



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:28 pm BST

PDB ID : 2DYS
Title : Bovine heart cytochrome C oxidase modified by DCCD
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2006-09-16
Resolution : 2.20 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

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

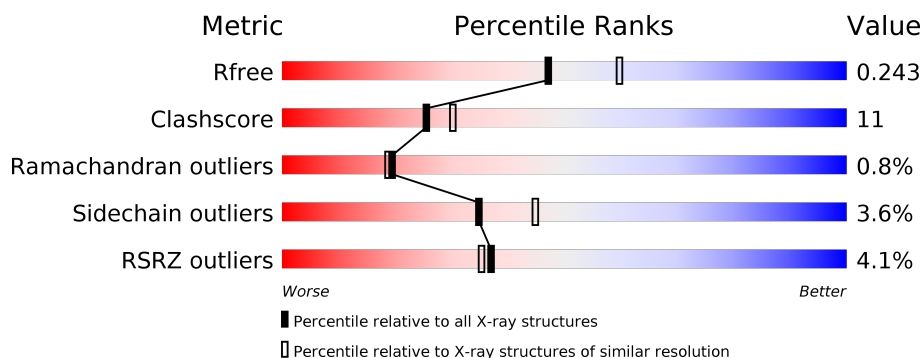
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 4898 (2.20-2.20) |
| Clashscore | 141614 | 5594 (2.20-2.20) |
| Ramachandran outliers | 138981 | 5503 (2.20-2.20) |
| Sidechain outliers | 138945 | 5504 (2.20-2.20) |
| RSRZ outliers | 127900 | 4800 (2.20-2.20) |

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 514 | <div> <div>84%</div> <div>15%</div> </div> |
| 1 | N | 514 | <div> <div>82%</div> <div>17%</div> <div>.</div> </div> |
| 2 | B | 227 | <div> <div>74%</div> <div>24%</div> <div>.</div> </div> |
| 2 | O | 227 | <div> <div>%</div> <div>67%</div> <div>29%</div> <div>.</div> </div> |
| 3 | C | 261 | <div> <div>82%</div> <div>16%</div> <div>.</div> </div> |
| 3 | P | 261 | <div> <div>84%</div> <div>15%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | D | 147 | |
| 4 | Q | 147 | |
| 5 | E | 109 | |
| 5 | R | 109 | |
| 6 | F | 98 | |
| 6 | S | 98 | |
| 7 | G | 85 | |
| 7 | T | 85 | |
| 8 | H | 85 | |
| 8 | U | 85 | |
| 9 | I | 73 | |
| 9 | V | 73 | |
| 10 | J | 59 | |
| 10 | W | 59 | |
| 11 | K | 56 | |
| 11 | X | 56 | |
| 12 | L | 47 | |
| 12 | Y | 47 | |
| 13 | M | 46 | |
| 13 | Z | 46 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17 | HEA | A | 604 | X | - | - | - |
| 17 | HEA | A | 605 | X | - | - | - |
| 17 | HEA | N | 604 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17 | HEA | N | 605 | X | - | - | - |
| 20 | TGL | L | 101 | - | - | X | - |
| 21 | PSC | B | 303 | - | - | X | - |
| 21 | PSC | O | 304 | - | - | X | - |
| 22 | CHD | C | 310 | X | - | - | - |
| 22 | CHD | J | 101 | X | - | - | - |
| 22 | CHD | P | 310 | X | - | - | - |
| 22 | CHD | W | 101 | X | - | - | - |
| 23 | DCW | C | 301 | - | - | X | - |
| 24 | DMU | C | 302 | X | - | - | X |
| 24 | DMU | M | 101 | X | - | - | - |
| 24 | DMU | P | 302 | X | - | - | X |
| 24 | DMU | Z | 101 | X | - | - | - |
| 26 | PEK | G | 102 | - | - | - | X |
| 26 | PEK | T | 101 | - | - | - | X |
| 27 | CDL | T | 102 | - | - | X | - |
| 9 | SAC | V | 1 | - | X | - | X |

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32170 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 Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4027 | 2691 | 623 | 678 | 35 | | | |
| 1 | N | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4027 | 2691 | 623 | 678 | 35 | | | |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 227 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1185 | 281 | 340 | 18 | | | |
| 2 | O | 227 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1185 | 281 | 340 | 18 | | | |

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 259 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2109 | 1412 | 336 | 349 | 12 | | | |
| 3 | P | 259 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2109 | 1412 | 336 | 349 | 12 | | | |

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 777 | 196 | 218 | 4 | | | |
| 4 | Q | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 777 | 196 | 218 | 4 | | | |

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 852 | 544 | 144 | 162 | 2 | | | |
| 5 | R | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 852 | 544 | 144 | 162 | 2 | | | |

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 748 | 464 | 134 | 145 | 5 | | | |
| 6 | S | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 748 | 464 | 134 | 145 | 5 | | | |

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 84 | Total | C | N | O | P | S | 0 | 0 |
| | | | 675 | 431 | 129 | 113 | 1 | 1 | | |
| 7 | T | 84 | Total | C | N | O | P | S | 0 | 0 |
| | | | 675 | 431 | 129 | 113 | 1 | 1 | | |

