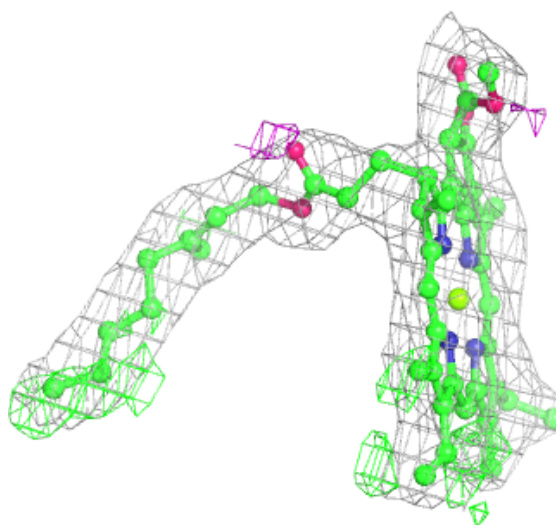
**Electron density around CLA Z 817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



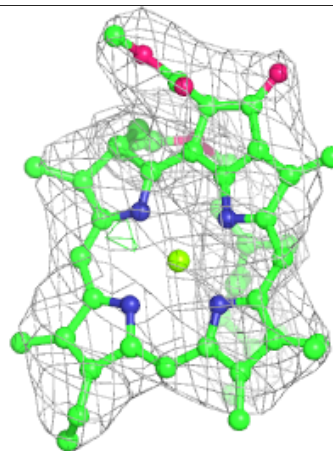
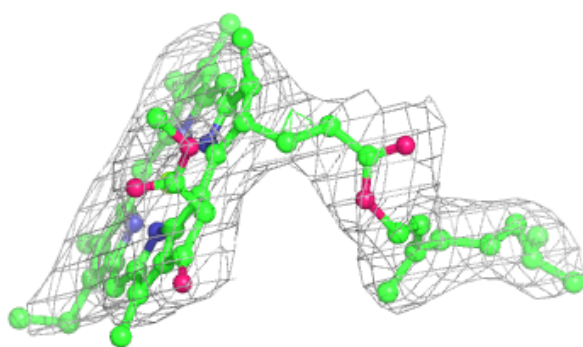
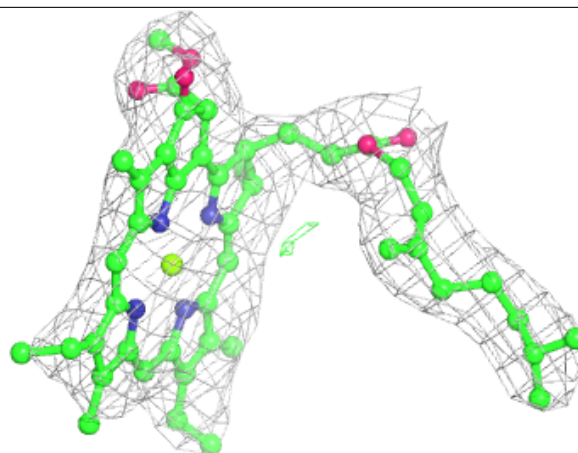
**Electron density around CLA Z 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

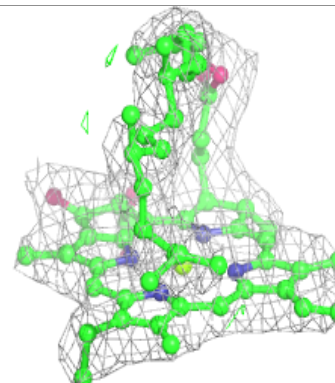
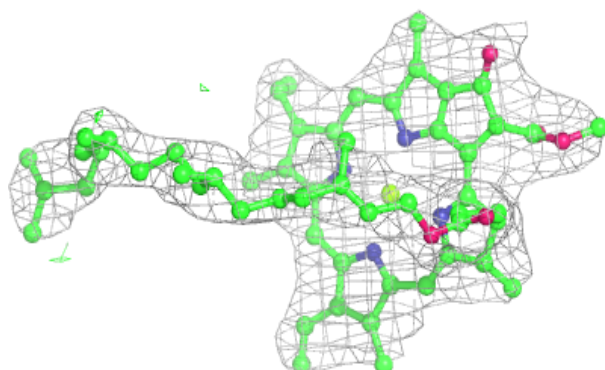
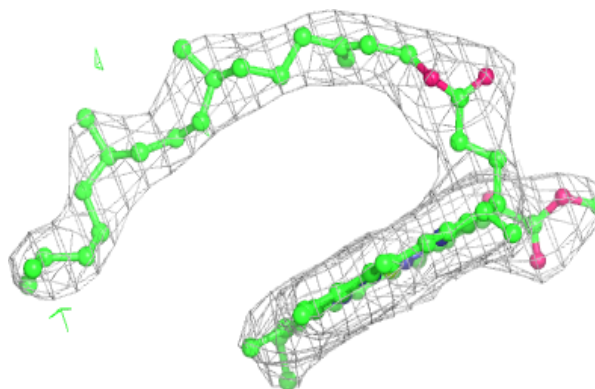


**Electron density around CLA Y 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

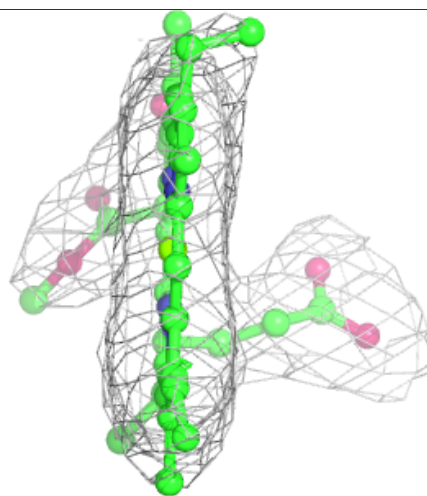
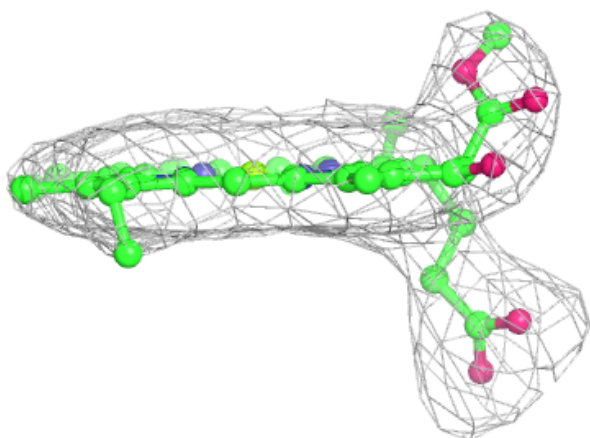
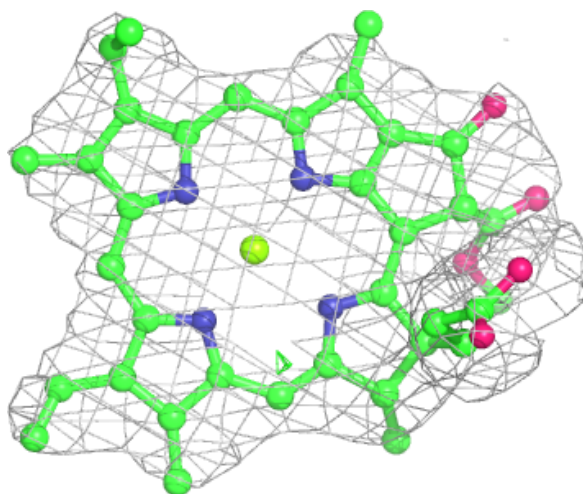
**Electron density around CLA h 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



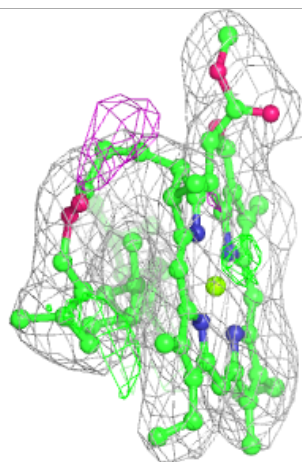
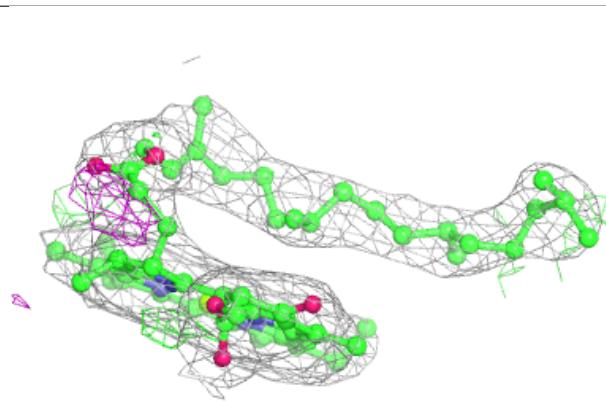
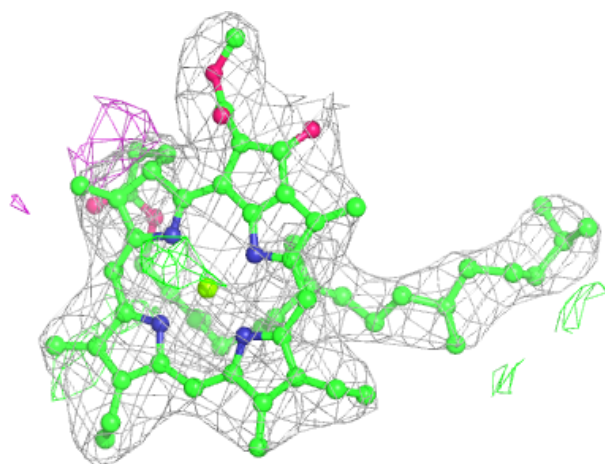
**Electron density around CLA Z 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 827:**

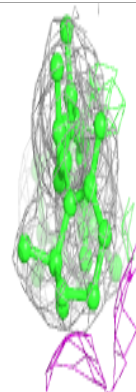
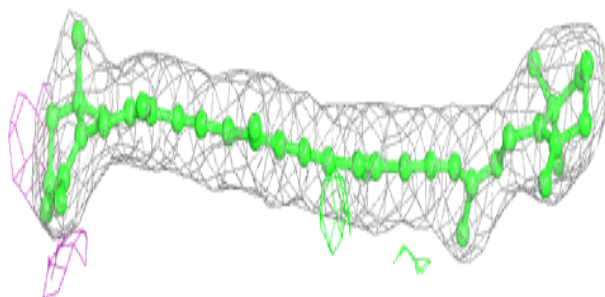
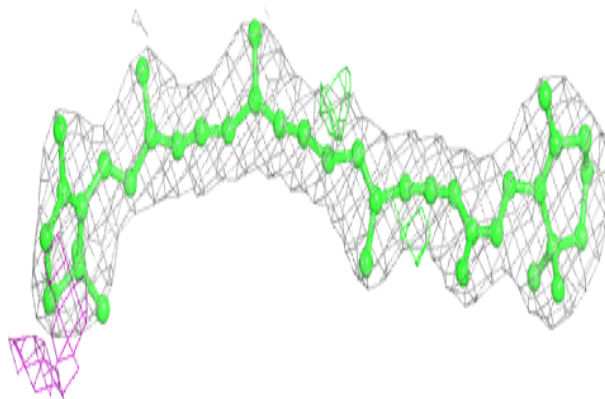
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



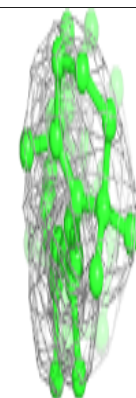
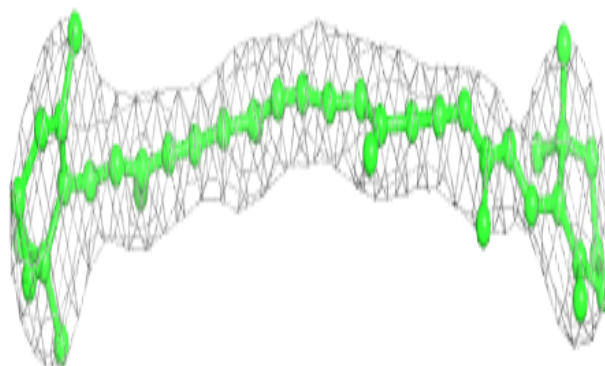
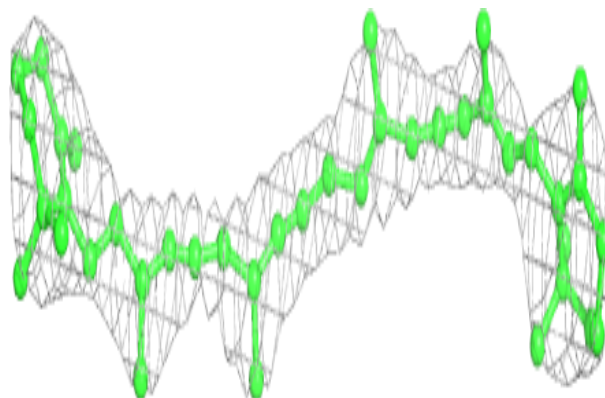


**Electron density around BCR B 847:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

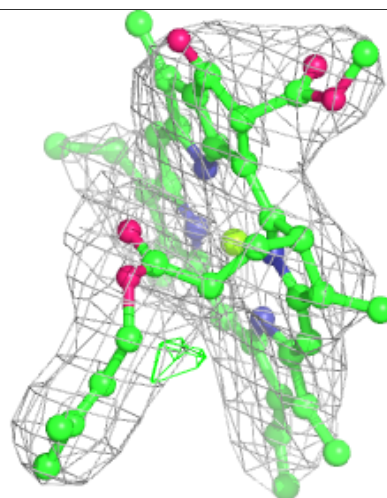
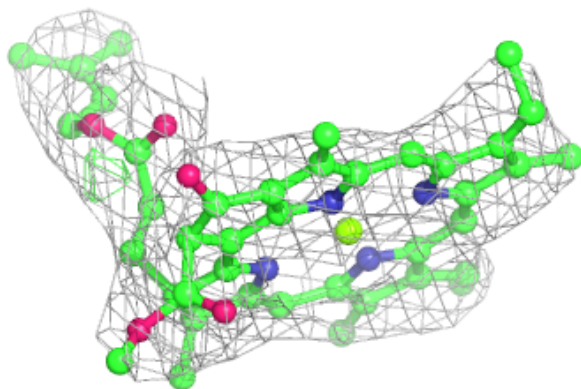
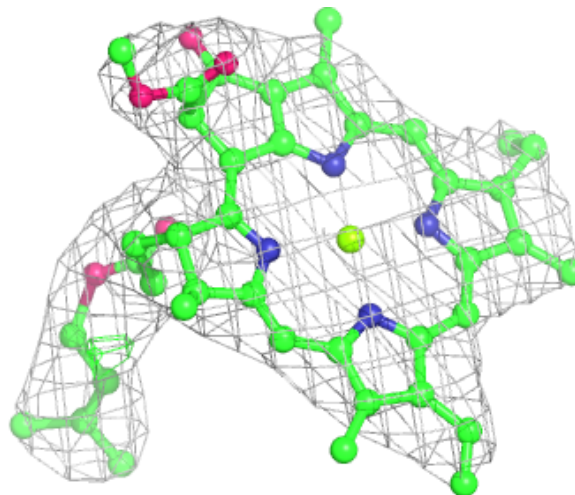
**Electron density around BCR G 847:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



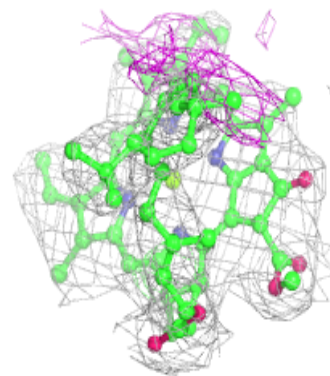
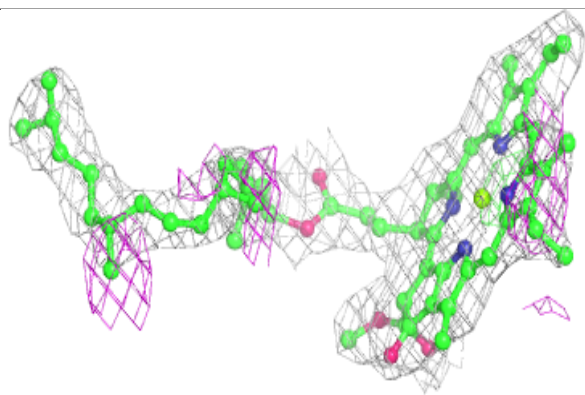
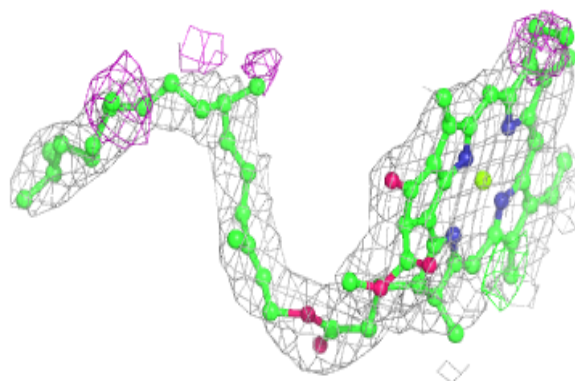
**Electron density around CLA Y 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 803:**

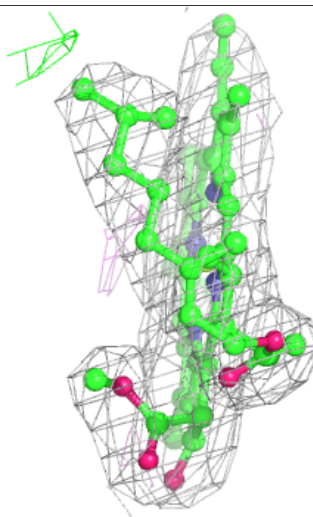
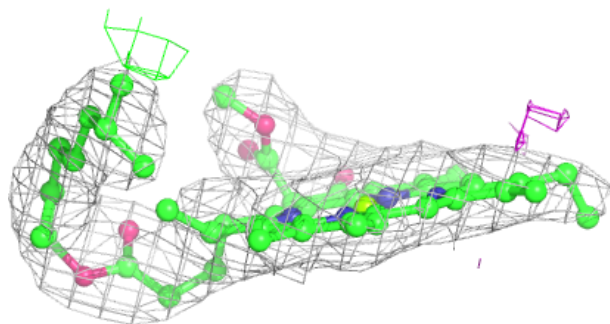
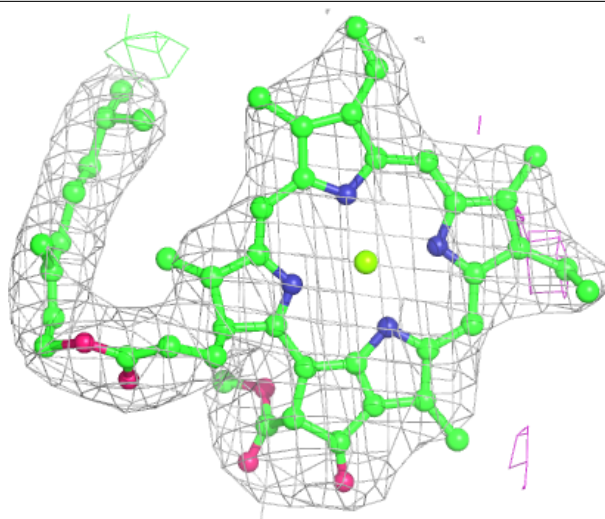
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





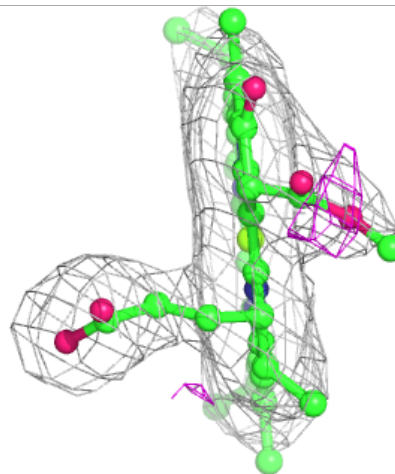
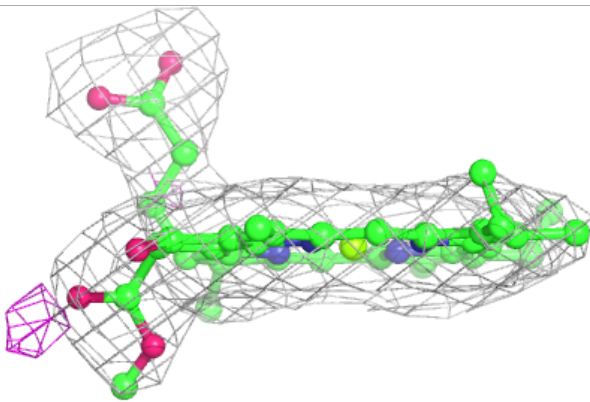
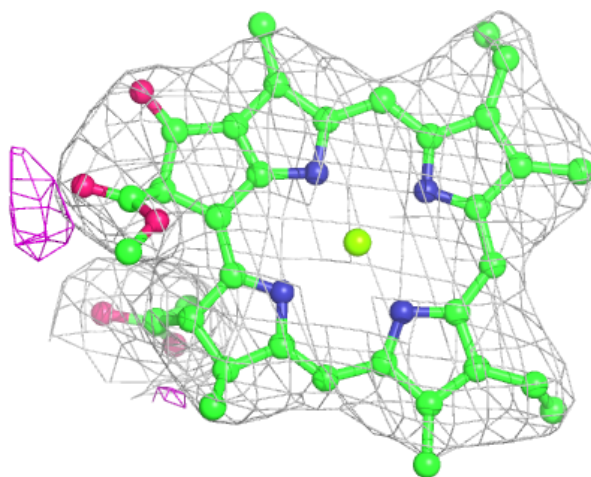
**Electron density around CLA B 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



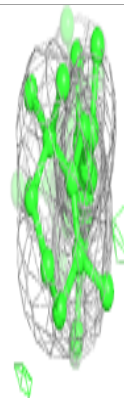
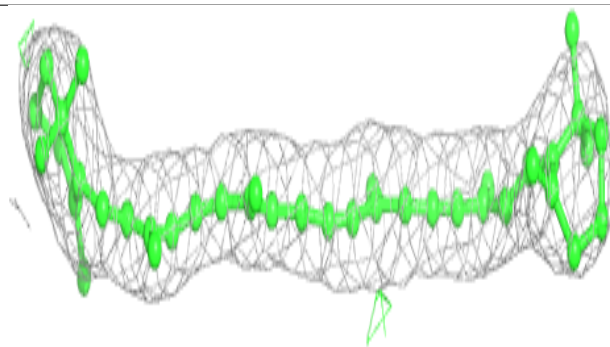
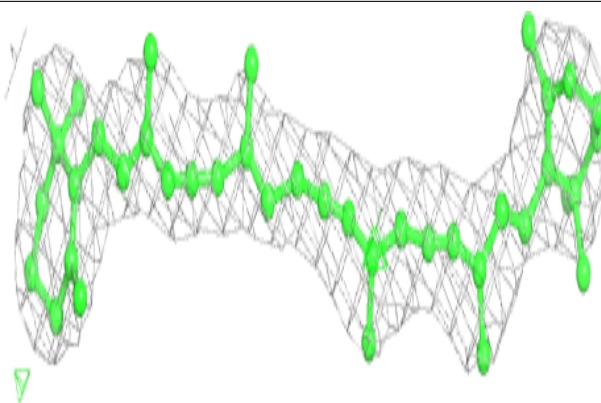
**Electron density around CLA B 821:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



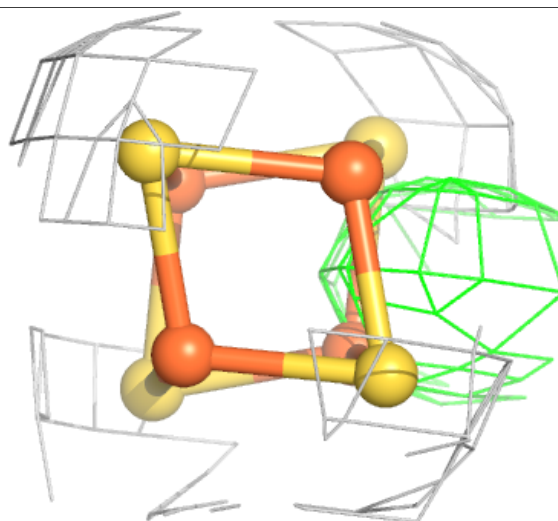
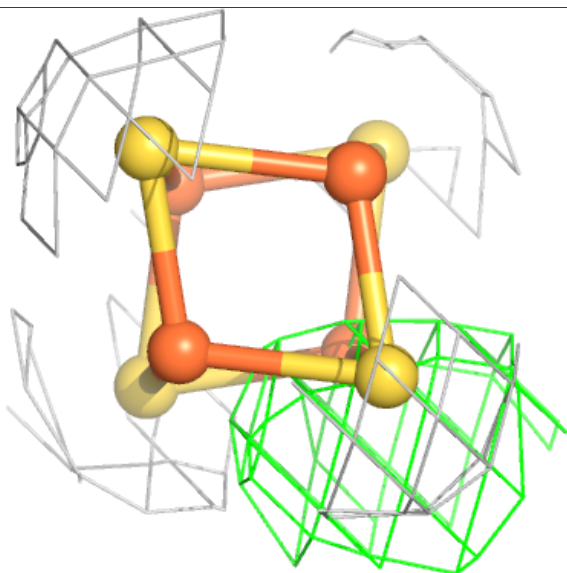
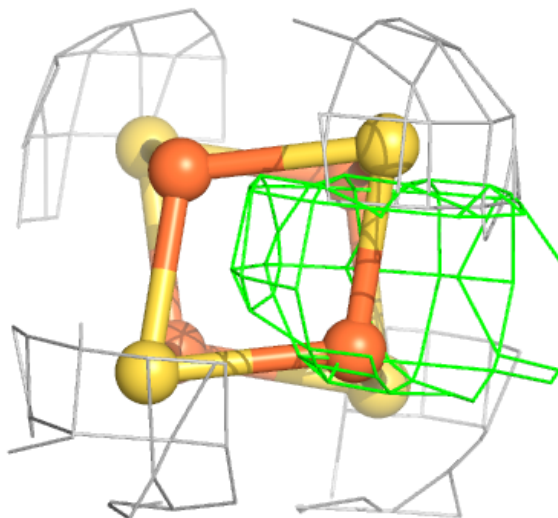
**Electron density around BCR Z 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



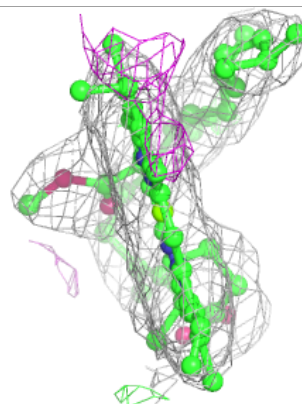
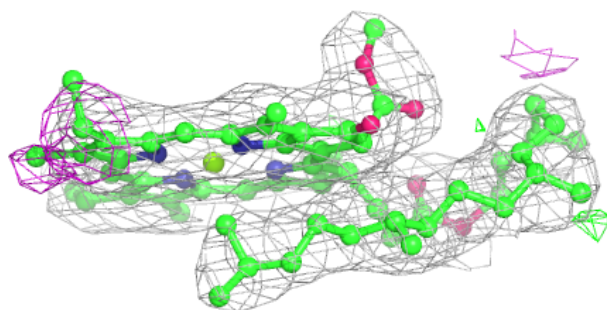
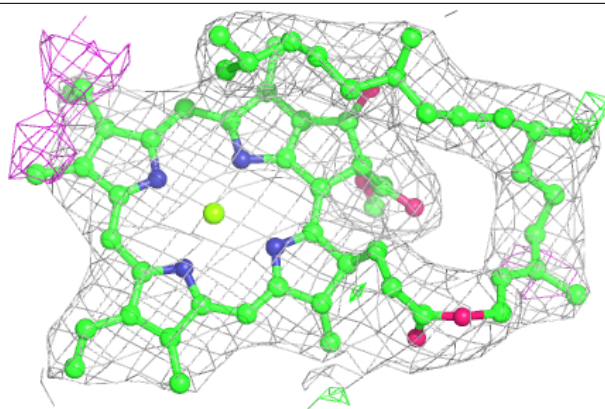
**Electron density around SF4 Y 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

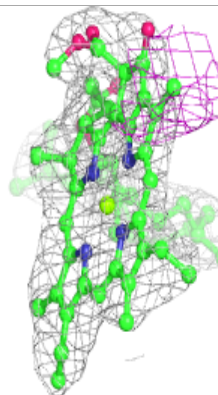
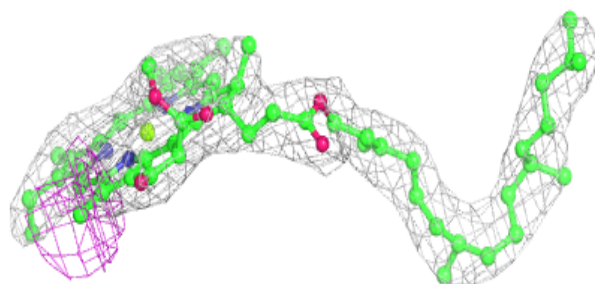
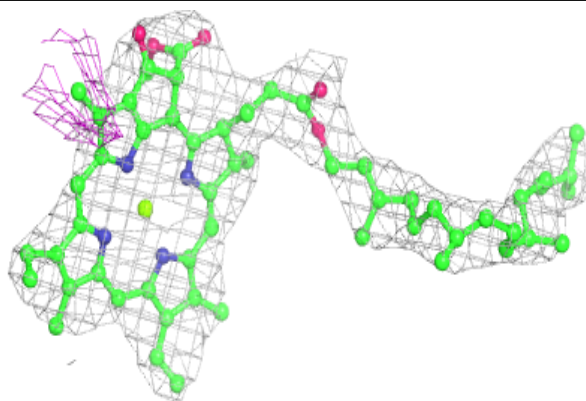


**Electron density around CLA Z 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA H 812:**

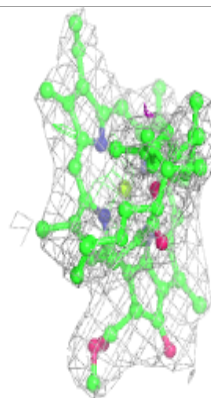
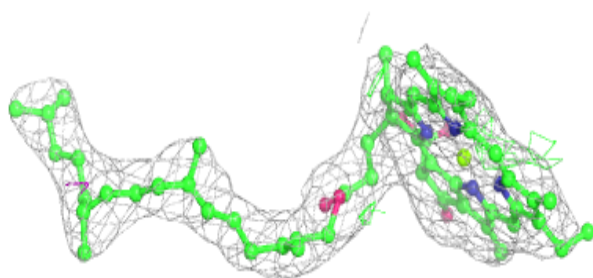
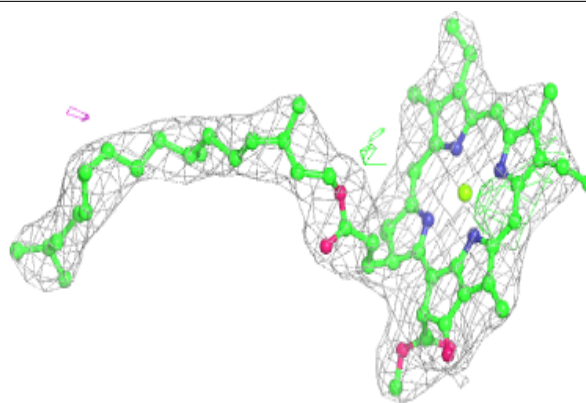
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



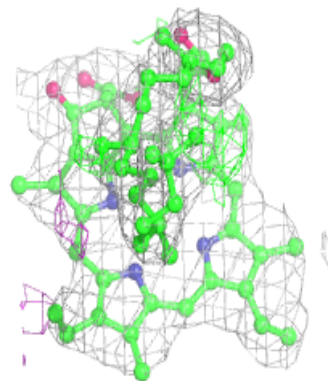
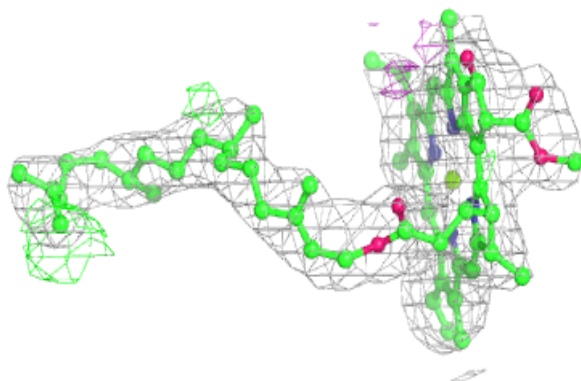
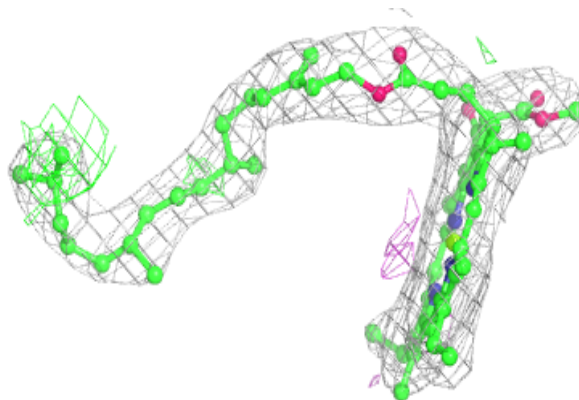


**Electron density around CLA A 821:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

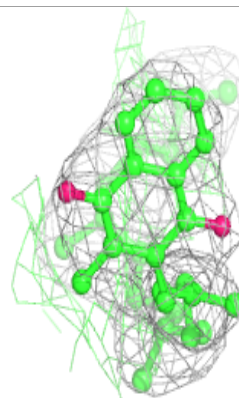
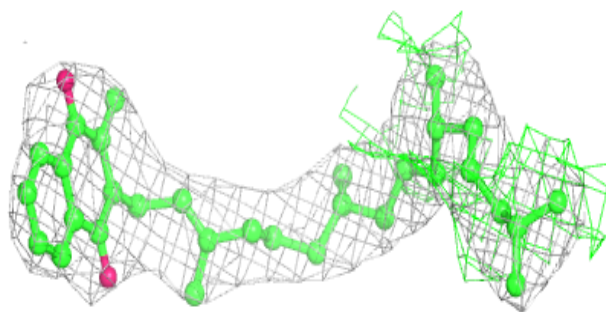
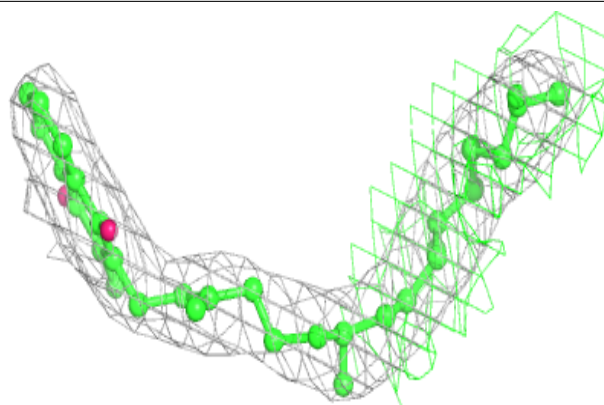
**Electron density around CLA G 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



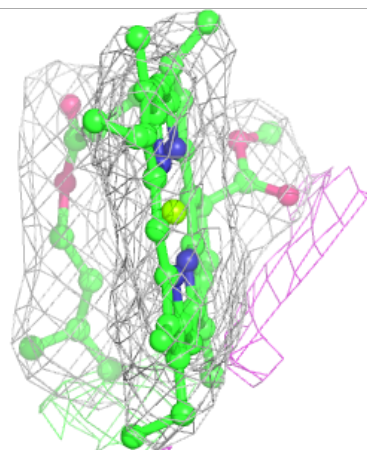
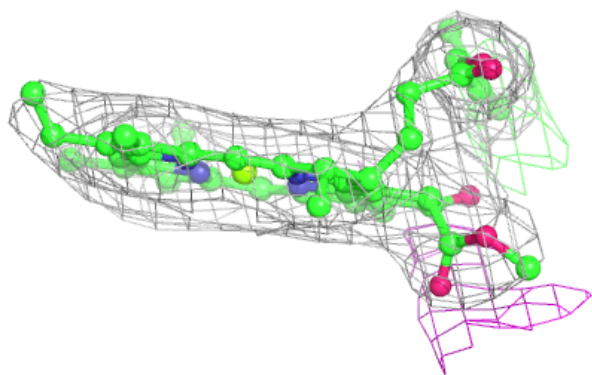
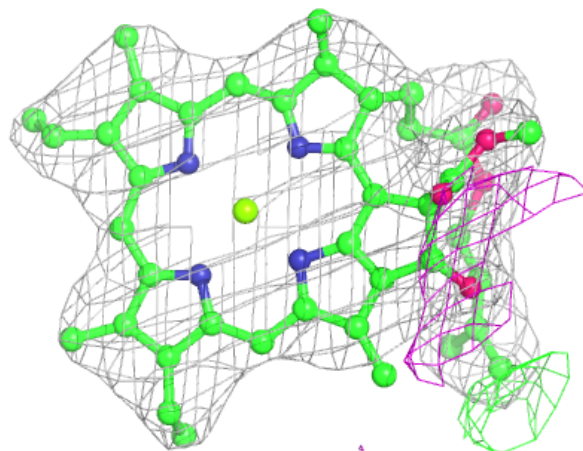
**Electron density around PQN H 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

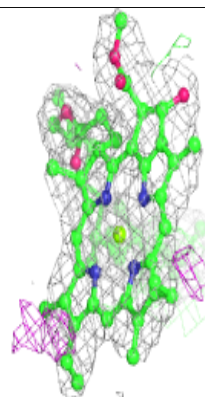
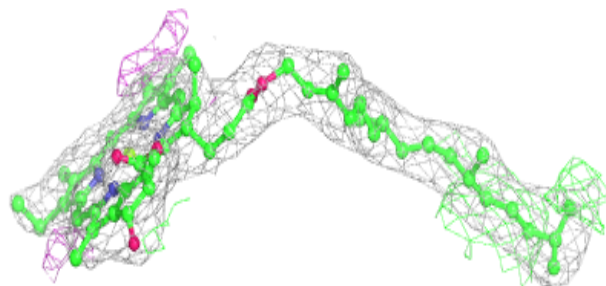
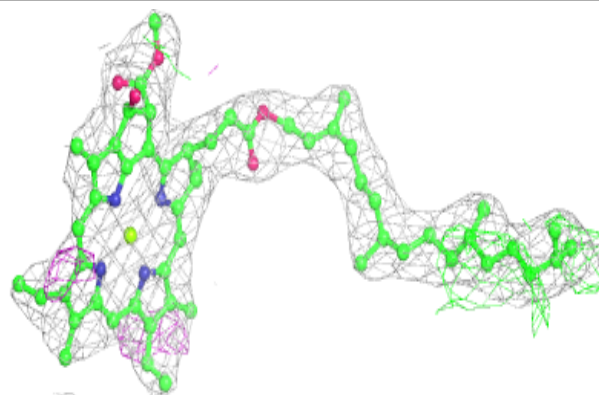


**Electron density around CLA A 842:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 802:**

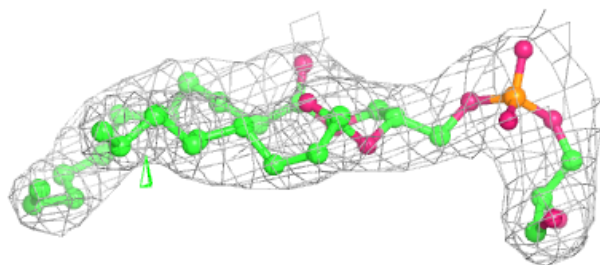
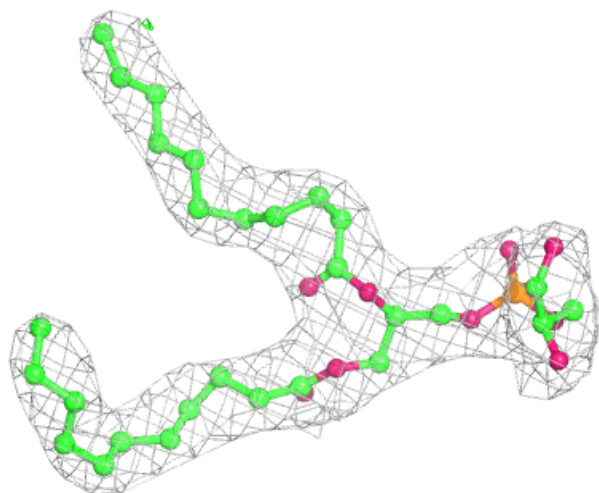
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





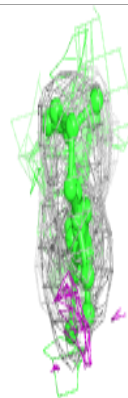
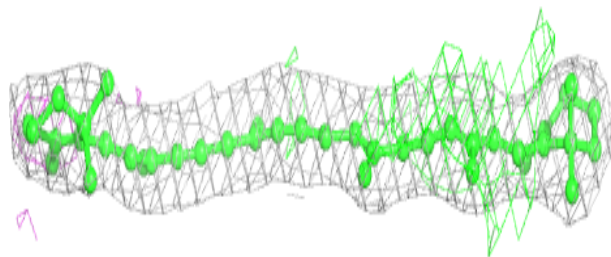
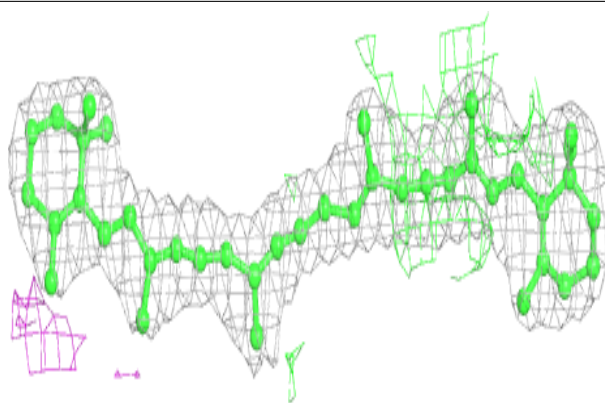
**Electron density around LHG B 850:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



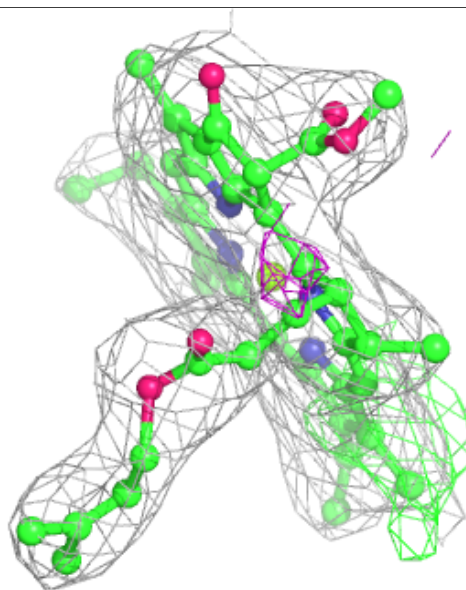
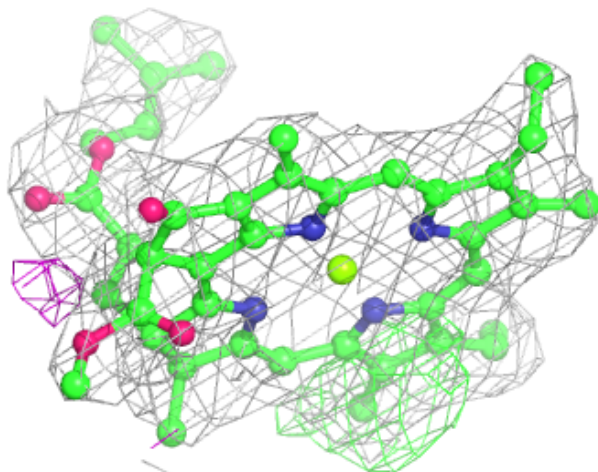
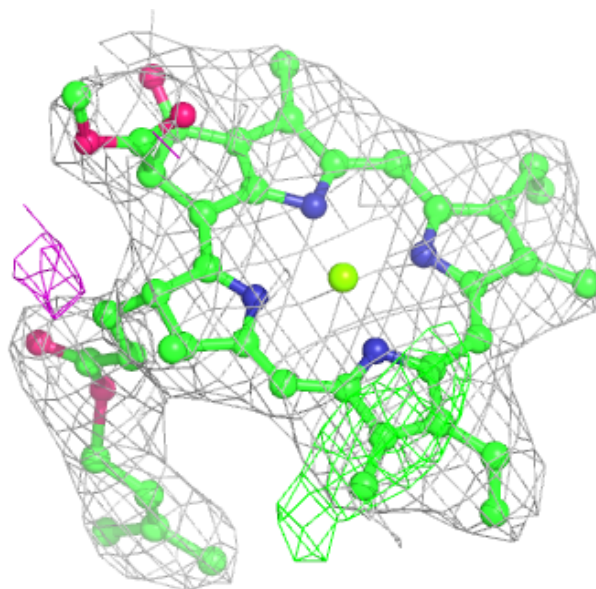
**Electron density around BCR L 208:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



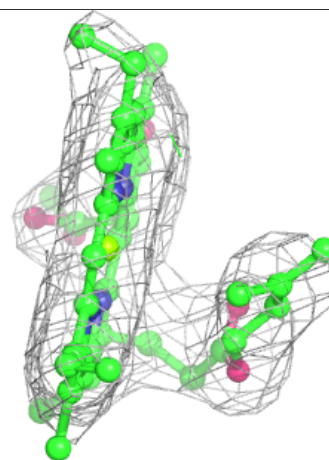
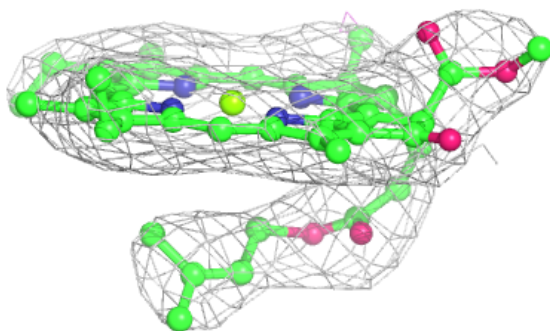
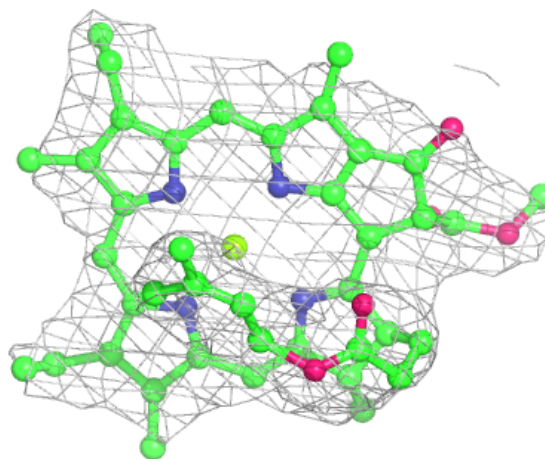
**Electron density around CLA A 831:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



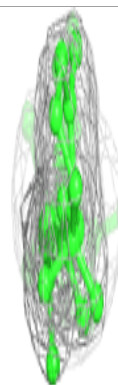
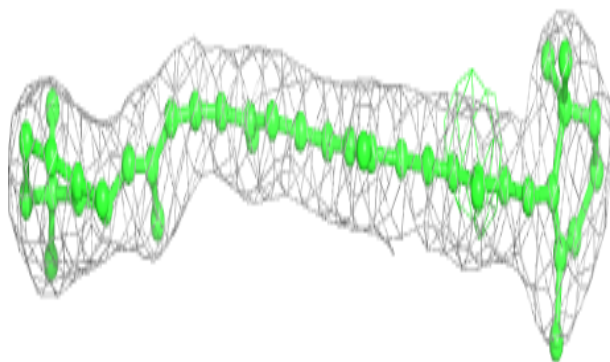
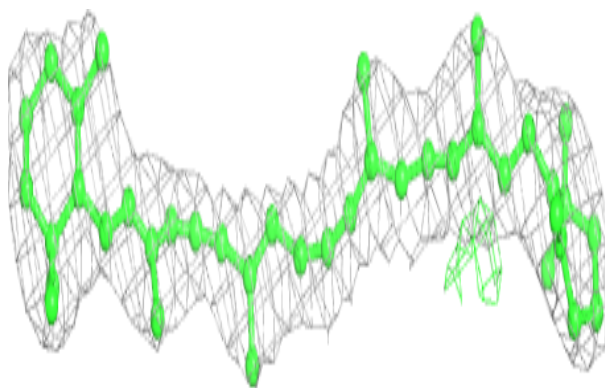
**Electron density around CLA Y 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

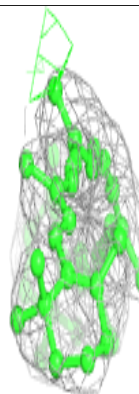
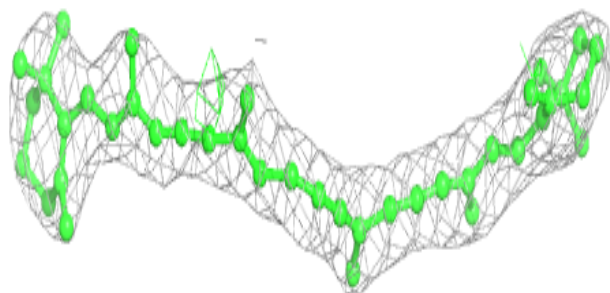
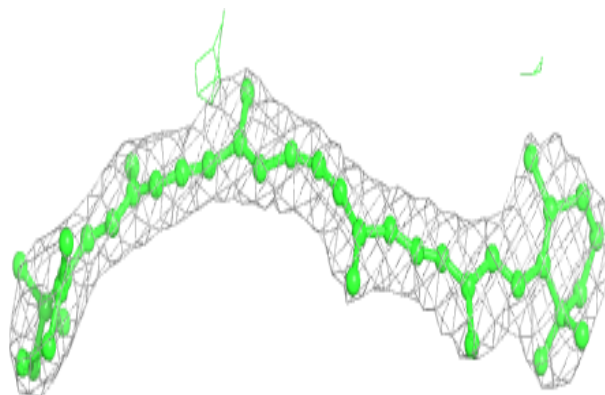


**Electron density around BCR f 105:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR Z 846:**

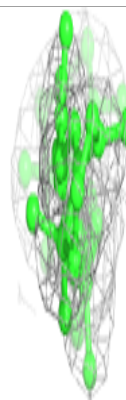
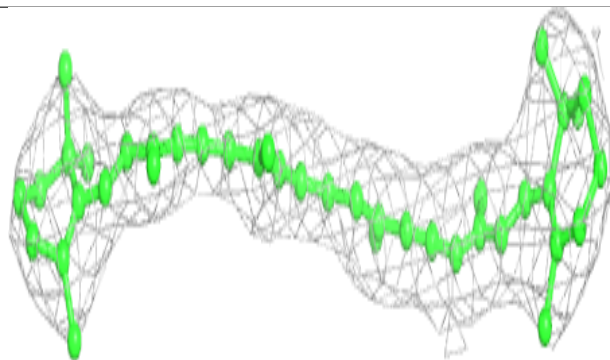
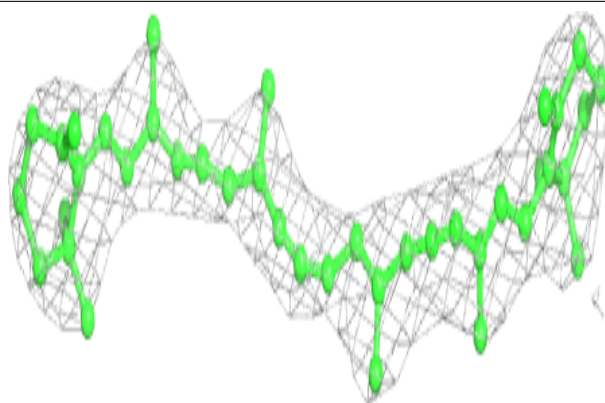
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