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 417 | 121 | 119 | 5 | | | |
| 8 | U | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 417 | 121 | 119 | 5 | | | |

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | I | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 601 | 390 | 107 | 100 | 4 | | | |
| 9 | V | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 601 | 390 | 107 | 100 | 4 | | | |

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | J | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 297 | 78 | 82 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | W | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 297 | 78 | 82 | 3 | | | |

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | K | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |
| 11 | X | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | L | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 380 | 254 | 64 | 60 | 2 | | | |
| 12 | Y | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 380 | 254 | 64 | 60 | 2 | | | |

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13 | M | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |
| 13 | Z | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | N | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

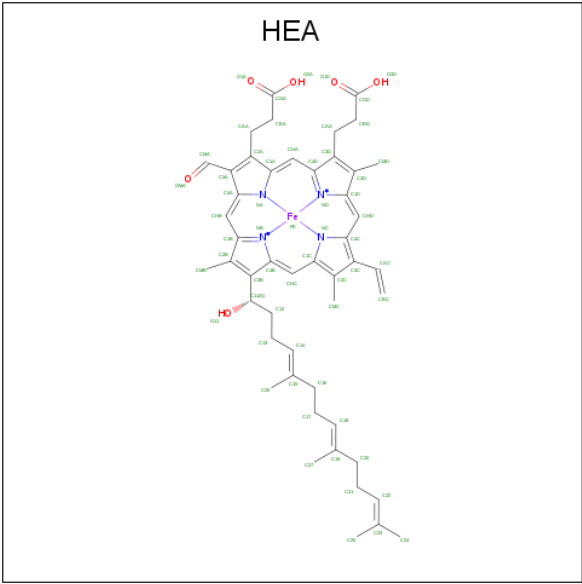
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

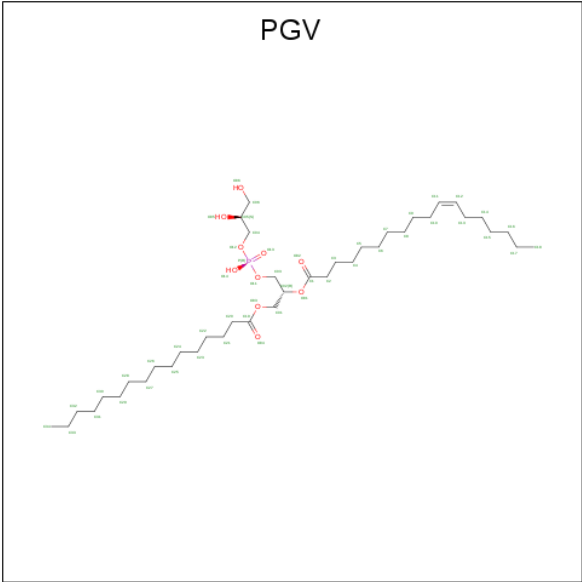
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 16 | N | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



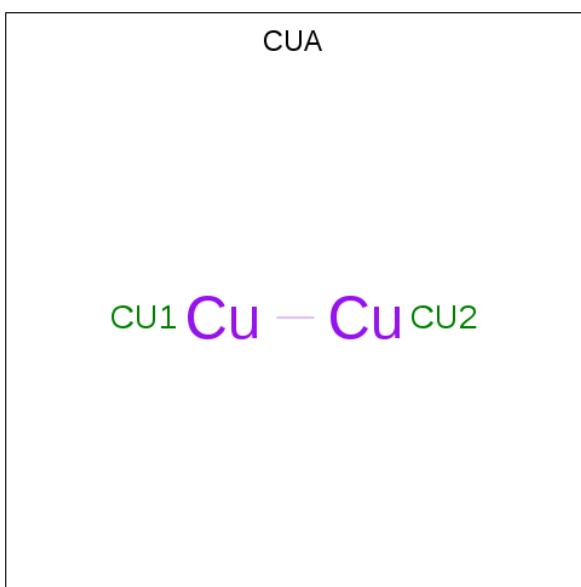
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 17 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 17 | N | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 17 | N | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |

- Molecule 18 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



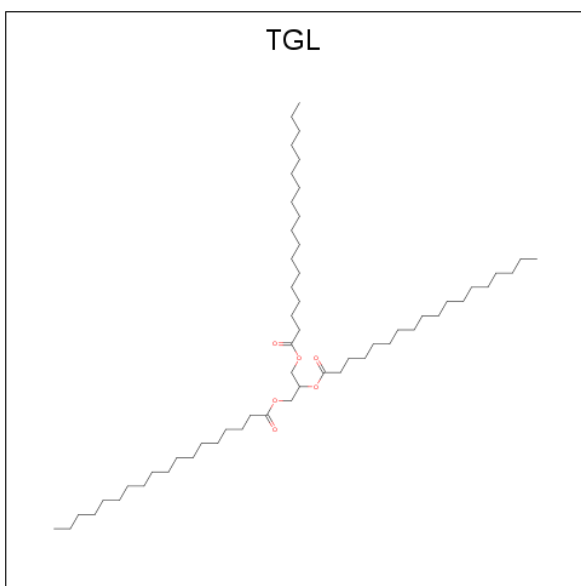
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | N | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | N | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 18 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19 | B | 1 | Total | Cu | 0 | 0 |
| | | | 2 | 2 | | |
| 19 | O | 1 | Total | Cu | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