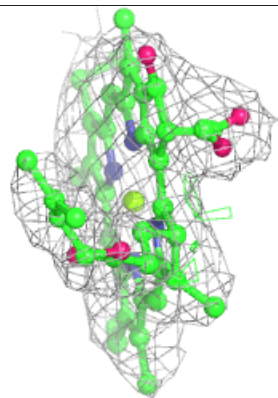
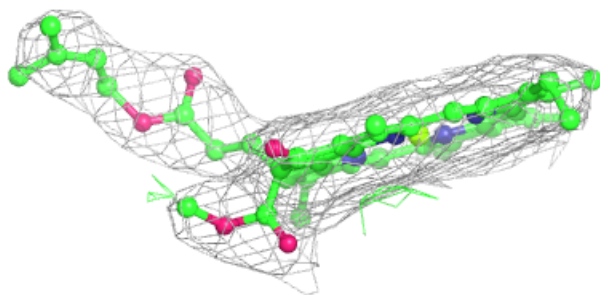
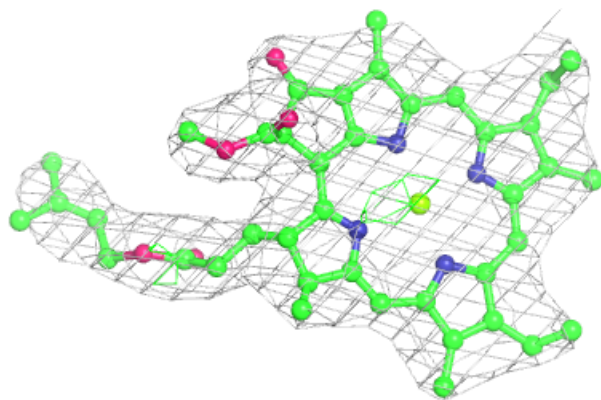


**Electron density around BCR Y 847:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

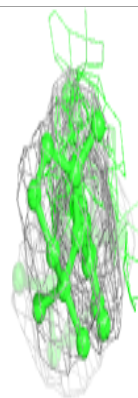
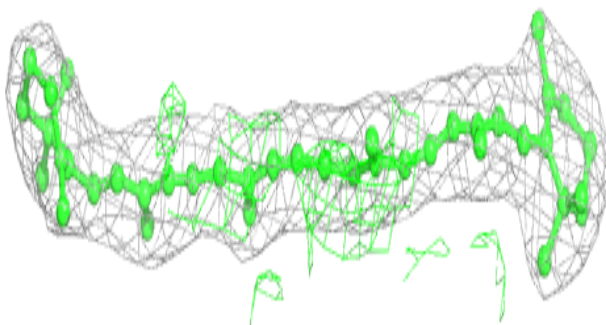
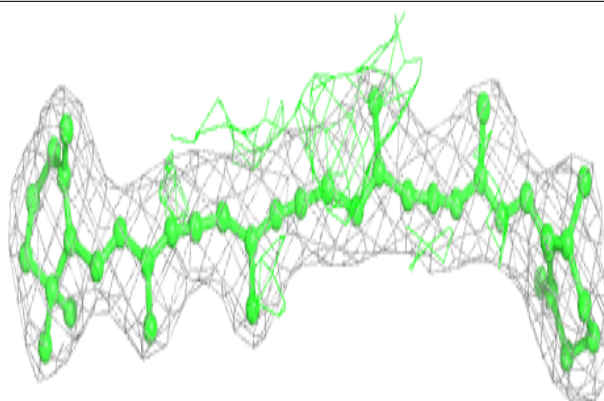
**Electron density around CLA A 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

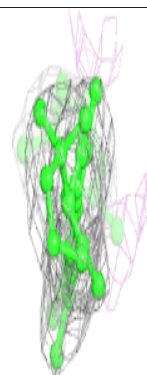
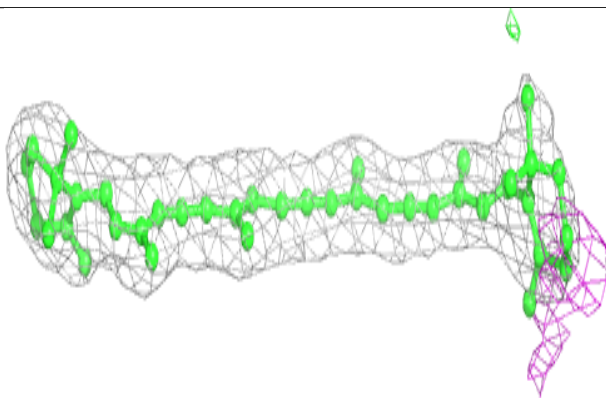
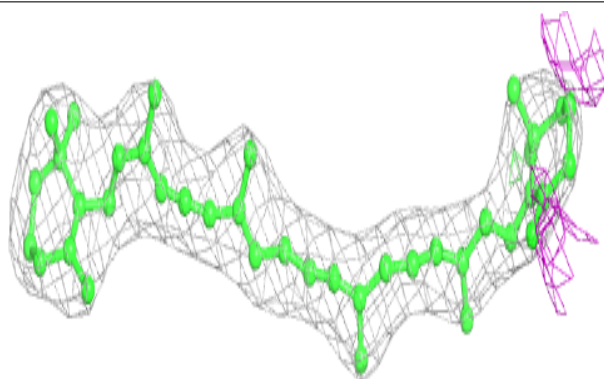


**Electron density around BCR Y 856:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

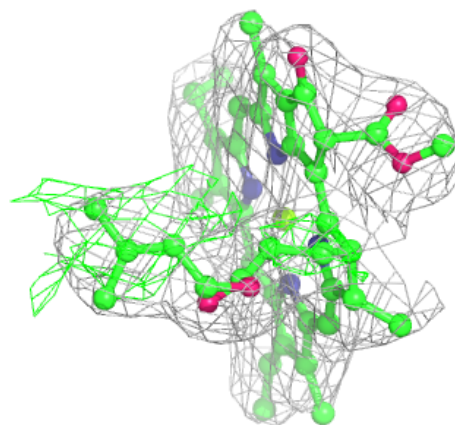
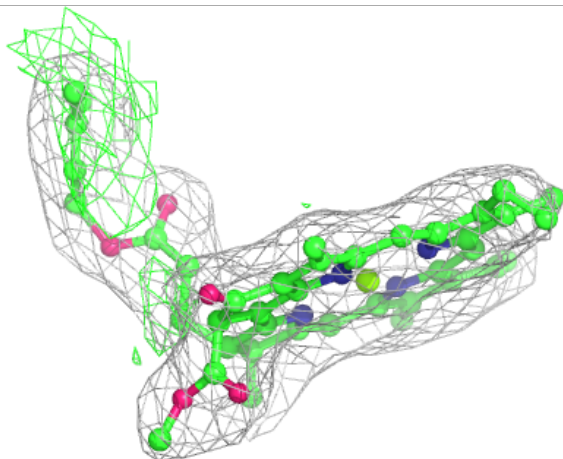
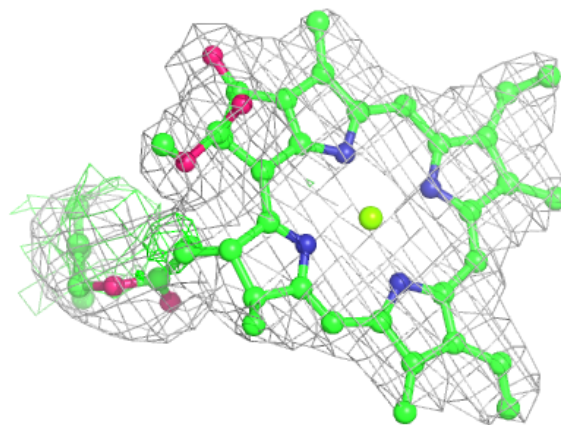
**Electron density around BCR Z 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 839:**

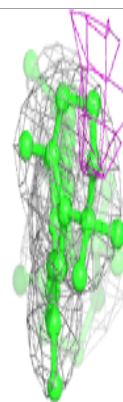
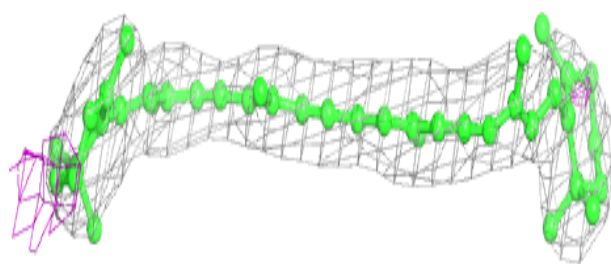
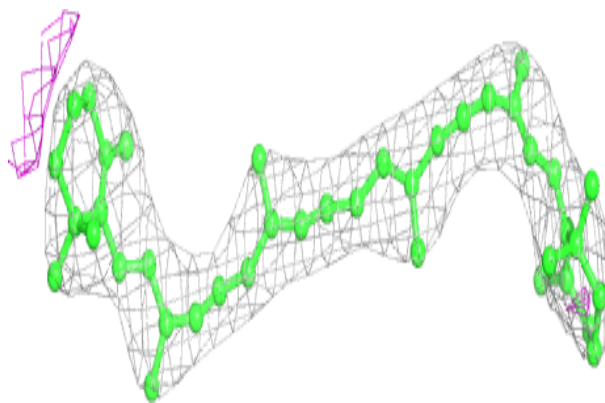
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





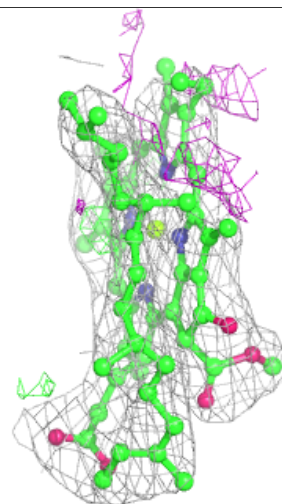
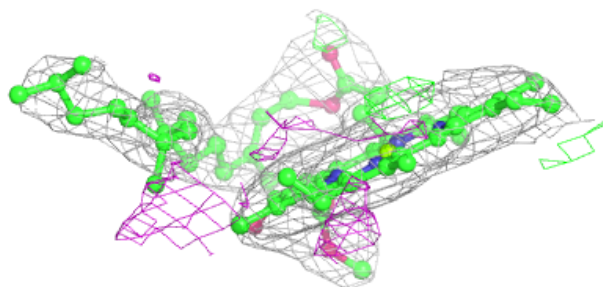
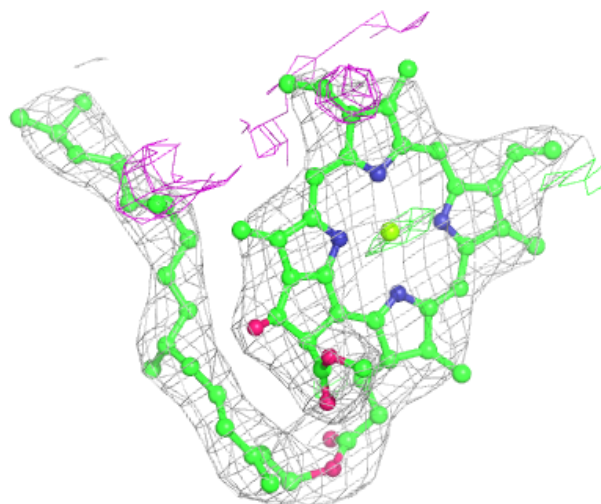
**Electron density around BCR B 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



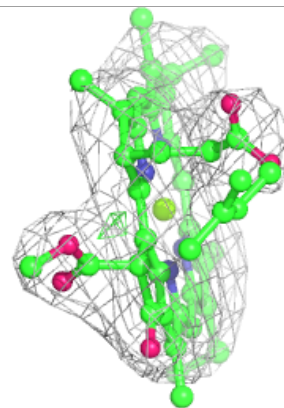
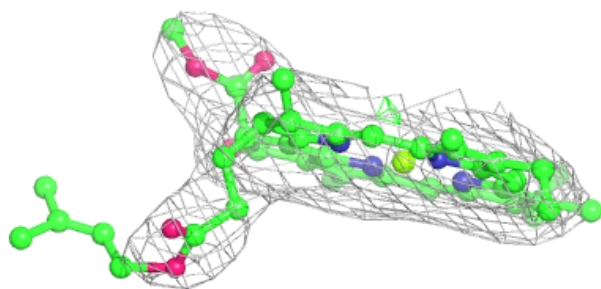
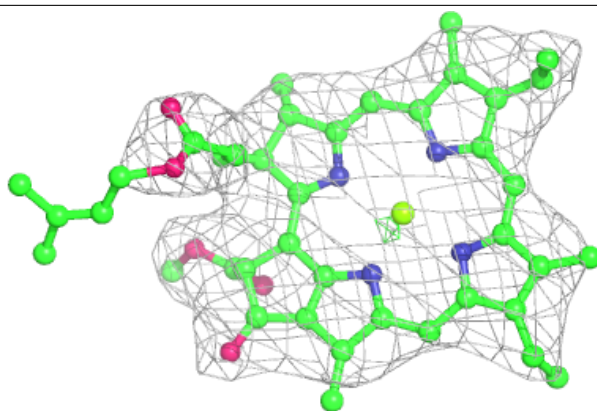
**Electron density around CLA G 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



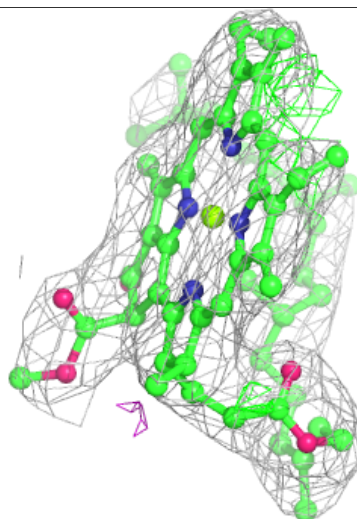
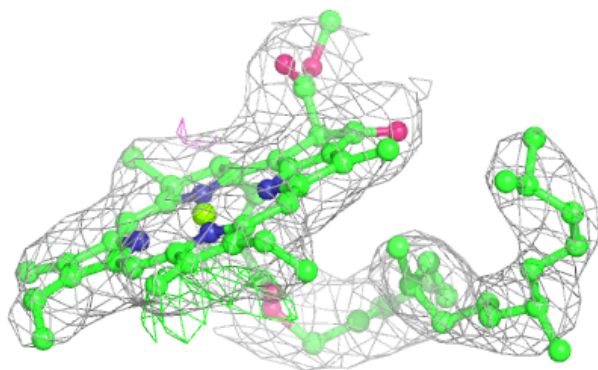
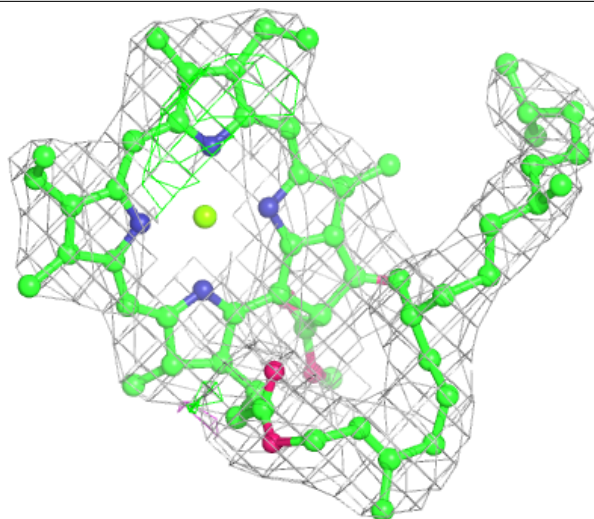
**Electron density around CLA Y 816:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



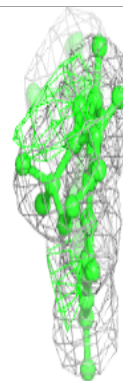
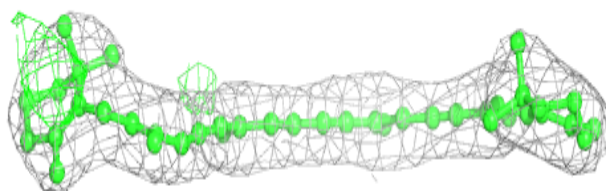
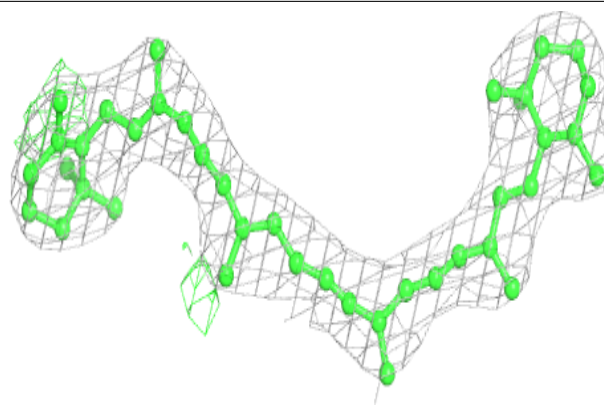
**Electron density around CLA Q 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



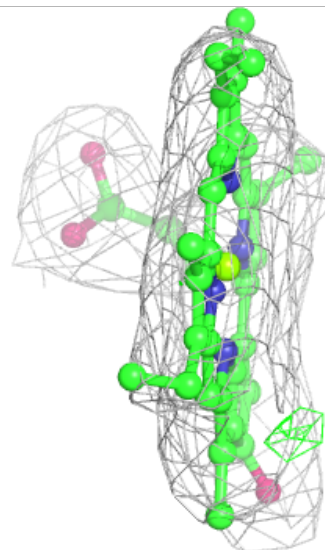
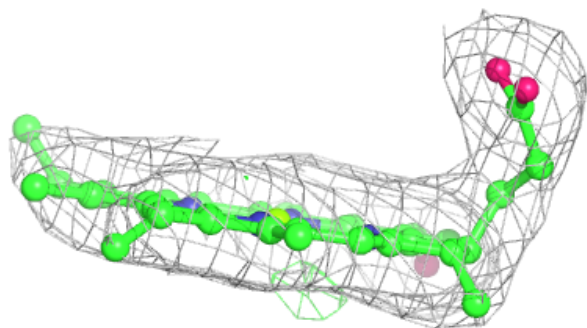
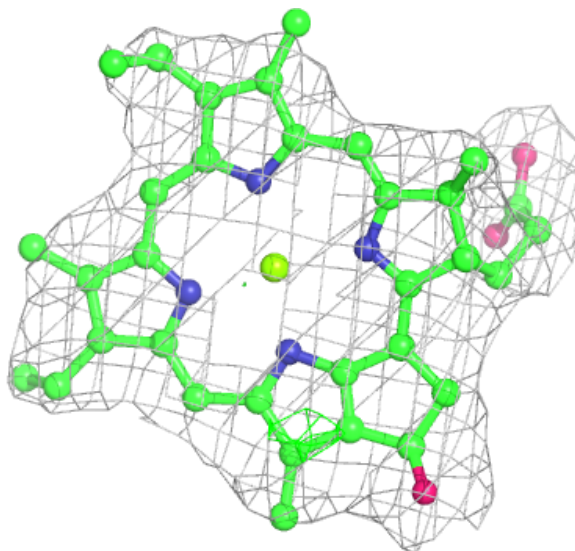
**Electron density around BCR G 850:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



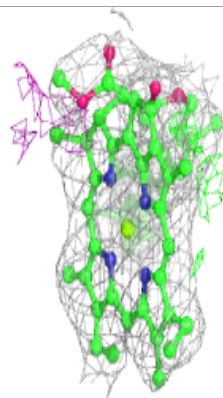
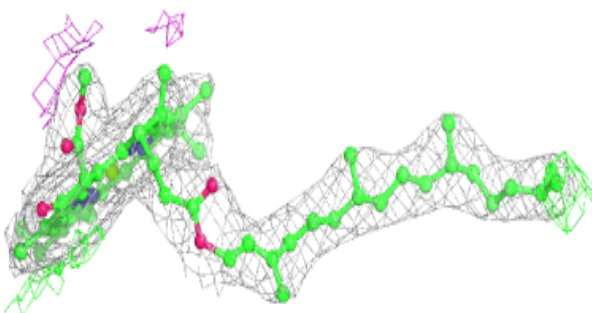
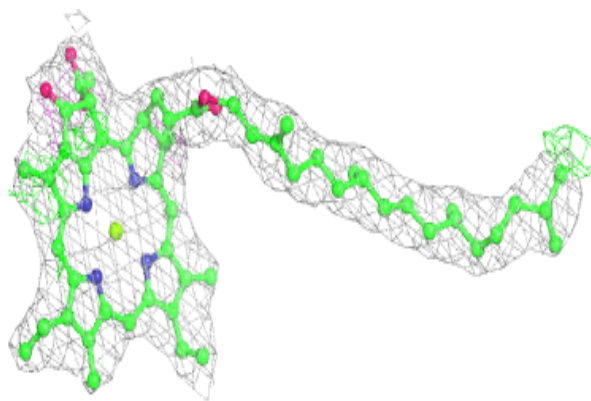
**Electron density around CLA K 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

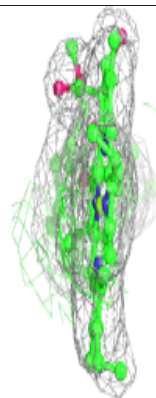
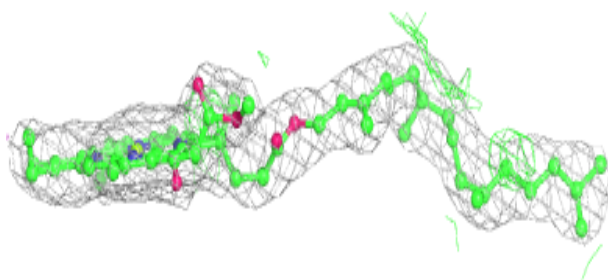
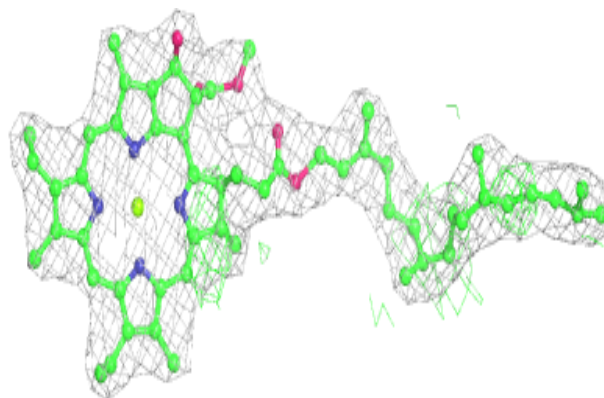


**Electron density around CLA L 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 833:**

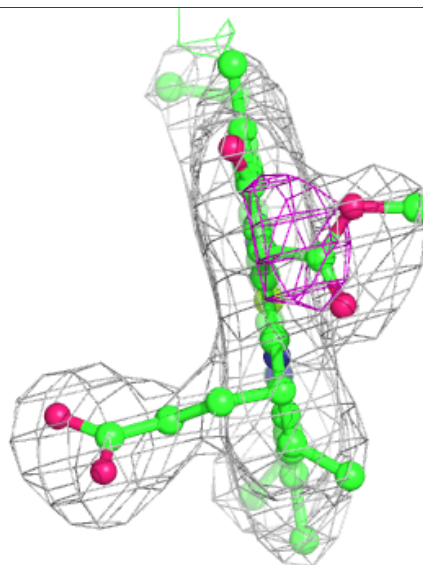
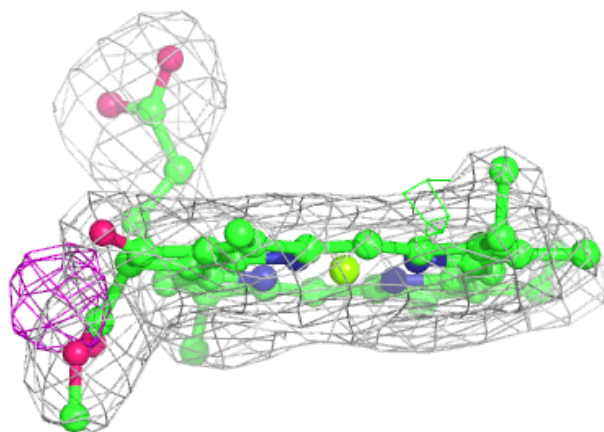
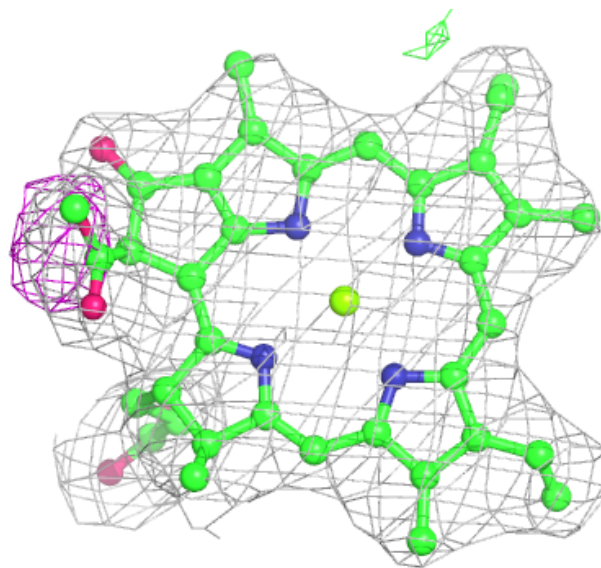
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA H 829:**

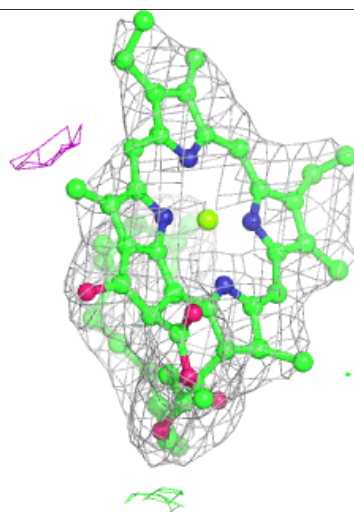
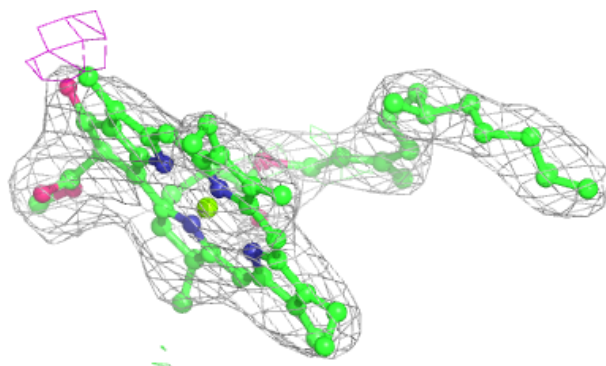
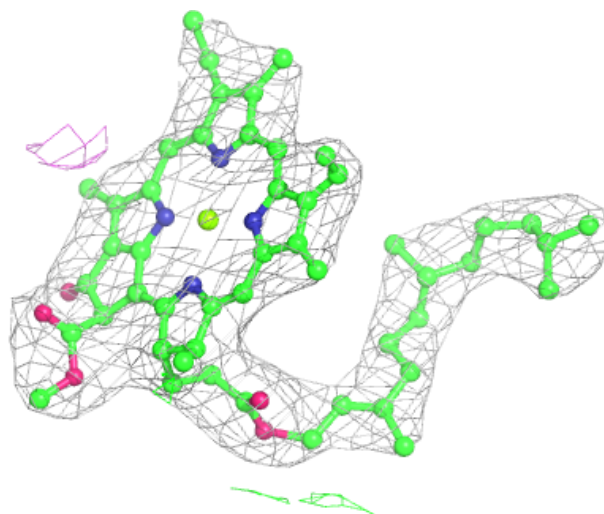
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





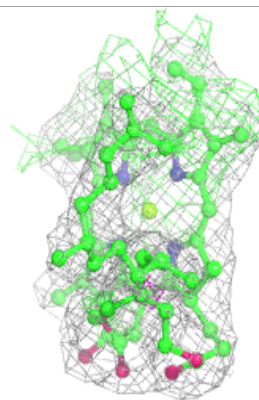
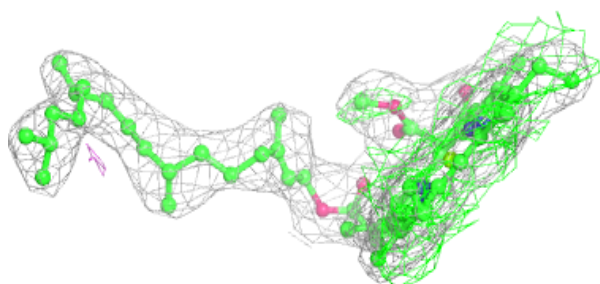
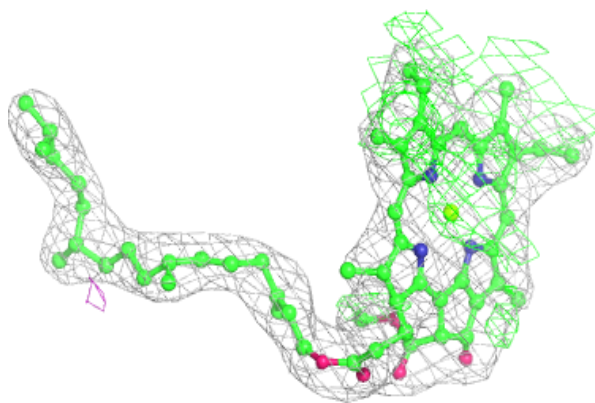
**Electron density around CLA A 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

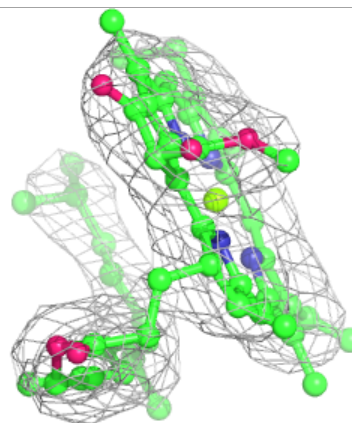
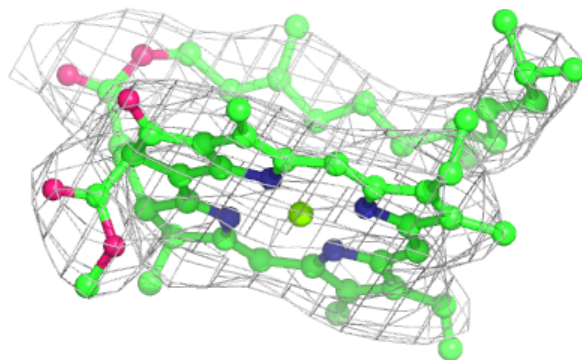
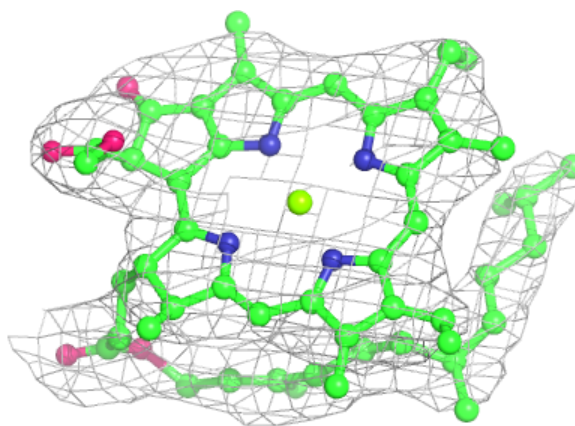


**Electron density around CLA L 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

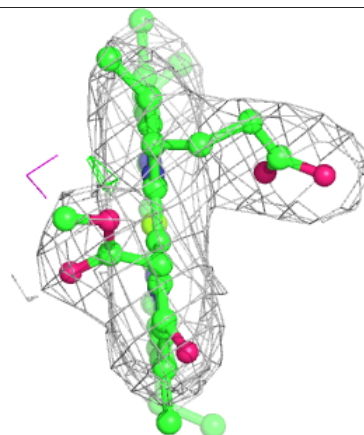
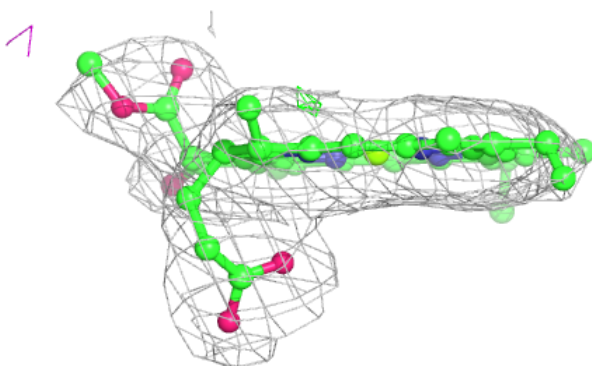
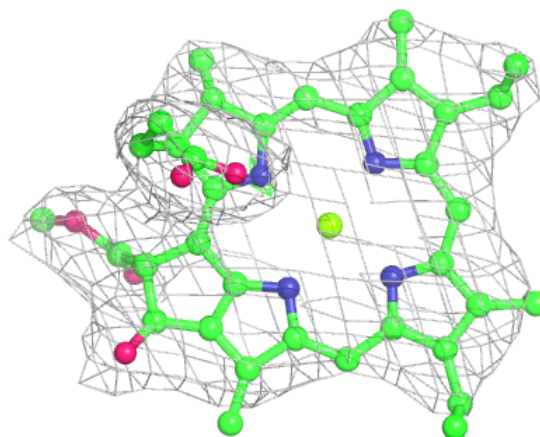
**Electron density around CLA G 820:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

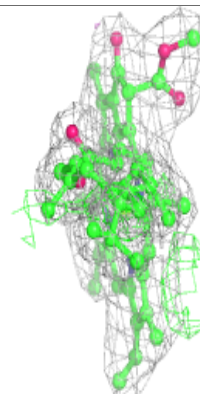
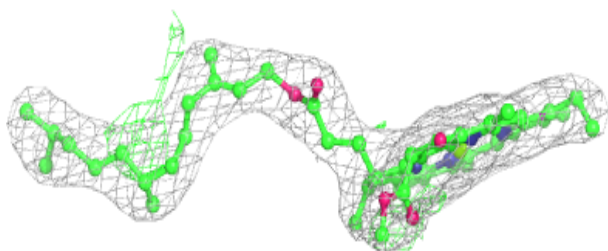
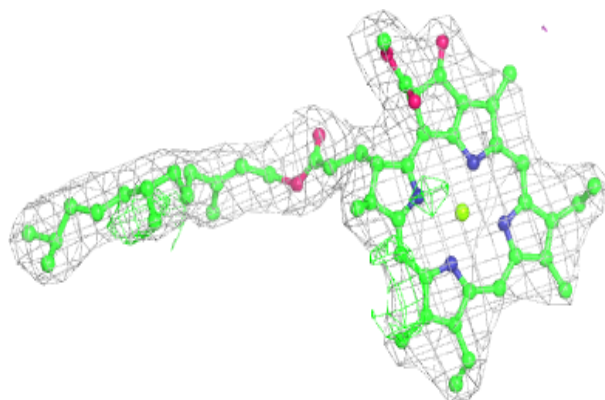


**Electron density around CLA G 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

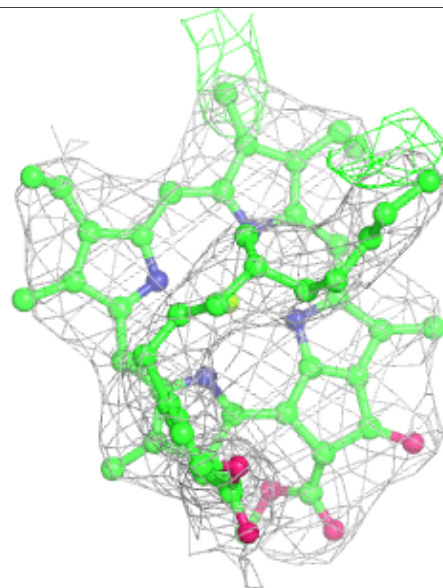
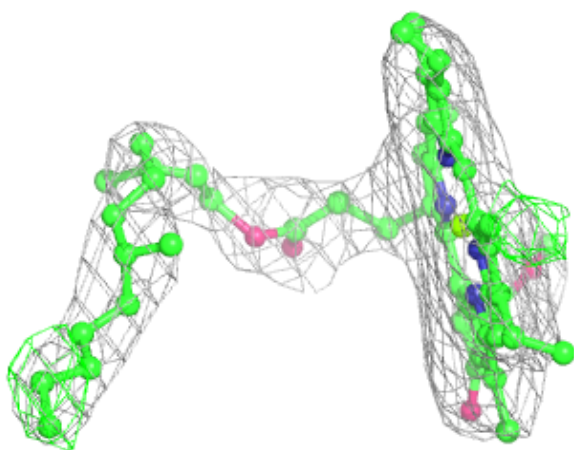
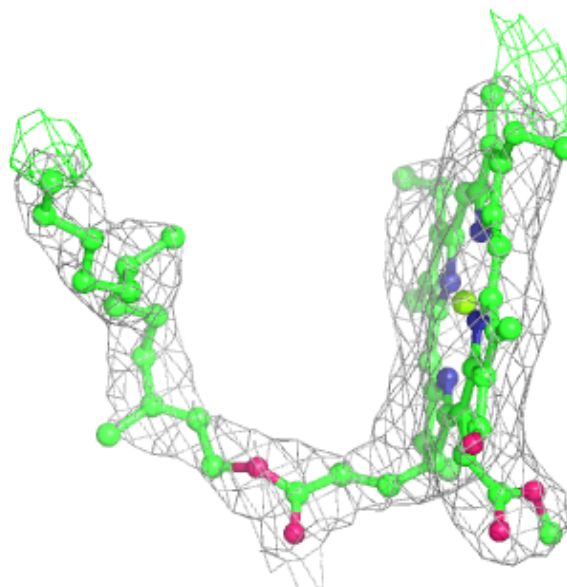
**Electron density around CLA Y 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 804:**

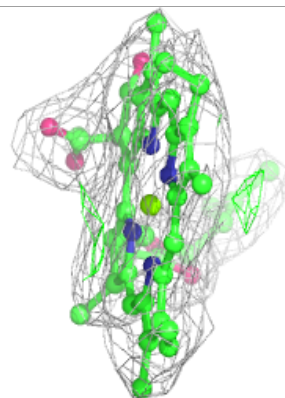
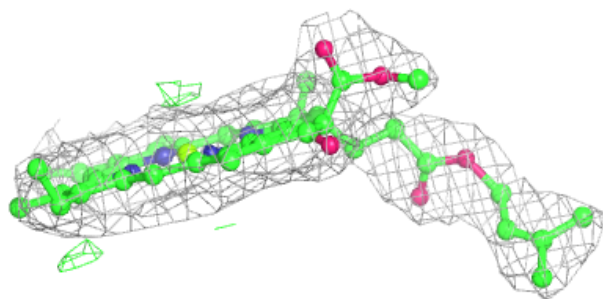
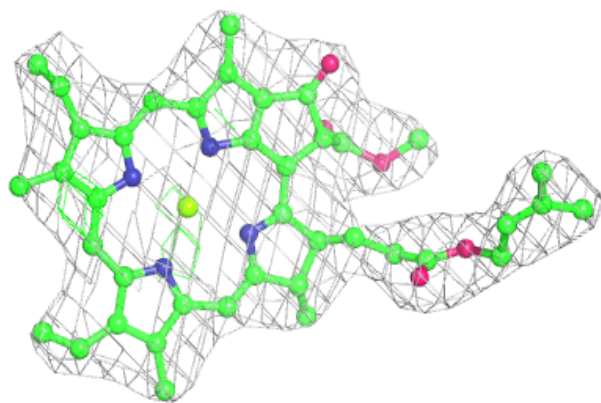
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



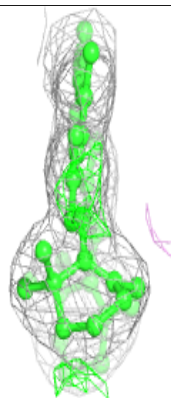
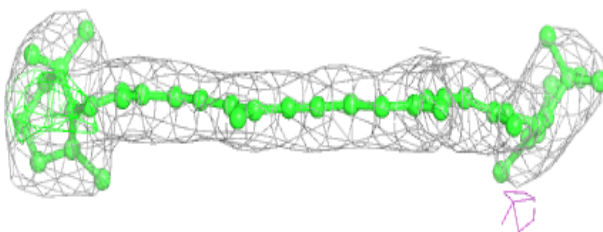
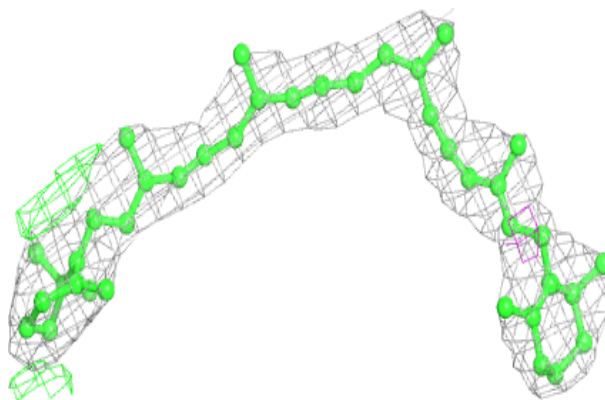


**Electron density around CLA d 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

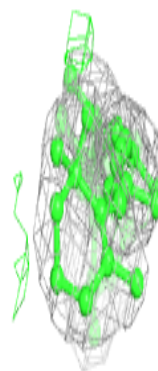
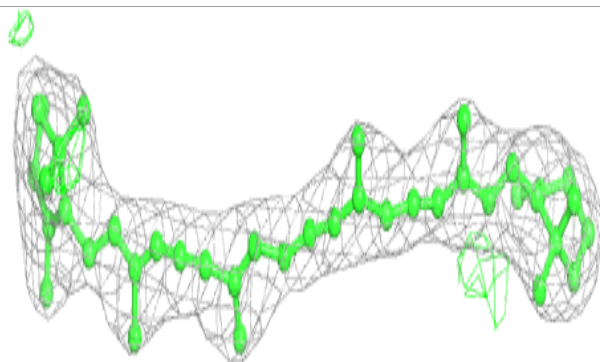
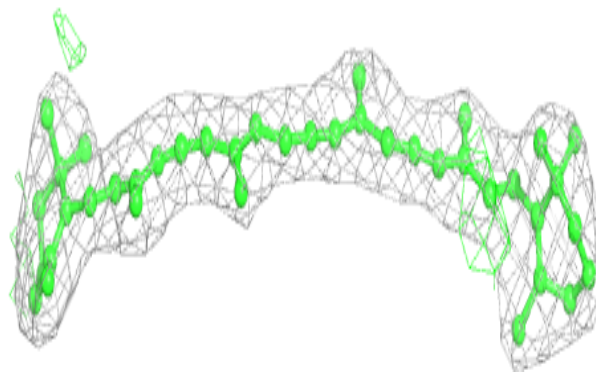
**Electron density around BCR Q 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



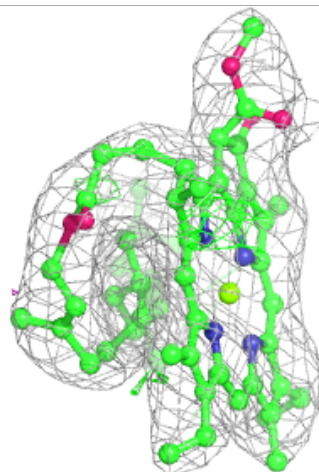
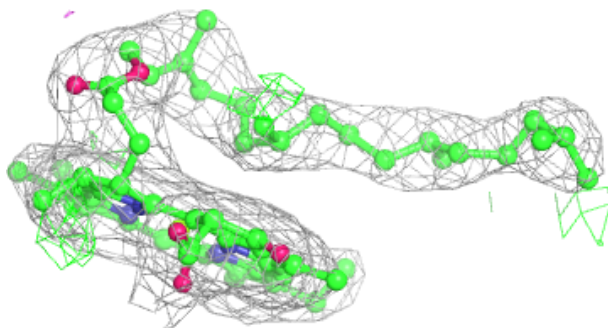
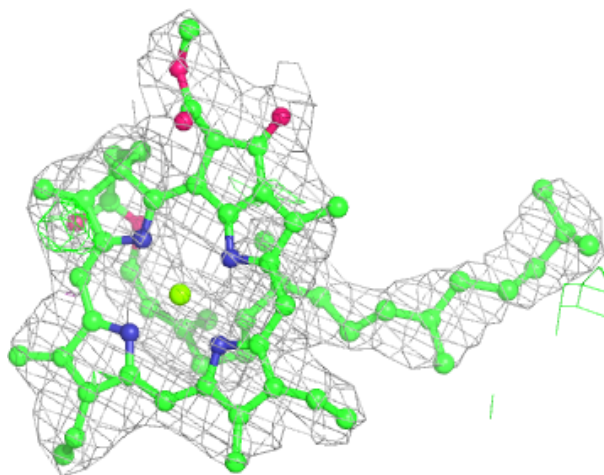
**Electron density around BCR V 1202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



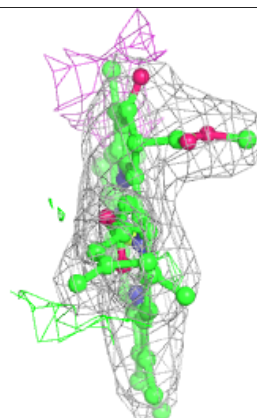
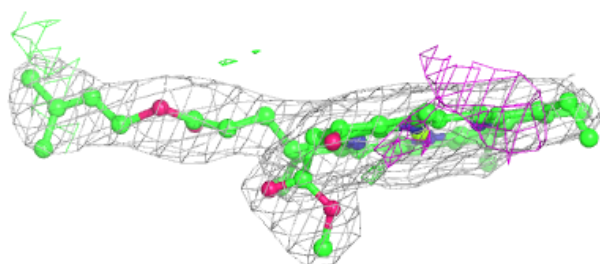
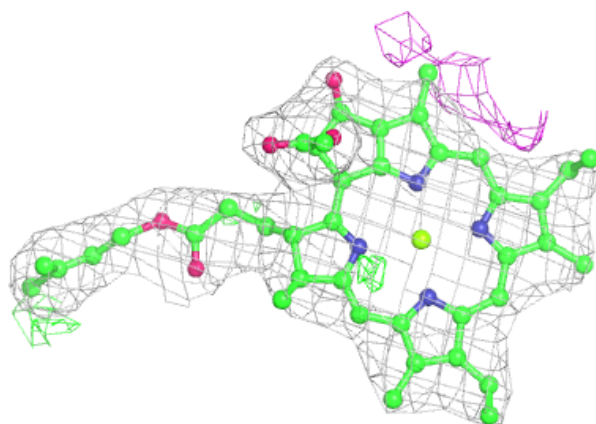
**Electron density around CLA Z 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 837:**

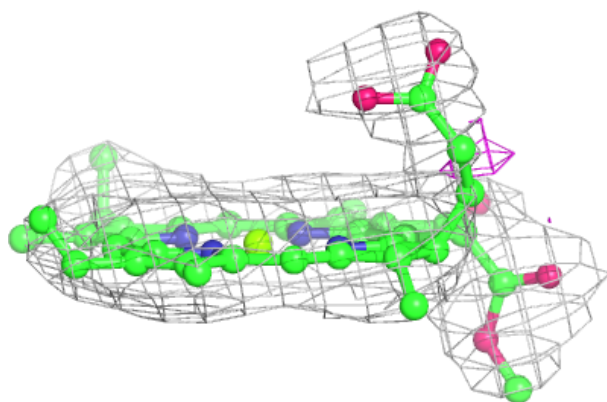
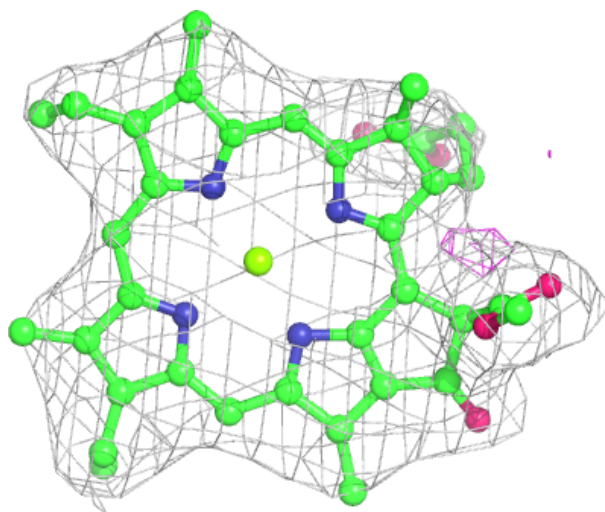
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





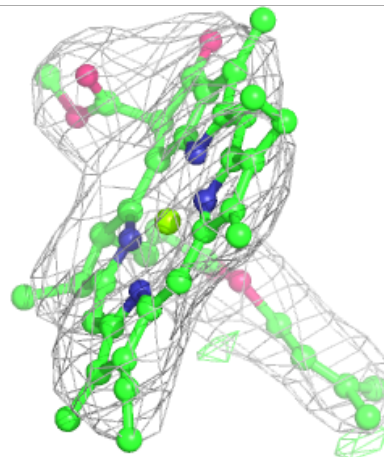
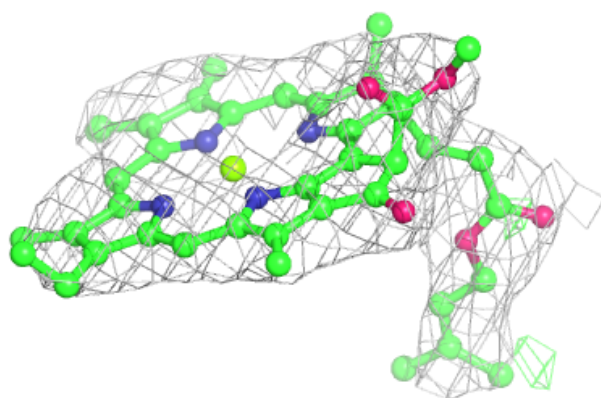
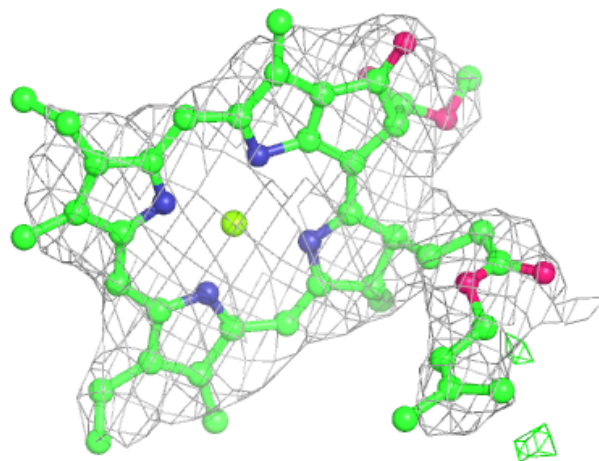
**Electron density around CLA Z 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