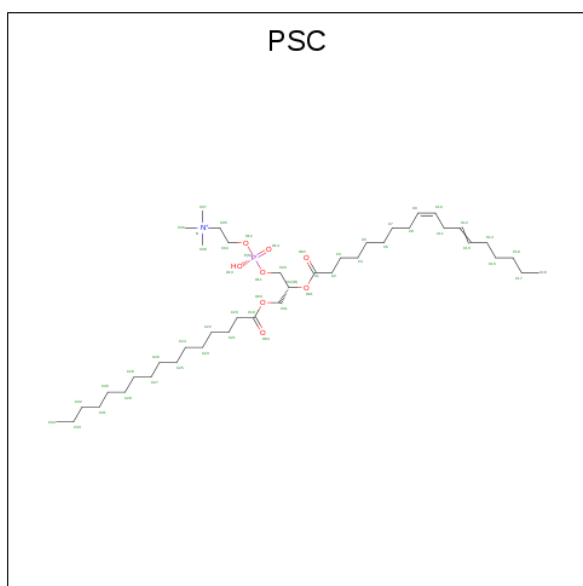
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20 | B | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 20 | D | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

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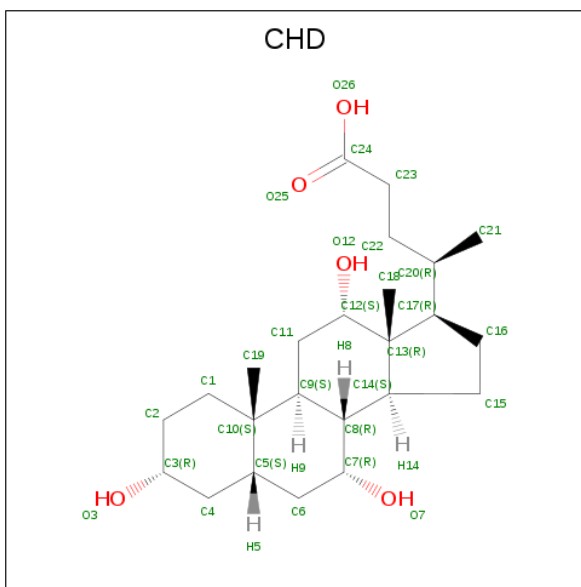
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20 | L | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 20 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 20 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 20 | O | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



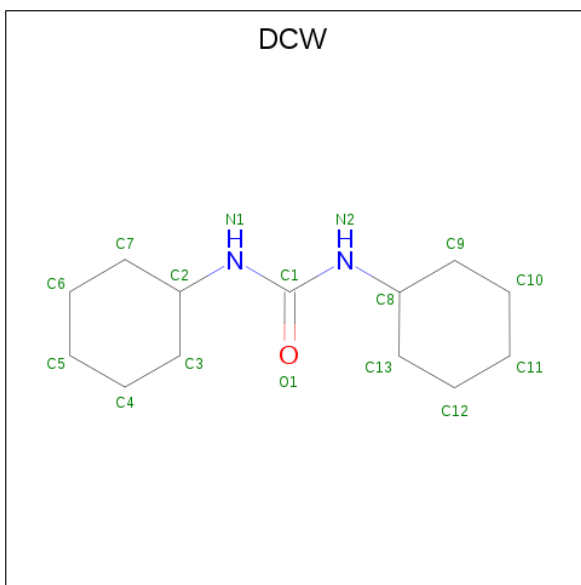
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 21 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 21 | O | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



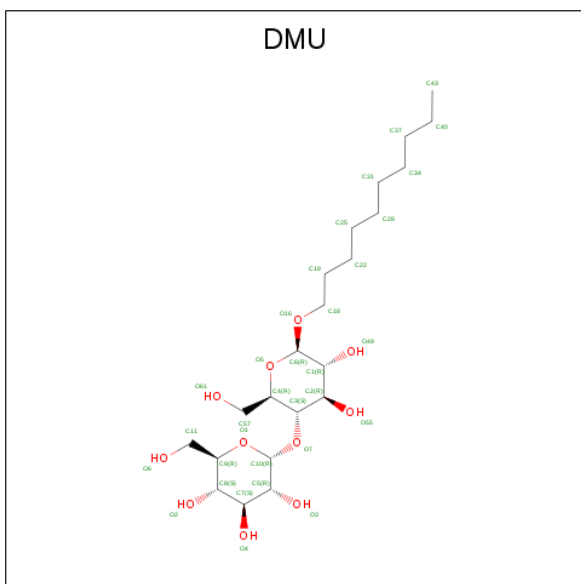
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22 | B | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | J | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | O | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 22 | W | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

- Molecule 23 is DICYCLOHEXYLUREA (three-letter code: DCW) (formula: $C_{13}H_{24}N_2O$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 23 | C | 1 | Total 16 | C 13 | N 2 | O 1 | 0 | 0 |
| 23 | P | 1 | Total 16 | C 13 | N 2 | O 1 | 0 | 0 |

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24 | C | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |