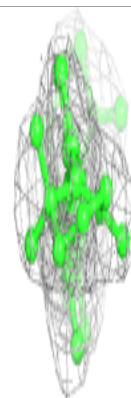
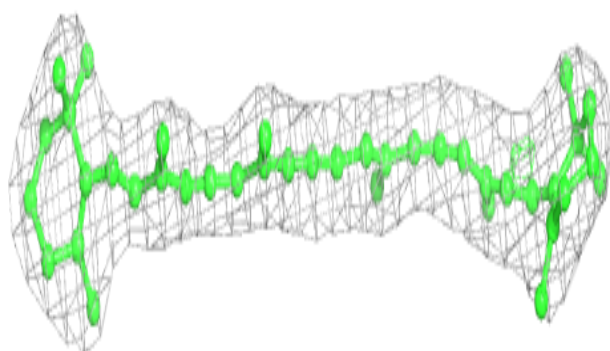
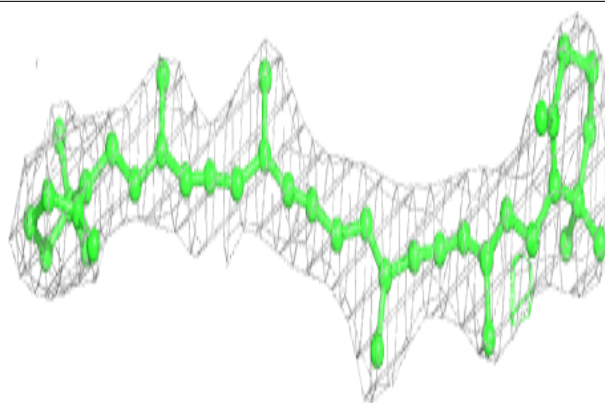
**Electron density around CLA A 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

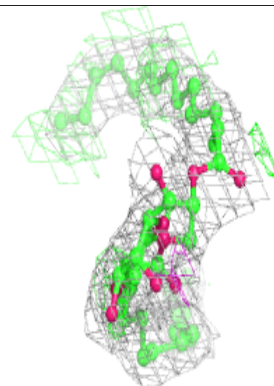
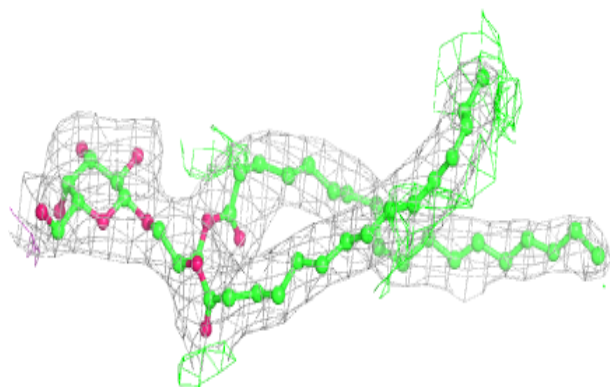
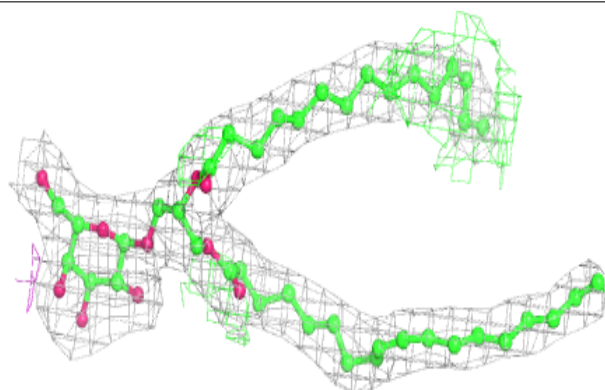


**Electron density around BCR U 1008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

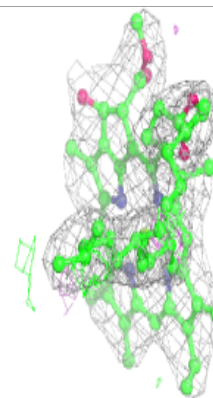
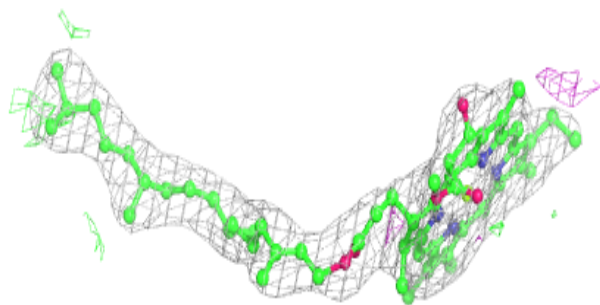
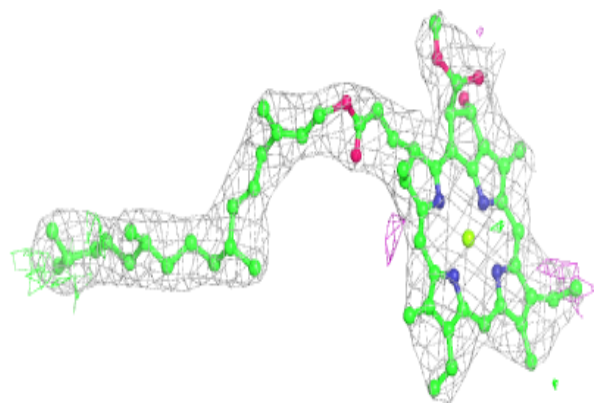
**Electron density around LMG B 849:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

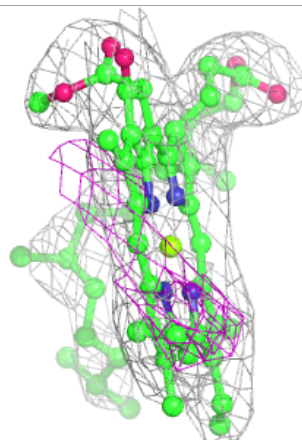
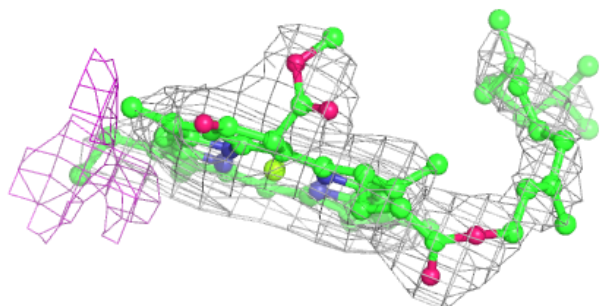
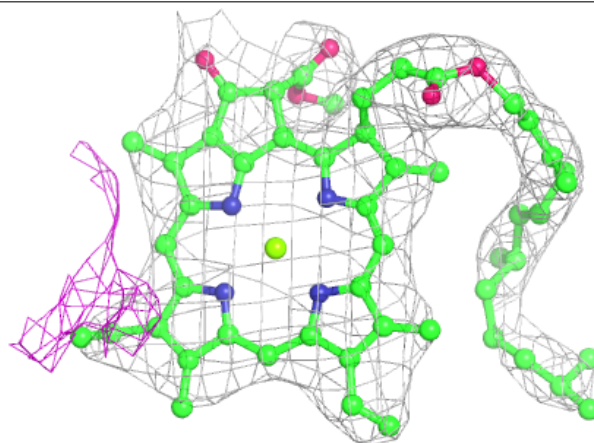


**Electron density around CLA G 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

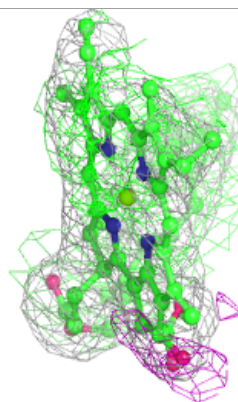
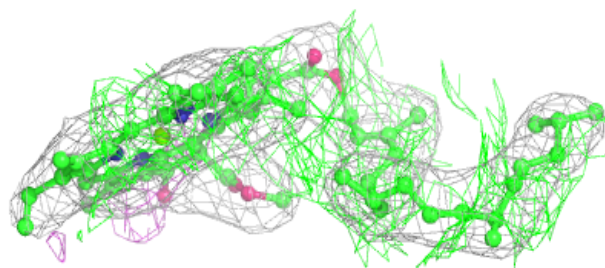
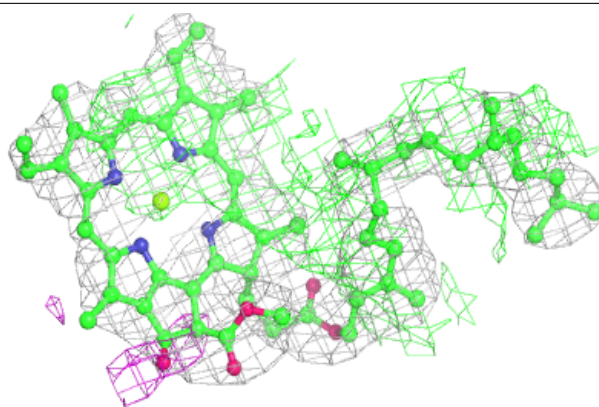
**Electron density around CLA Y 813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

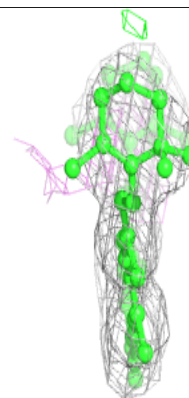
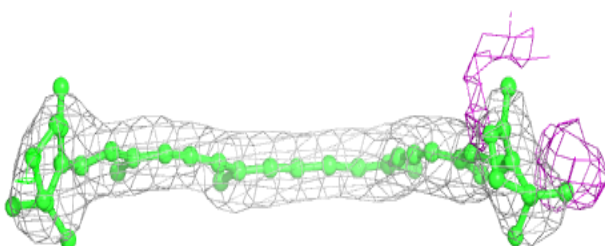
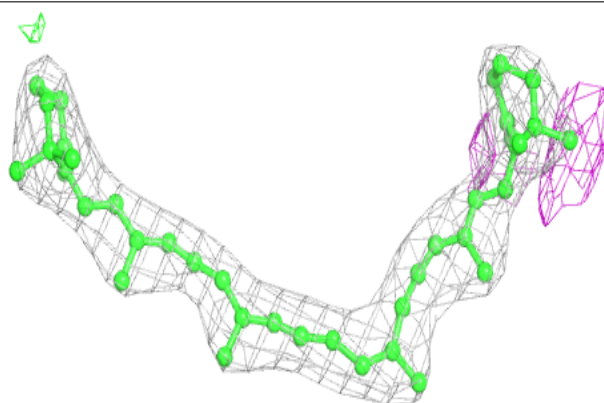


**Electron density around CLA S 1101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR F 203:**

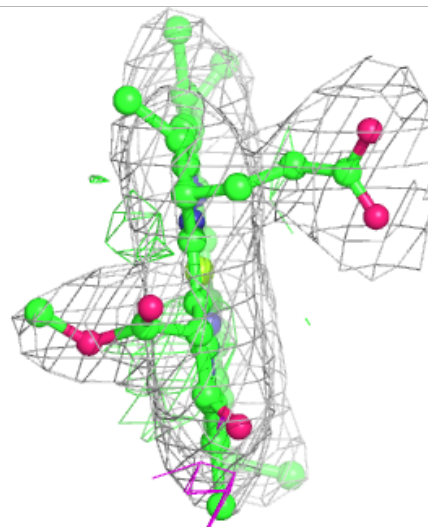
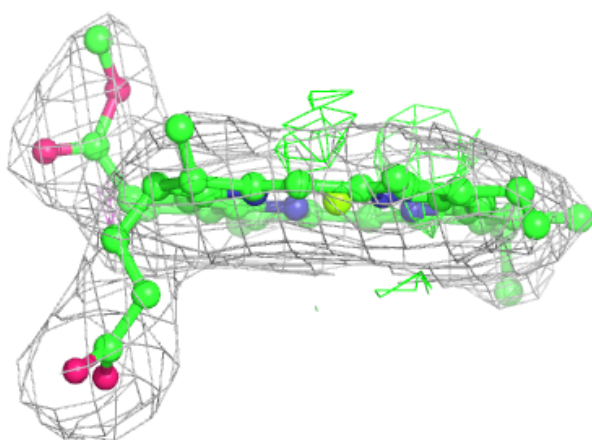
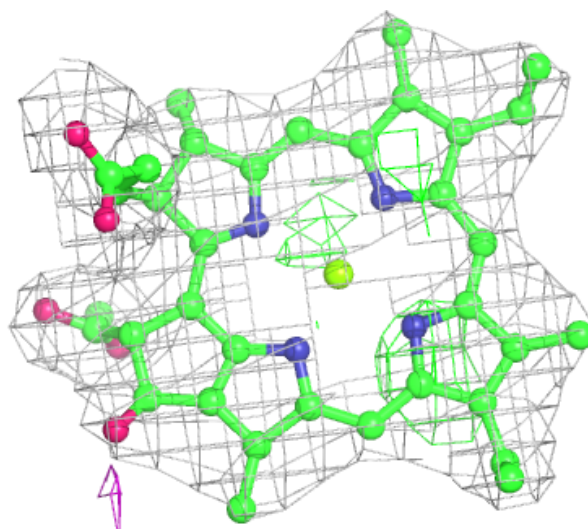
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





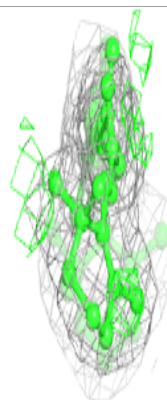
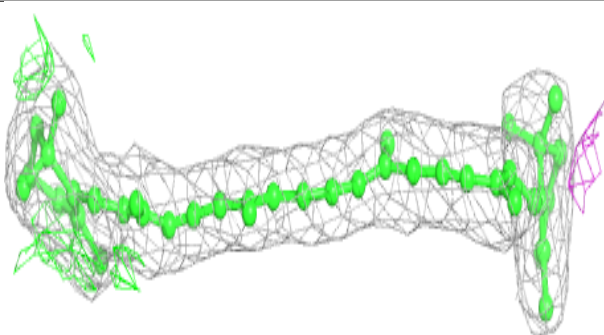
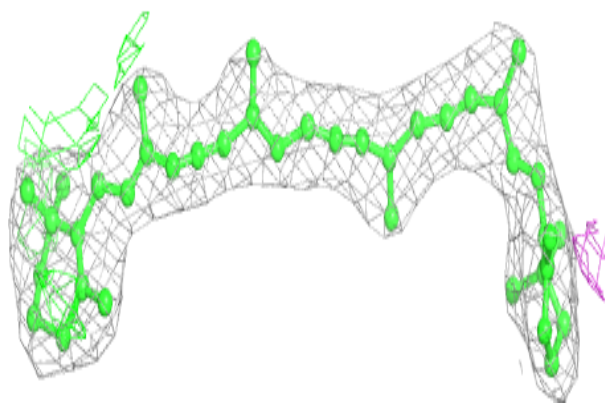
**Electron density around CLA B 820:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

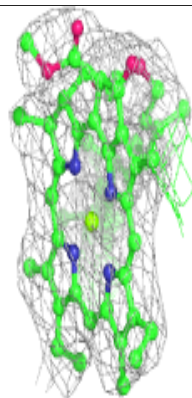
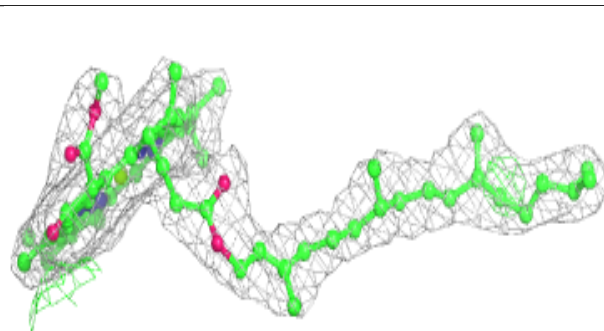
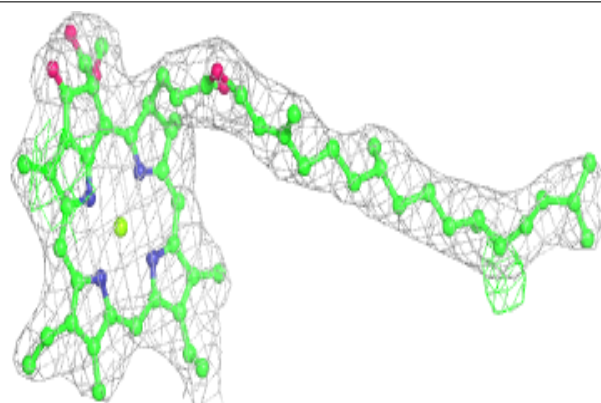


**Electron density around BCR U 1007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

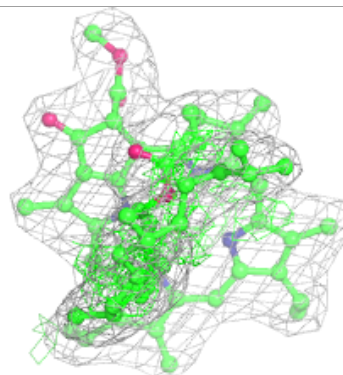
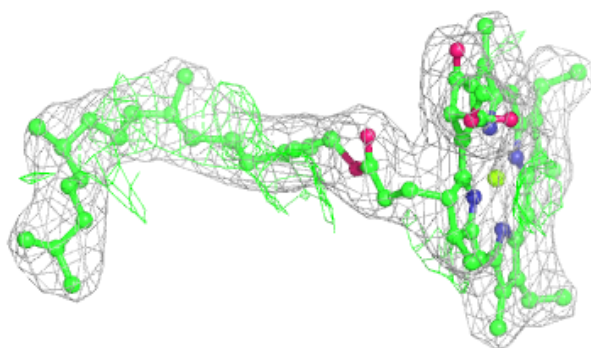
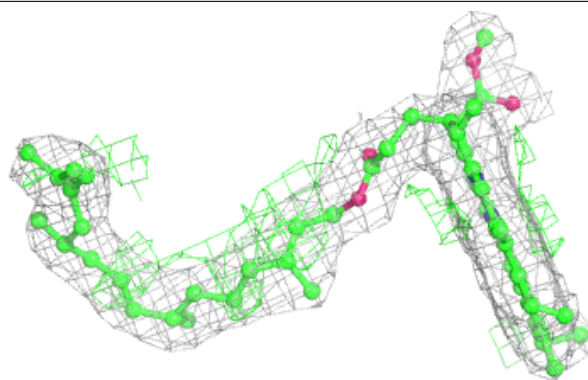
**Electron density around CLA G 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

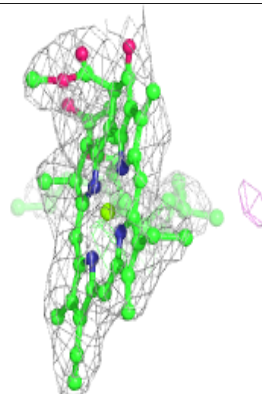
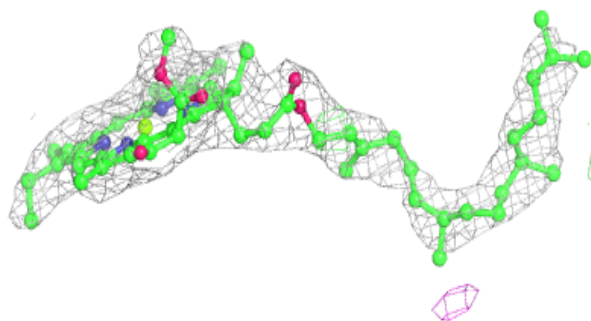
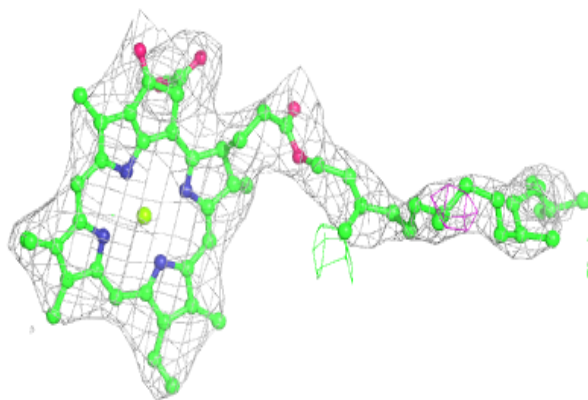


**Electron density around CLA Z 838:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Z 811:**

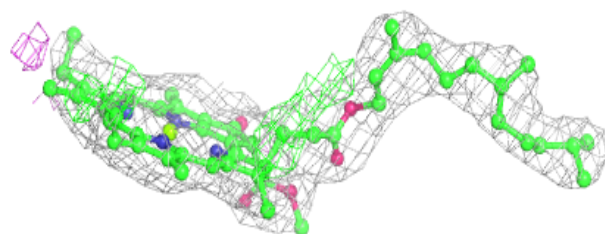
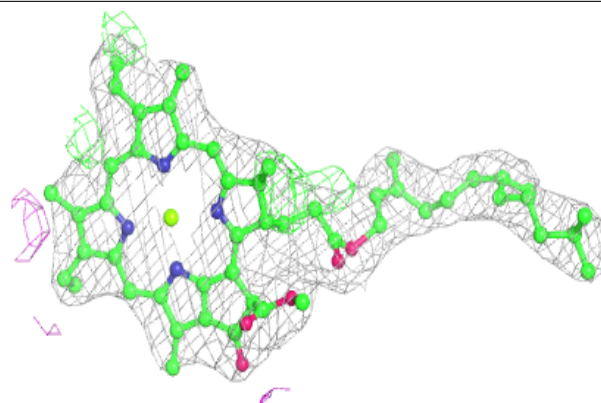
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



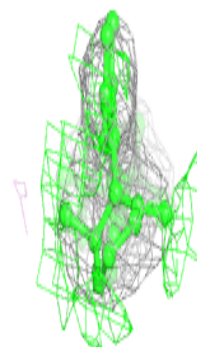
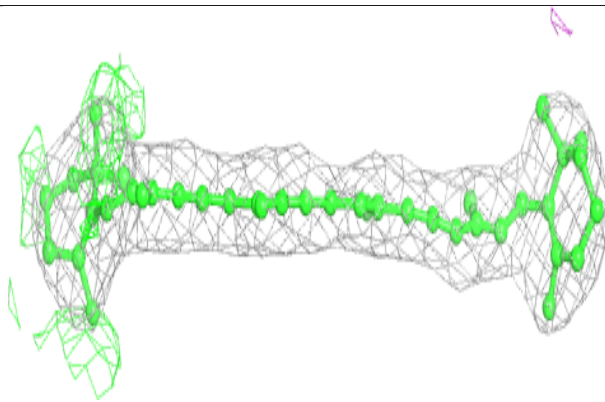
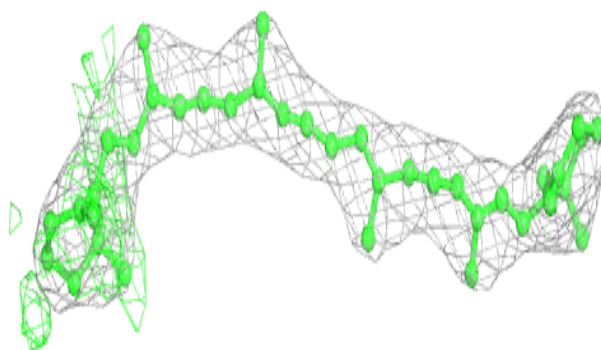


**Electron density around CLA H 822:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

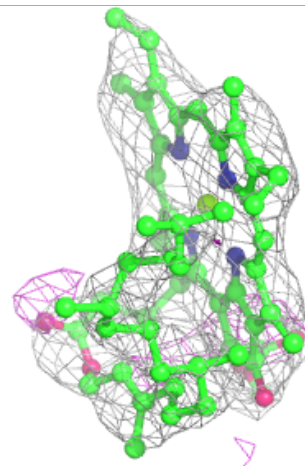
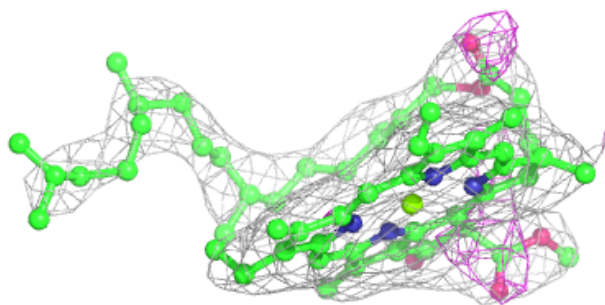
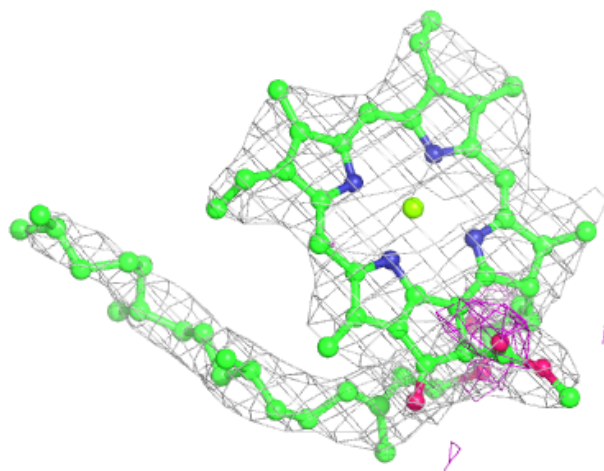
**Electron density around BCR G 848:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



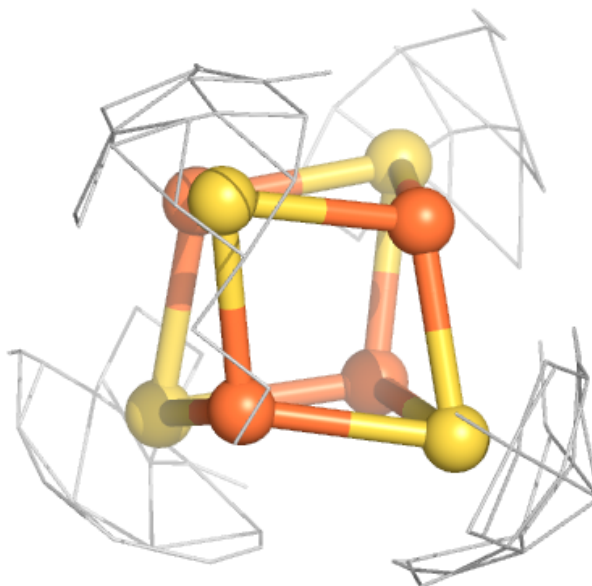
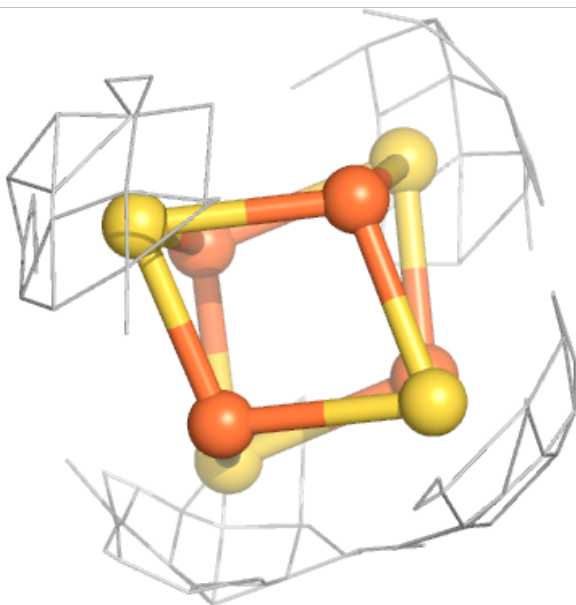
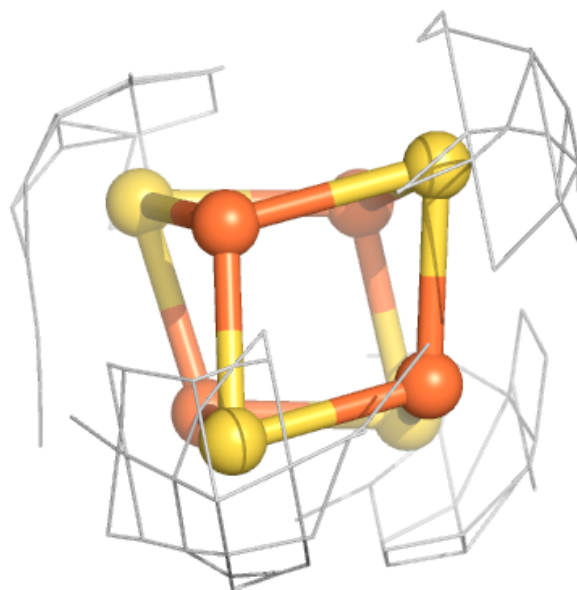
**Electron density around CLA G 829:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



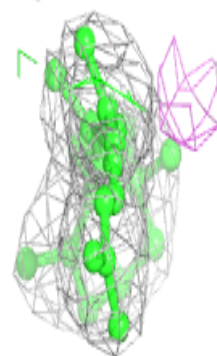
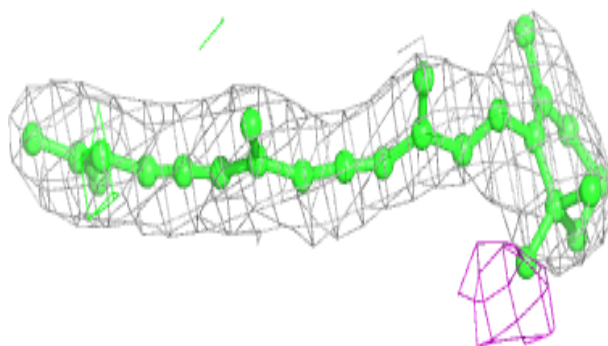
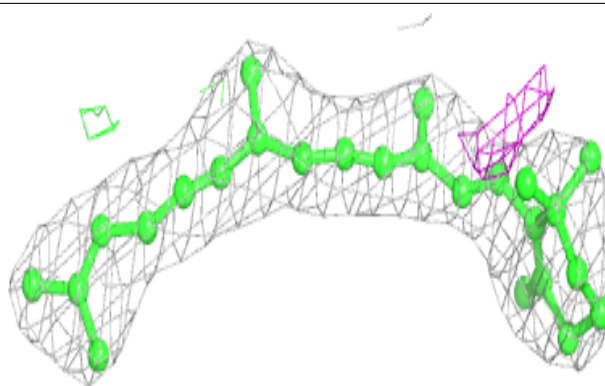
**Electron density around SF4 C 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

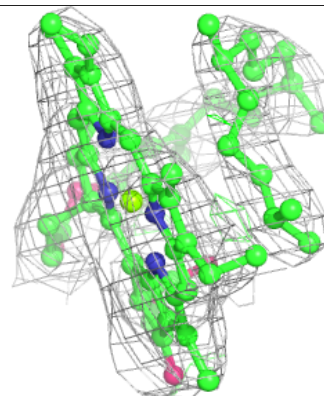
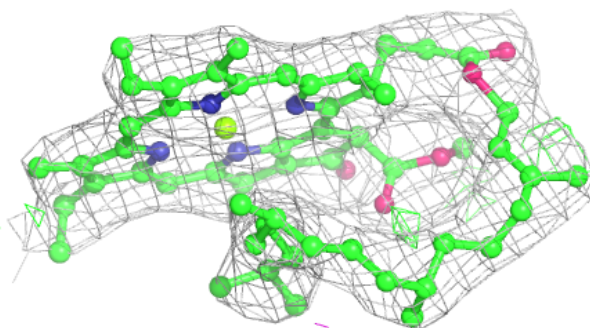
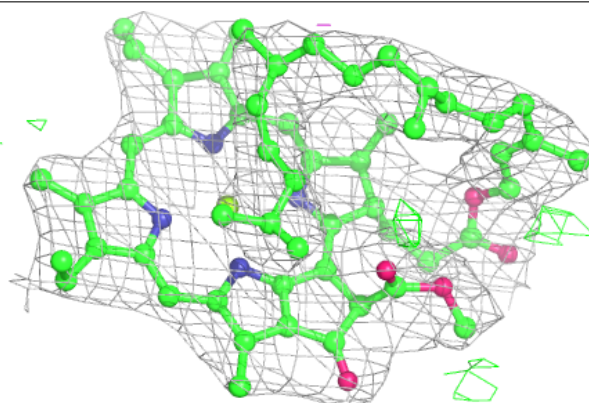


**Electron density around BCR H 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

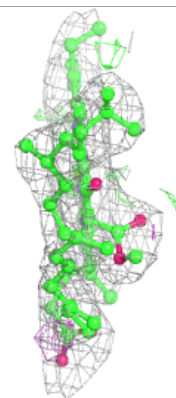
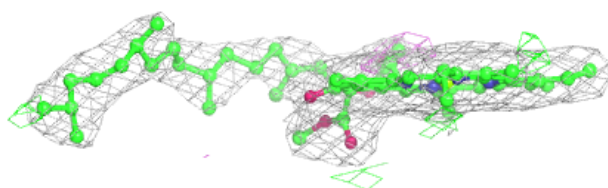
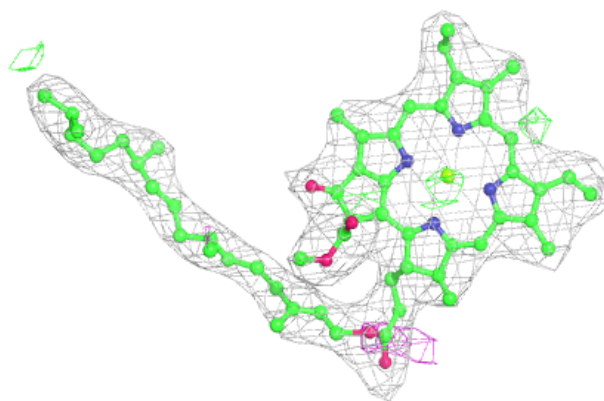
**Electron density around CLA Y 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

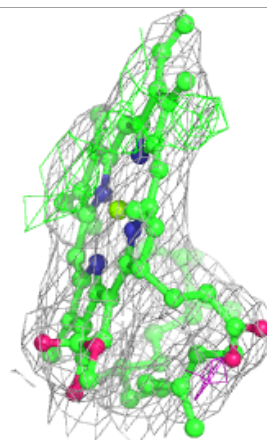
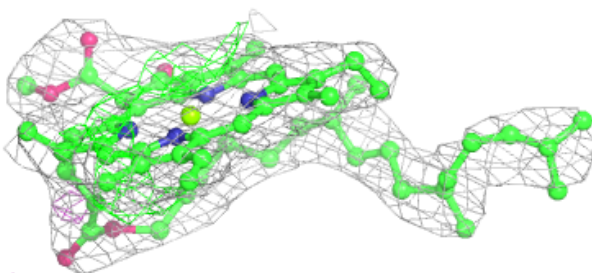
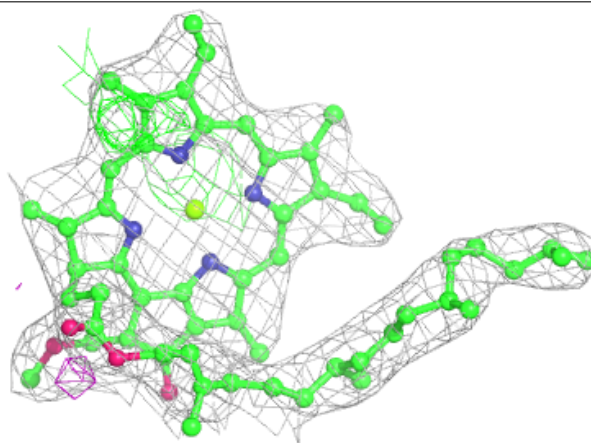


**Electron density around CLA h 207:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Y 829:**

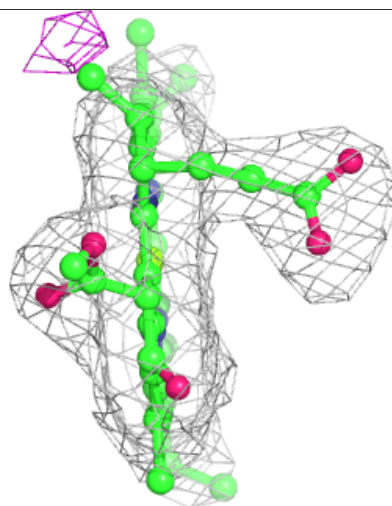
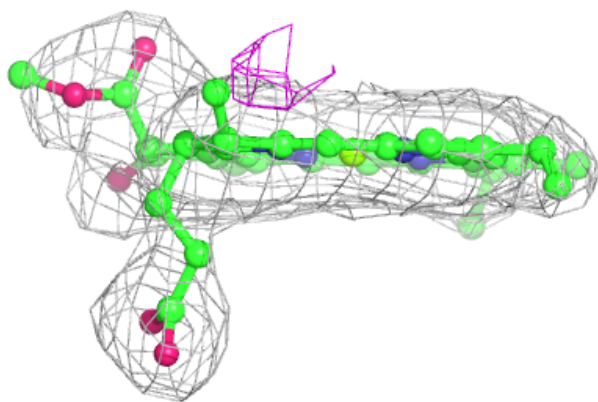
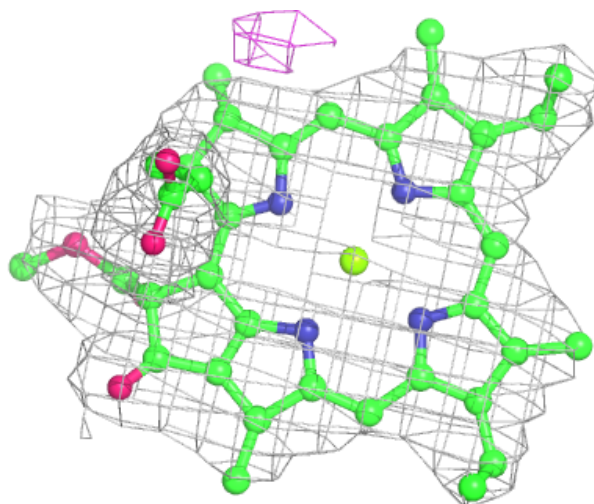
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





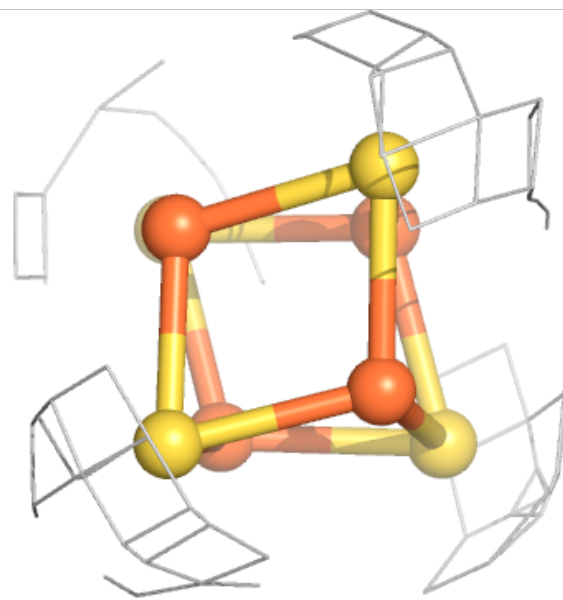
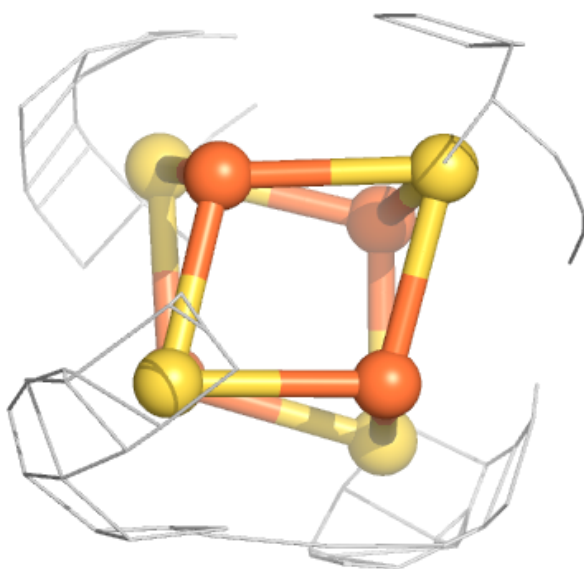
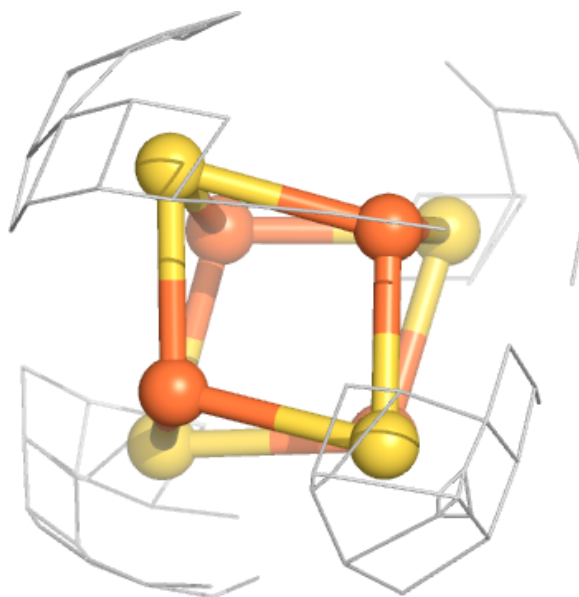
**Electron density around CLA G 853:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



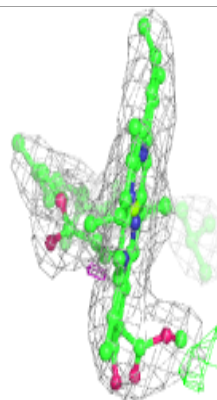
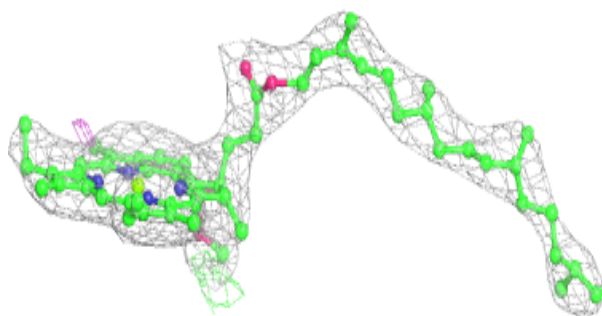
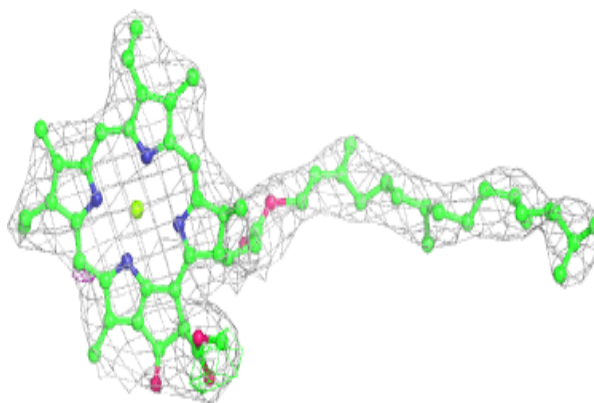
**Electron density around SF4 C 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

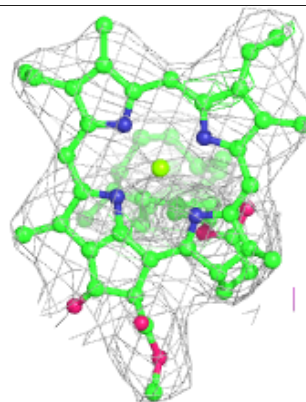
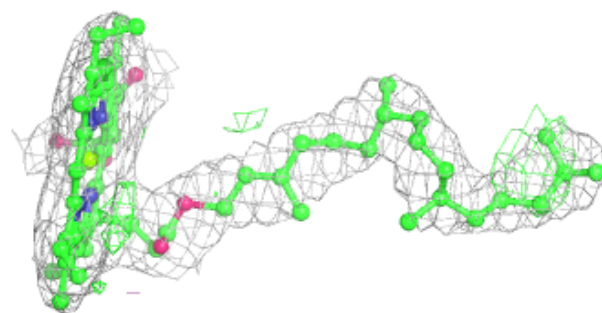
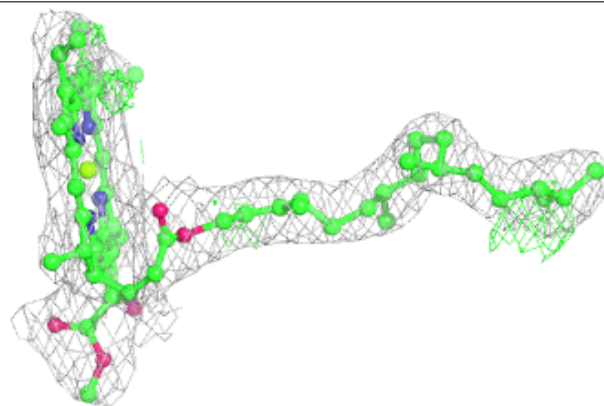


**Electron density around CLA Z 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 828:**

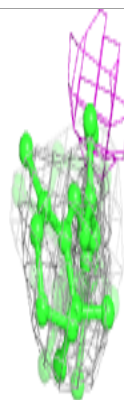
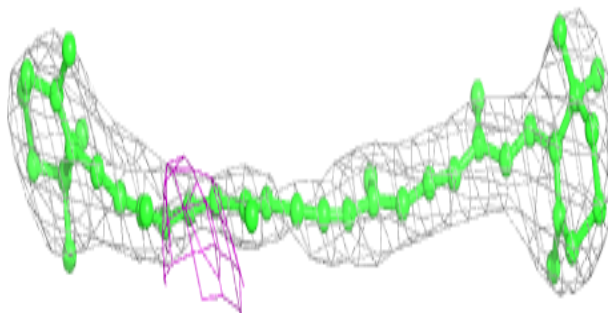
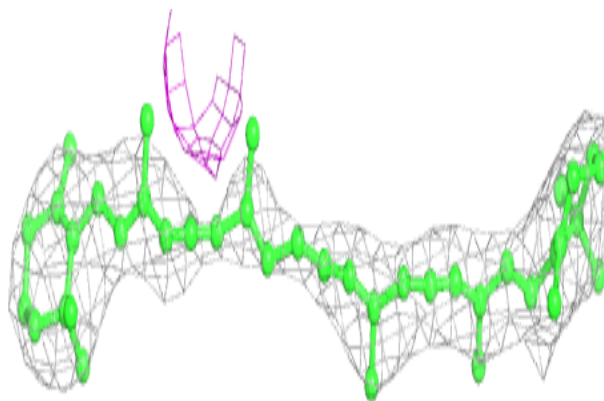
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



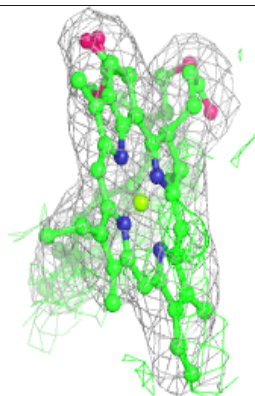
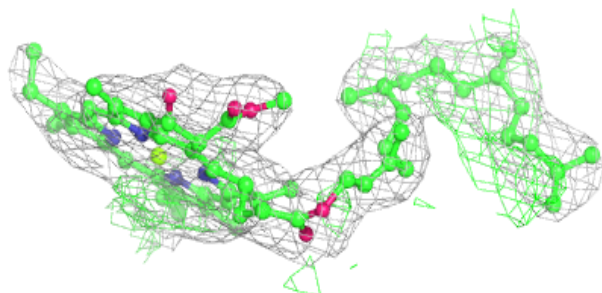
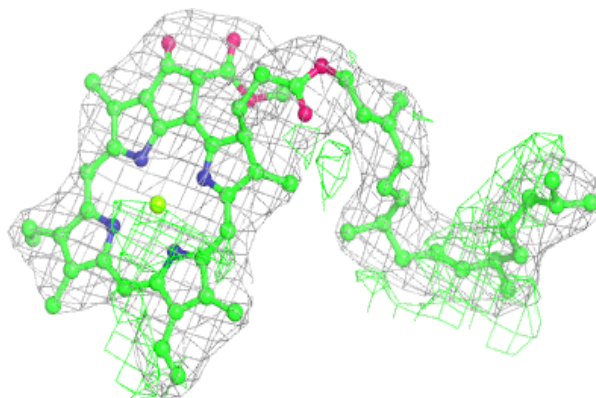


**Electron density around BCR A 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

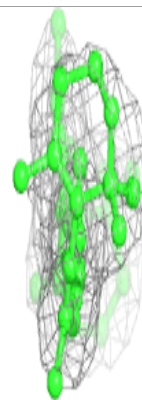
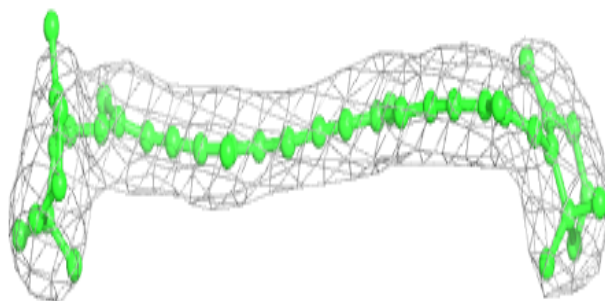
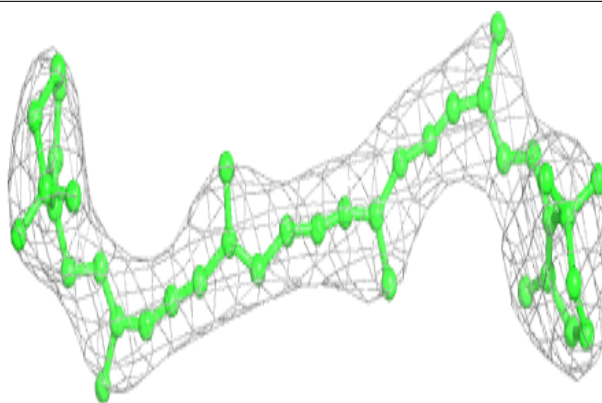
**Electron density around CLA A 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



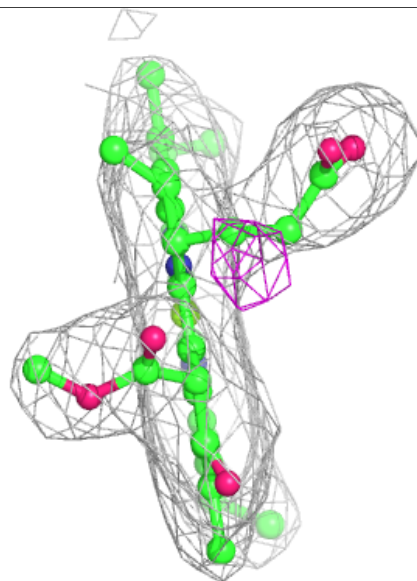
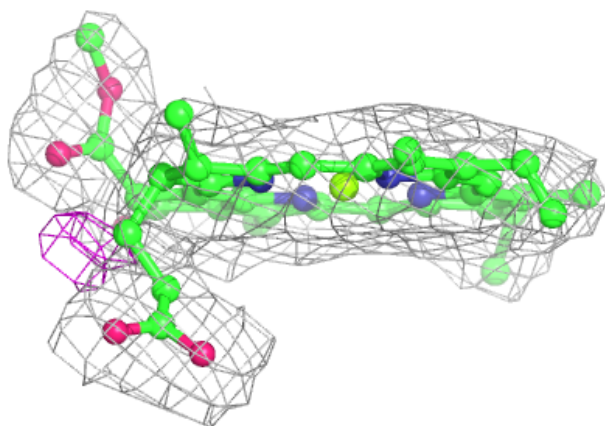
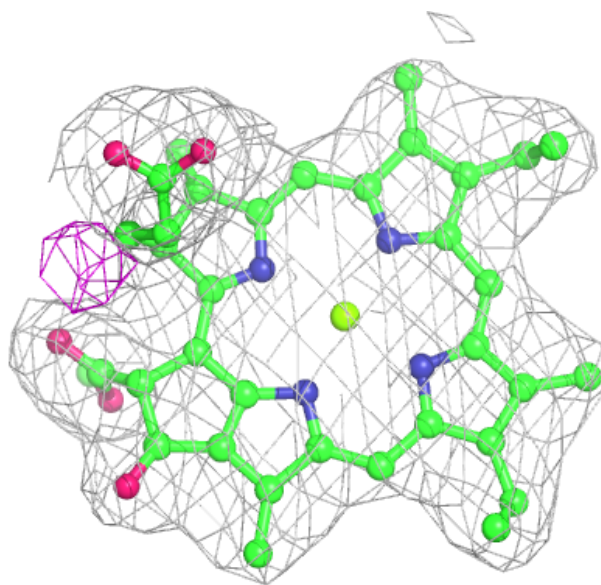
**Electron density around BCR Z 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



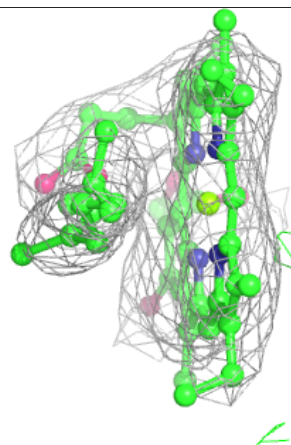
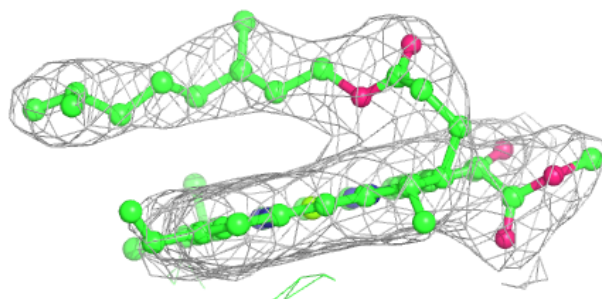
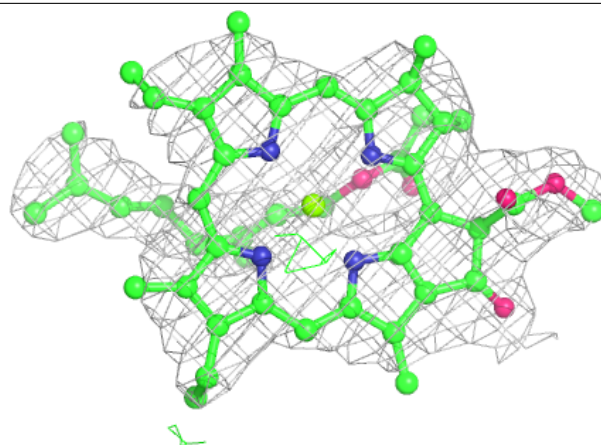
**Electron density around CLA B 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



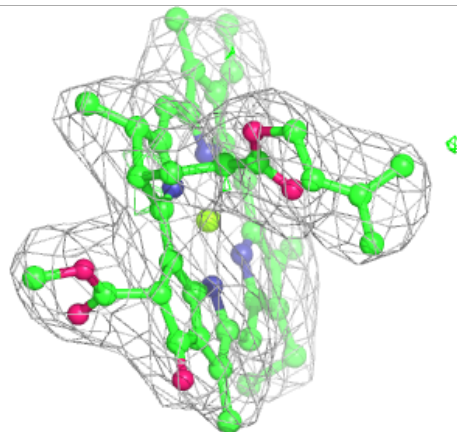
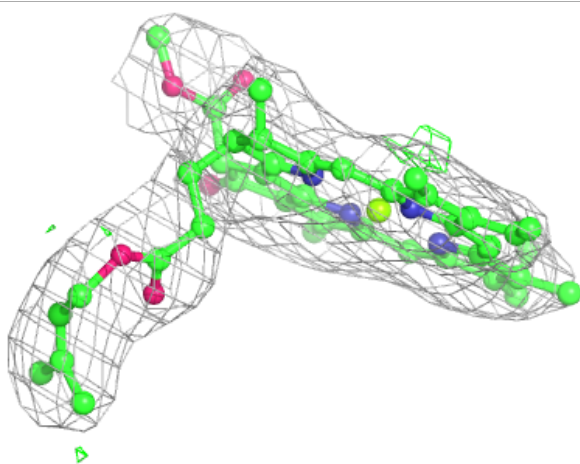
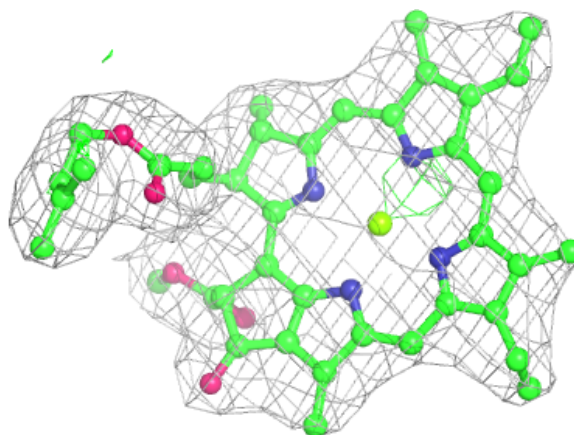
**Electron density around CLA Z 820:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA G 838:**

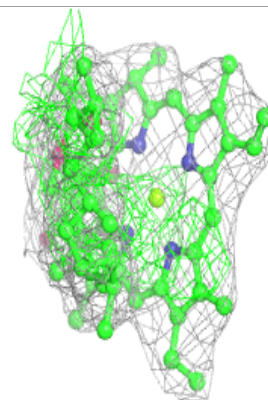
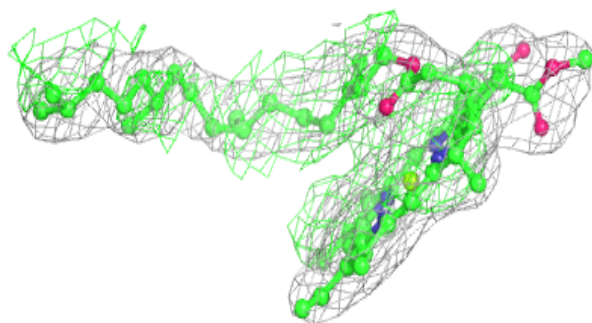
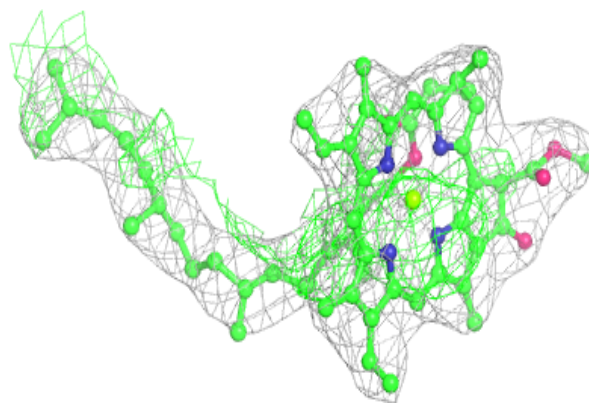
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



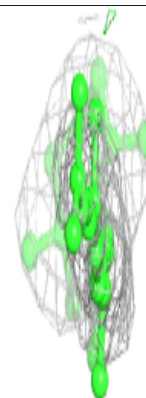
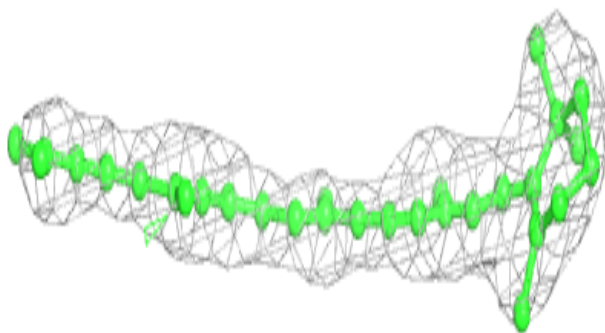
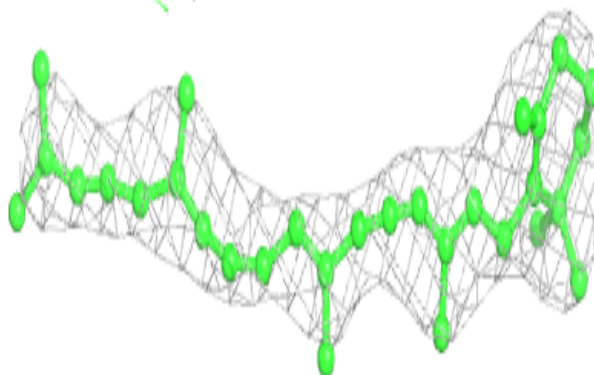


**Electron density around CLA Y 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

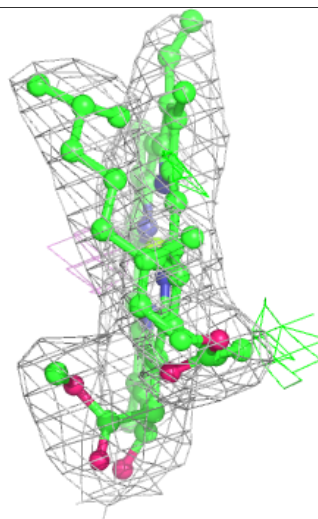
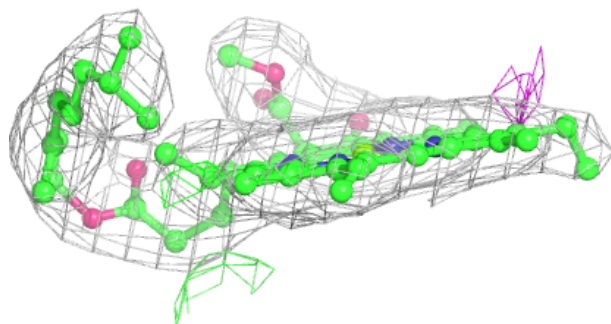
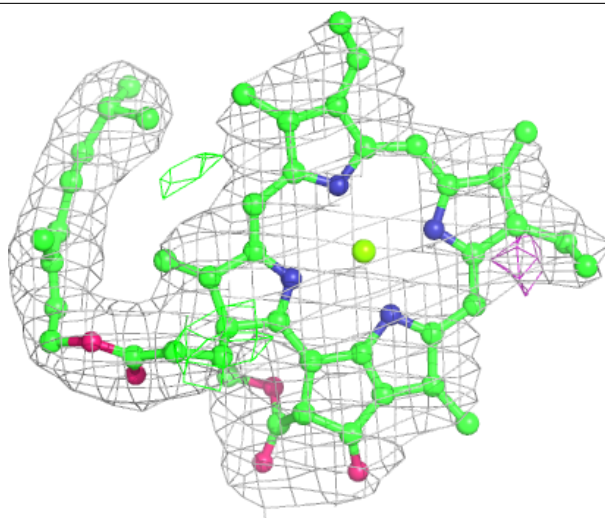
**Electron density around BCR B 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



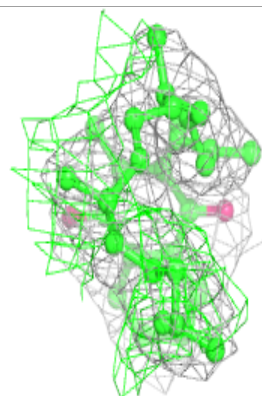
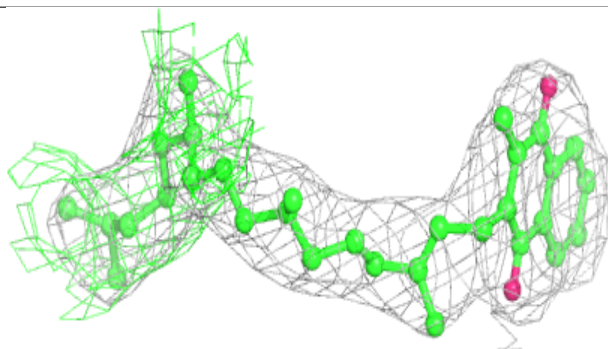
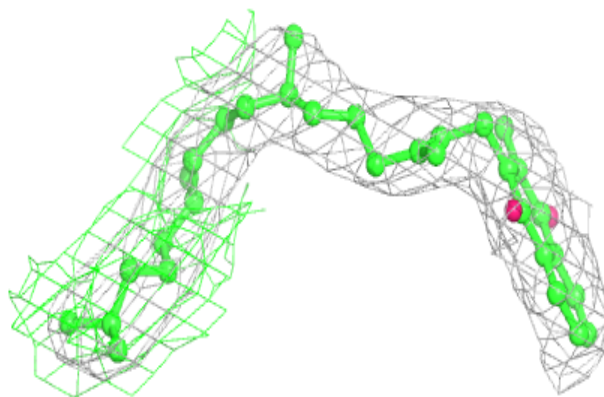
**Electron density around CLA Z 822:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

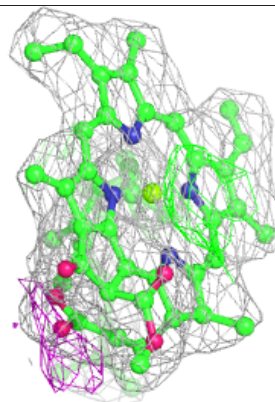
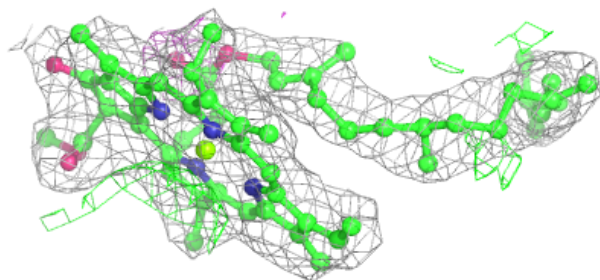
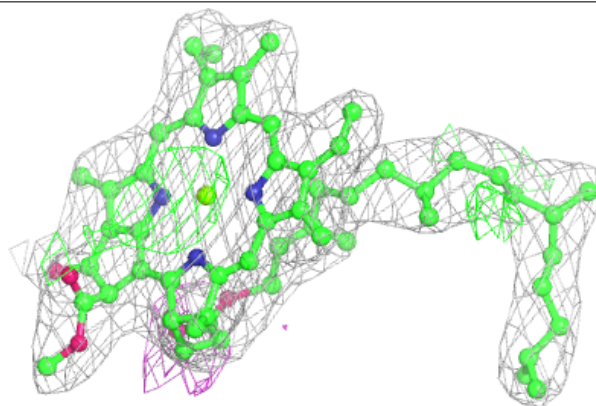


**Electron density around PQN B 842:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA Y 842:**

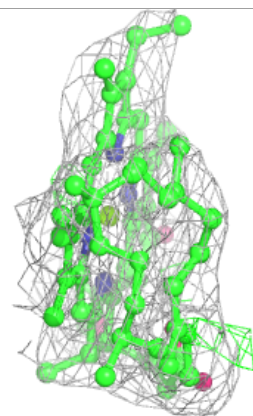
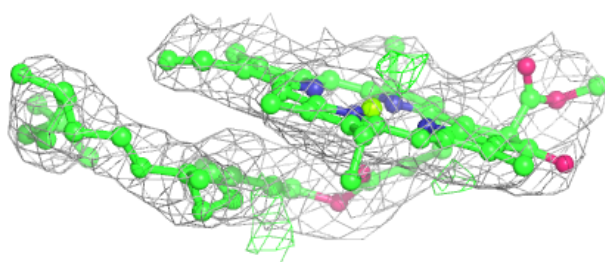
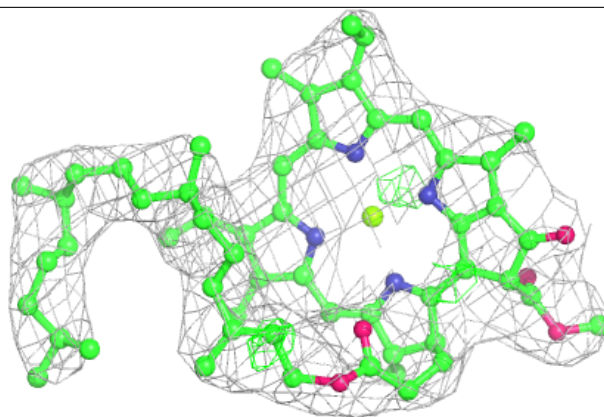
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





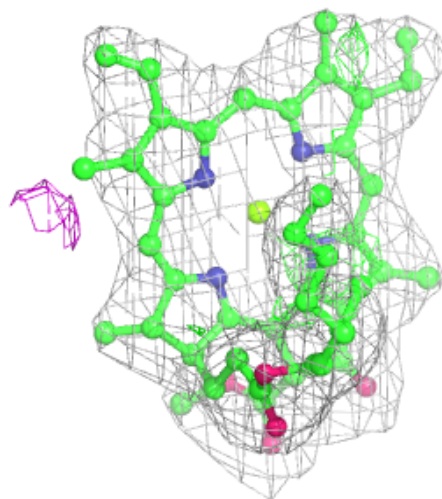
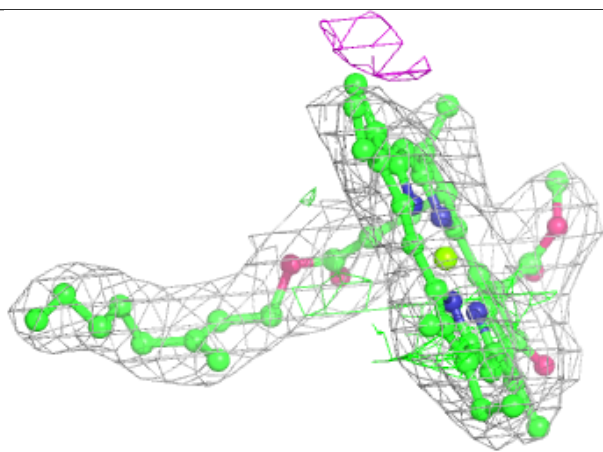
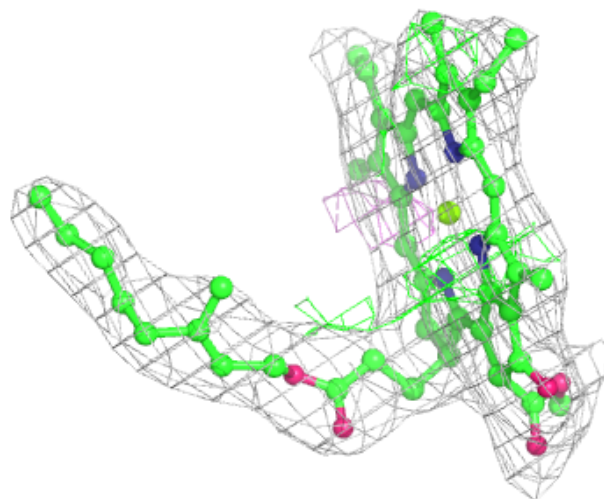
**Electron density around CLA A 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



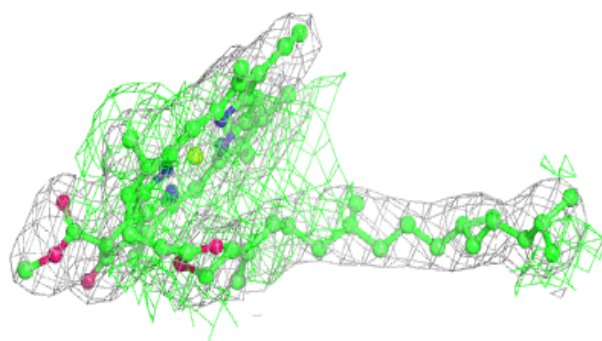
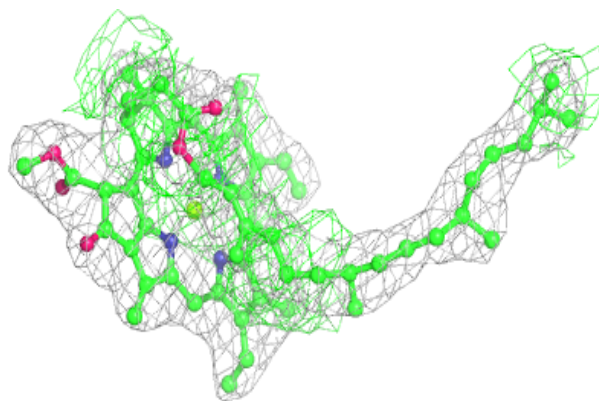
**Electron density around CLA V 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

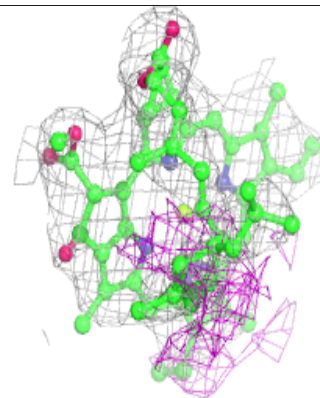
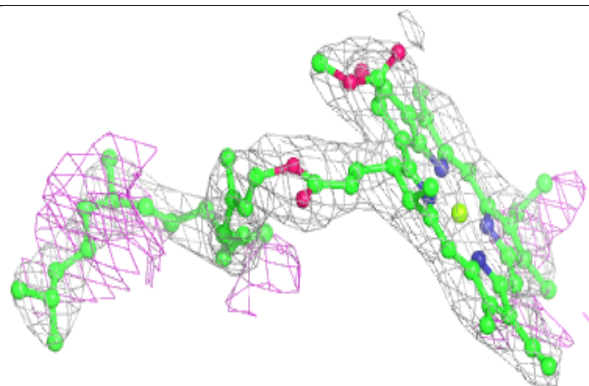
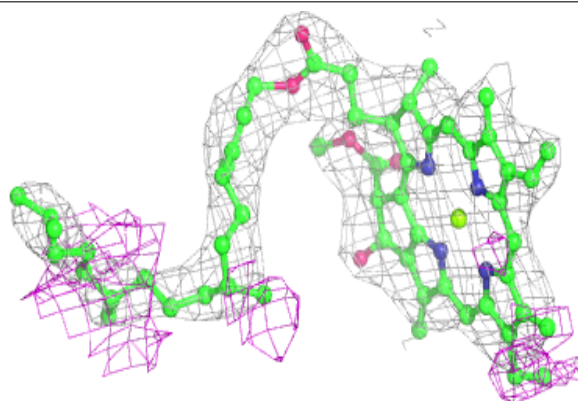


**Electron density around CLA A 840:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

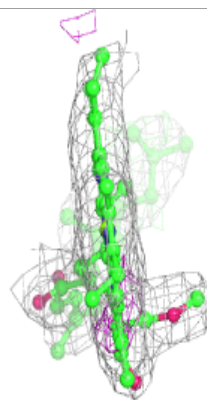
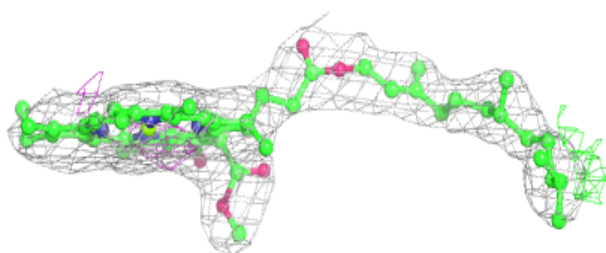
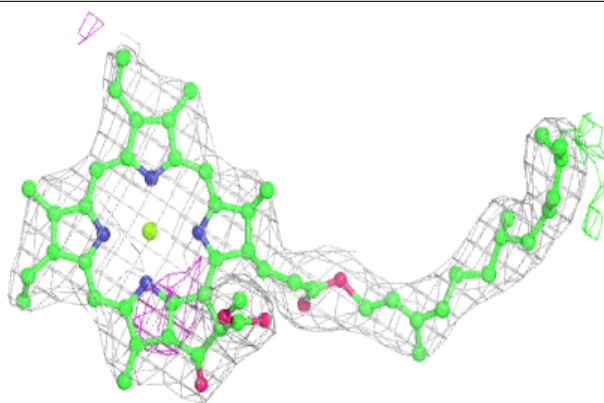
**Electron density around CLA Z 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

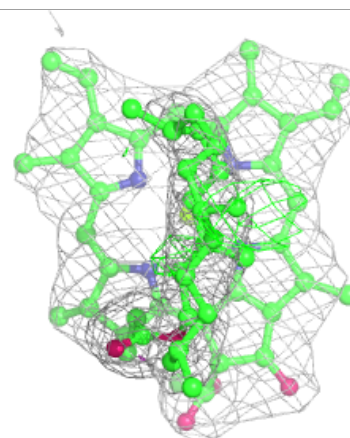
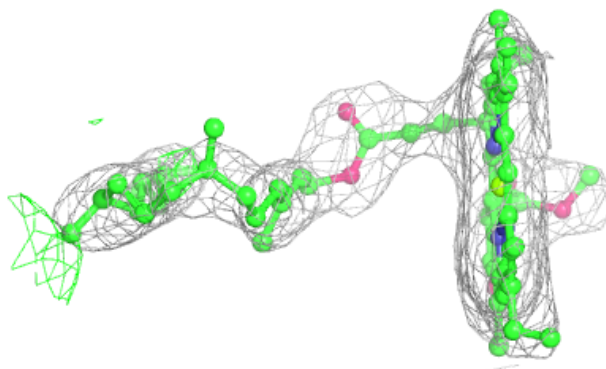
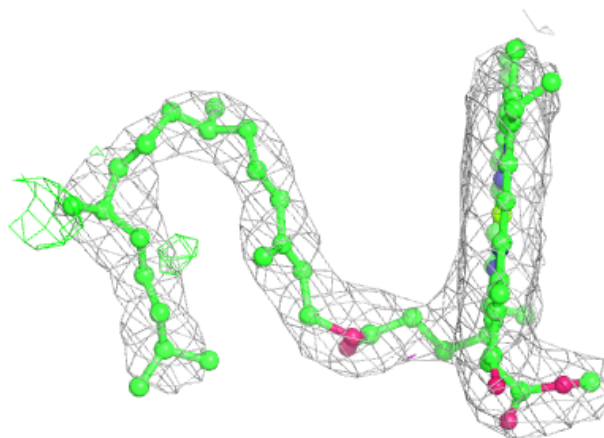


**Electron density around CLA H 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 814:**

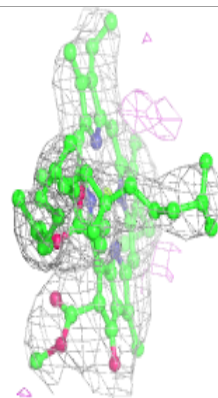
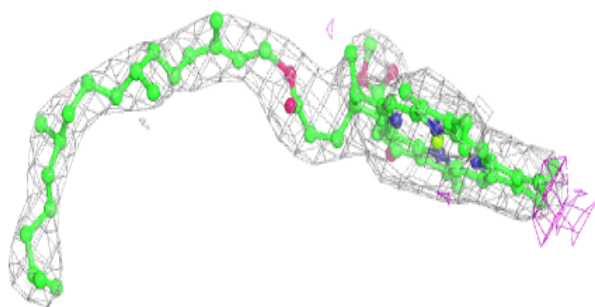
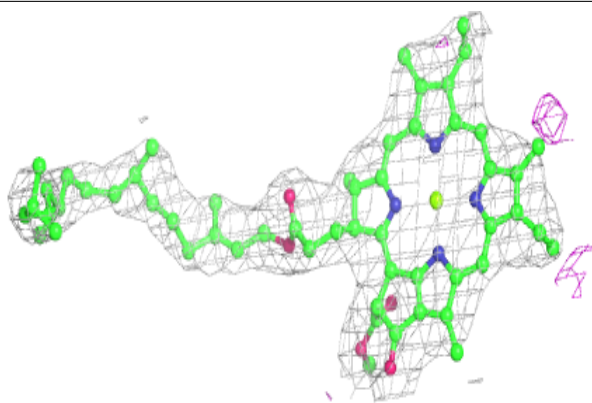
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



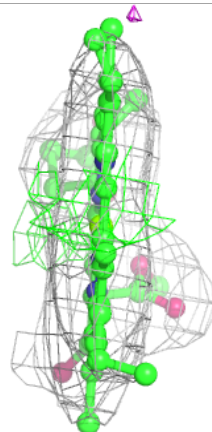
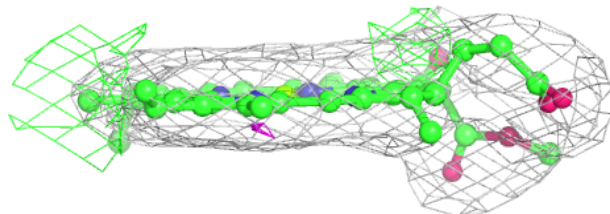
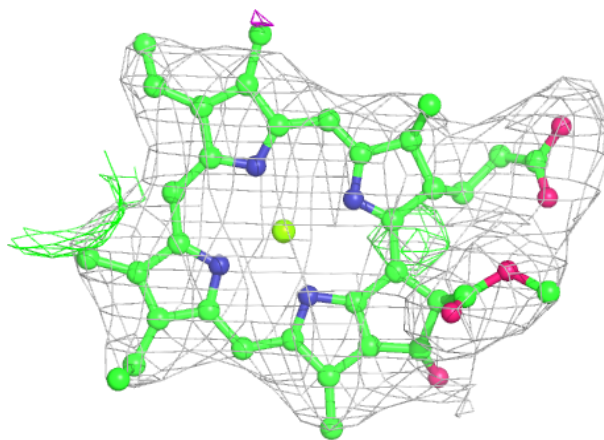


**Electron density around CLA Y 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

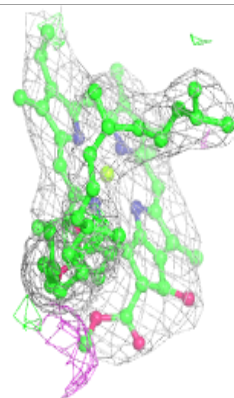
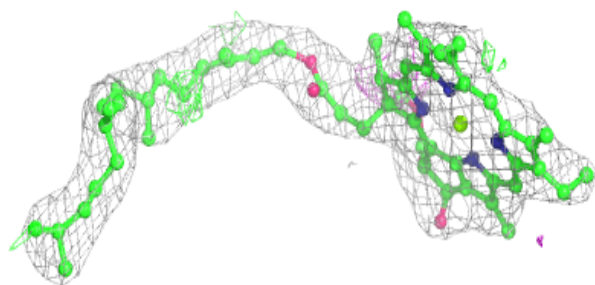
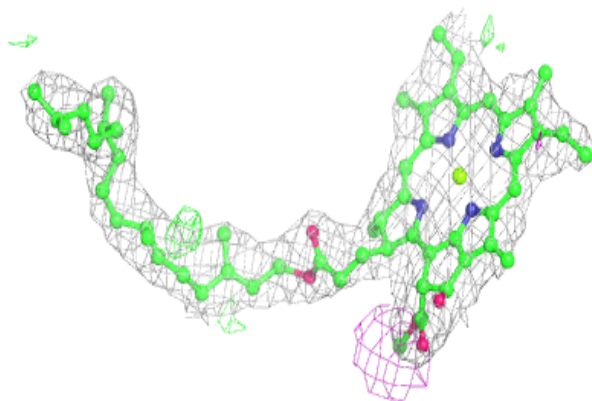
**Electron density around CLA Q 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



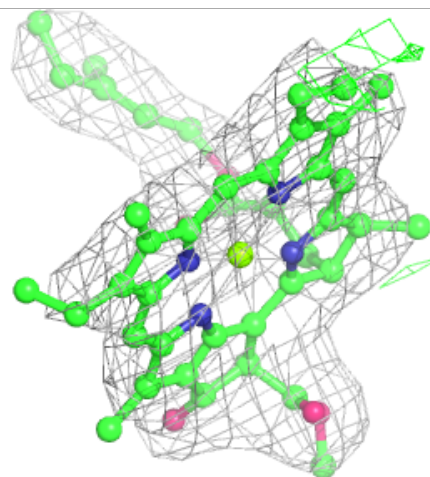
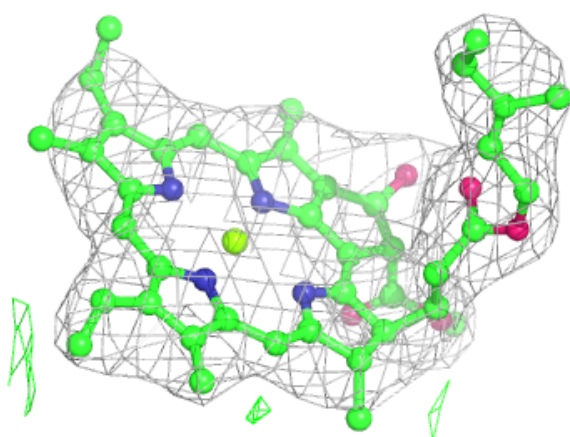
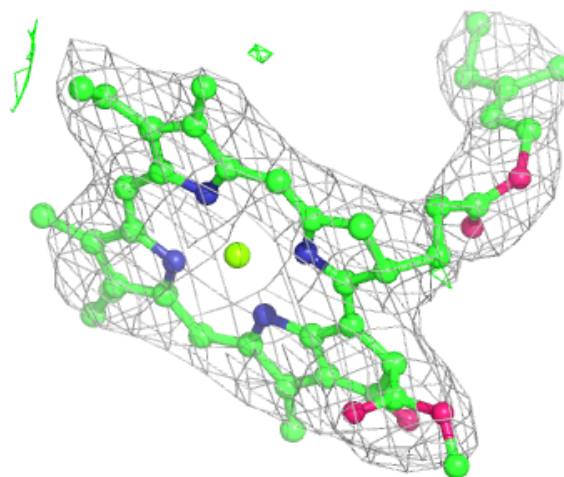
**Electron density around CLA Y 854:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



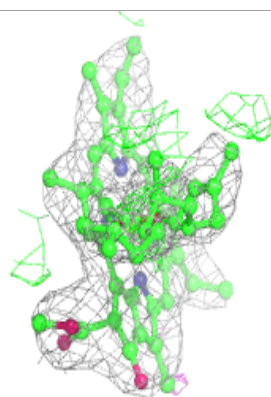
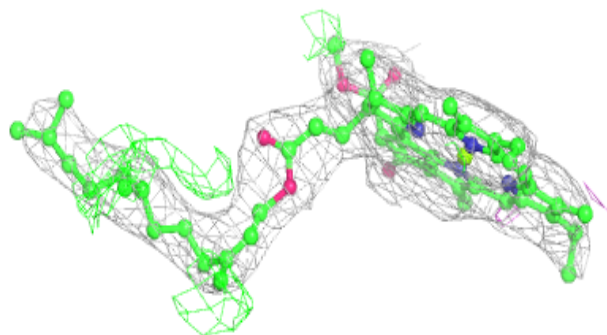
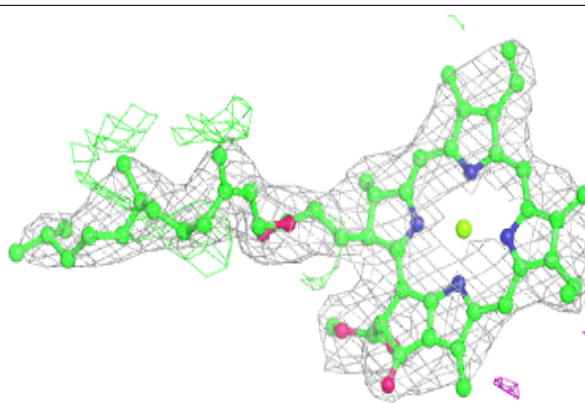
**Electron density around CLA G 807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Z 821:**

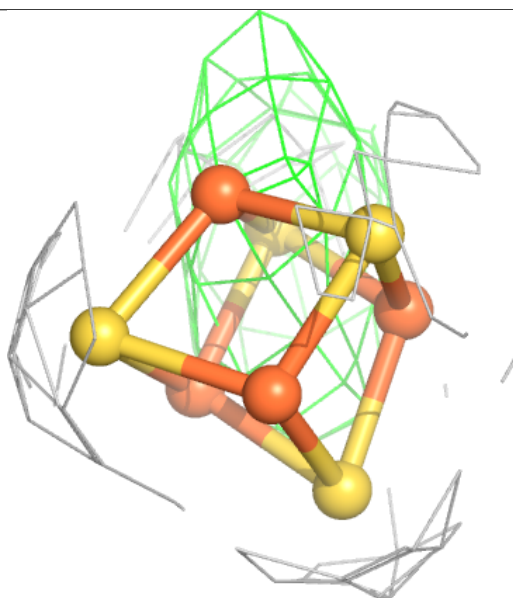
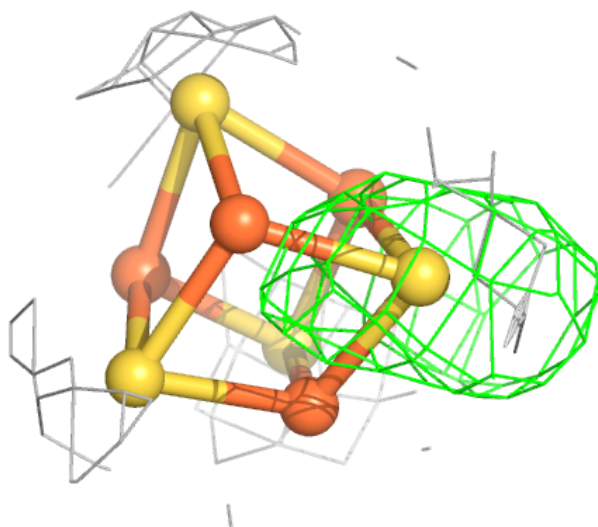
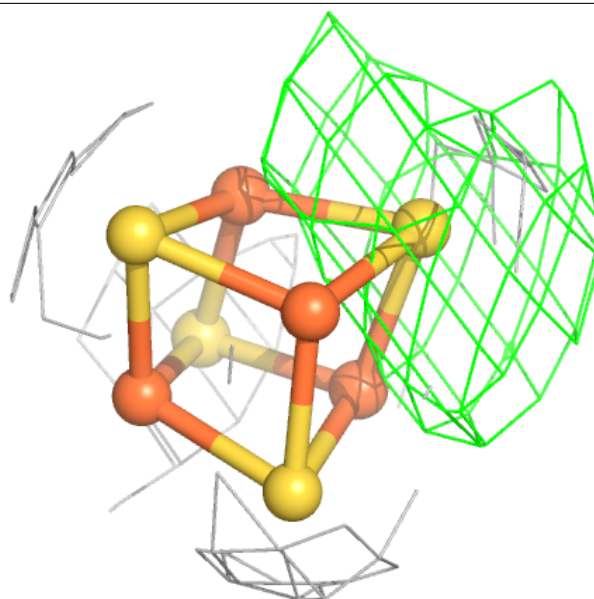
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





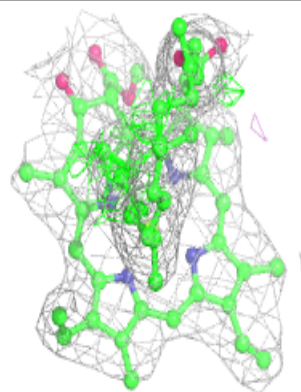
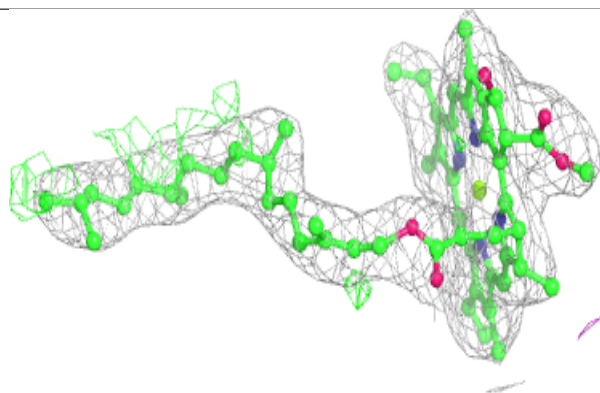
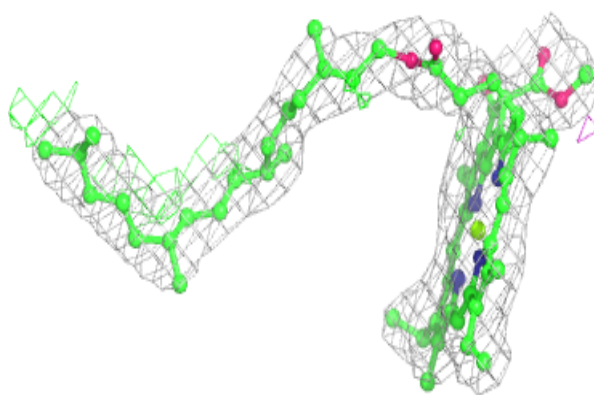
**Electron density around SF4 N 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

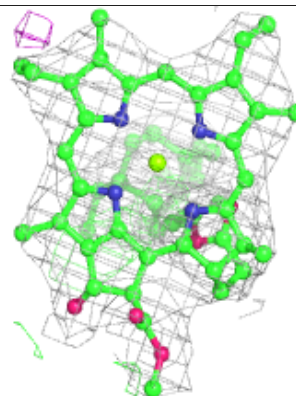
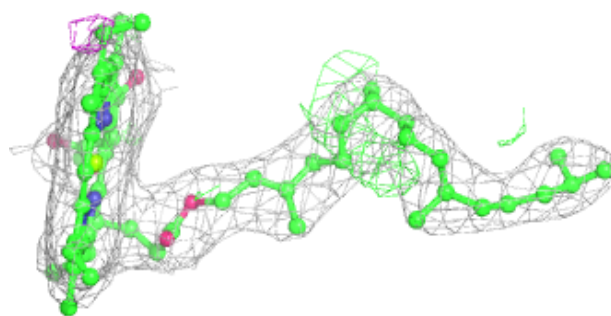
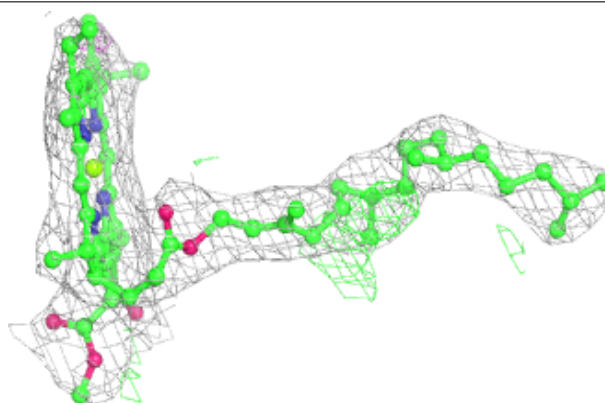


**Electron density around CLA A 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

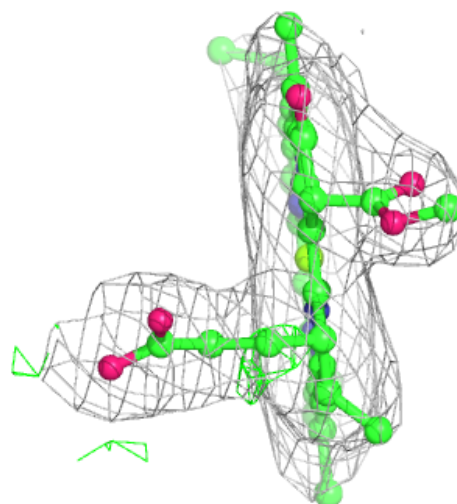
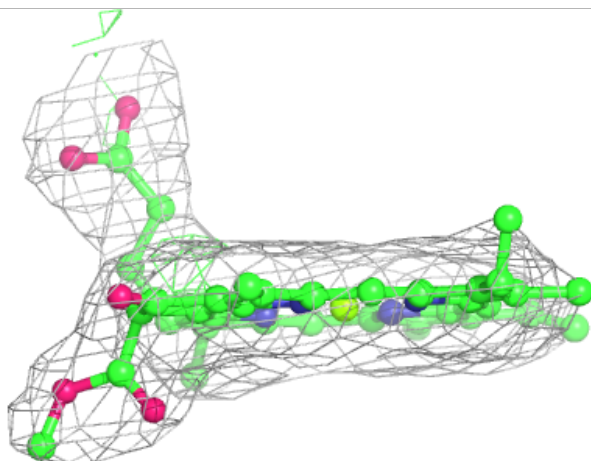
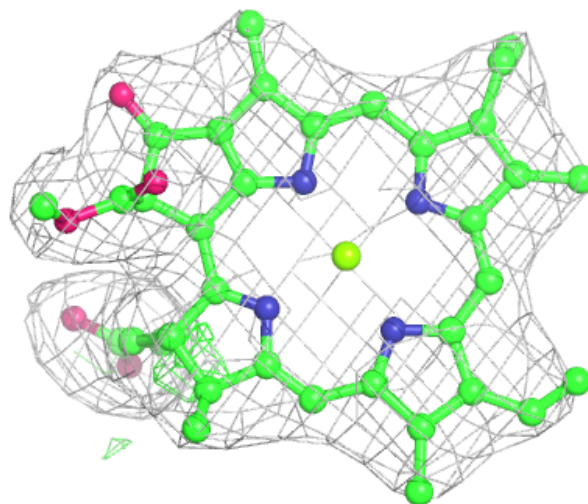
**Electron density around CLA G 828:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



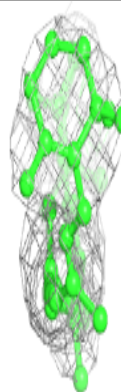
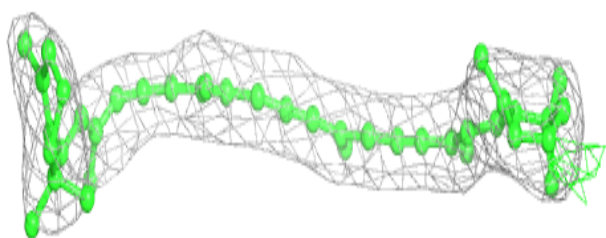
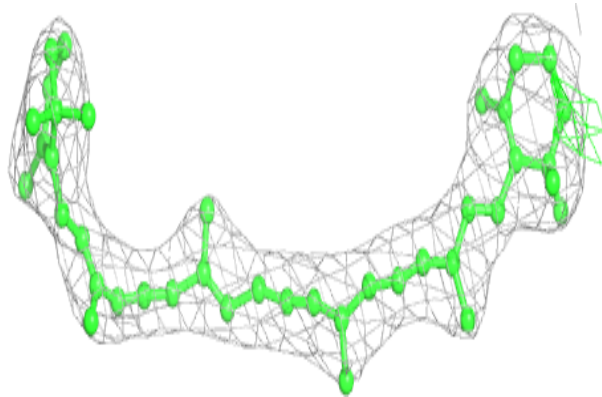
**Electron density around CLA H 836:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

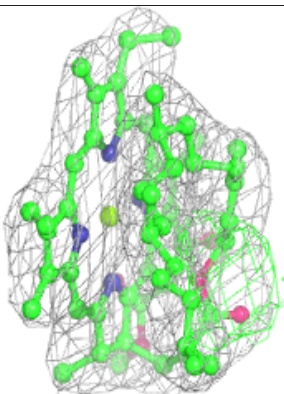
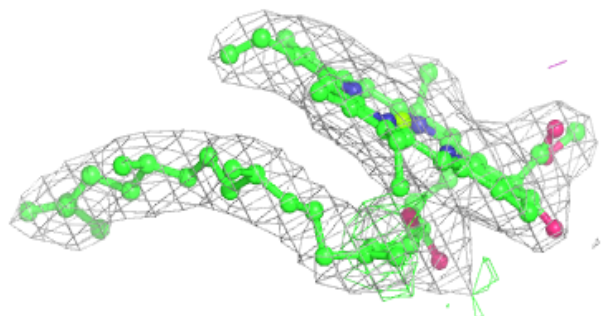
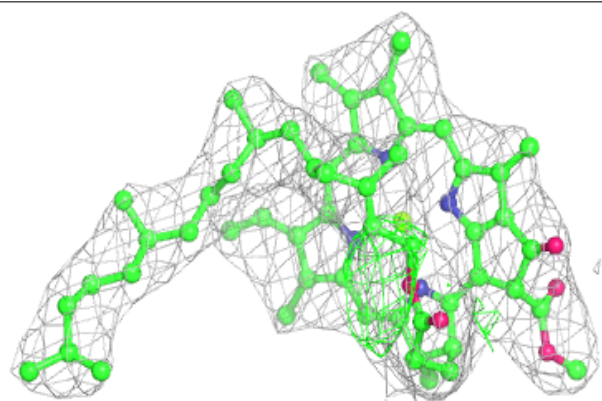


**Electron density around BCR Z 842:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

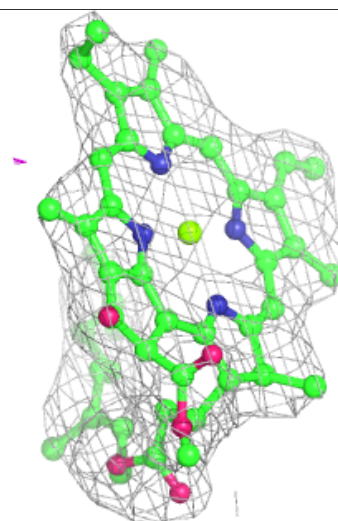
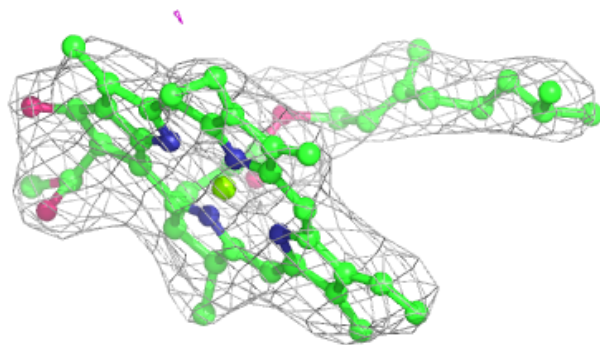
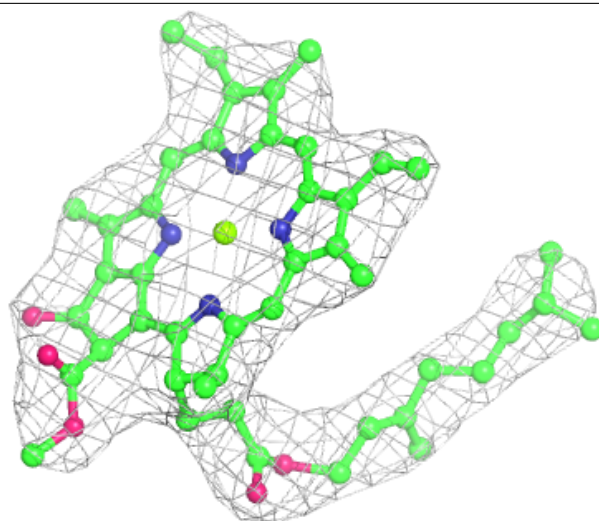
**Electron density around CLA B 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 816:**