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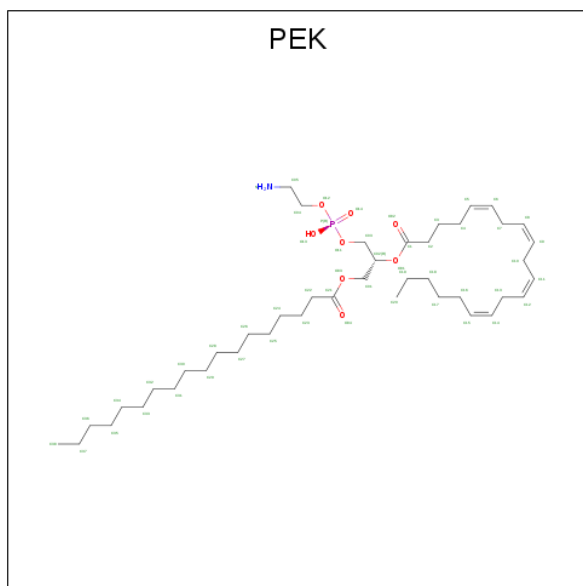
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24 | M | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 24 | P | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 24 | Z | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 25 | P | 1 | Total | X | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | C | 1 | Total | X | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 26 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



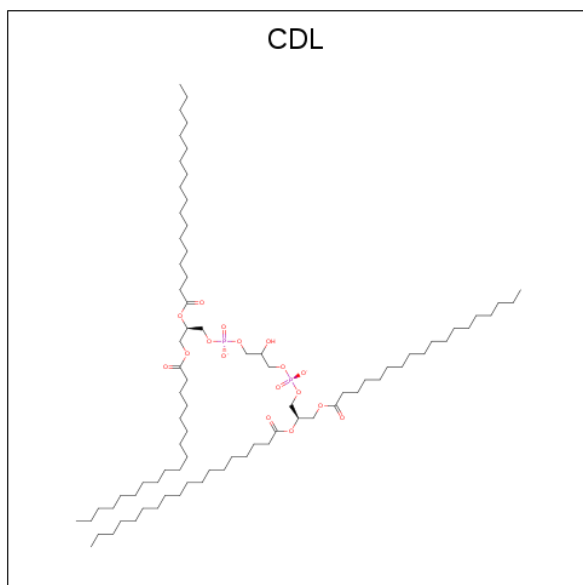
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 26 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 26 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 27 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 27 | G | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 27 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 27 | T | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 28 | S | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 28 | F | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 29 | A | 199 | Total O 199 199 | 0 | 0 |
| 29 | B | 119 | Total O 119 119 | 0 | 0 |
| 29 | C | 82 | Total O 82 82 | 0 | 0 |
| 29 | D | 79 | Total O 79 79 | 0 | 0 |
| 29 | E | 58 | Total O 58 58 | 0 | 0 |
| 29 | F | 64 | Total O 64 64 | 0 | 0 |
| 29 | G | 35 | Total O 35 35 | 0 | 0 |
| 29 | H | 39 | Total O 39 39 | 0 | 0 |
| 29 | I | 29 | Total O 29 29 | 0 | 0 |
| 29 | J | 14 | Total O 14 14 | 0 | 0 |
| 29 | K | 21 | Total O 21 21 | 0 | 0 |
| 29 | L | 17 | Total O 17 17 | 0 | 0 |
| 29 | M | 14 | Total O 14 14 | 0 | 0 |
| 29 | N | 176 | Total O 176 176 | 0 | 0 |
| 29 | O | 103 | Total O 103 103 | 0 | 0 |
| 29 | P | 74 | Total O 74 74 | 0 | 0 |
| 29 | Q | 46 | Total O 46 46 | 0 | 0 |
| 29 | R | 41 | Total O 41 41 | 0 | 0 |
| 29 | S | 56 | Total O 56 56 | 0 | 0 |
| 29 | T | 30 | Total O 30 30 | 0 | 0 |
| 29 | U | 39 | Total O 39 39 | 0 | 0 |

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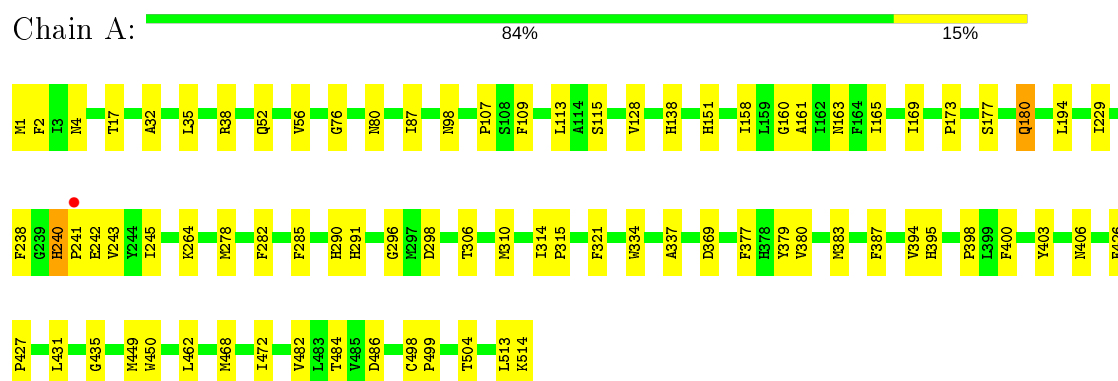
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 29 | V | 19 | Total 19 | O 19 | 0 | 0 |
| 29 | W | 14 | Total 14 | O 14 | 0 | 0 |
| 29 | X | 17 | Total 17 | O 17 | 0 | 0 |
| 29 | Y | 13 | Total 13 | O 13 | 0 | 0 |
| 29 | Z | 10 | Total 10 | O 10 | 0 | 0 |

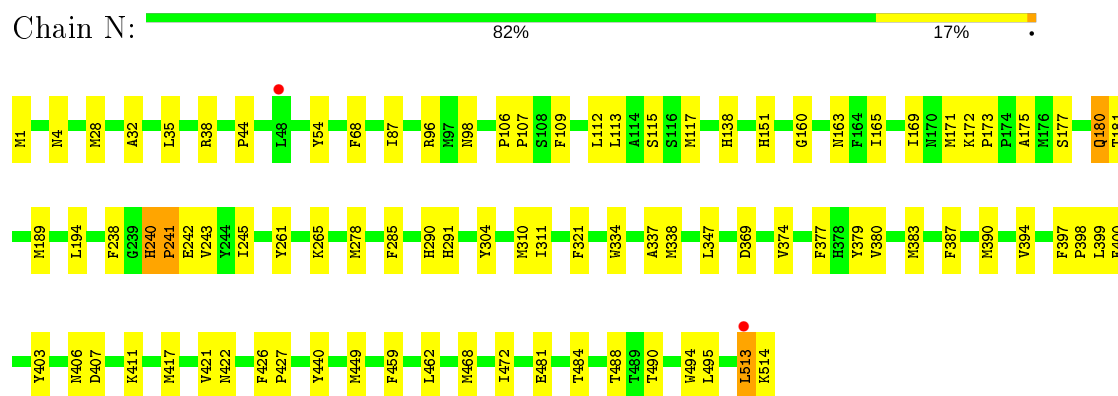
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

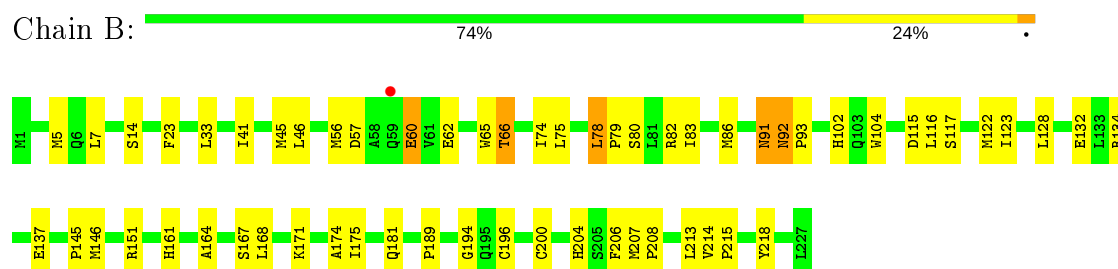
• Molecule 1: Cytochrome c oxidase subunit 1



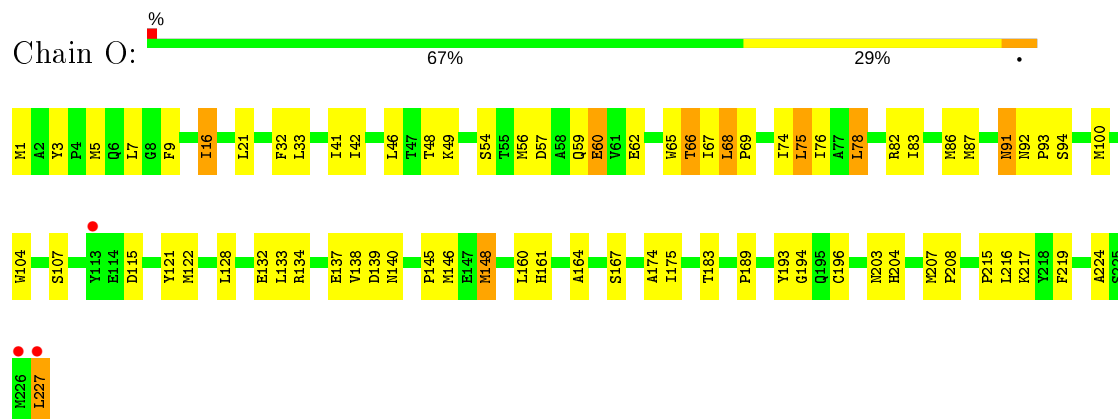
• Molecule 1: Cytochrome c oxidase subunit 1



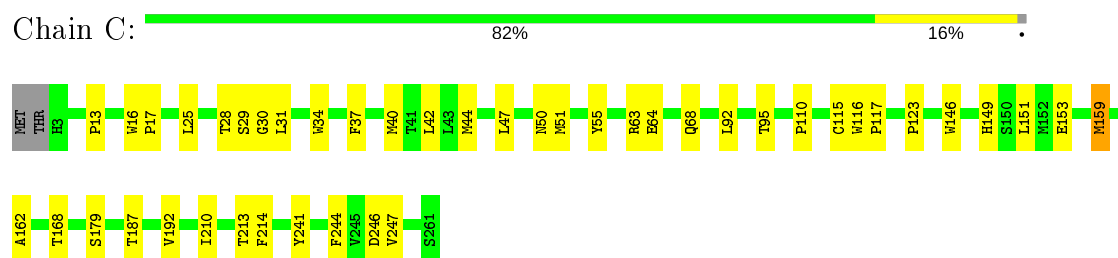
• Molecule 2: Cytochrome c oxidase subunit 2