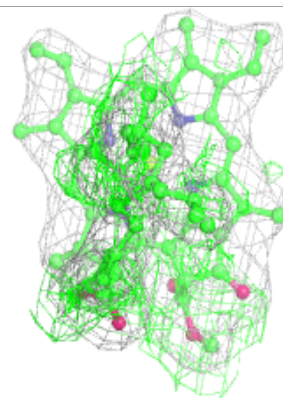
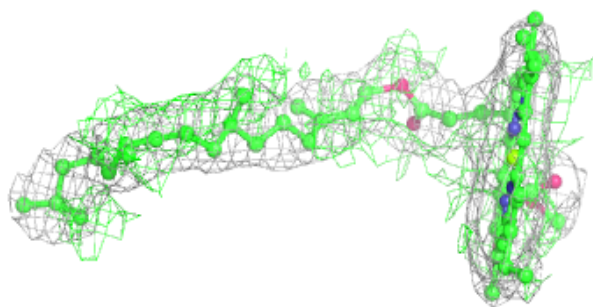
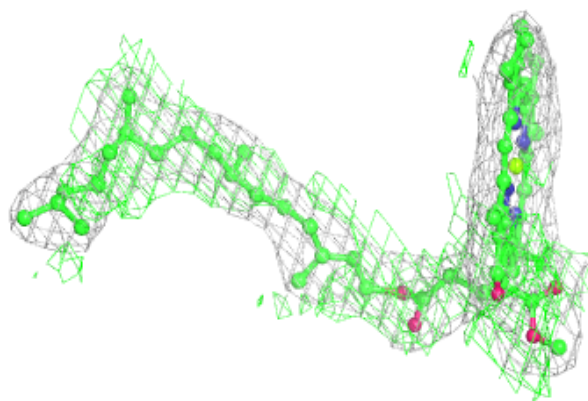
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



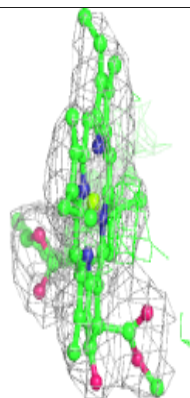
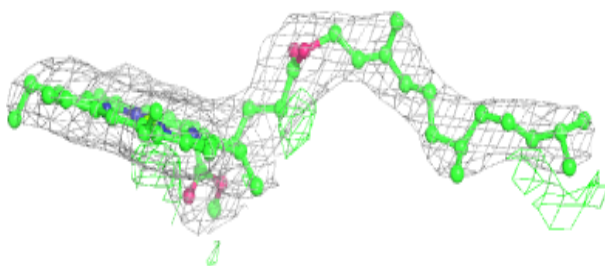
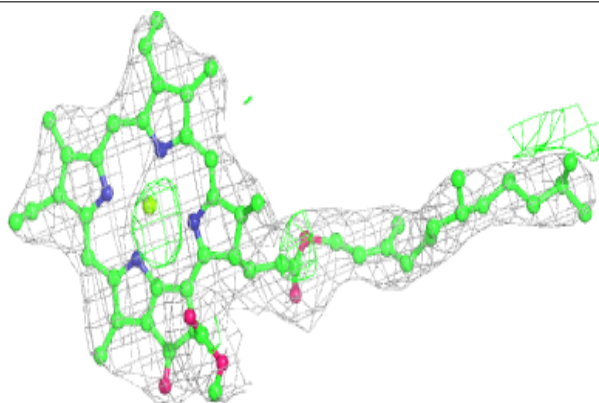


**Electron density around CLA Z 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

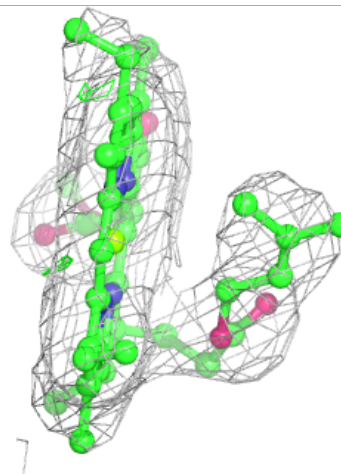
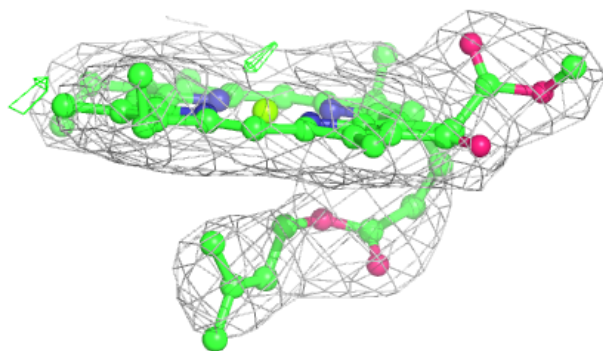
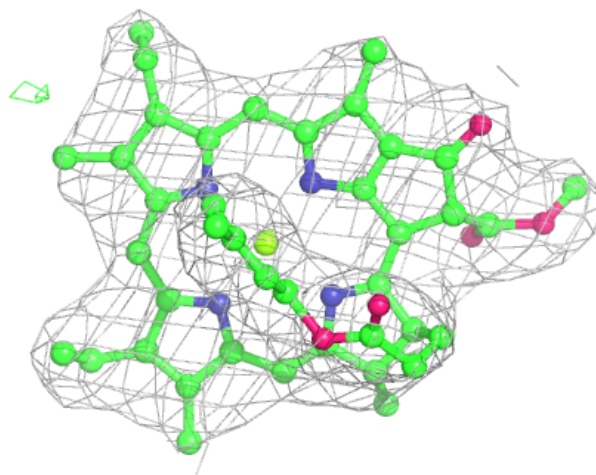
**Electron density around CLA G 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



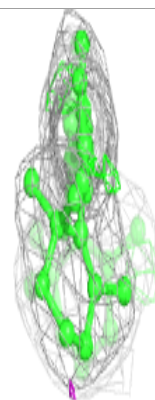
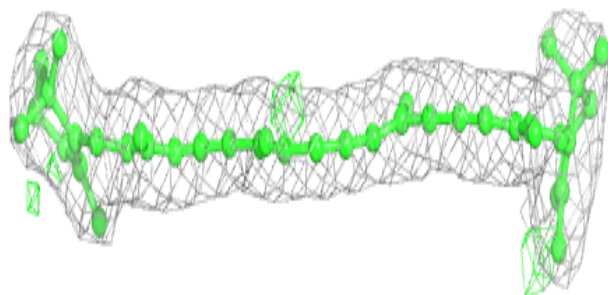
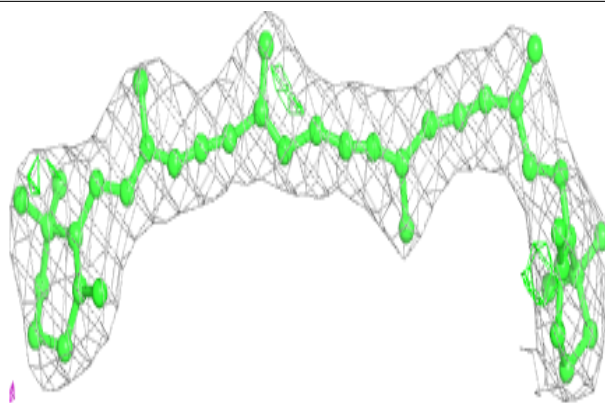
**Electron density around CLA A 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

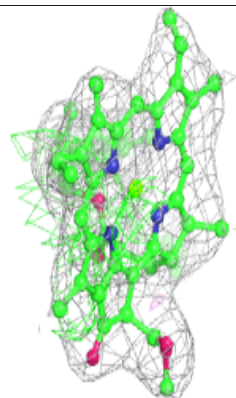
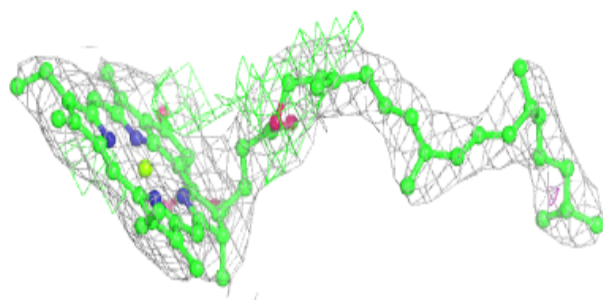
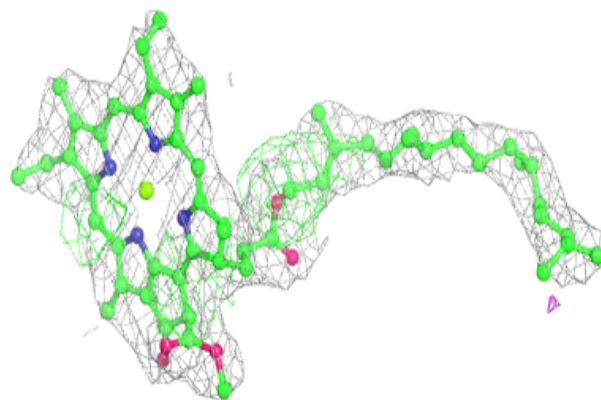


**Electron density around BCR h 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 821:**

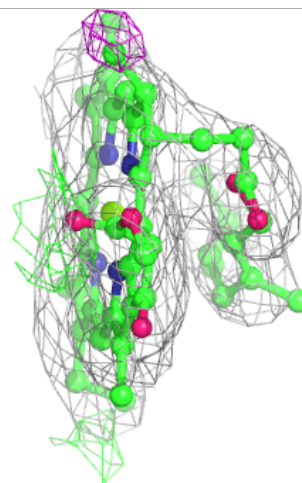
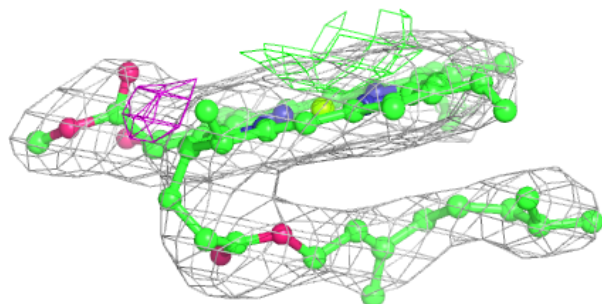
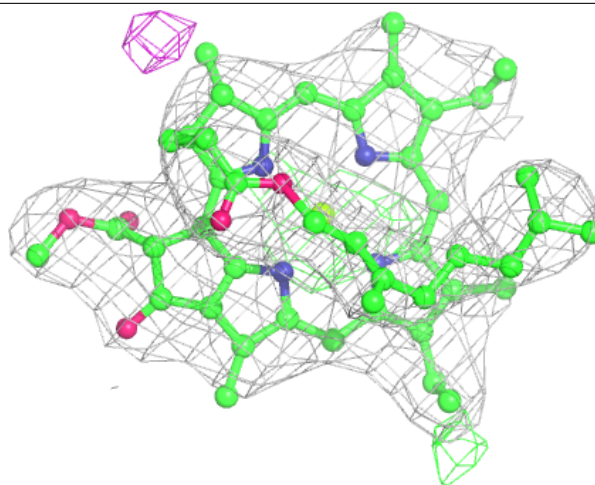
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





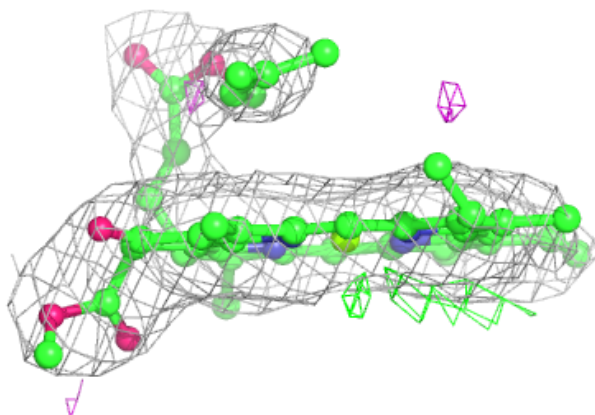
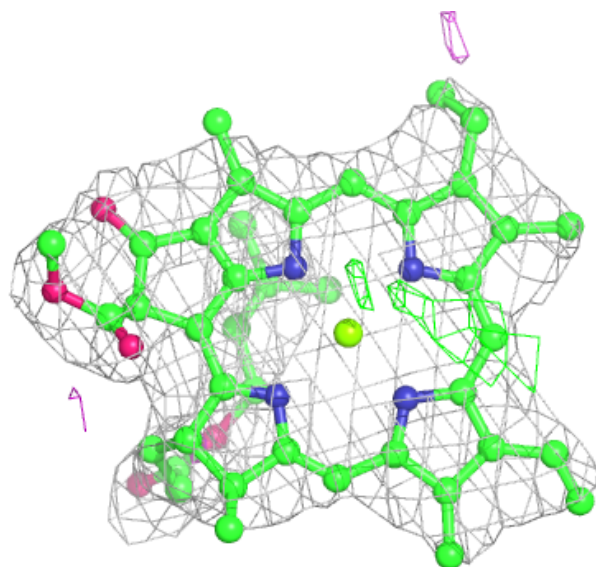
**Electron density around CLA B 822:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



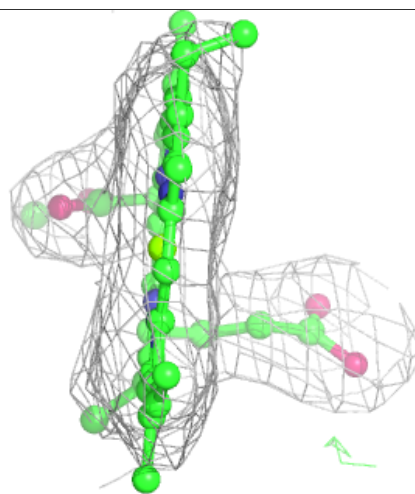
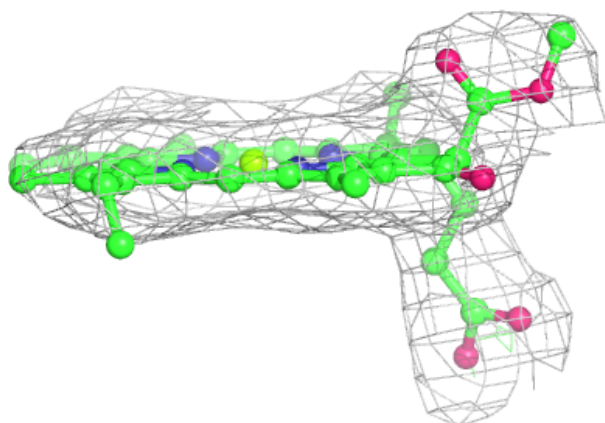
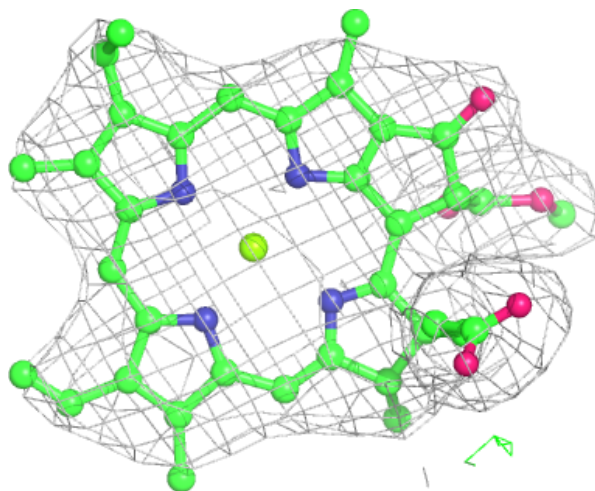
**Electron density around CLA Y 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



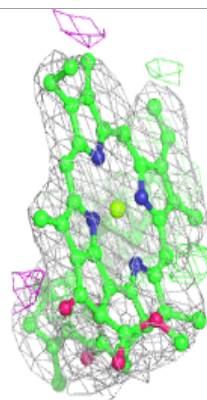
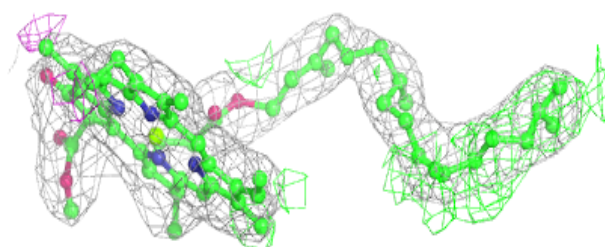
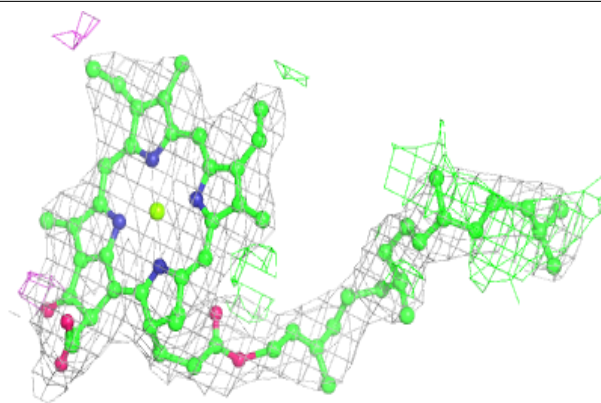
**Electron density around CLA B 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



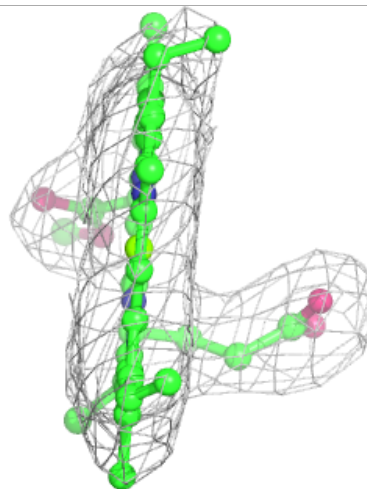
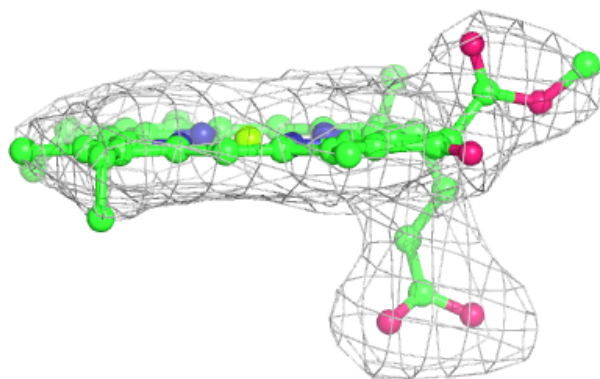
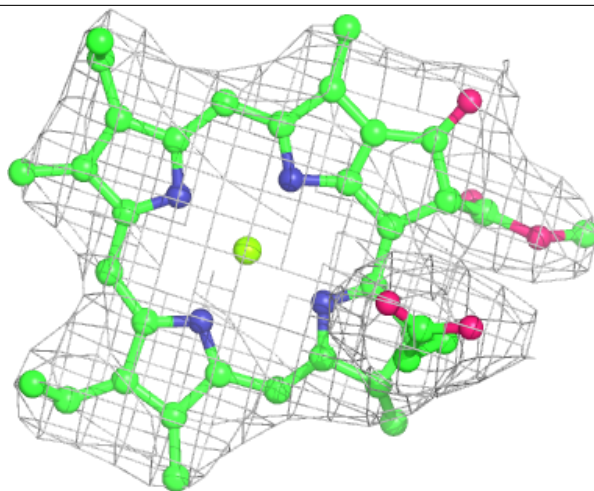
**Electron density around CLA A 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



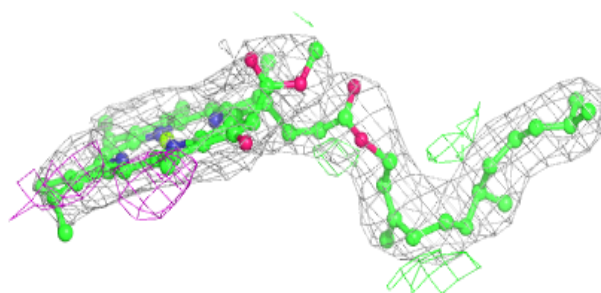
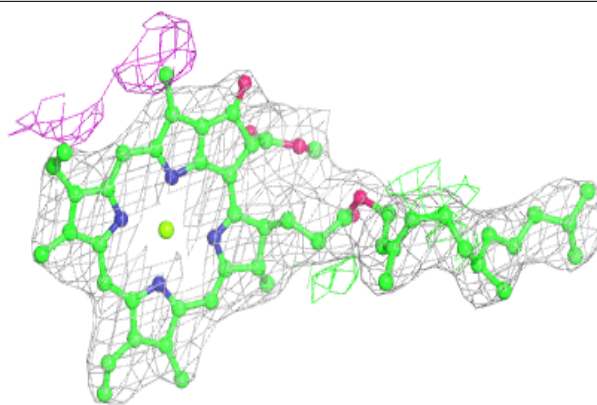
**Electron density around CLA H 811:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

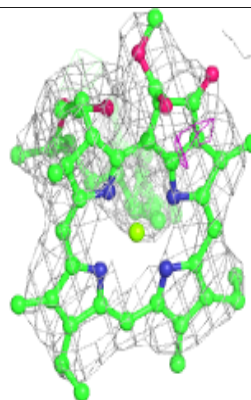
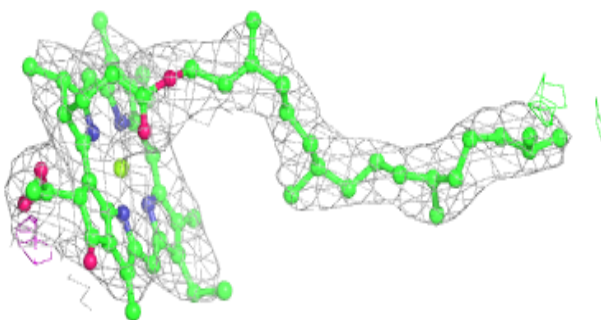
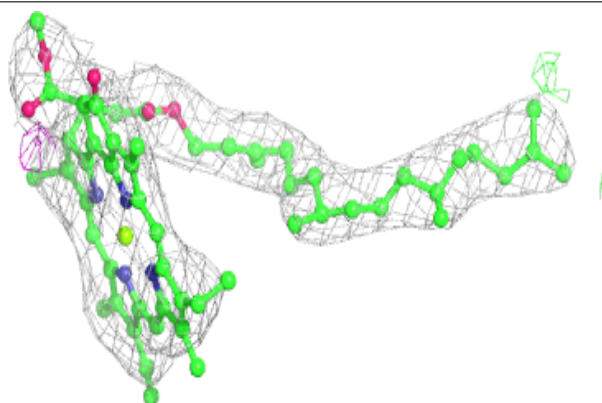


**Electron density around CLA B 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 811:**

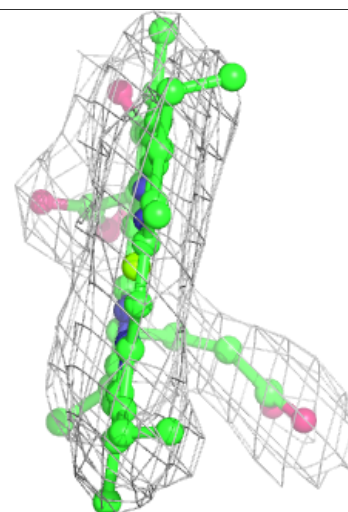
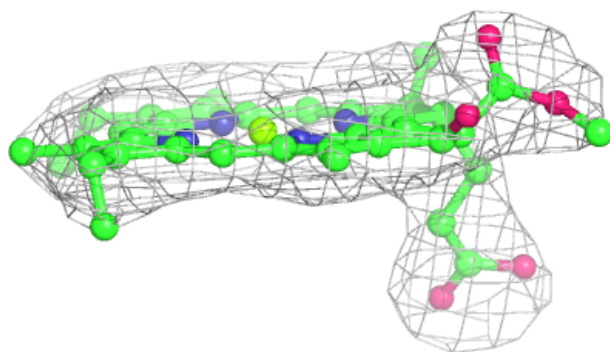
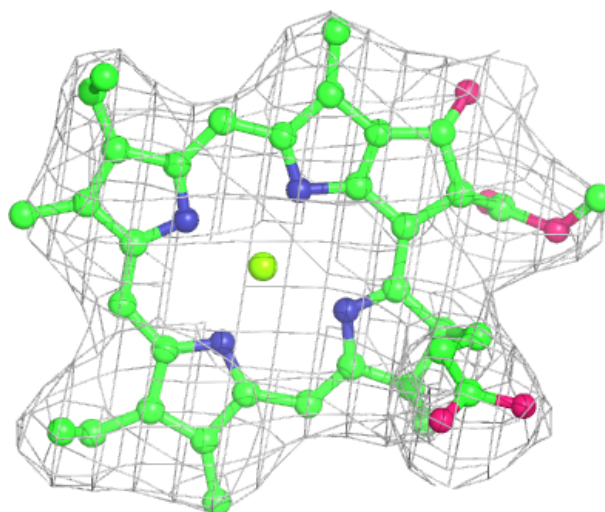
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





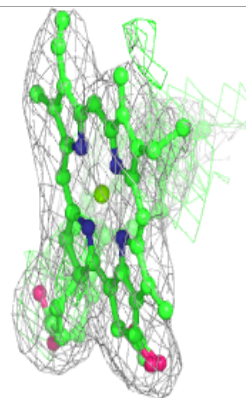
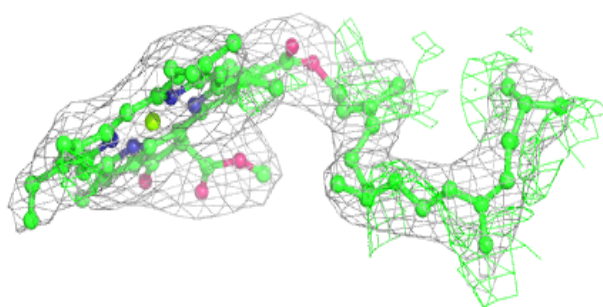
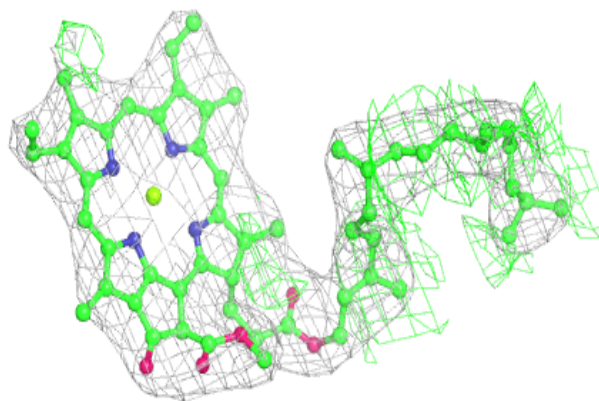
**Electron density around CLA Z 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 803:**

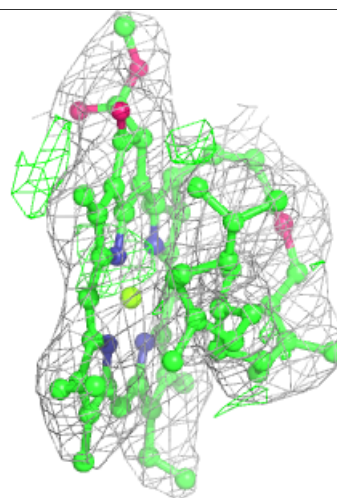
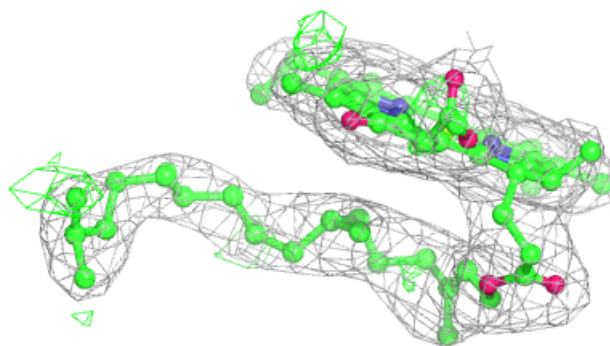
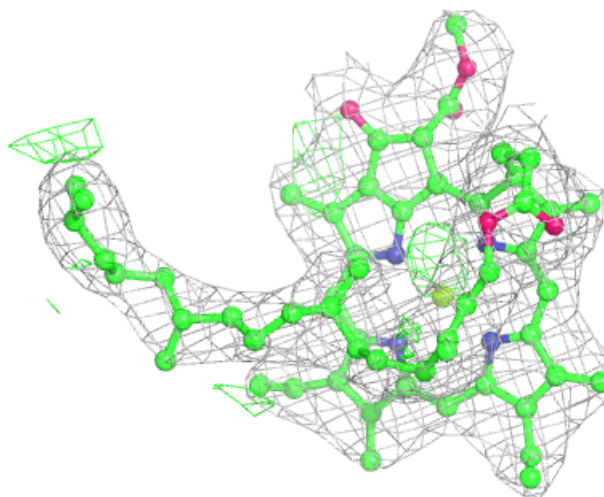
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





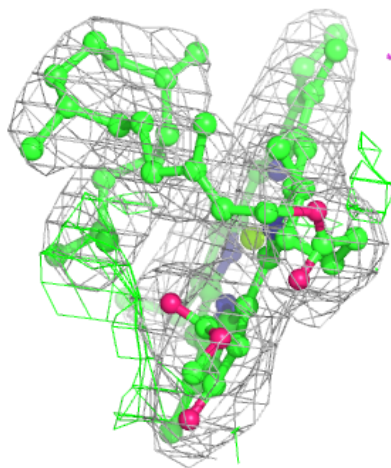
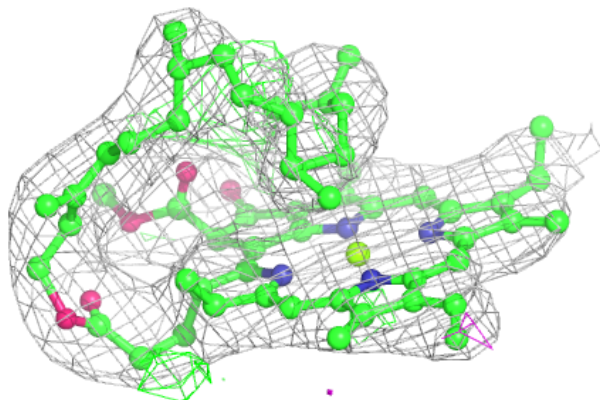
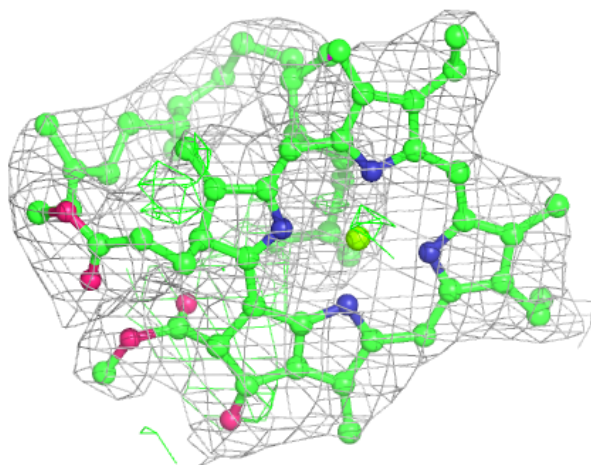
**Electron density around CLA H 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



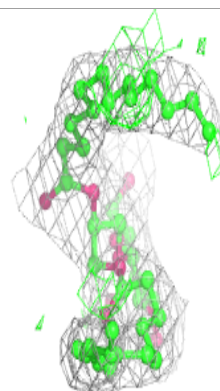
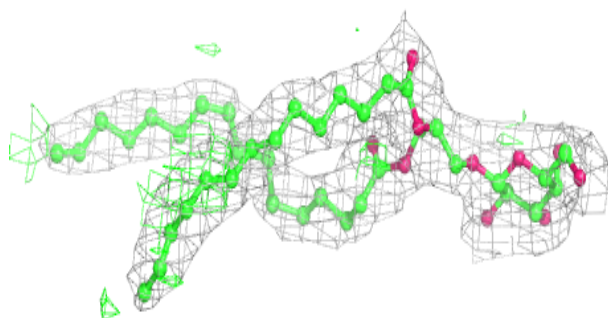
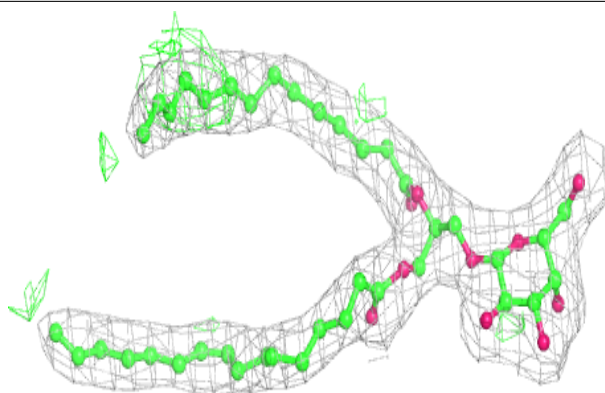
**Electron density around CLA B 807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

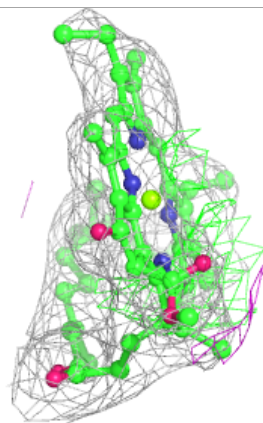
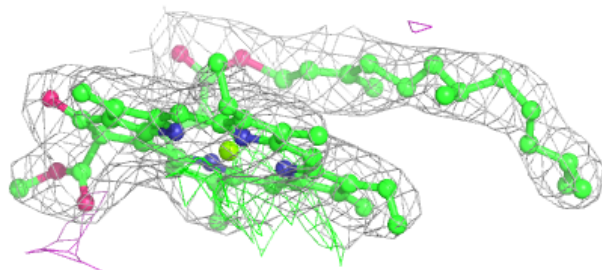
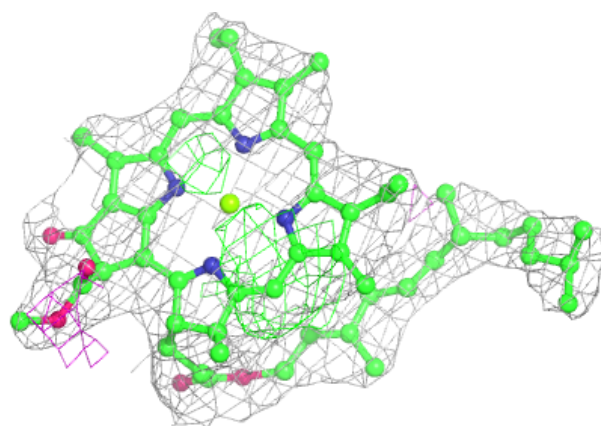


**Electron density around LMG H 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

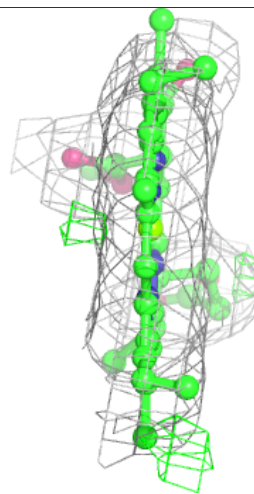
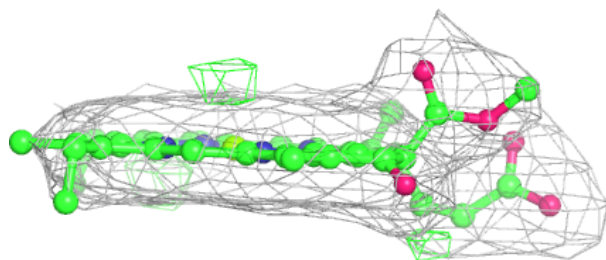
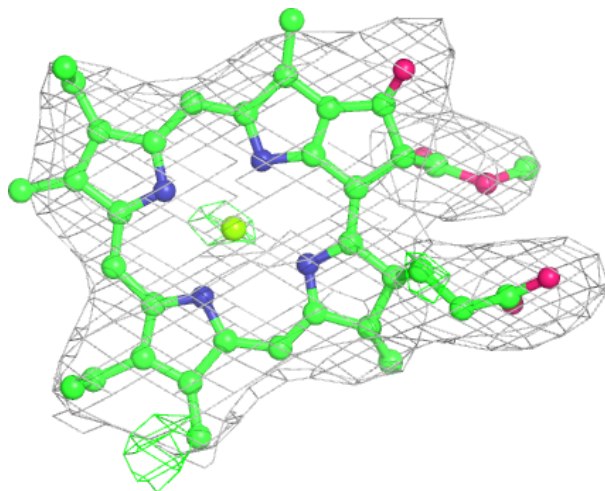
**Electron density around CLA Z 816:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



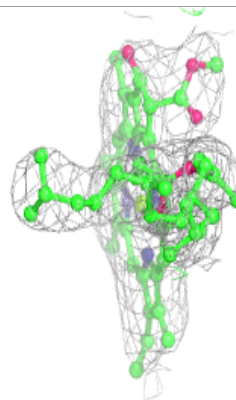
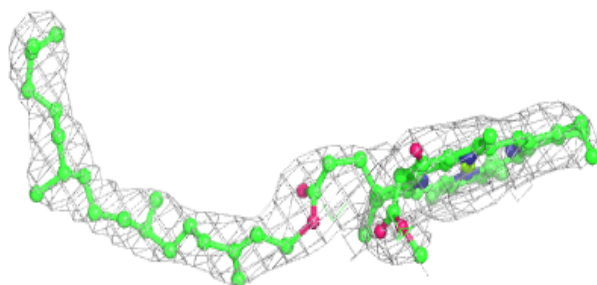
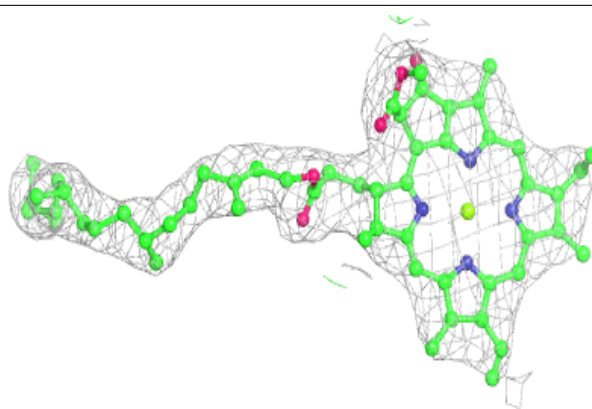
**Electron density around CLA B 836:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

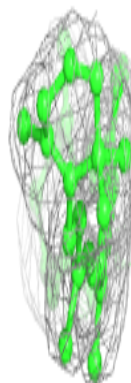
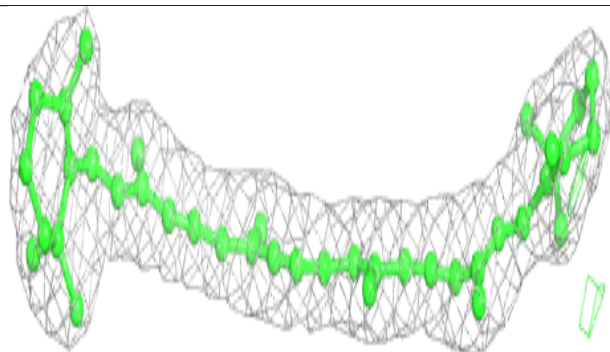
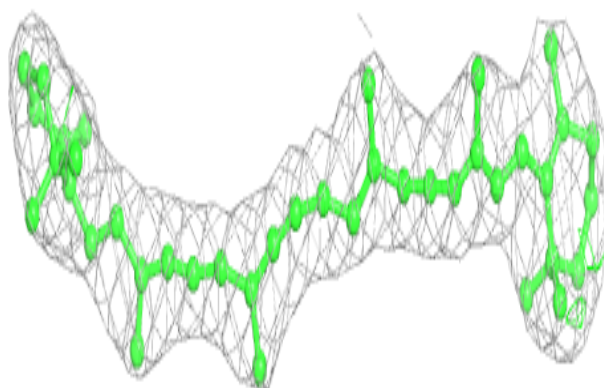


**Electron density around CLA G 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR i 101:**

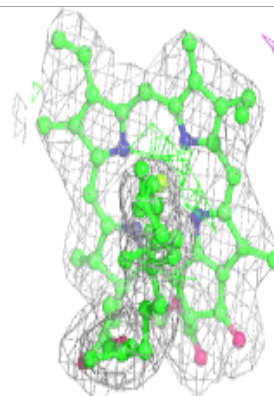
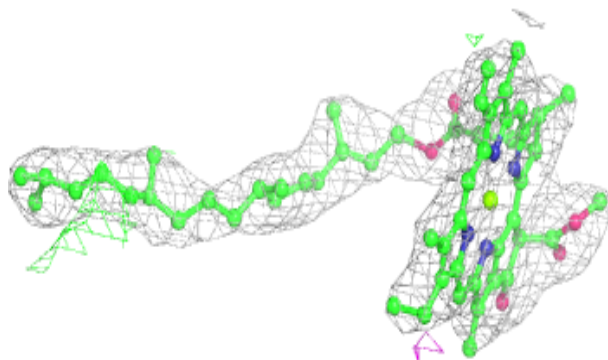
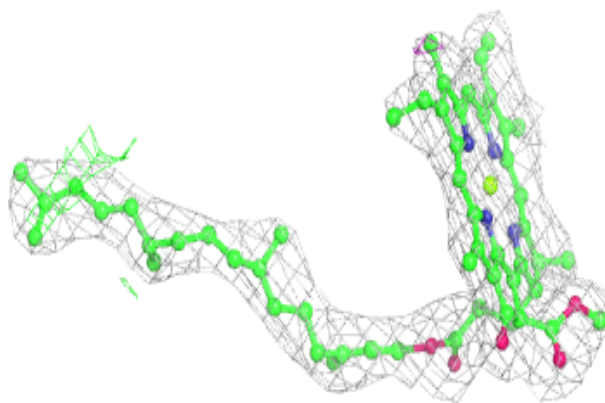
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





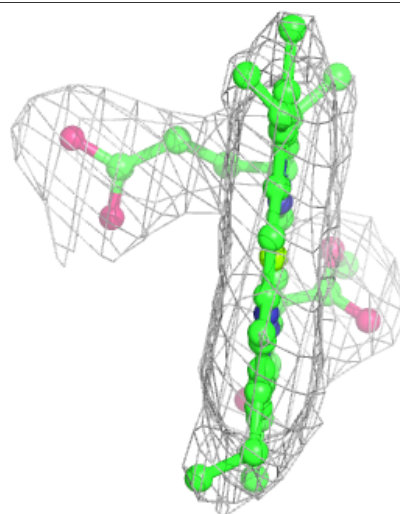
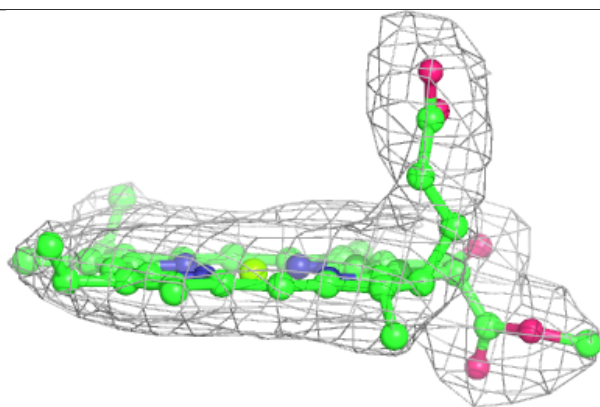
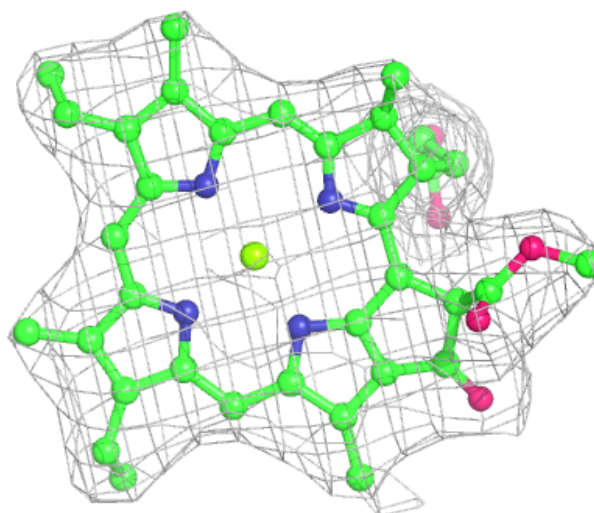
**Electron density around CLA H 828:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



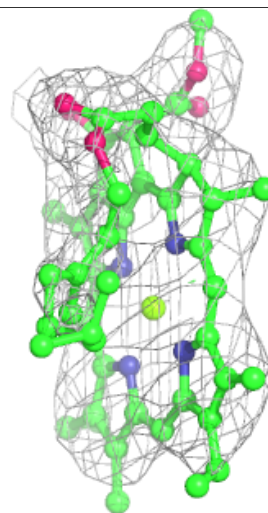
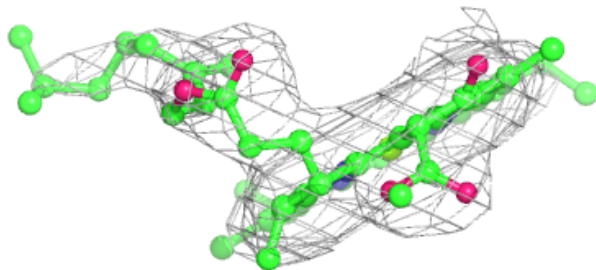
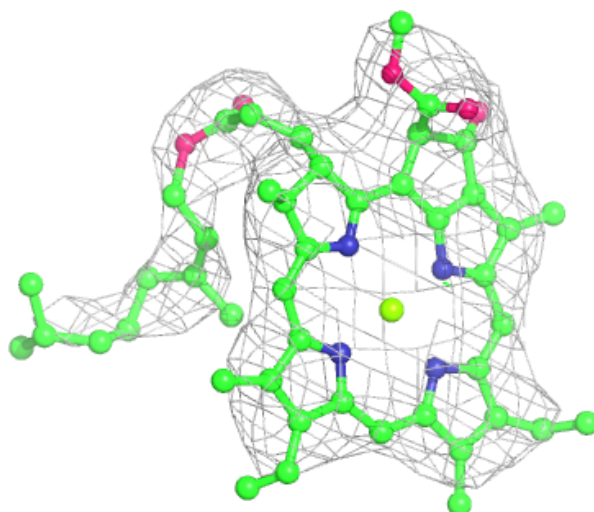
**Electron density around CLA B 831:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA f 102:**

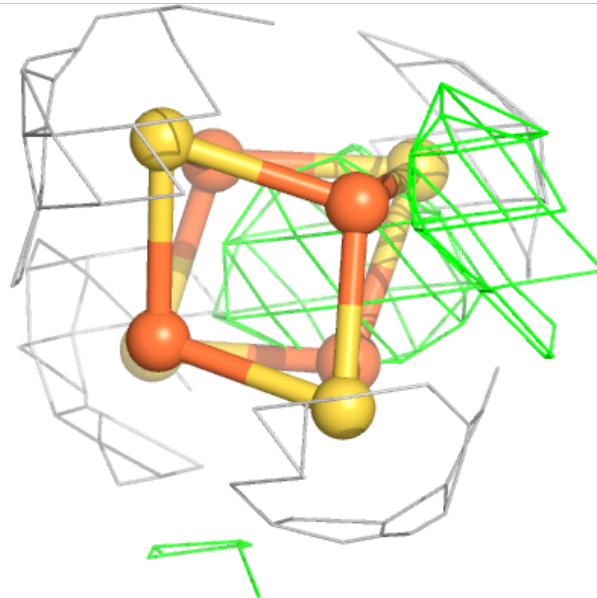
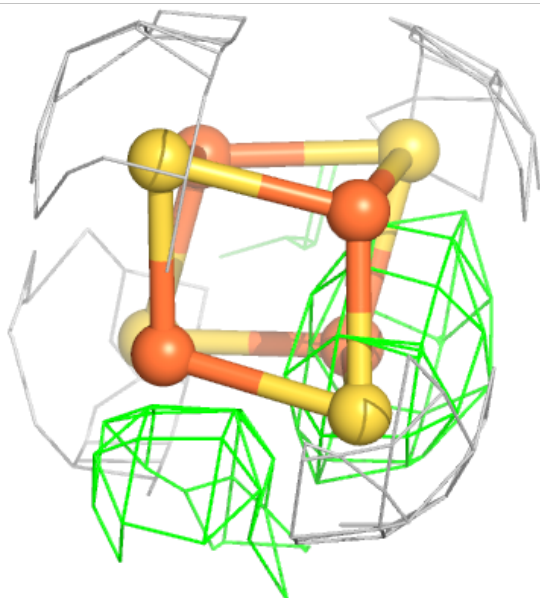
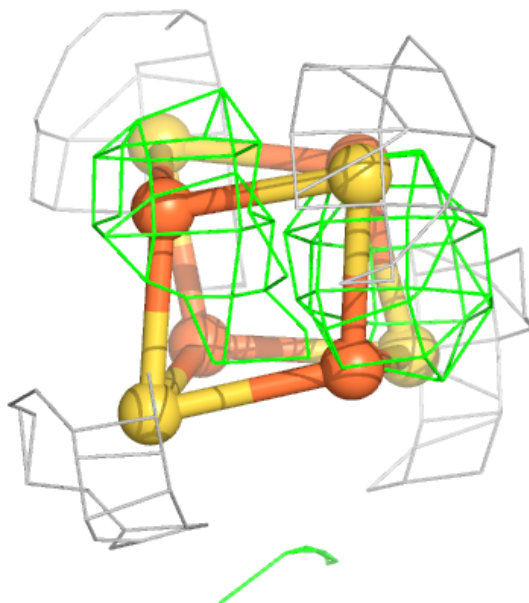
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





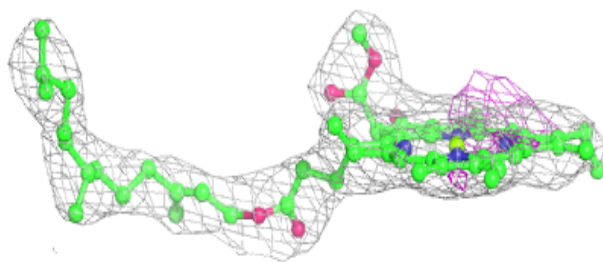
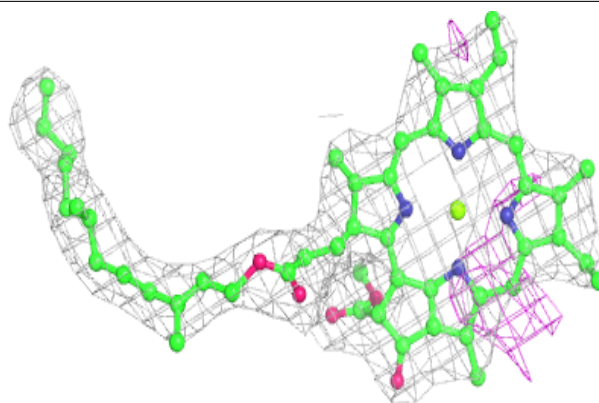
**Electron density around SF4 A 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

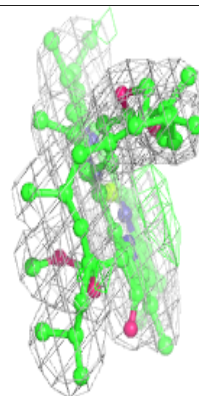
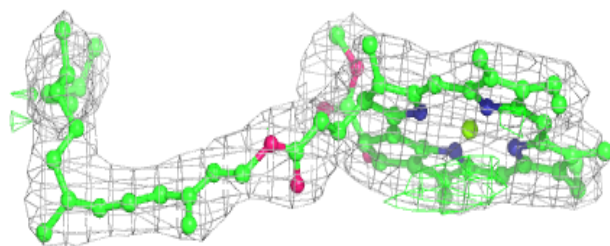
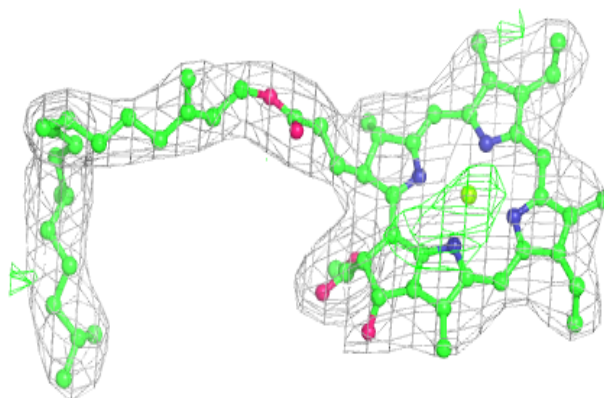


**Electron density around CLA Z 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

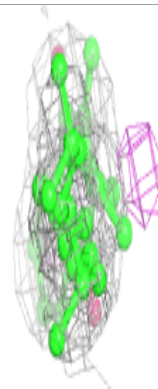
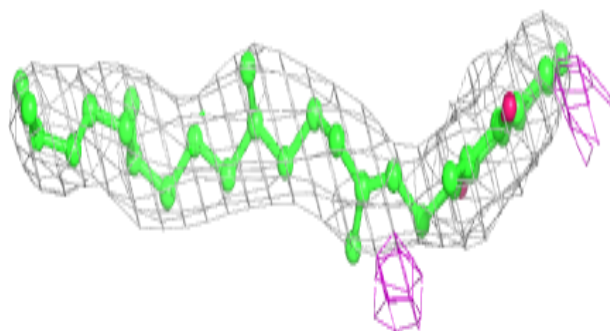
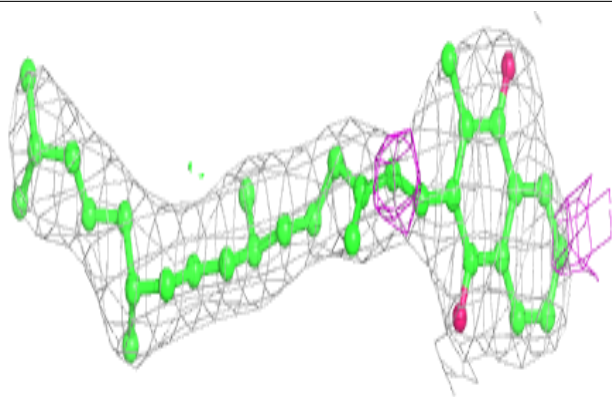
**Electron density around CLA B 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



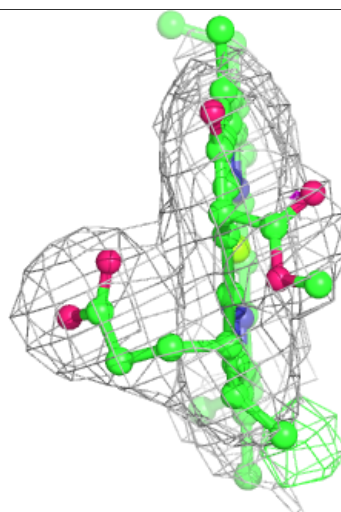
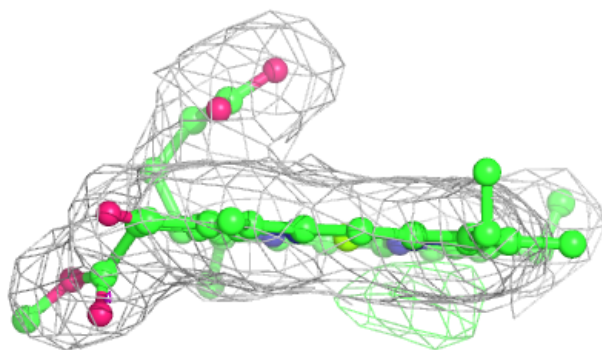
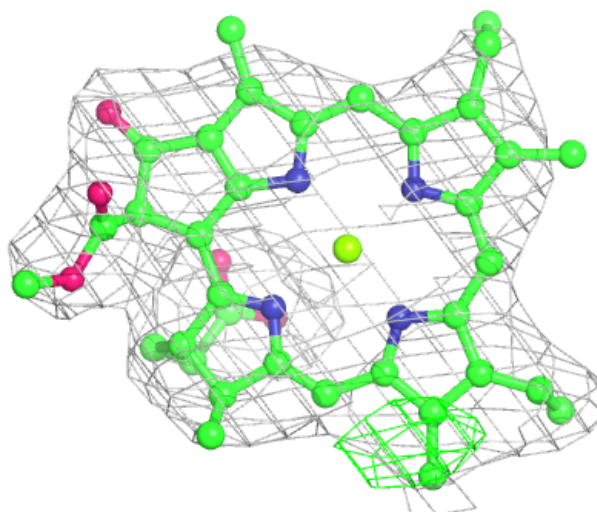
**Electron density around PQN A 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



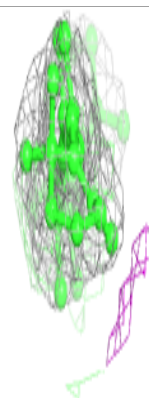
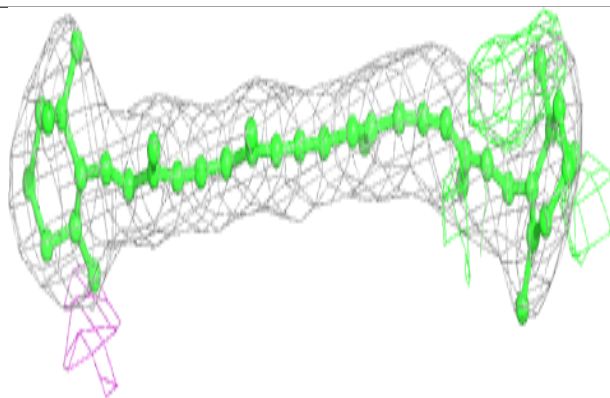
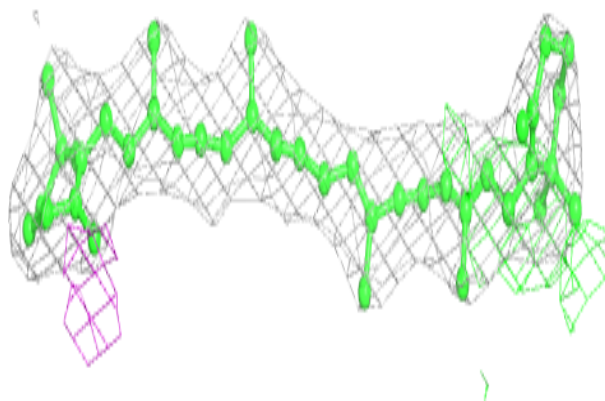
**Electron density around CLA A 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



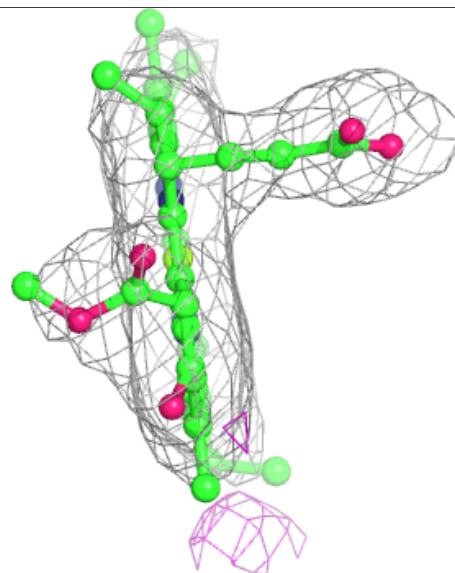
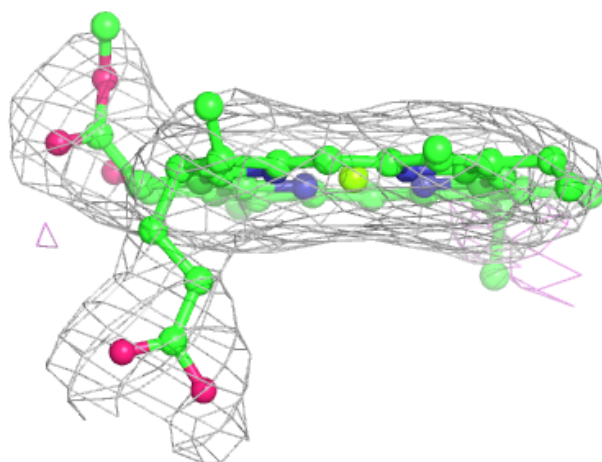
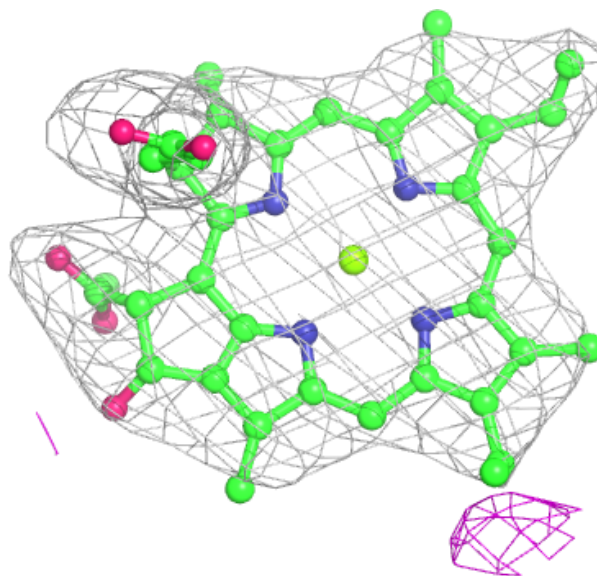
**Electron density around BCR L 209:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 815:**

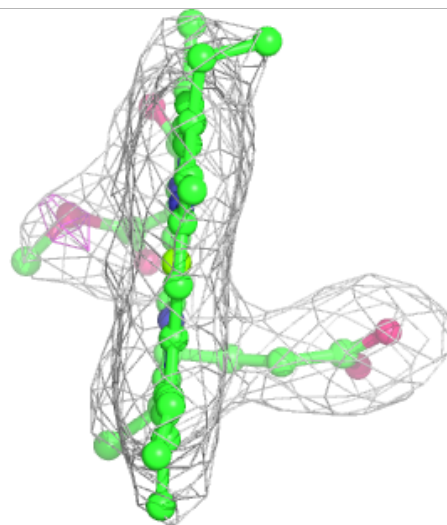
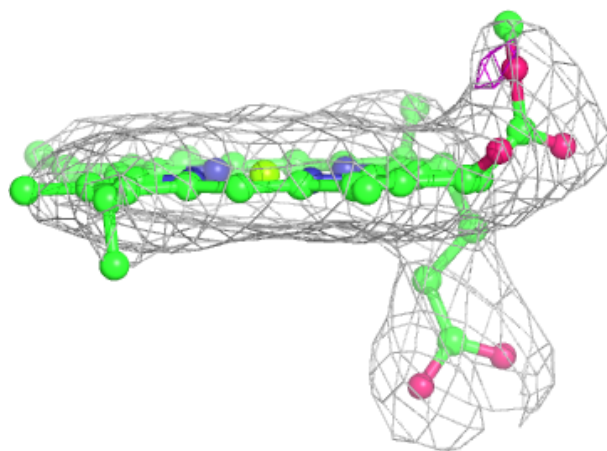
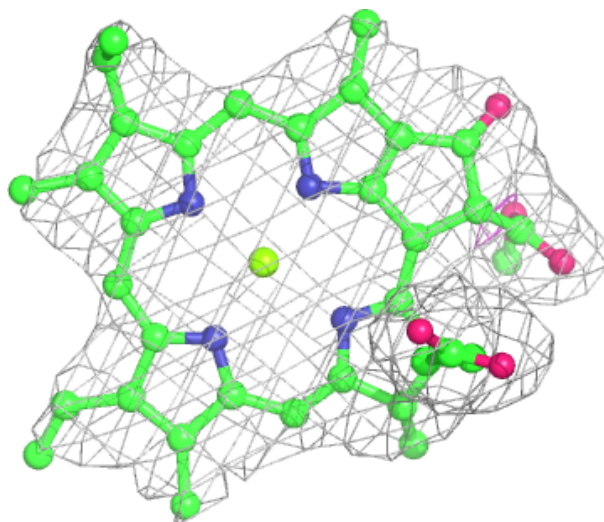
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





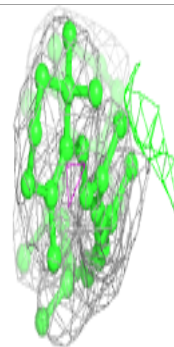
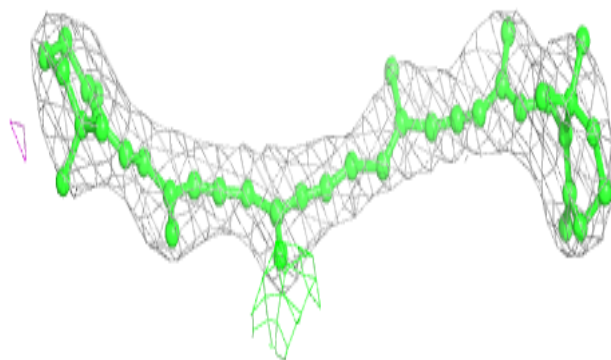
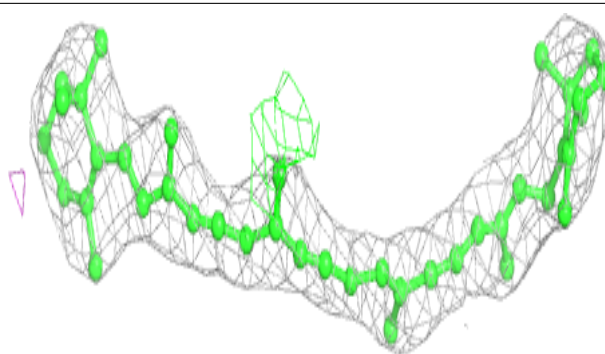
**Electron density around CLA Z 813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR F 201:**

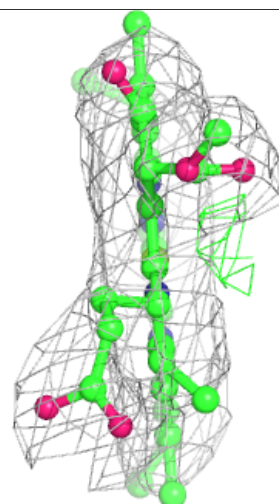
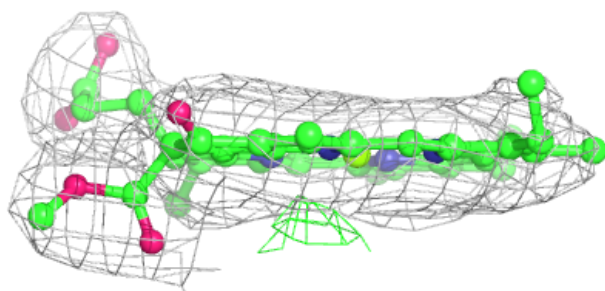
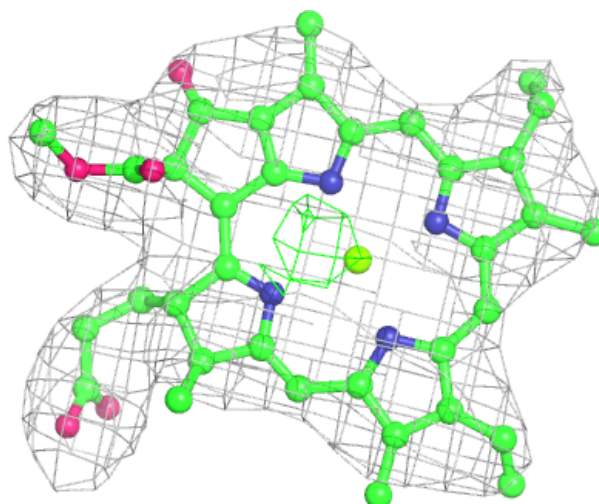
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





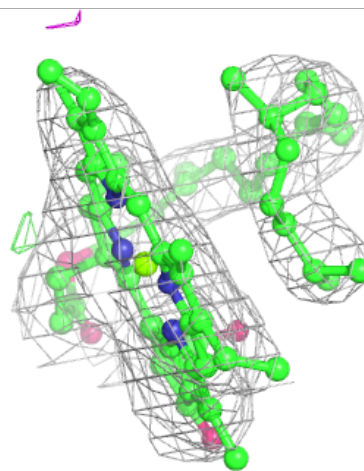
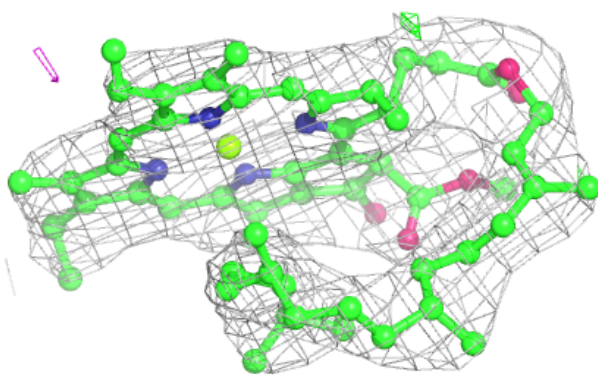
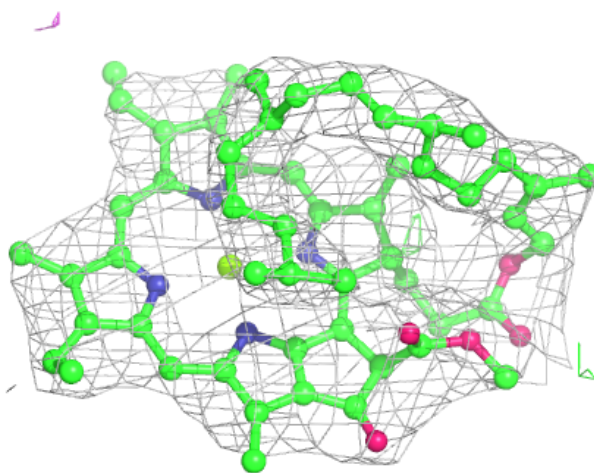
**Electron density around CLA X 1701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



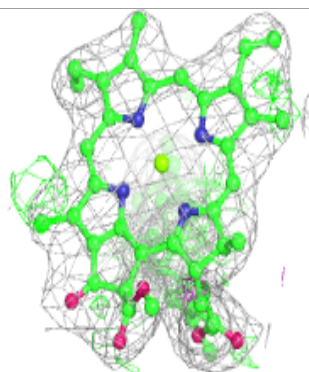
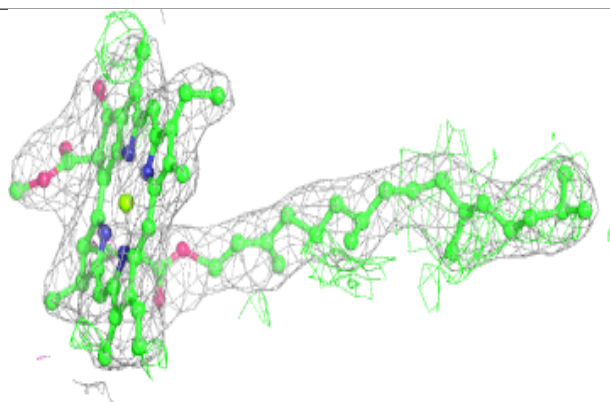
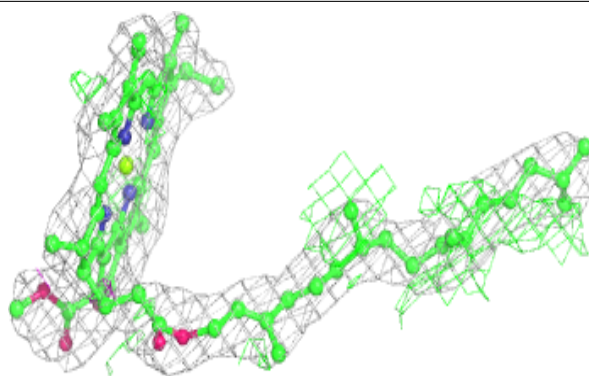
**Electron density around CLA A 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

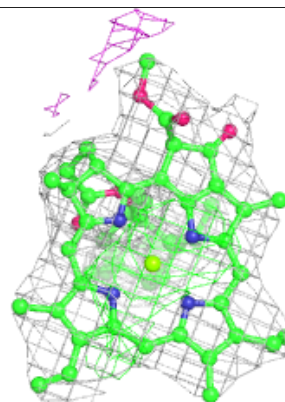
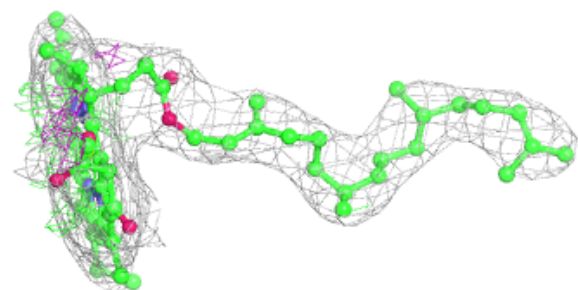
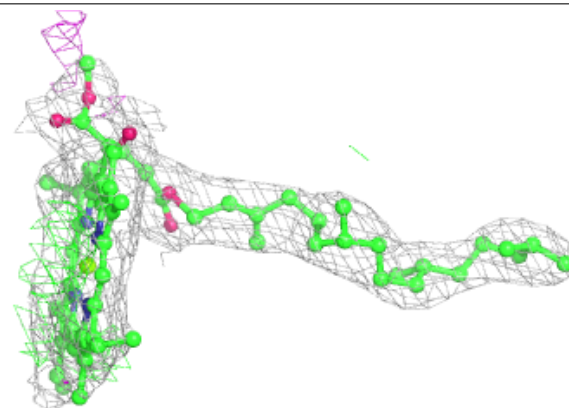


**Electron density around CLA B 829:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

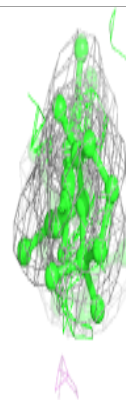
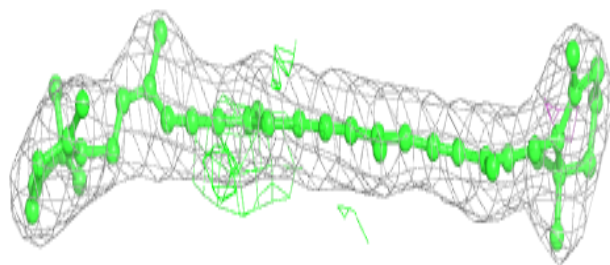
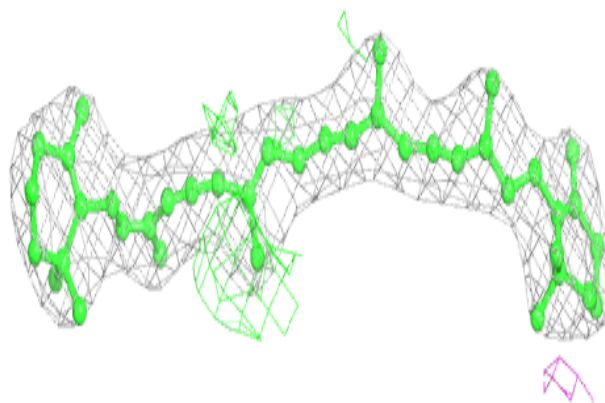
**Electron density around CLA Y 828:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

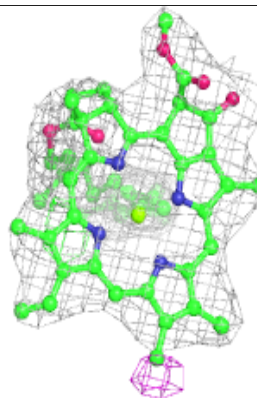
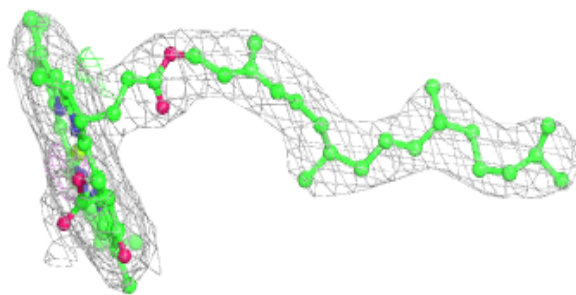
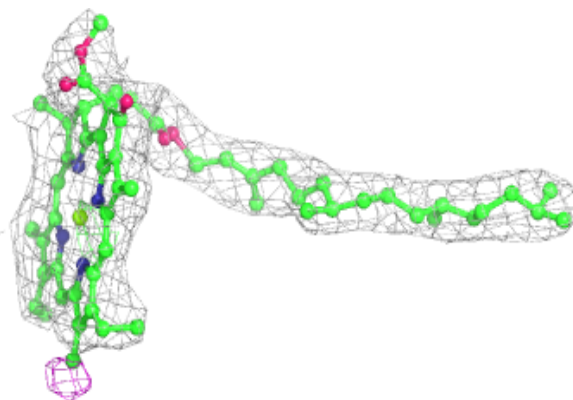


**Electron density around BCR H 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

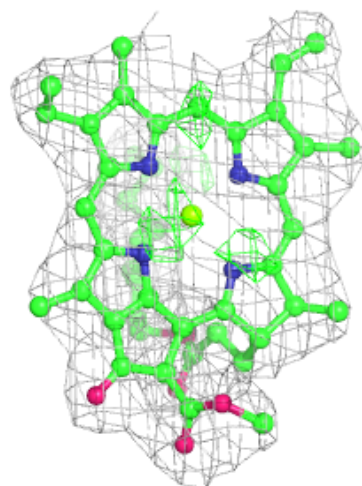
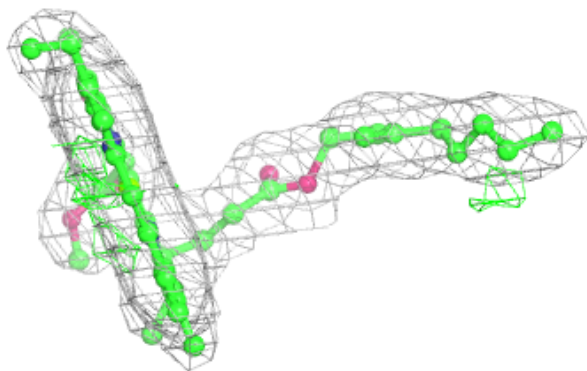
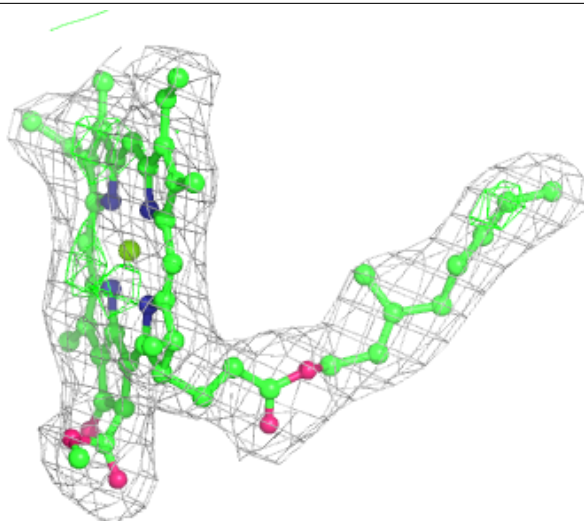
**Electron density around CLA Z 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 805:**

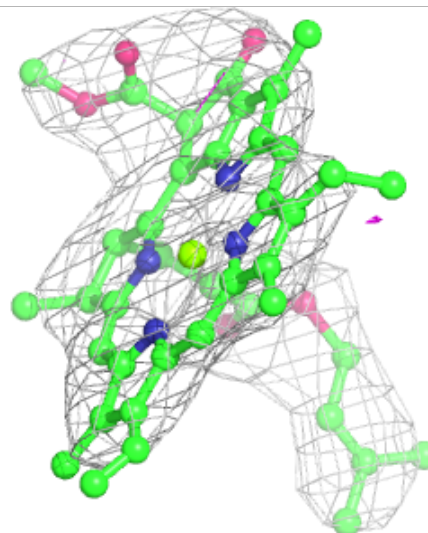
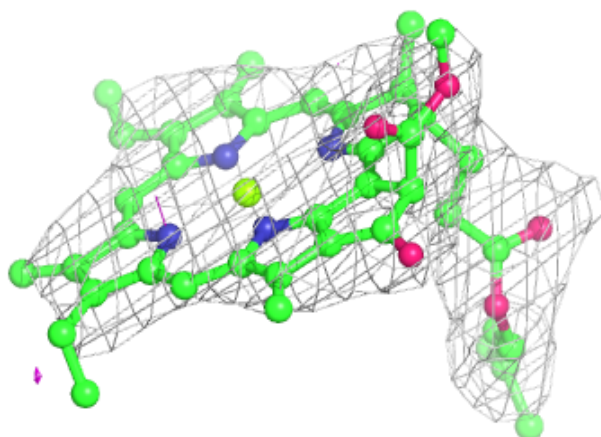
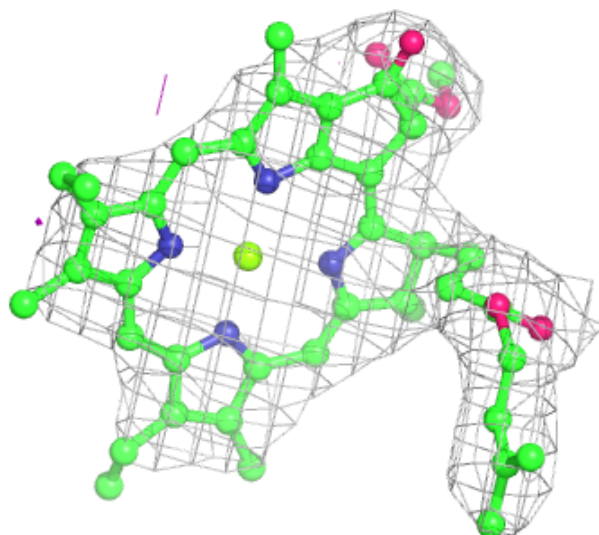
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





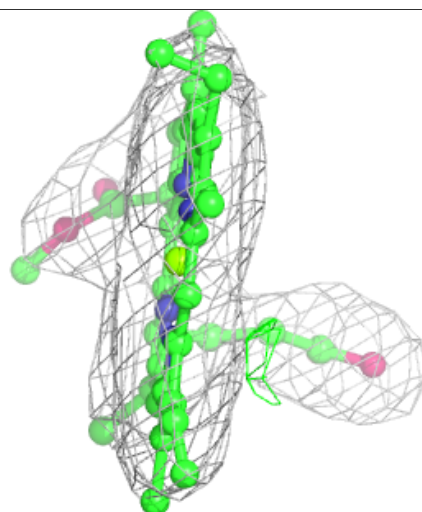
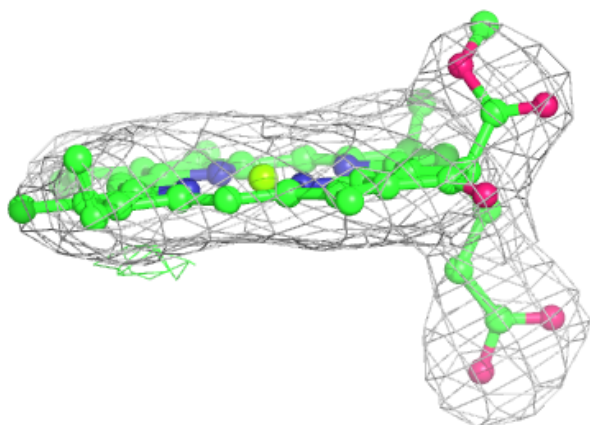
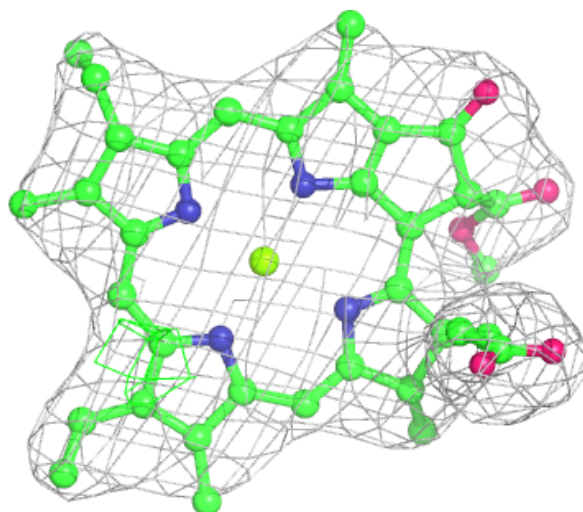
**Electron density around CLA G 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



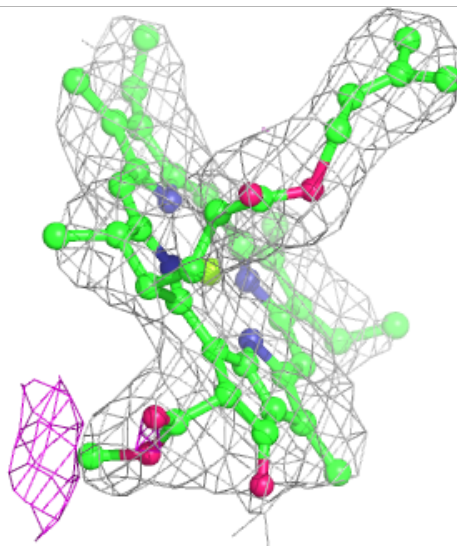
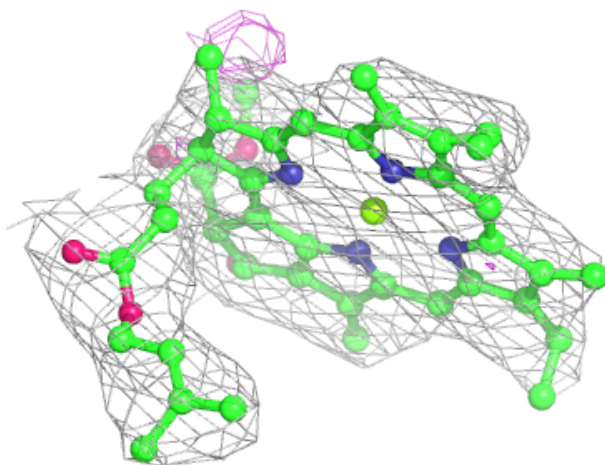
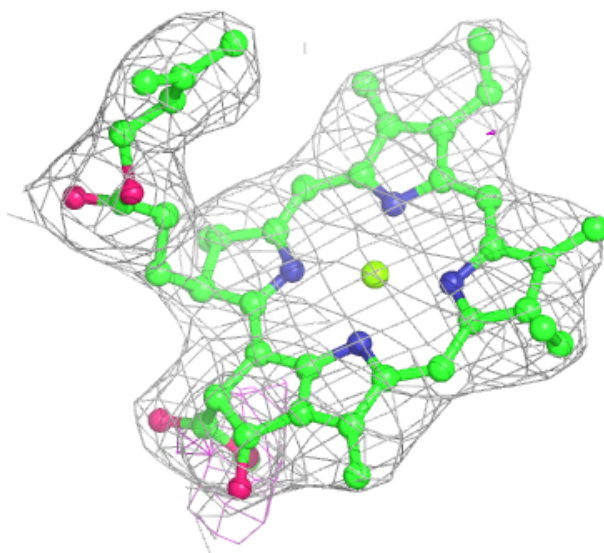
**Electron density around CLA g 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA G 831:**

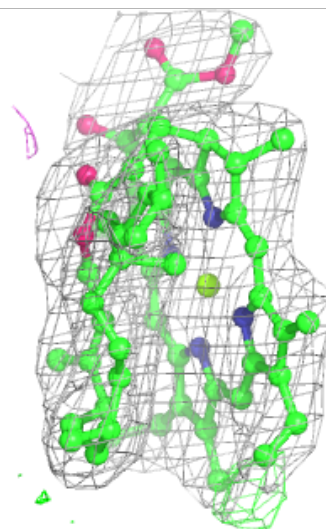
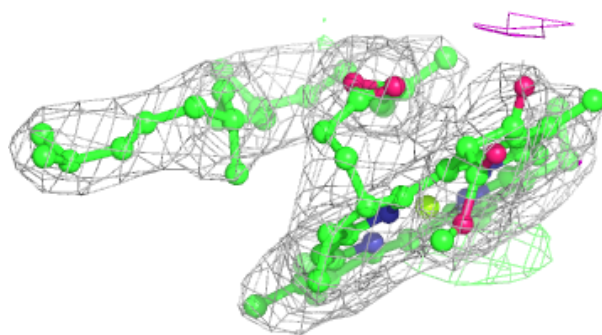
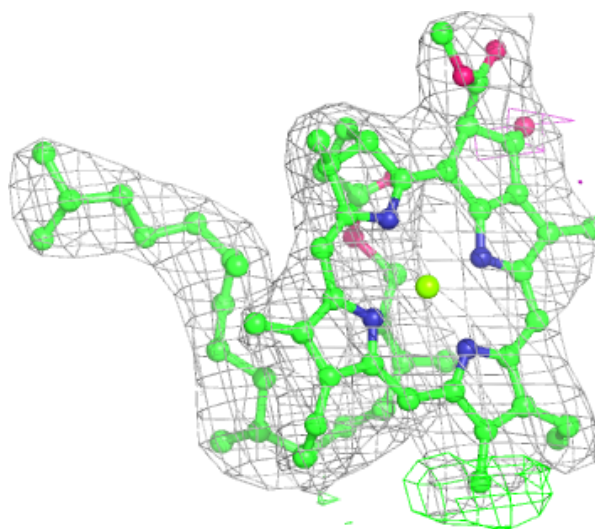
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





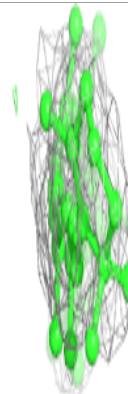
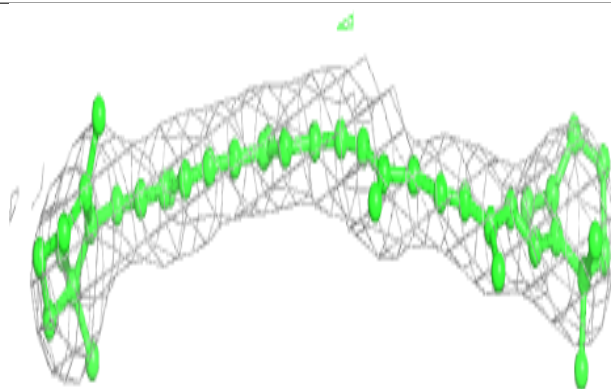
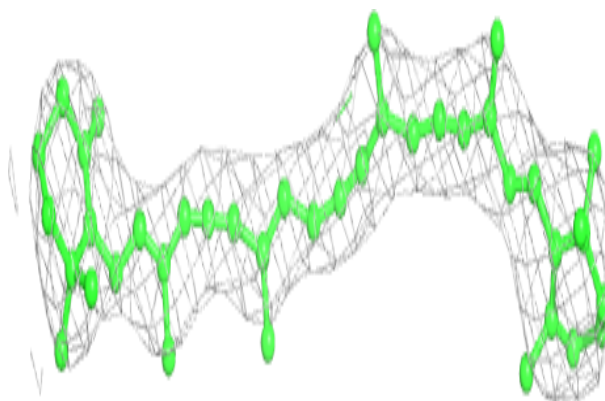
**Electron density around CLA B 809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



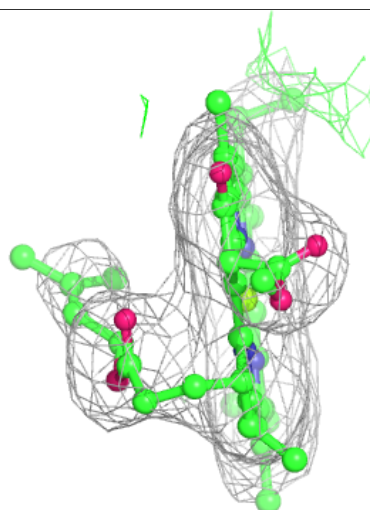
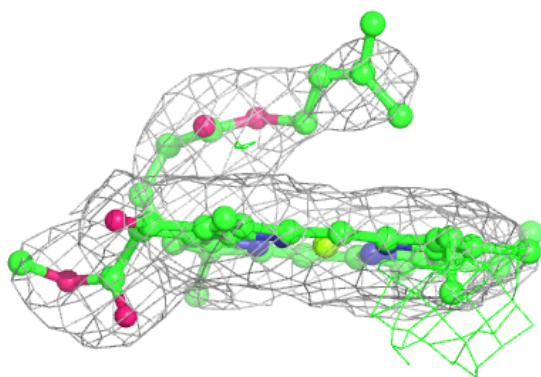
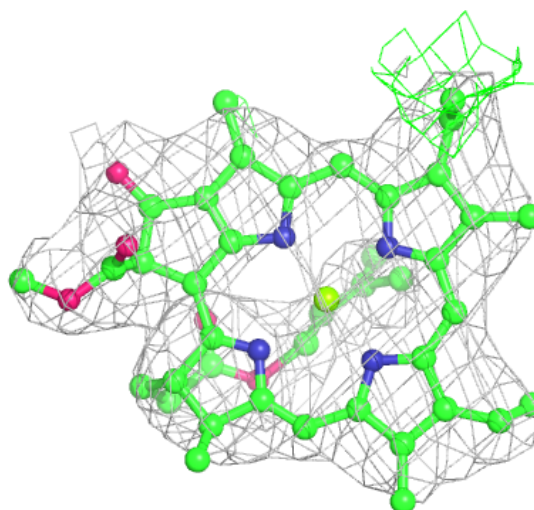
**Electron density around BCR H 840:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



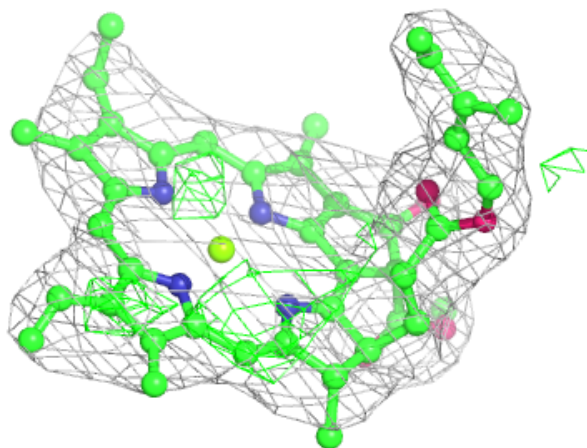
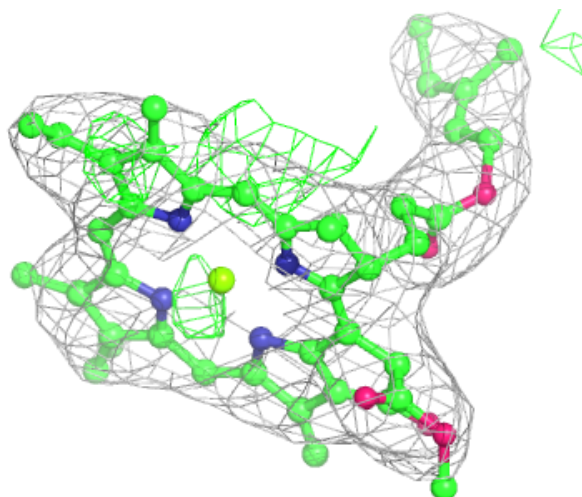
**Electron density around CLA G 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



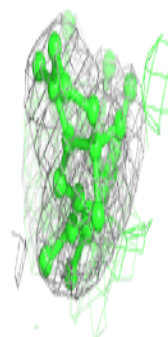
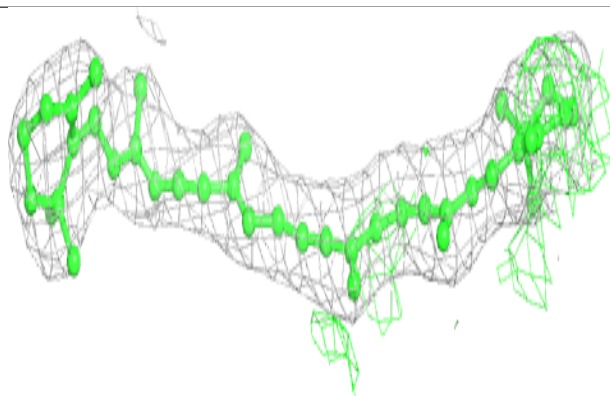
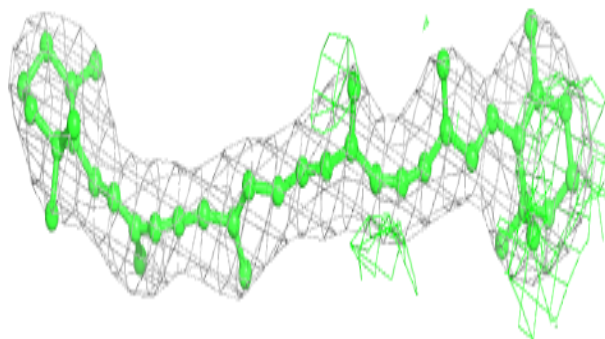
**Electron density around CLA Y 807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



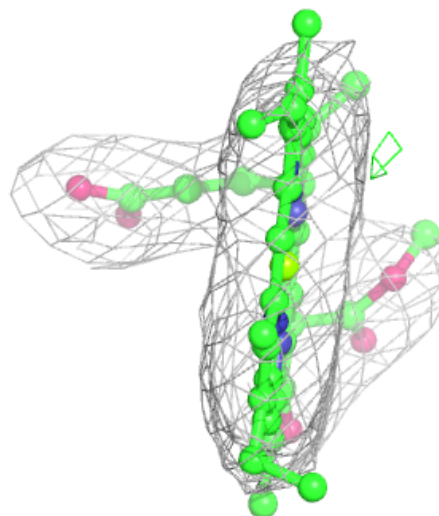
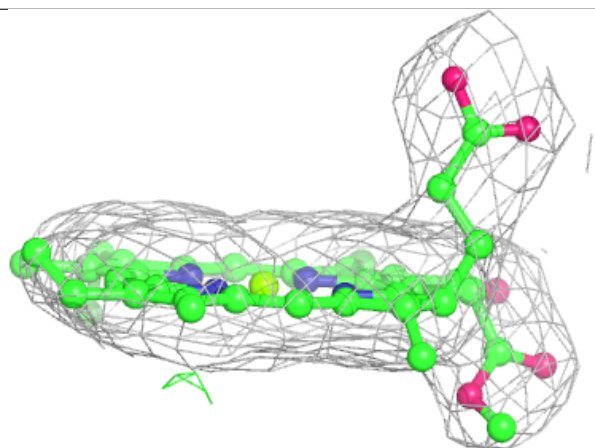
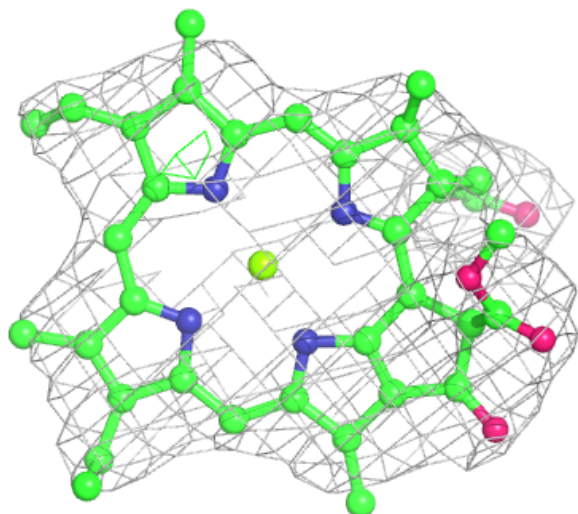
**Electron density around BCR S 1104:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA K 103:**

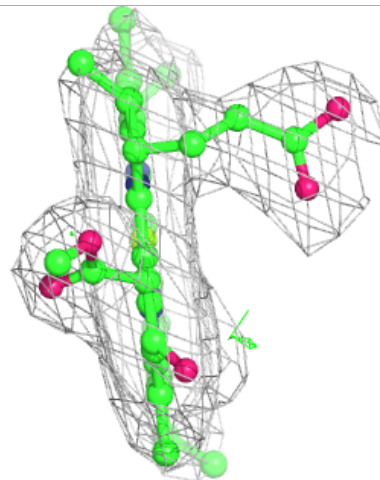
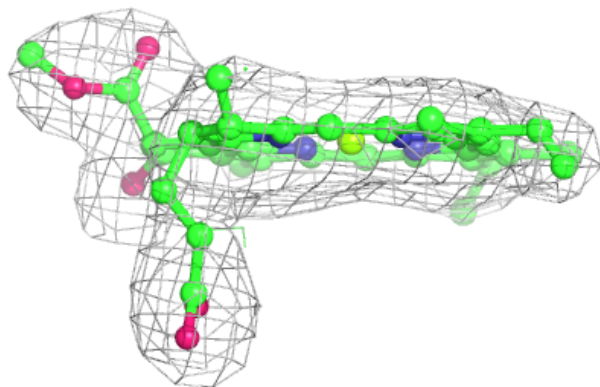
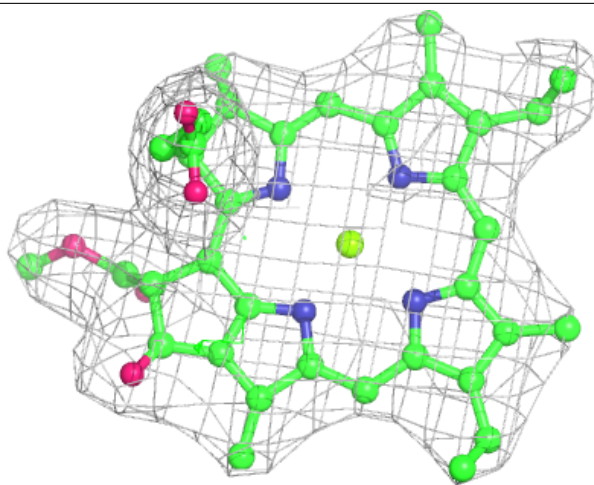
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