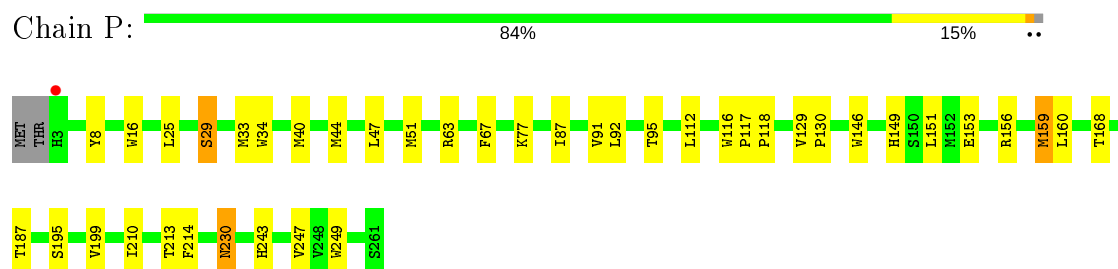
- Molecule 2: Cytochrome c oxidase subunit 2



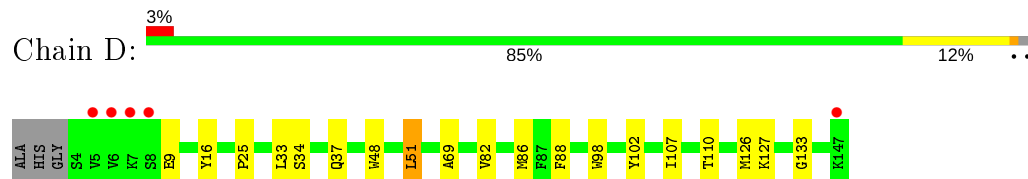
- Molecule 3: Cytochrome c oxidase subunit 3



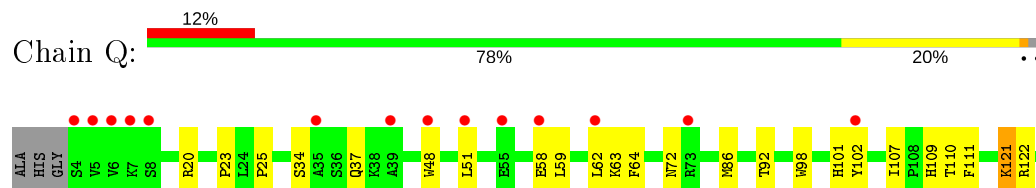
- Molecule 3: Cytochrome c oxidase subunit 3

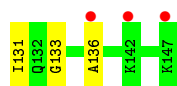


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

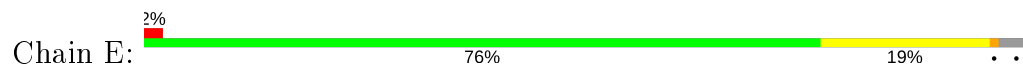


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1





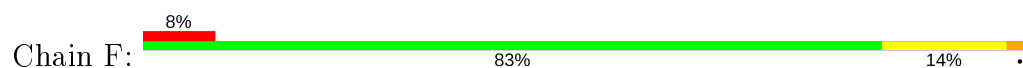
- Molecule 5: Cytochrome c oxidase polypeptide Va



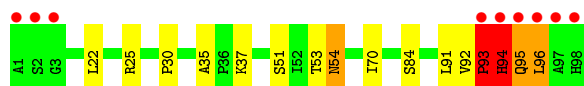
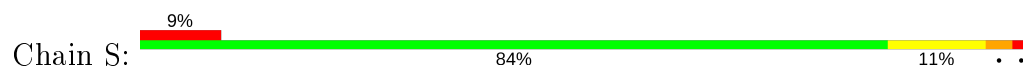
- Molecule 5: Cytochrome c oxidase polypeptide Va



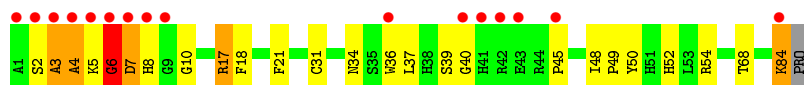
- Molecule 6: Cytochrome c oxidase polypeptide Vb



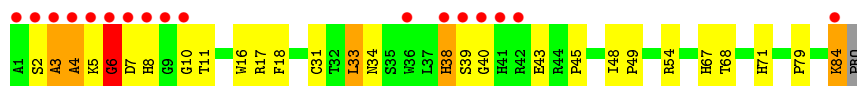
- Molecule 6: Cytochrome c oxidase polypeptide Vb