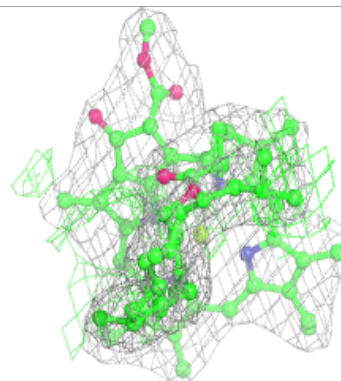
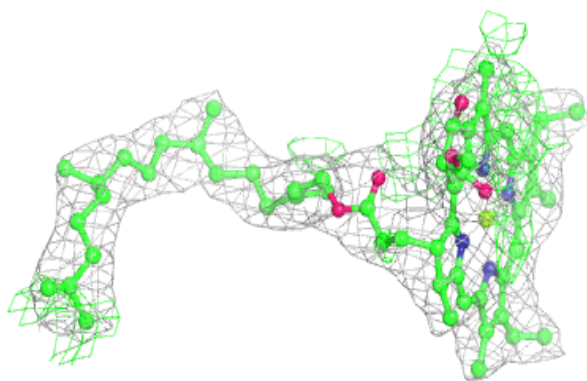
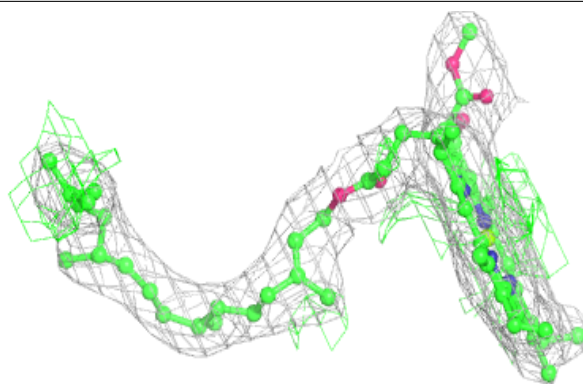
**Electron density around CLA Z 829:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

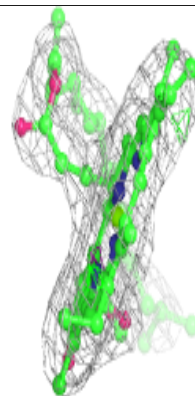
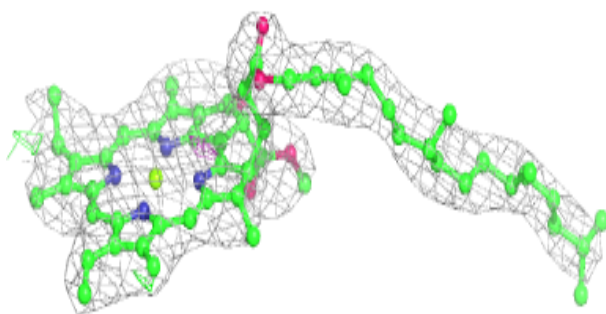
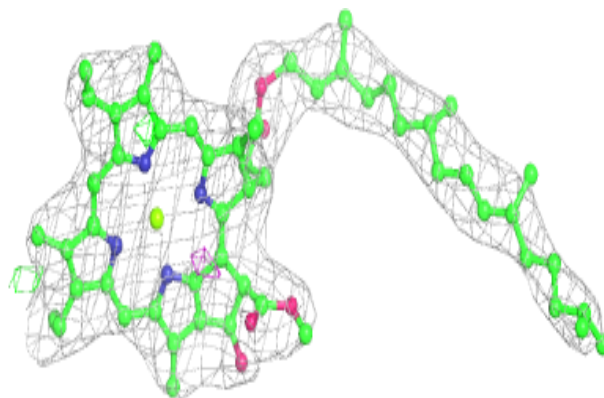


**Electron density around CLA B 840:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 822:**

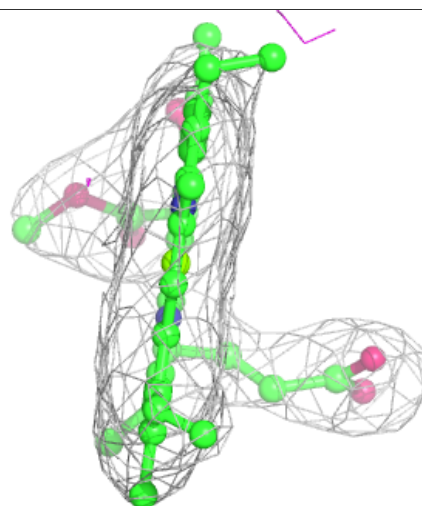
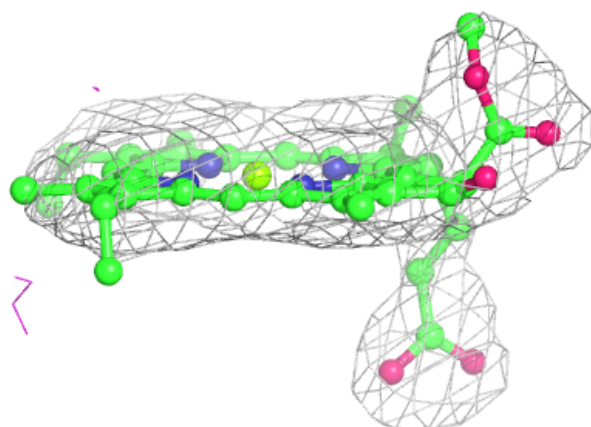
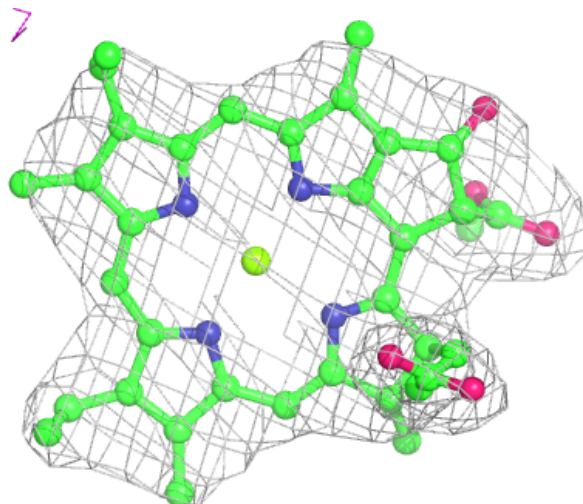
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





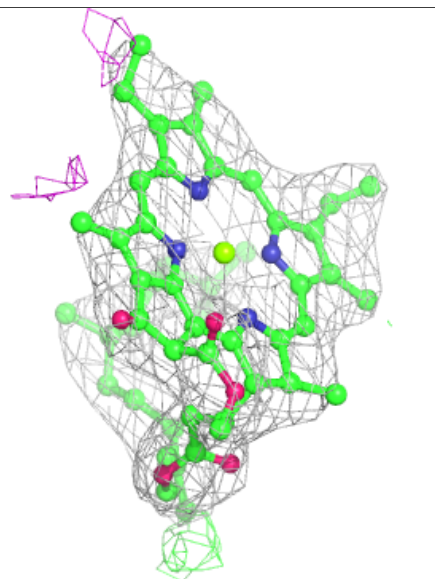
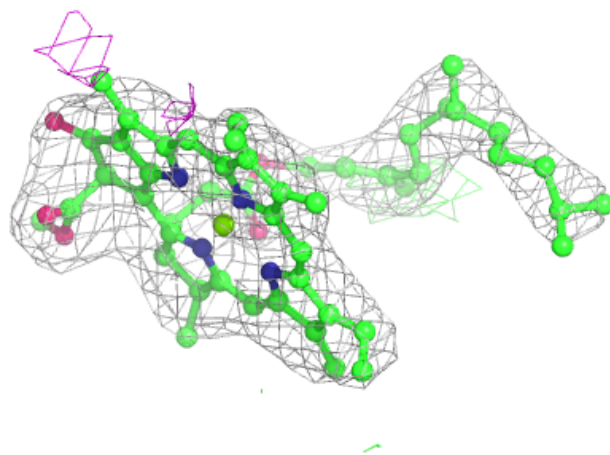
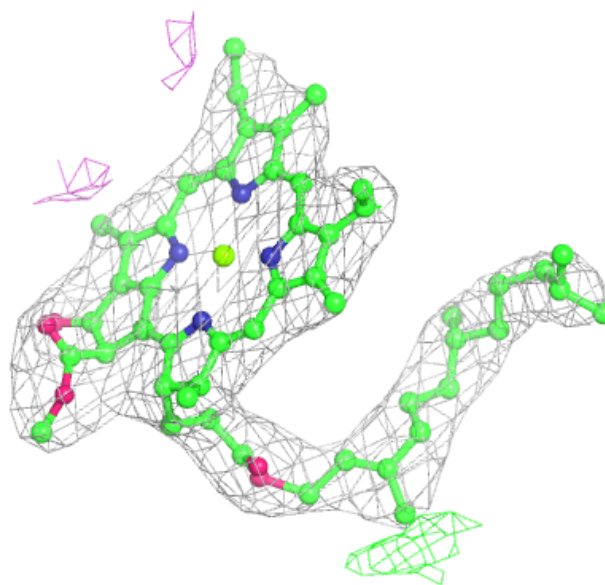
**Electron density around CLA H 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



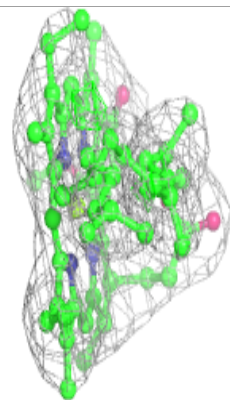
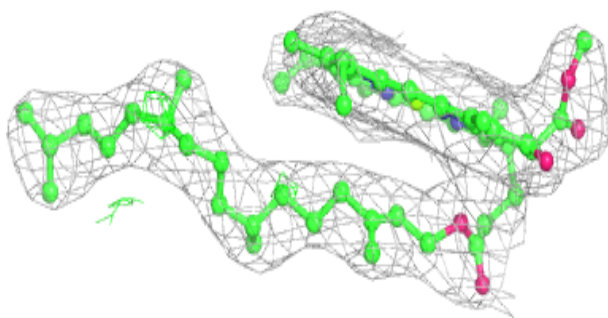
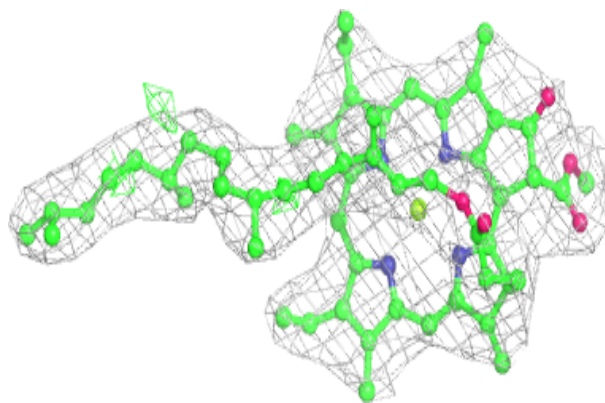
**Electron density around CLA Y 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

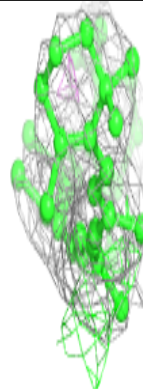
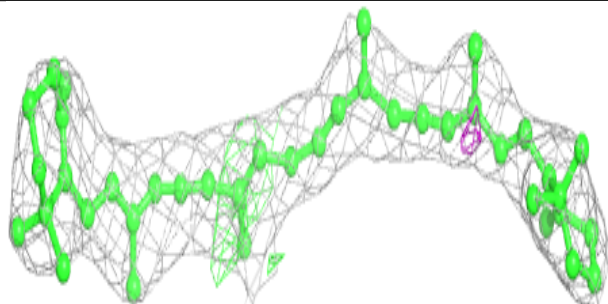
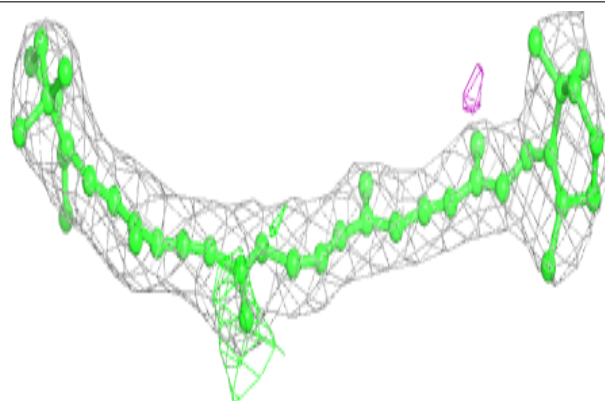


**Electron density around CLA A 837:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

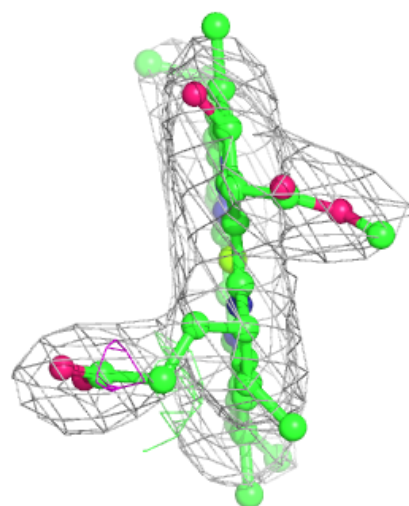
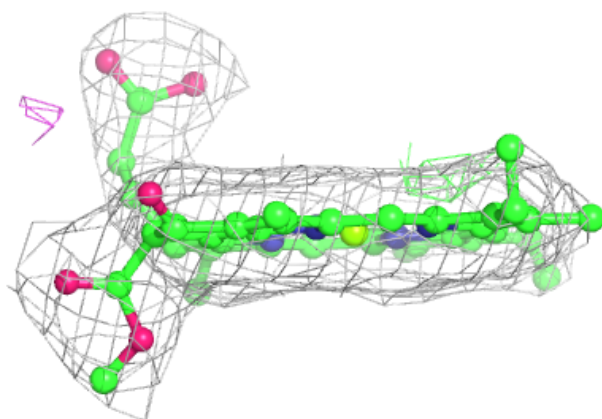
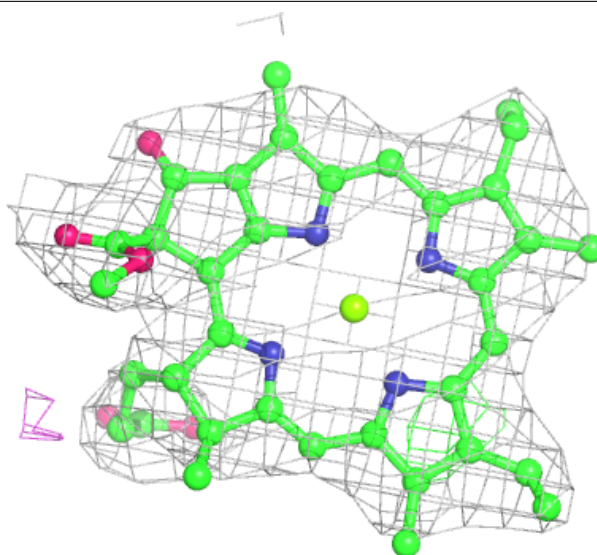
**Electron density around BCR Q 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



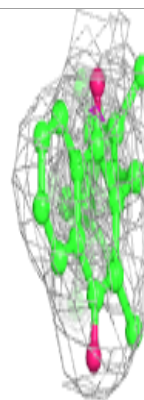
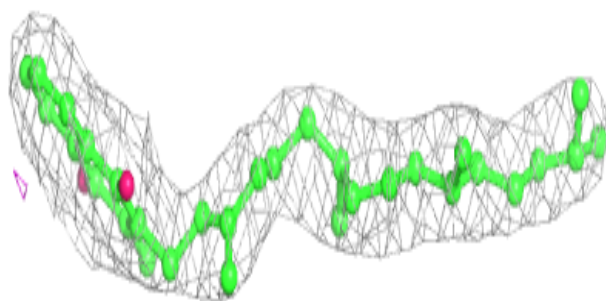
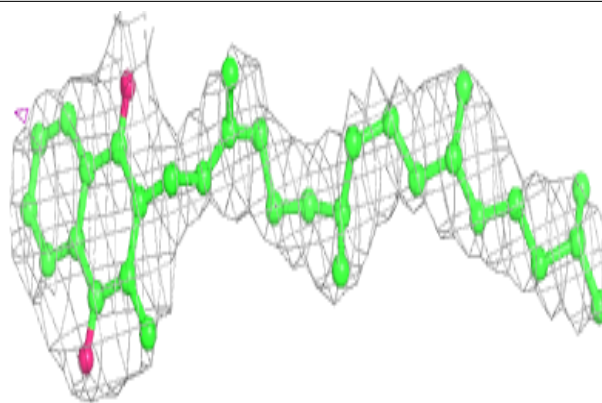
**Electron density around CLA H 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



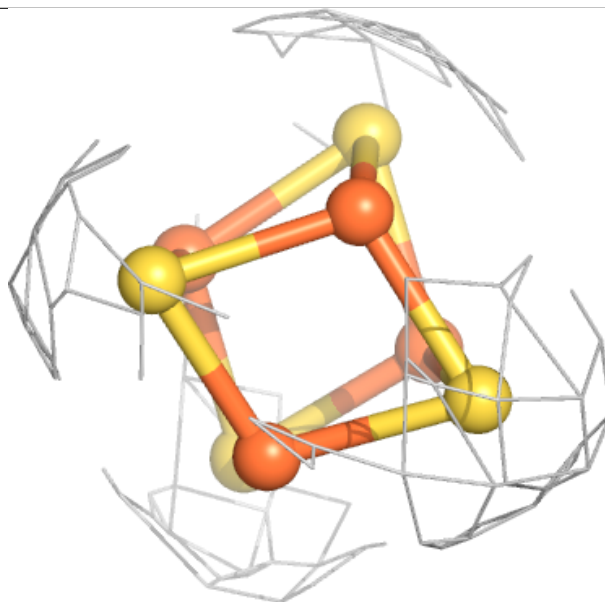
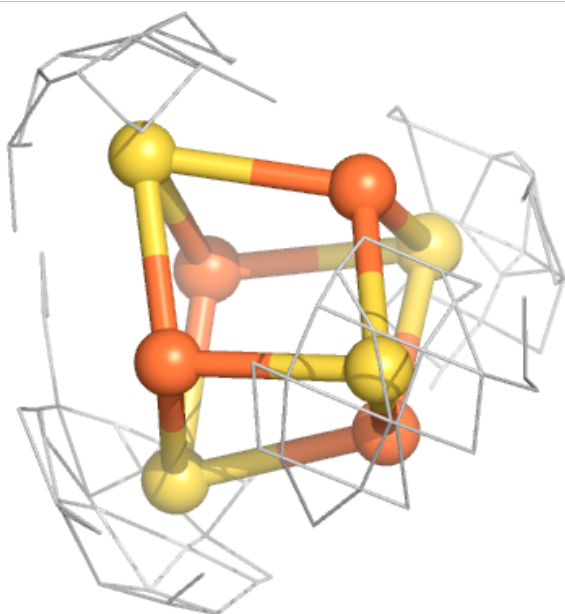
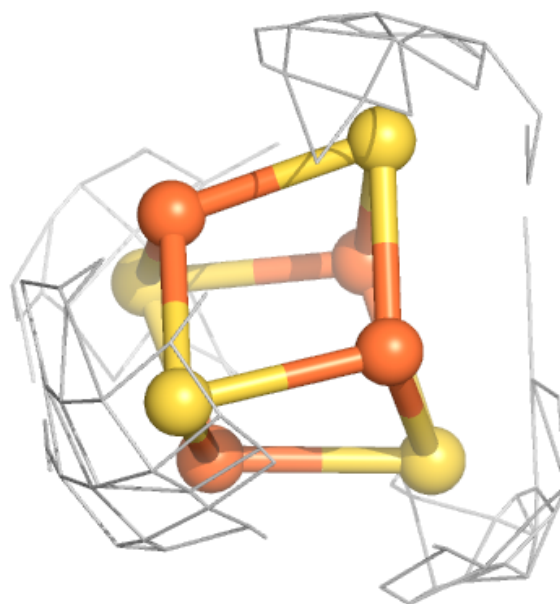
**Electron density around PQN Y 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SF4 a 102:**

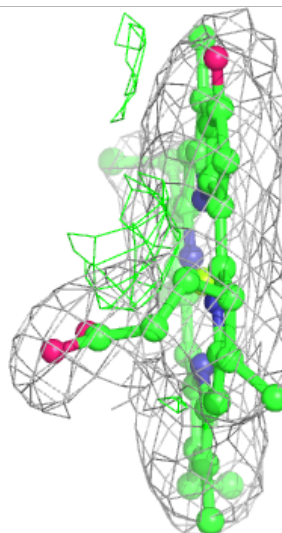
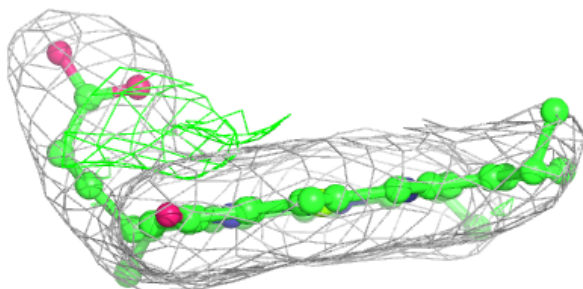
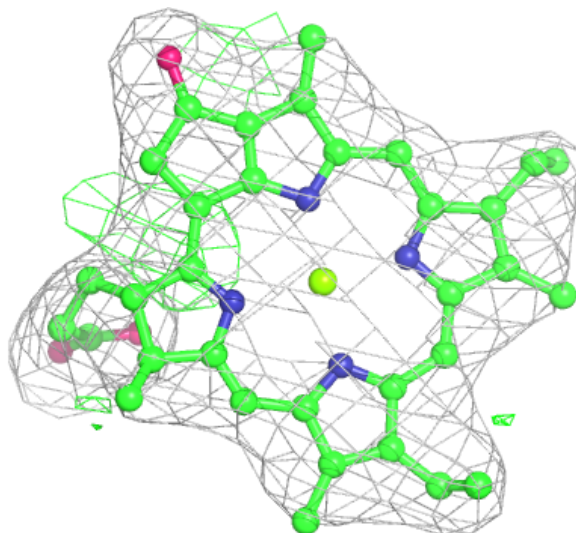
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





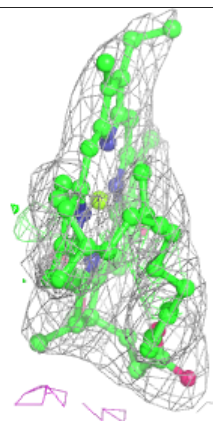
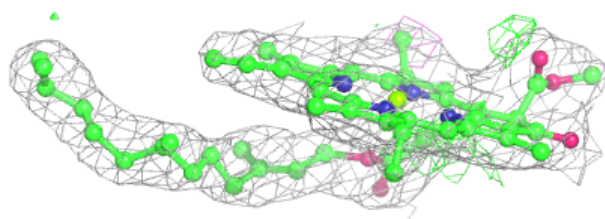
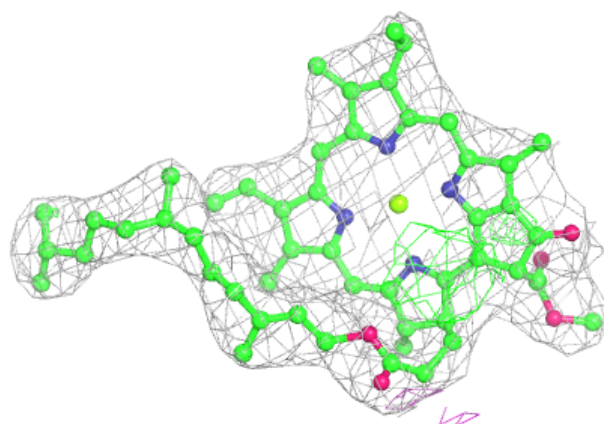
**Electron density around CLA g 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

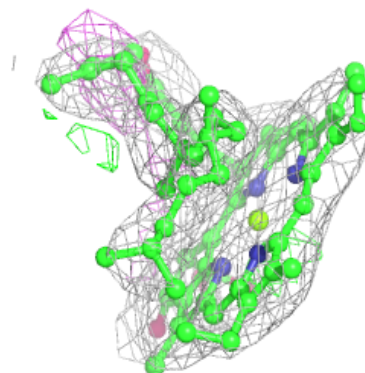
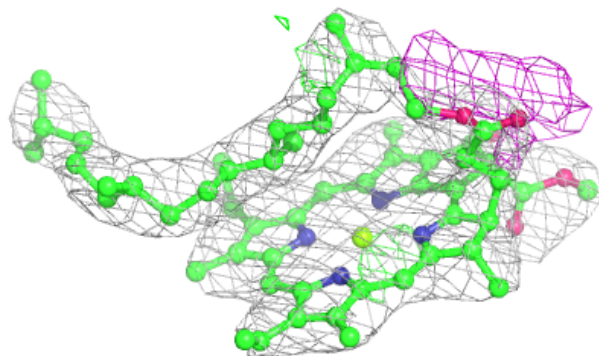
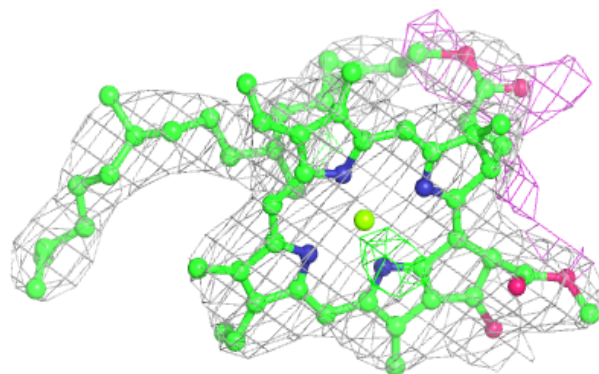


**Electron density around CLA B 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA H 816:**

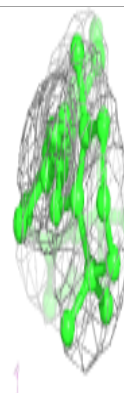
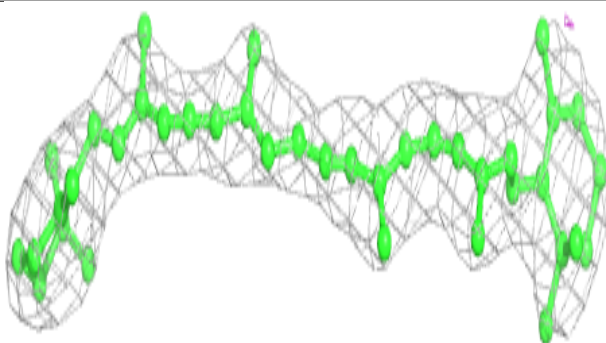
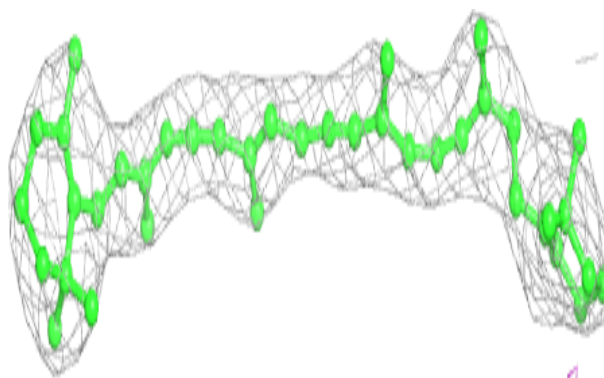
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



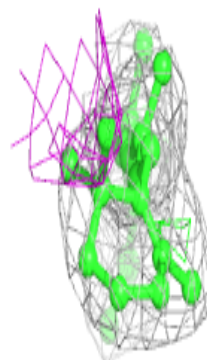
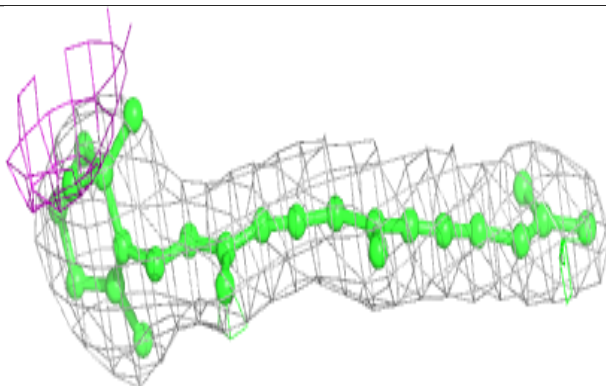
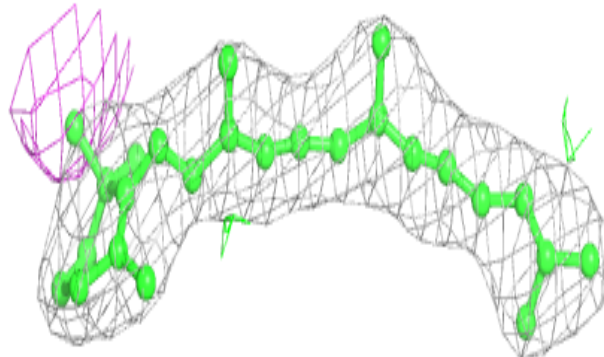


**Electron density around BCR T 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

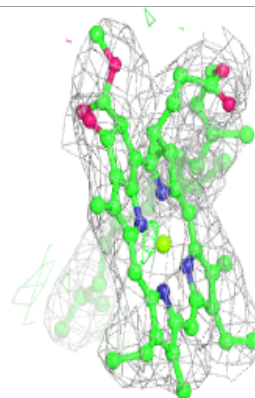
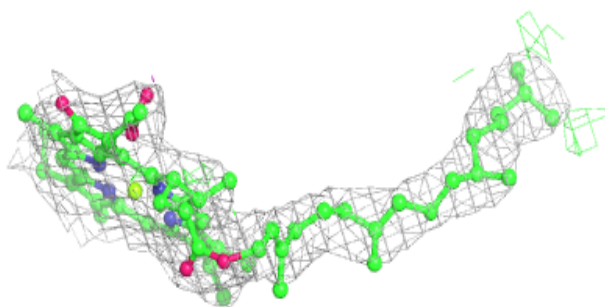
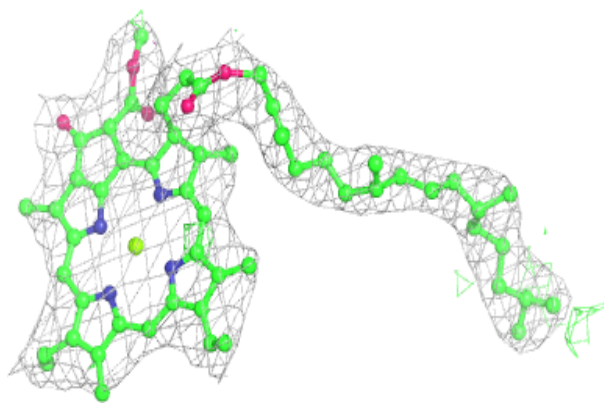
**Electron density around BCR B 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

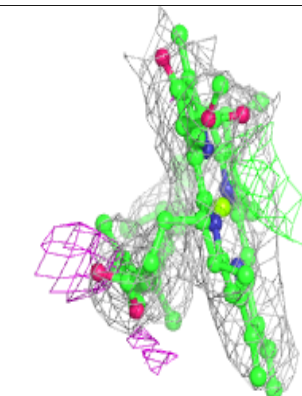
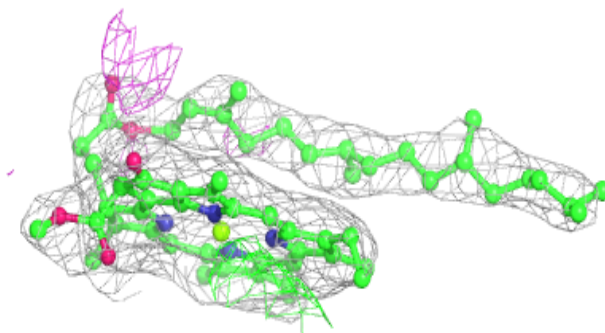
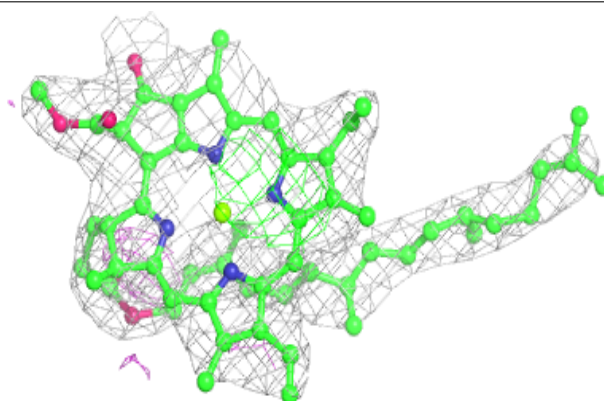


**Electron density around CLA G 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

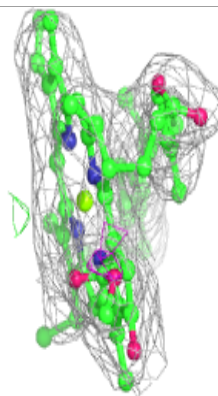
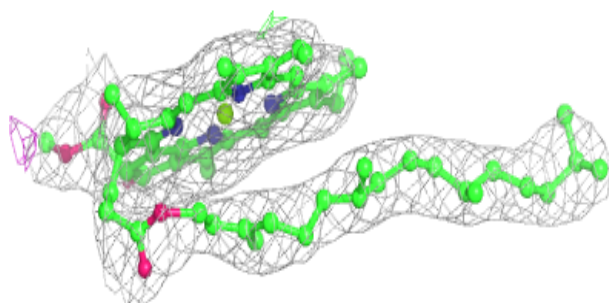
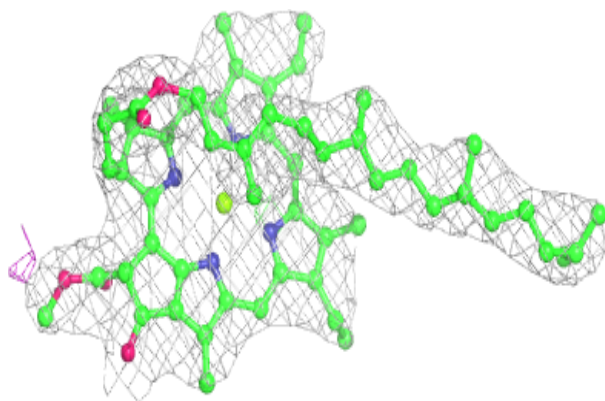
**Electron density around CLA G 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

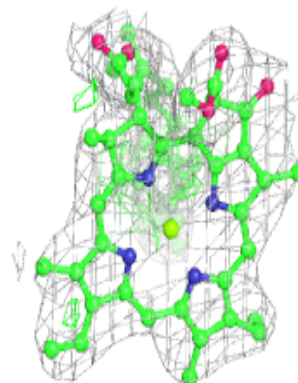
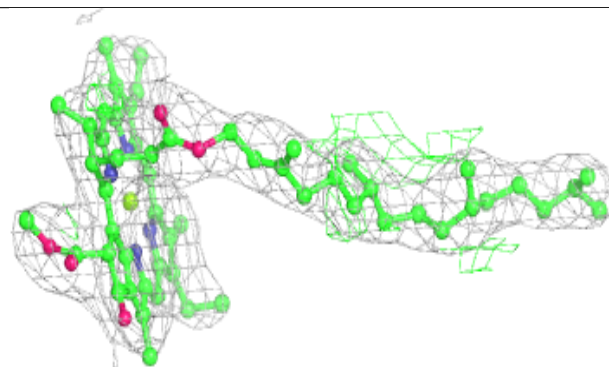
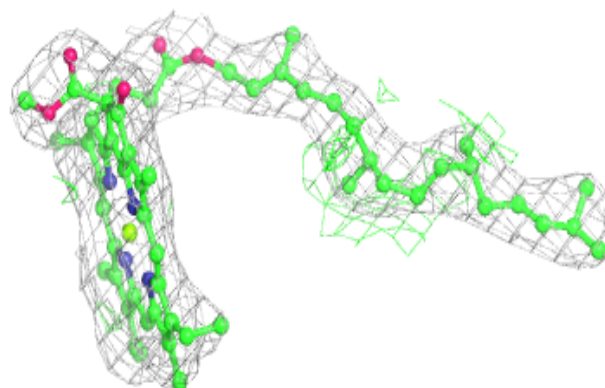


**Electron density around CLA A 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

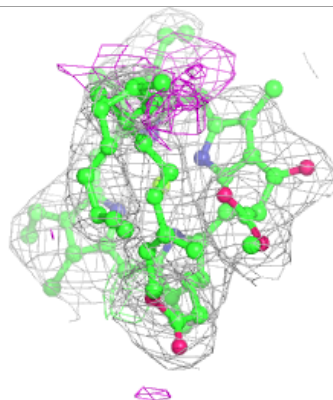
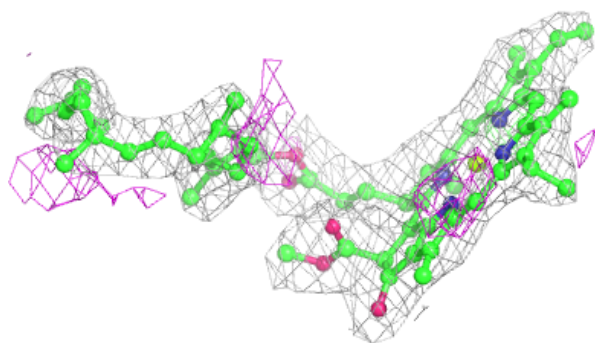
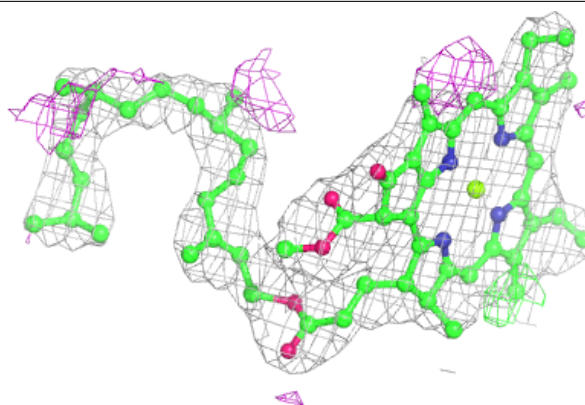
**Electron density around CLA Z 827:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

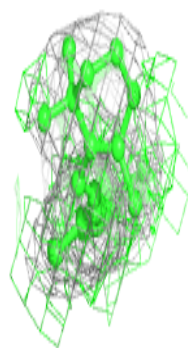
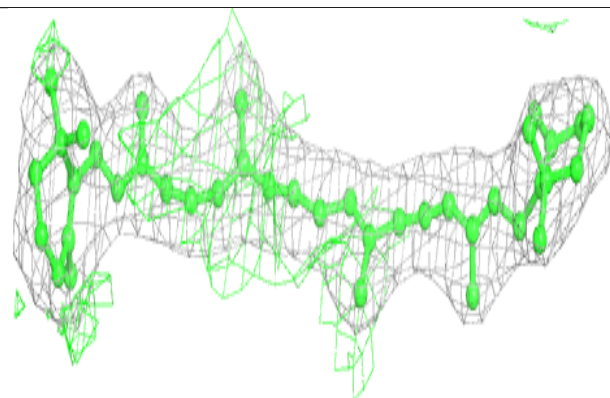
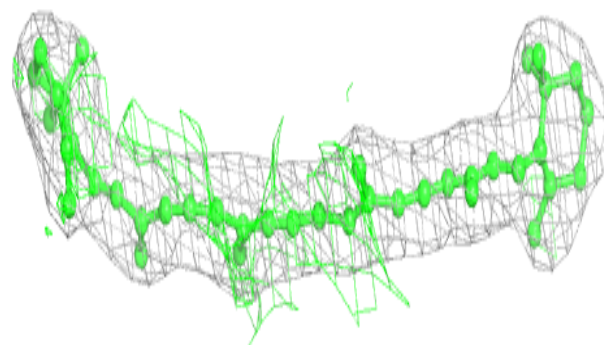


**Electron density around CL0 A 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR I 101:**

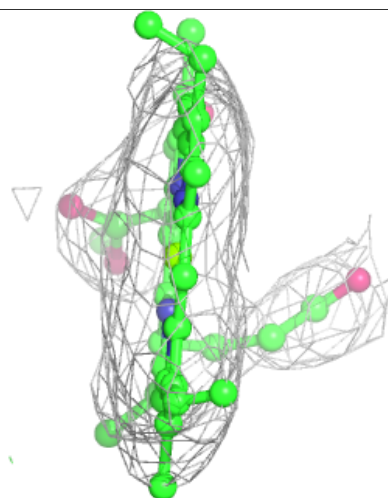
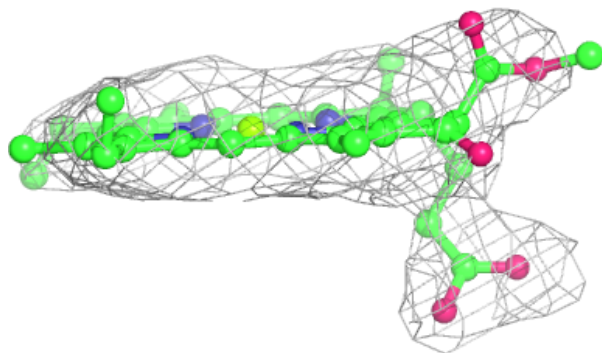
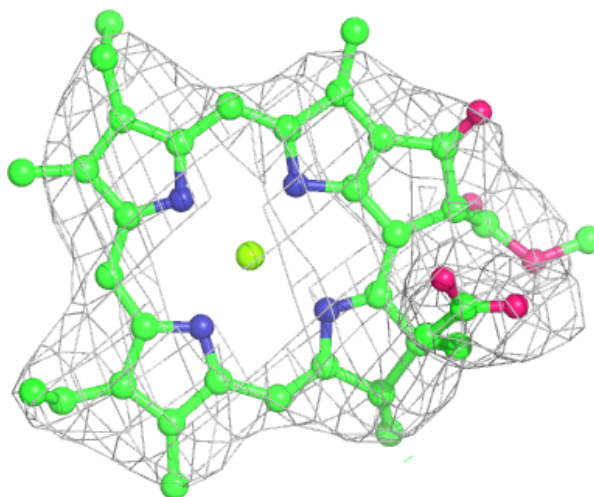
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





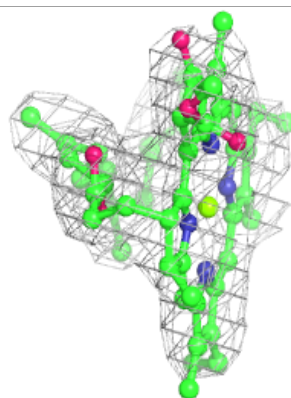
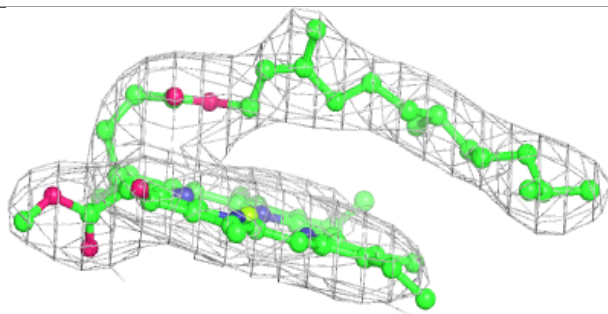
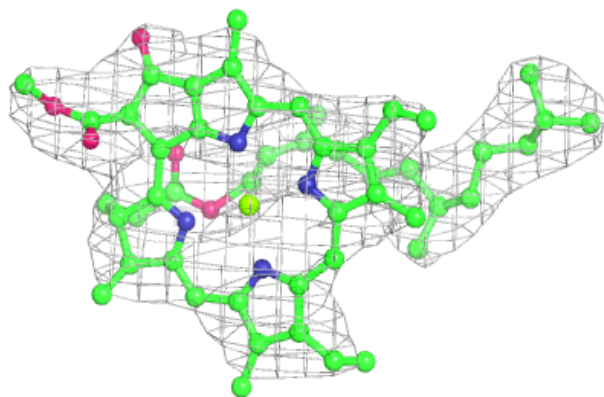
**Electron density around CLA f 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

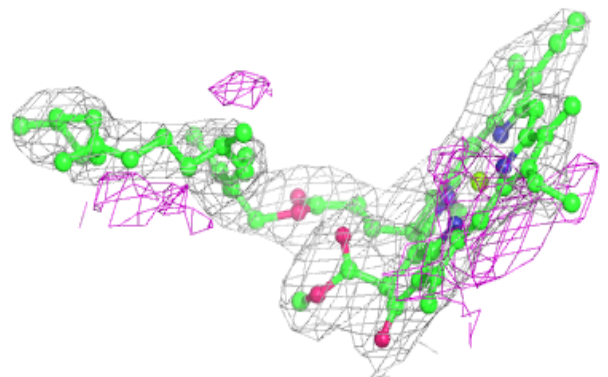
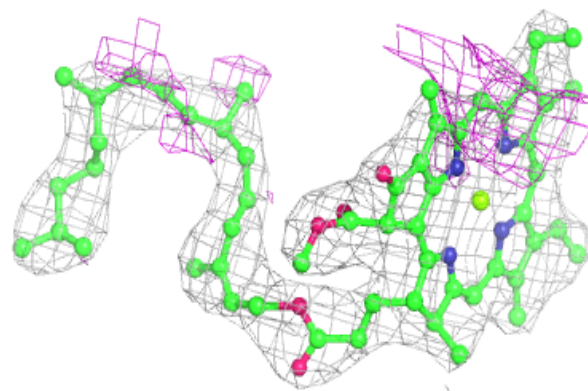


**Electron density around CLA Y 817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

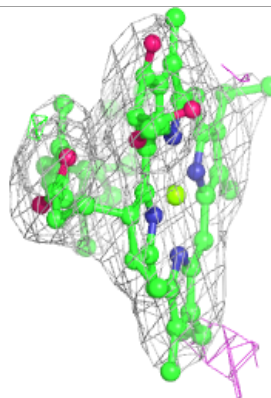
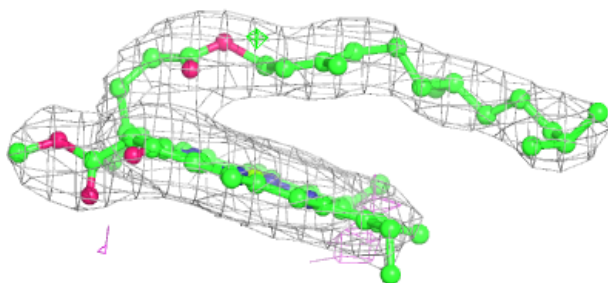
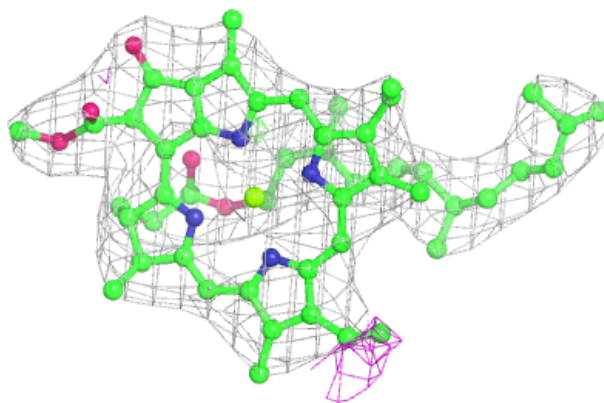
**Electron density around CL0 Y 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

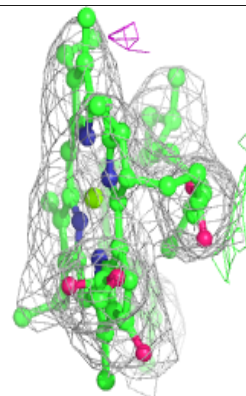
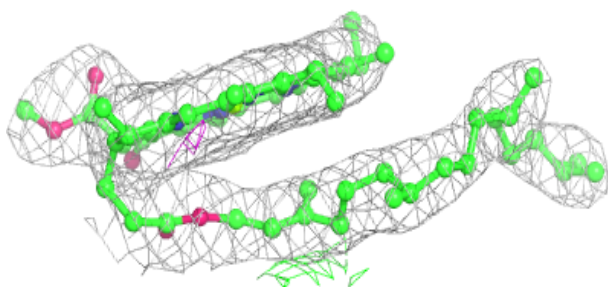
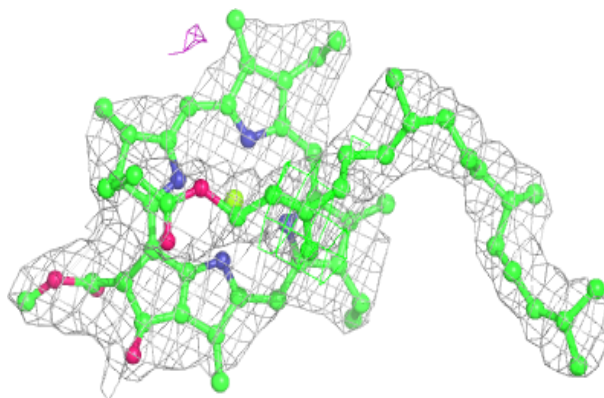


**Electron density around CLA A 817:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

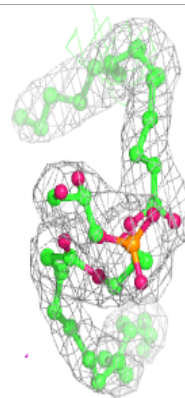
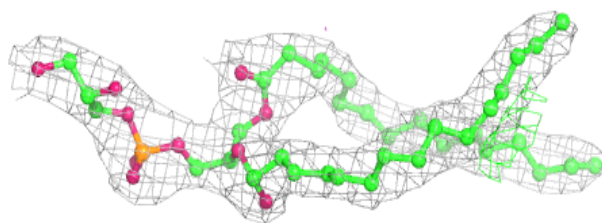
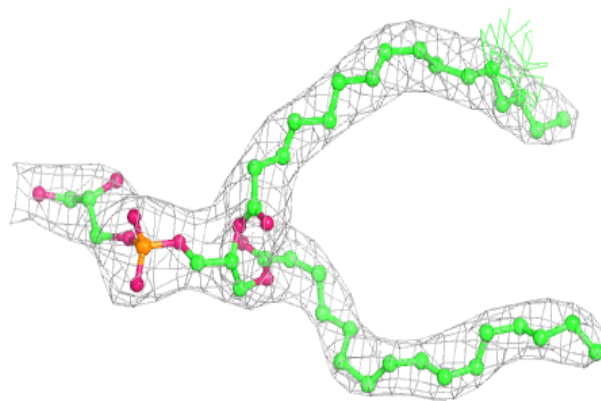
**Electron density around CLA Z 836:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG G 851:**

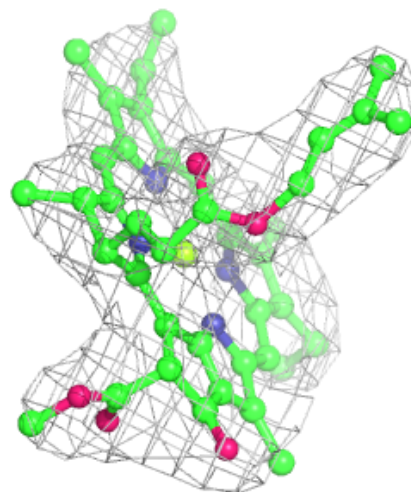
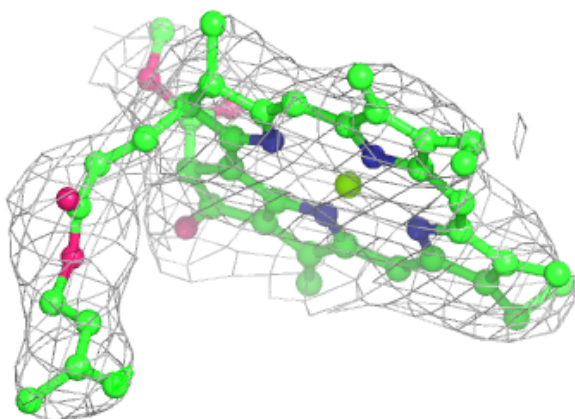
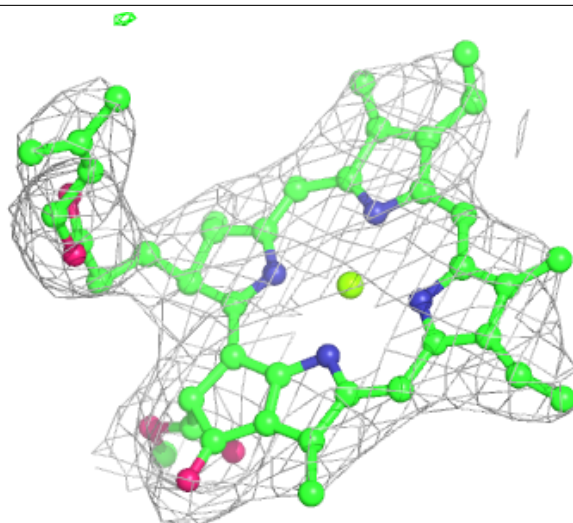
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





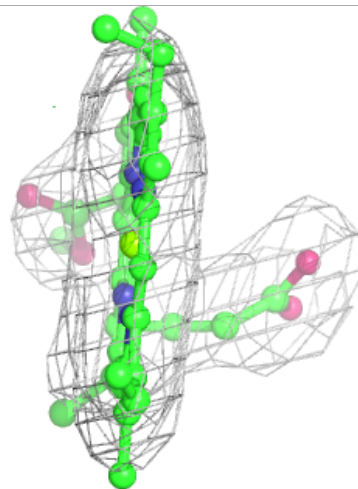
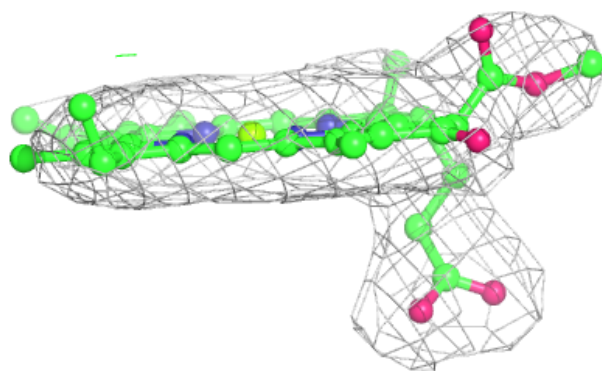
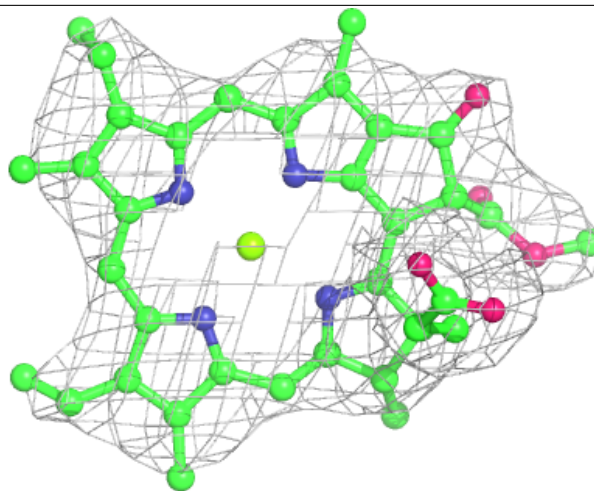
**Electron density around CLA G 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



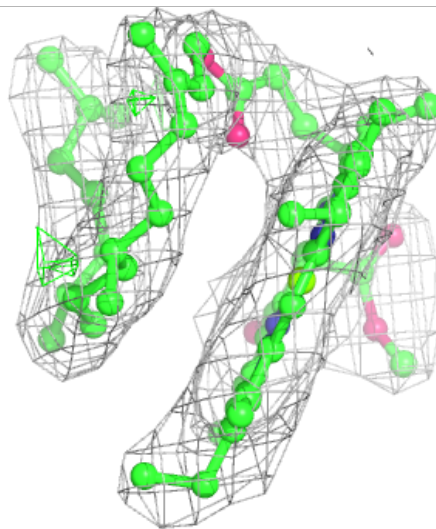
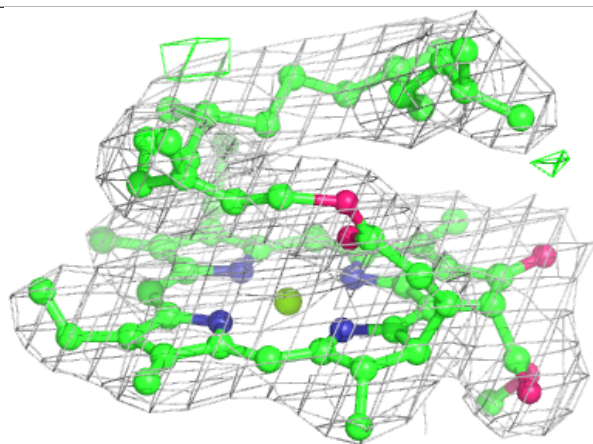
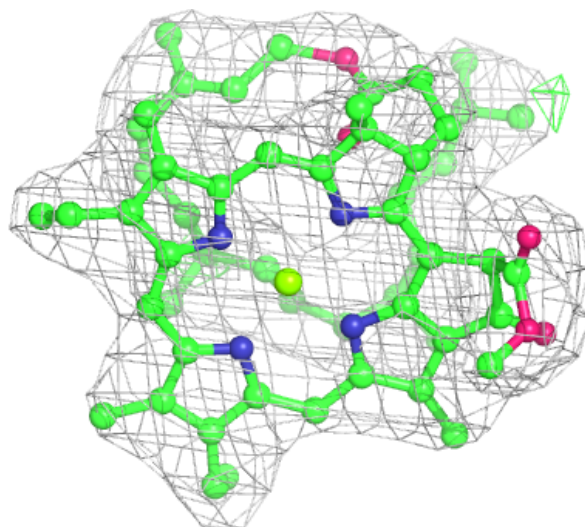
**Electron density around CLA A 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



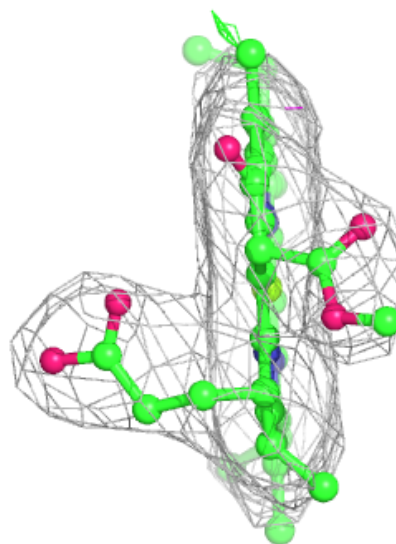
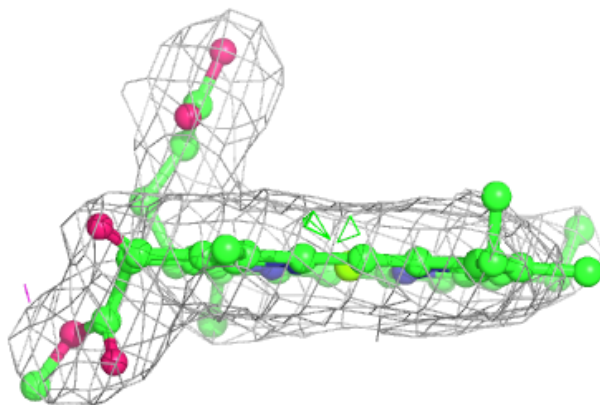
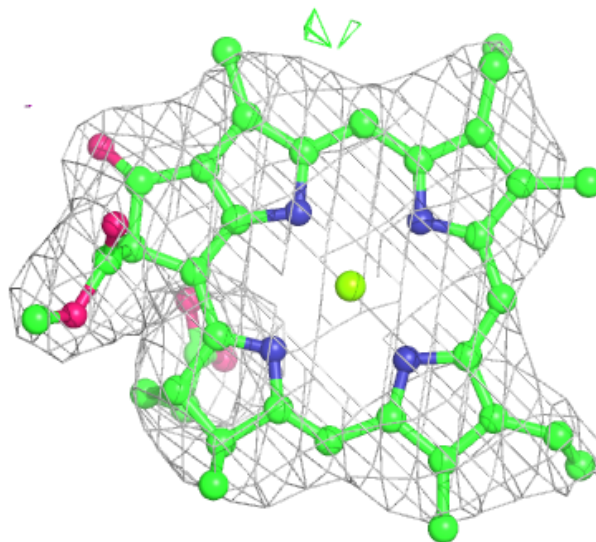
**Electron density around CLA h 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



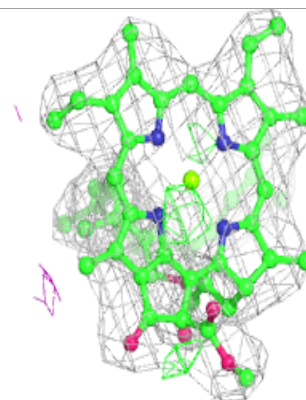
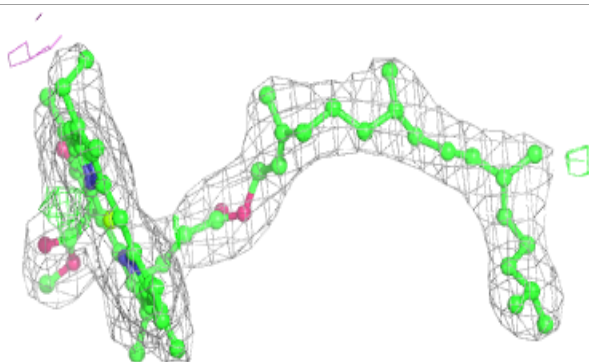
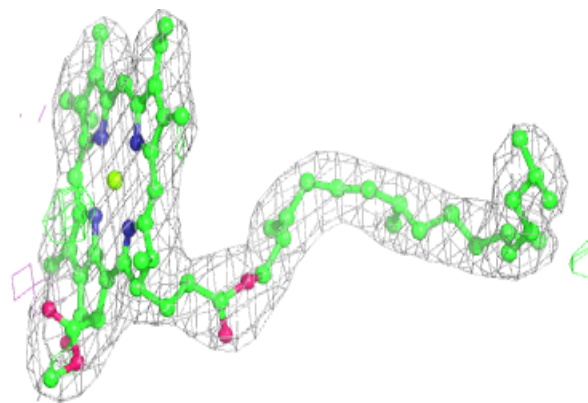
**Electron density around CLA Y 836:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

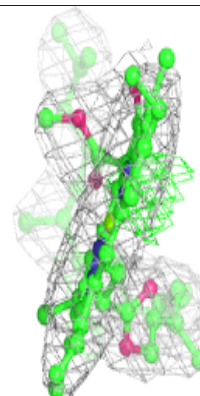
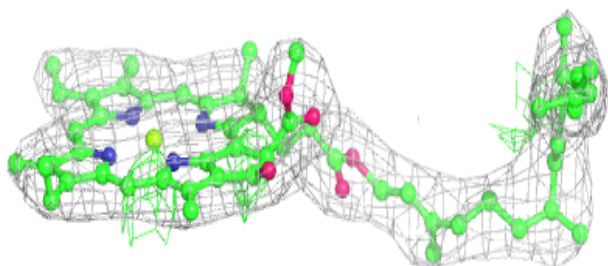
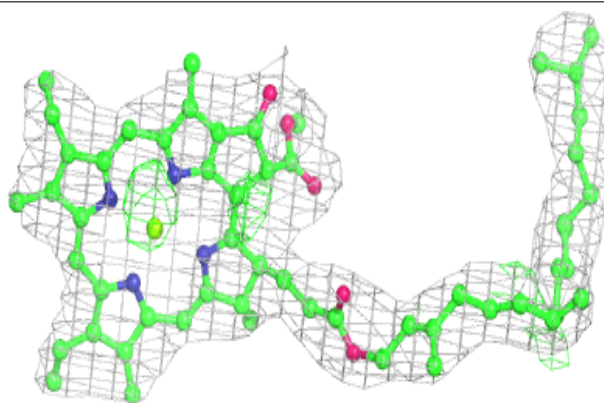


**Electron density around CLA h 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA H 825:**

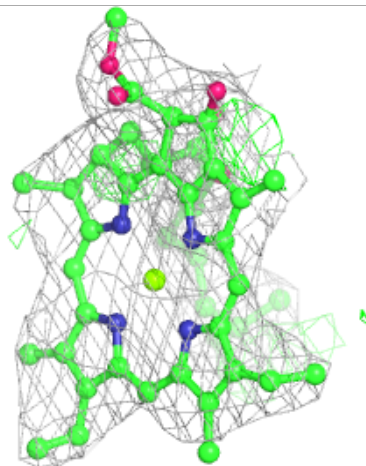
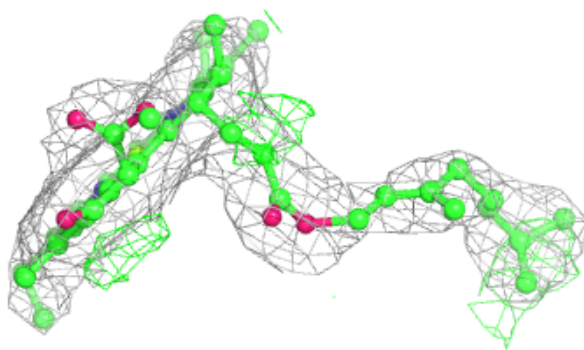
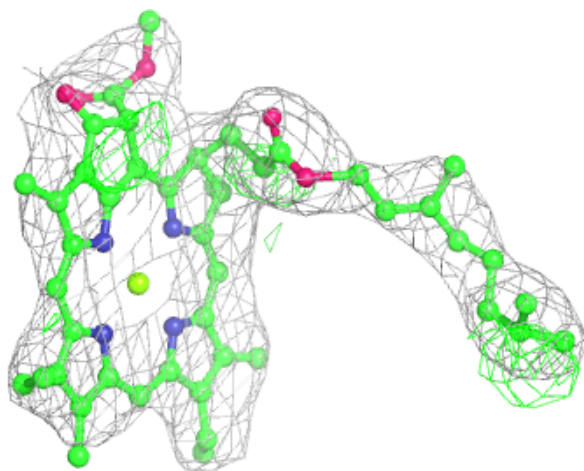
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





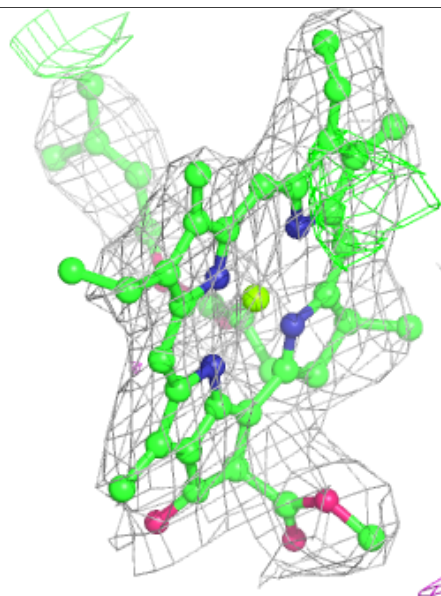
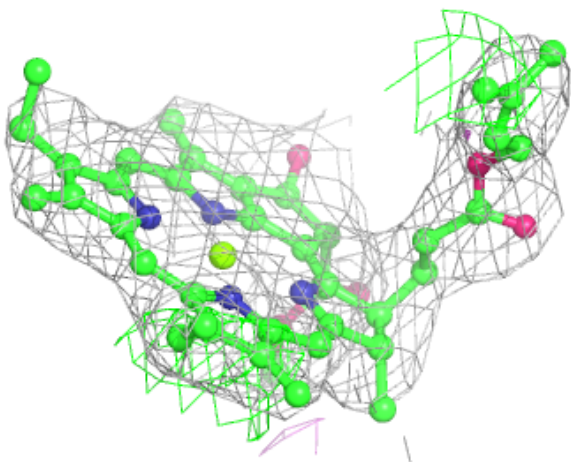
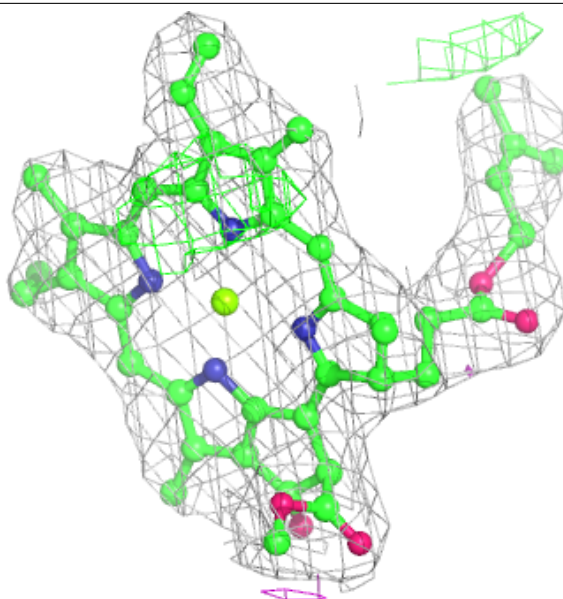
**Electron density around CLA A 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



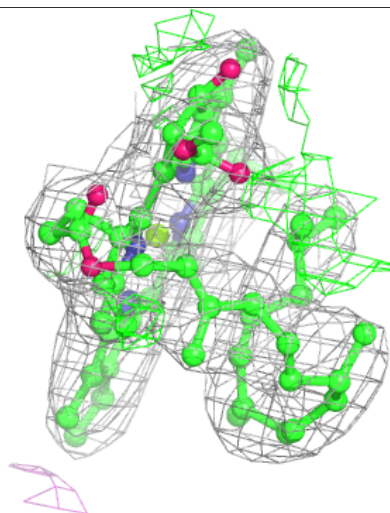
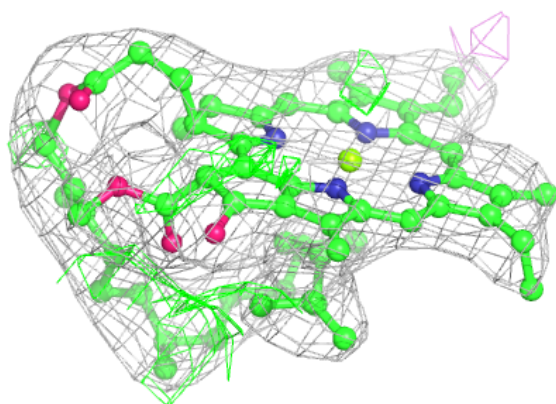
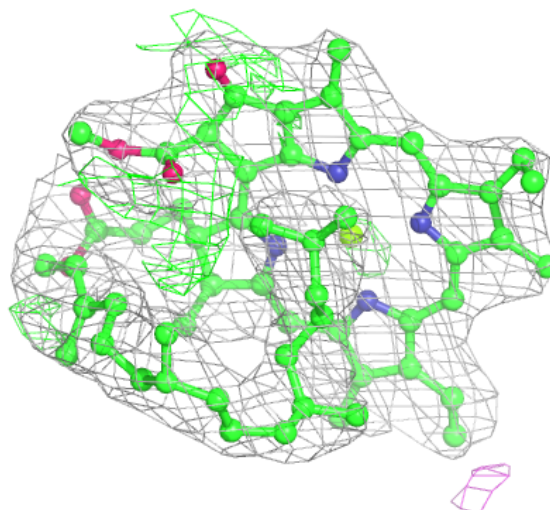
**Electron density around CLA Y 831:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Z 805:**

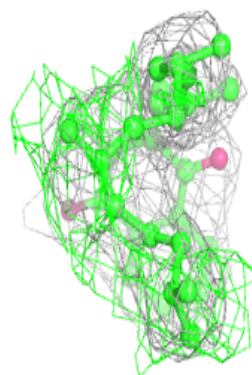
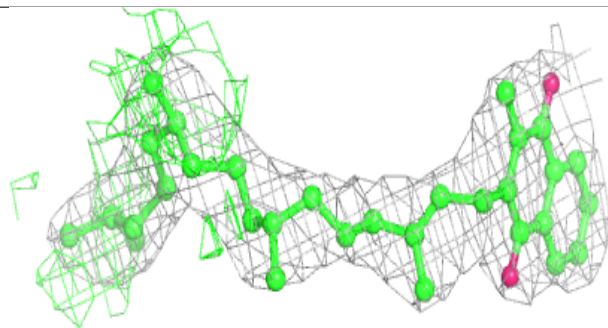
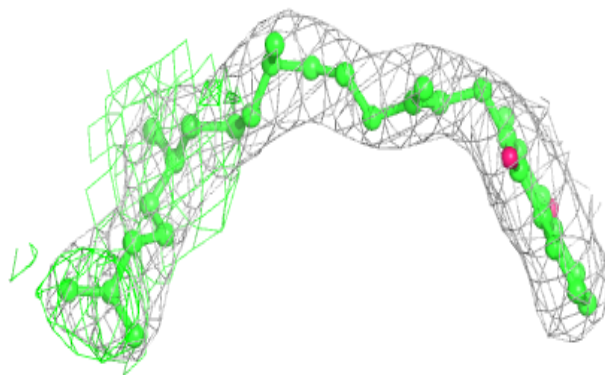
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



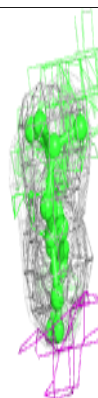
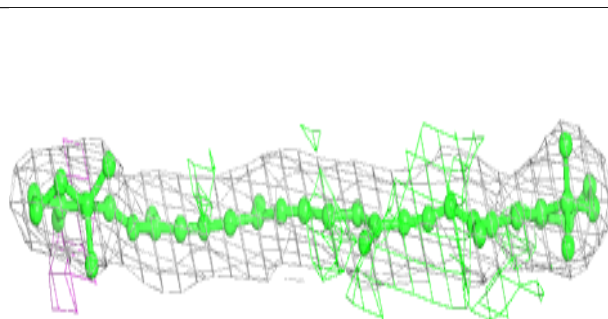
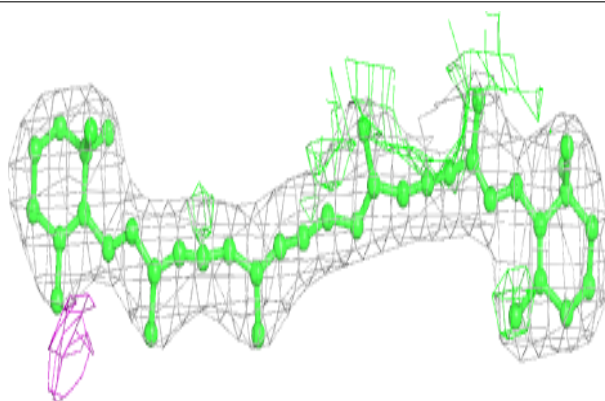


**Electron density around PQN Z 840:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

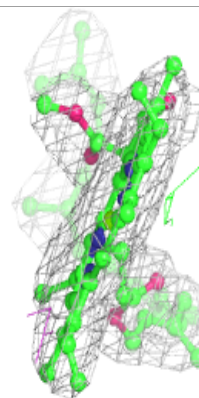
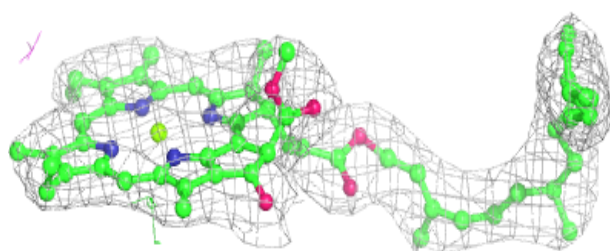
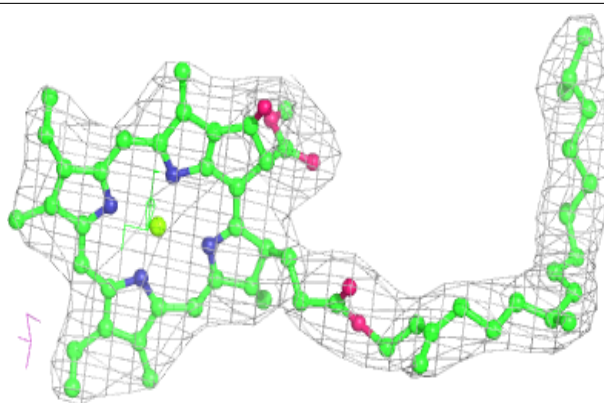
**Electron density around BCR R 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

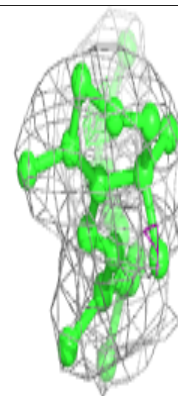
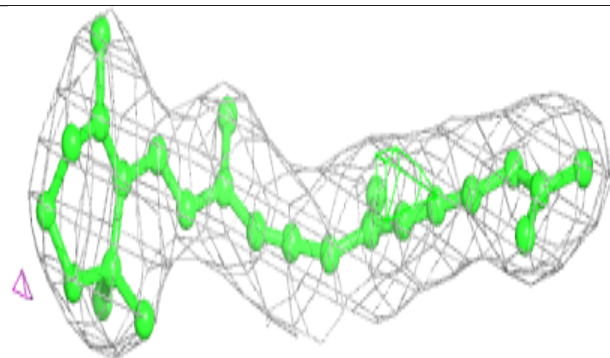
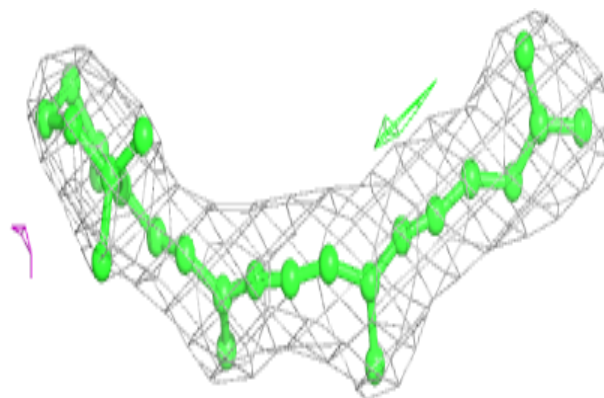


**Electron density around CLA Z 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

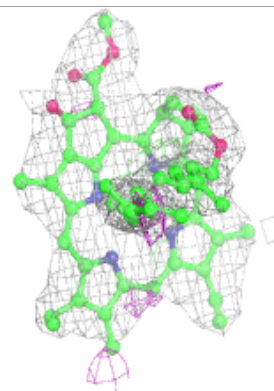
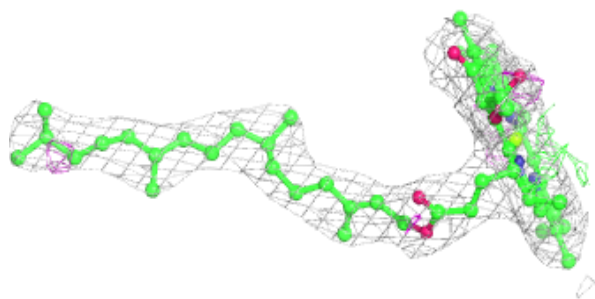
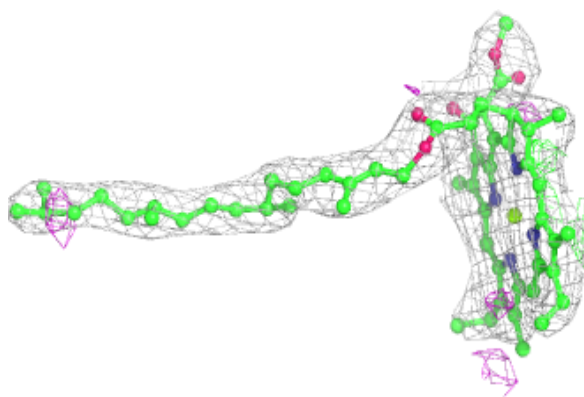
**Electron density around BCR Z 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

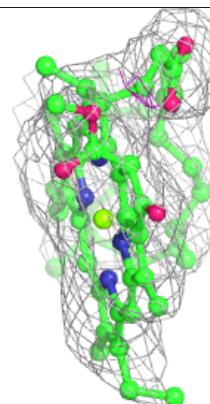
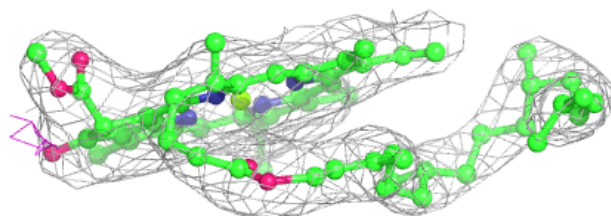
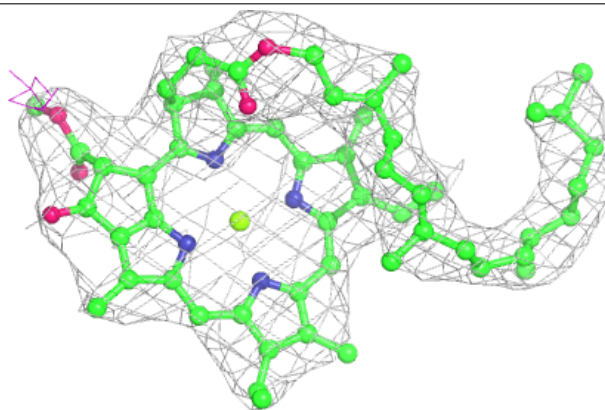


**Electron density around CLA B 828:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

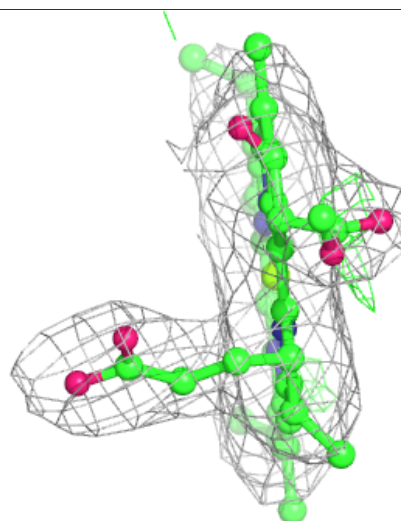
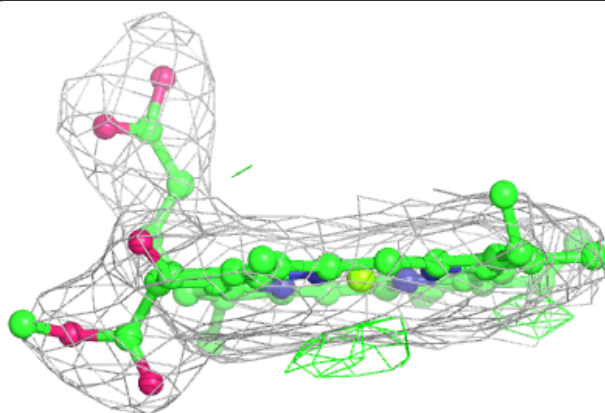
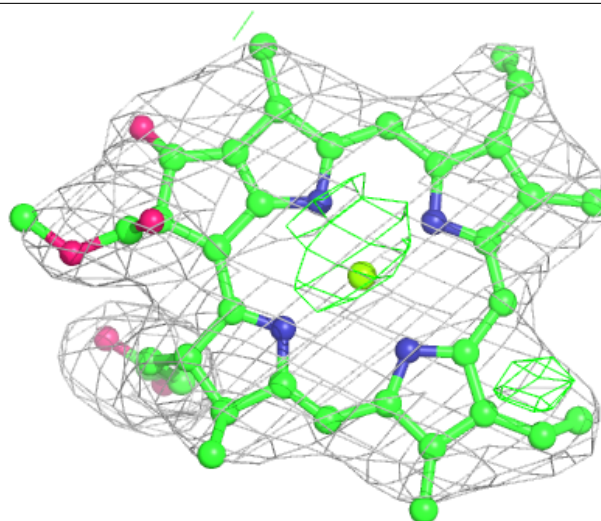
**Electron density around CLA G 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 835:**

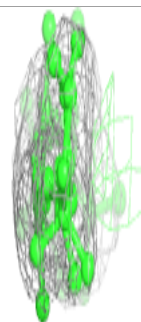
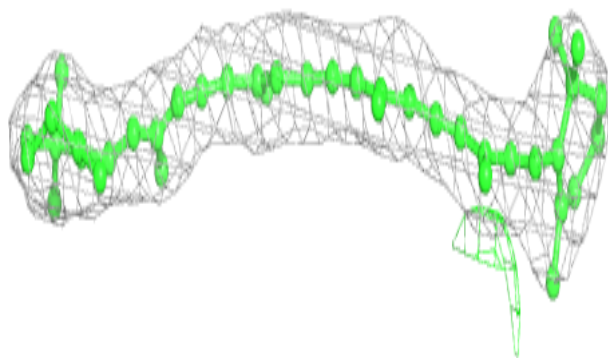
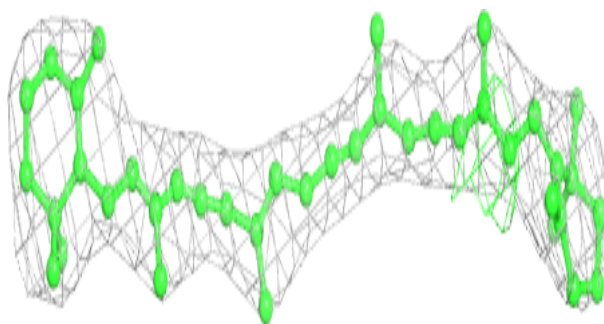
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



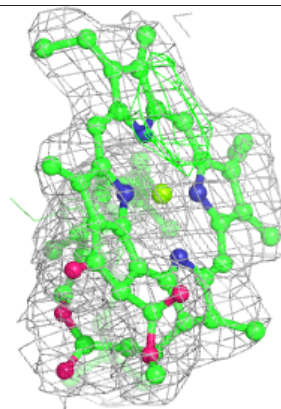
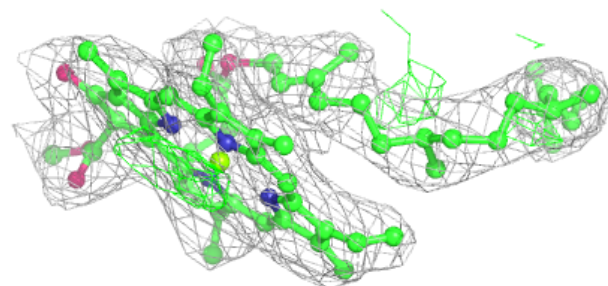
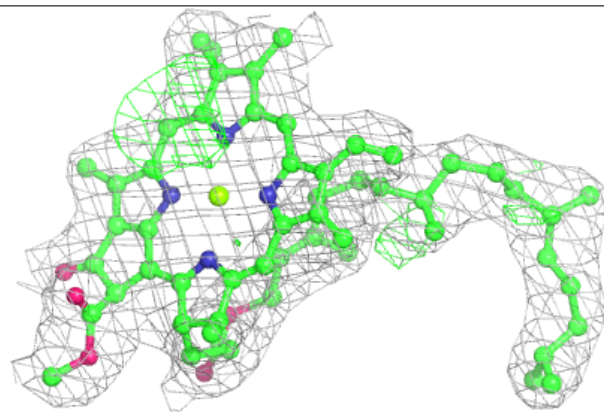


**Electron density around BCR H 848:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

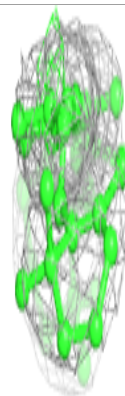
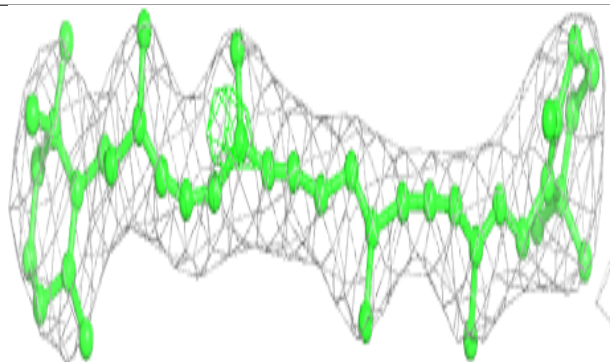
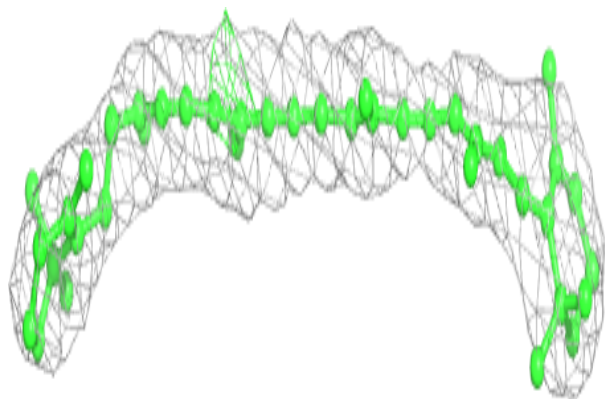
**Electron density around CLA G 842:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



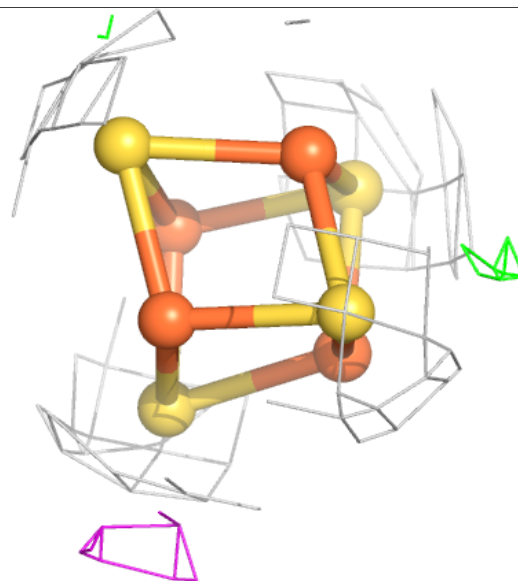
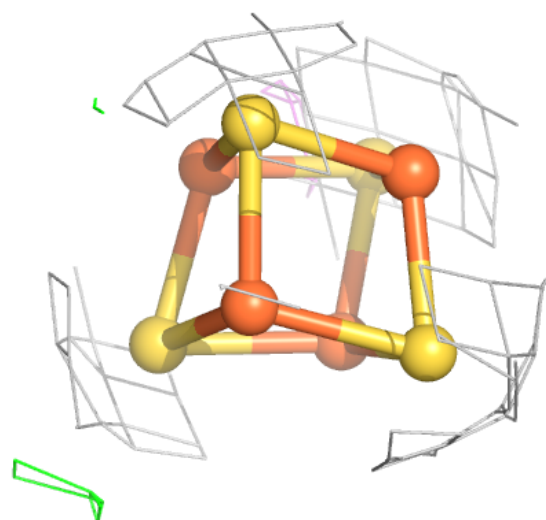
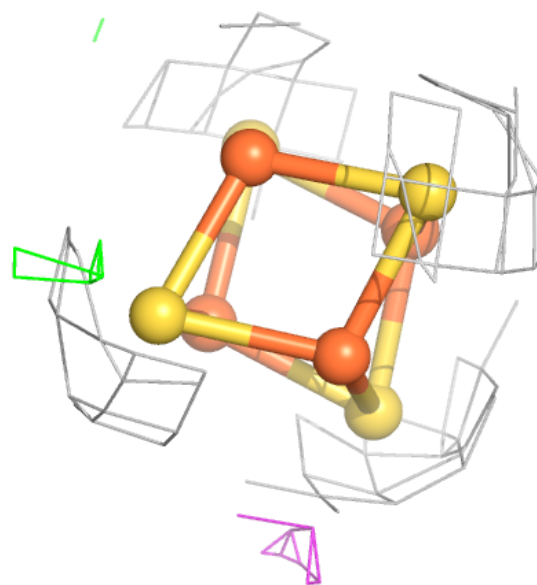
**Electron density around BCR K 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



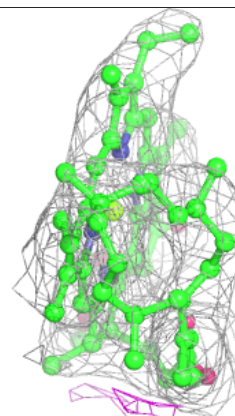
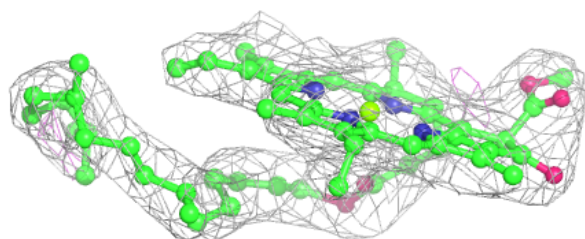
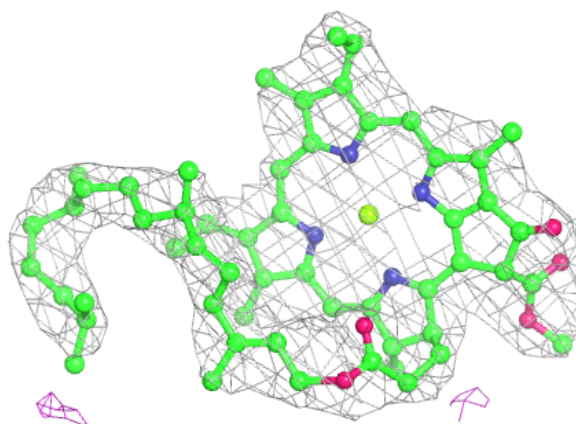
**Electron density around SF4 G 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

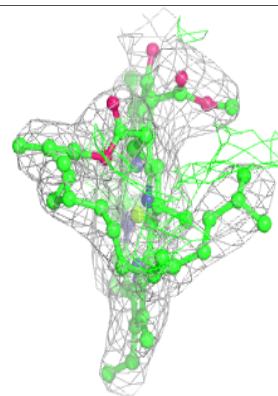
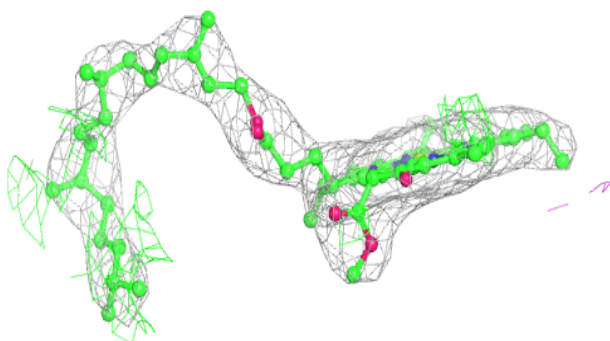
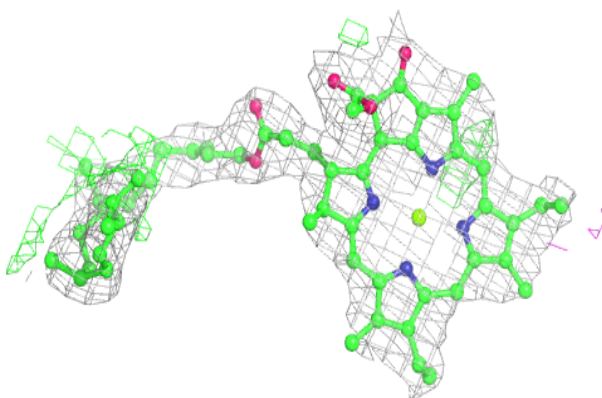


**Electron density around CLA Y 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 827:**

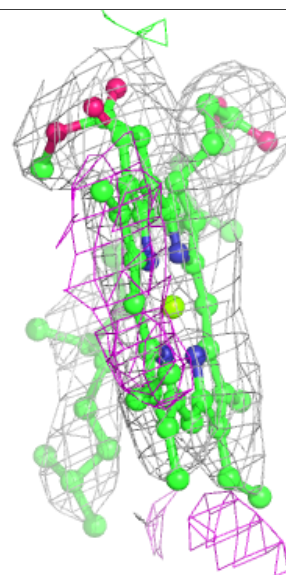
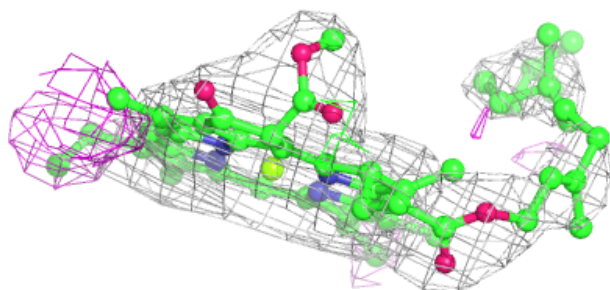
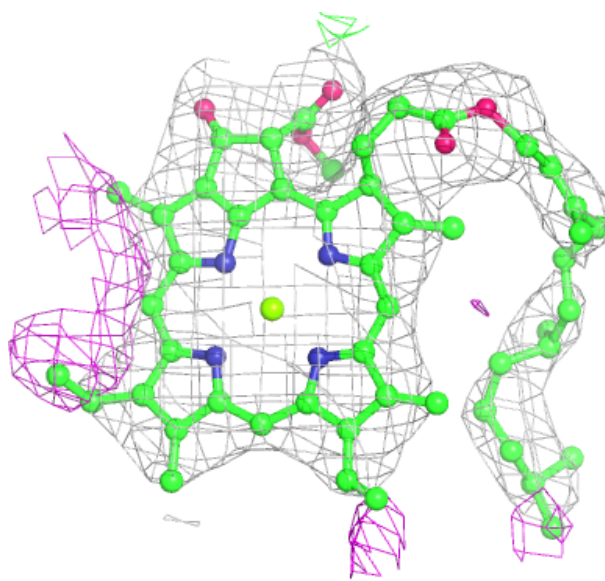
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





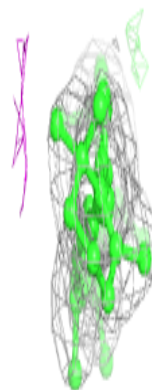
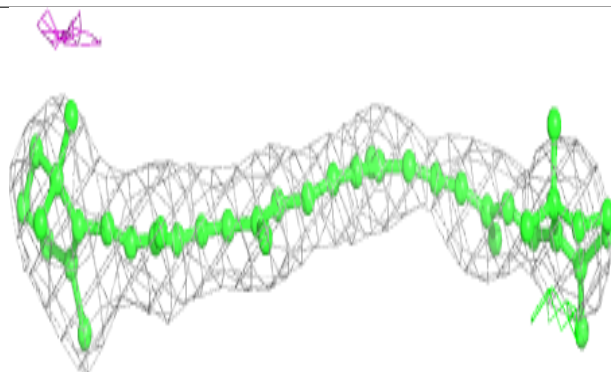
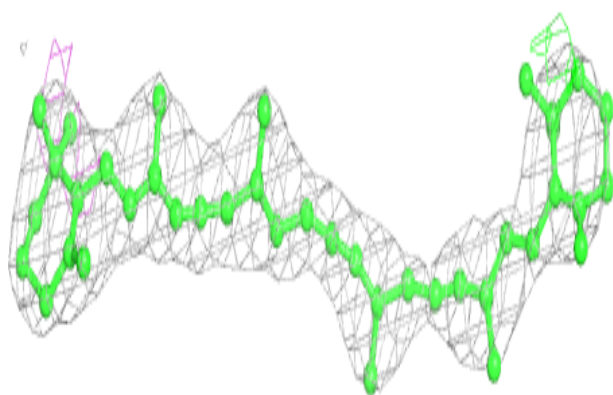
**Electron density around CLA A 813:**

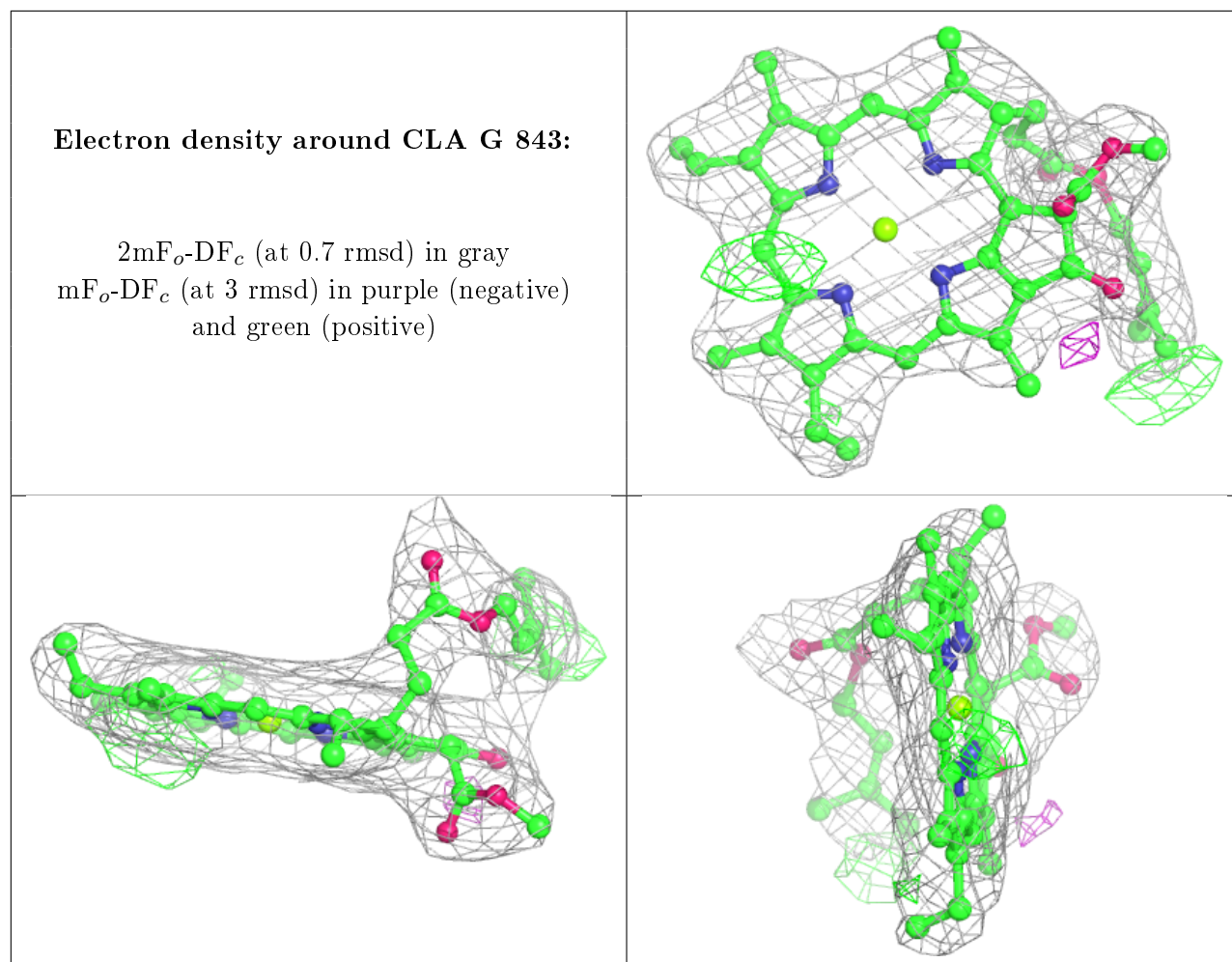
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR Y 849:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.