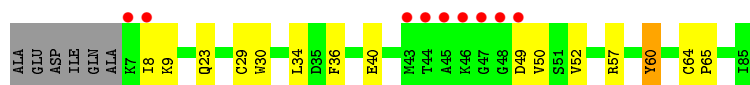
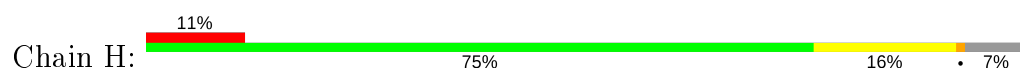
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



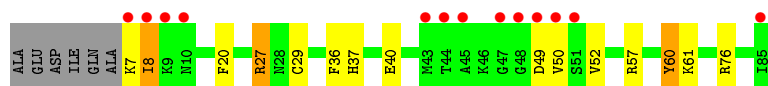
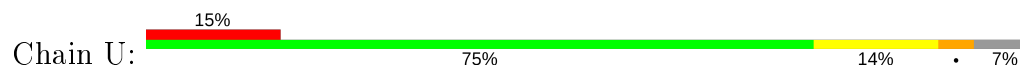
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



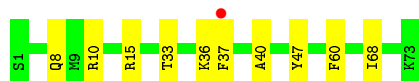
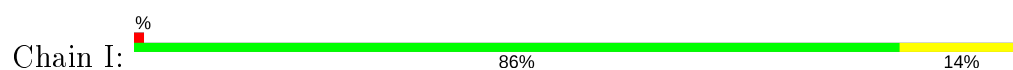
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



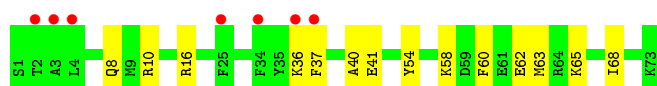
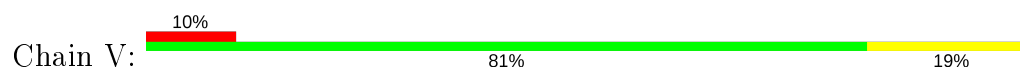
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



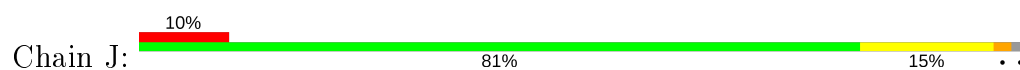
- Molecule 9: Cytochrome c oxidase polypeptide VIc



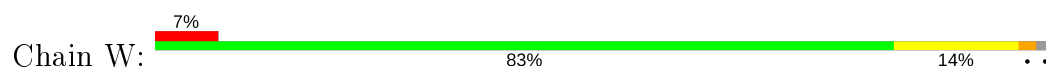
- Molecule 9: Cytochrome c oxidase polypeptide VIc



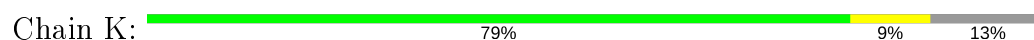
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



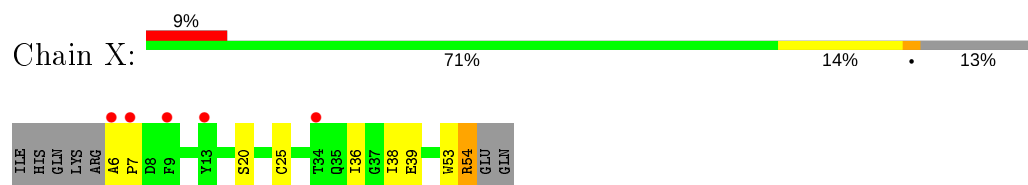
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



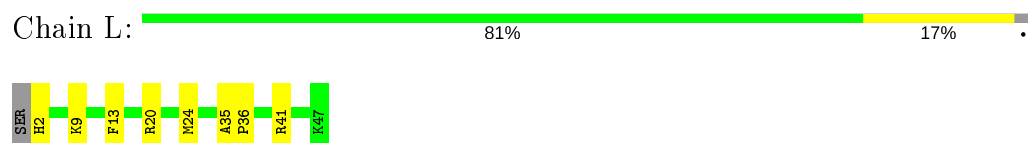
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



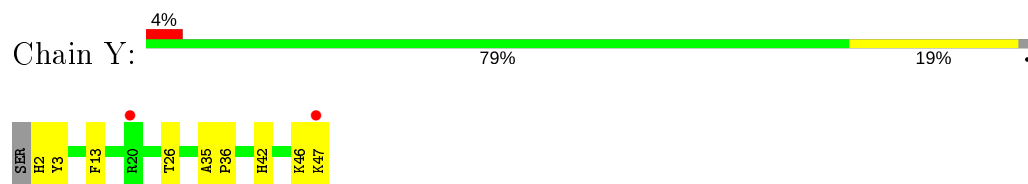
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



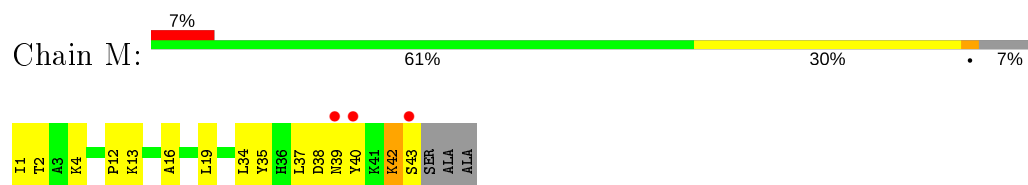
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



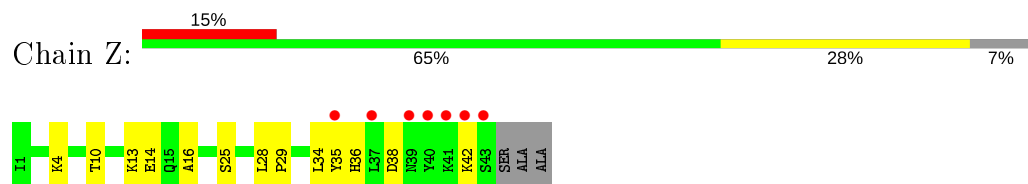
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 184.13Å 207.23Å 178.24Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.20 58.85 – 2.20 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (40.00-2.20) 99.3 (58.85-2.20) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.57 (at 2.20Å) | Xtriage |
| Refinement program | X-PLOR 3.851 | Depositor |
| R, R_{free} | 0.197 , 0.242 0.207 , 0.243 | Depositor DCC |
| R_{free} test set | 16860 reflections (4.95%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 33.2 | Xtriage |
| Anisotropy | 0.058 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 62.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | 0.006 for l,-k,h | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 32170 | wwPDB-VP |
| Average B, all atoms (Å ²) | 42.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, DCW, FME, CU, DMU

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 | 0.59 | 0/4156 | 0.72 | 1/5678 (0.0%) |
| 1 | N | 0.55 | 0/4156 | 0.69 | 0/5678 |
| 2 | B | 0.56 | 0/1860 | 0.79 | 0/2534 |
| 2 | O | 0.55 | 0/1860 | 0.80 | 1/2534 (0.0%) |
| 3 | C | 0.59 | 0/2196 | 0.64 | 0/3003 |
| 3 | P | 0.56 | 0/2196 | 0.64 | 0/3003 |
| 4 | D | 0.59 | 0/1229 | 0.73 | 2/1658 (0.1%) |
| 4 | Q | 0.59 | 0/1229 | 0.69 | 1/1658 (0.1%) |
| 5 | E | 0.53 | 0/871 | 0.69 | 0/1182 |
| 5 | R | 0.54 | 0/871 | 0.71 | 1/1182 (0.1%) |
| 6 | F | 0.54 | 0/765 | 0.84 | 2/1038 (0.2%) |
| 6 | S | 0.54 | 0/765 | 0.85 | 2/1038 (0.2%) |
| 7 | G | 0.61 | 0/690 | 0.76 | 1/937 (0.1%) |
| 7 | T | 0.60 | 0/690 | 0.79 | 2/937 (0.2%) |
| 8 | H | 0.53 | 0/682 | 0.70 | 0/921 |
| 8 | U | 0.49 | 0/682 | 0.68 | 0/921 |
| 9 | I | 0.56 | 0/605 | 0.65 | 0/802 |
| 9 | V | 0.57 | 0/605 | 0.62 | 0/802 |
| 10 | J | 0.51 | 0/471 | 0.67 | 0/636 |
| 10 | W | 0.51 | 0/471 | 0.72 | 0/636 |
| 11 | K | 0.56 | 0/398 | 0.70 | 0/546 |
| 11 | X | 0.50 | 0/398 | 0.68 | 0/546 |
| 12 | L | 0.59 | 0/393 | 0.61 | 0/526 |
| 12 | Y | 0.52 | 0/393 | 0.64 | 0/526 |
| 13 | M | 0.55 | 0/345 | 0.65 | 0/470 |
| 13 | Z | 0.53 | 0/345 | 0.66 | 0/470 |
| All | All | 0.56 | 0/29322 | 0.71 | 13/39862 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | N | 0 | 2 |
| 9 | I | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7 | T | 33 | LEU | CA-CB-CG | 6.86 | 131.08 | 115.30 |
| 6 | S | 94 | HIS | N-CA-C | 6.48 | 128.49 | 111.00 |
| 6 | F | 94 | HIS | N-CA-C | 6.21 | 127.75 | 111.00 |
| 4 | D | 51 | LEU | CA-CB-CG | 6.02 | 129.15 | 115.30 |
| 6 | F | 93 | PRO | N-CA-C | 5.85 | 127.30 | 112.10 |
| 5 | R | 42 | VAL | N-CA-C | -5.42 | 96.38 | 111.00 |
| 2 | O | 227 | LEU | CA-CB-CG | 5.38 | 127.67 | 115.30 |
| 1 | A | 435 | GLY | N-CA-C | 5.36 | 126.50 | 113.10 |
| 4 | Q | 133 | GLY | N-CA-C | 5.33 | 126.43 | 113.10 |
| 4 | D | 133 | GLY | N-CA-C | 5.28 | 126.30 | 113.10 |
| 7 | G | 6 | GLY | N-CA-C | 5.15 | 125.98 | 113.10 |
| 6 | S | 93 | PRO | N-CA-C | 5.15 | 125.49 | 112.10 |
| 7 | T | 6 | GLY | N-CA-C | 5.09 | 125.84 | 113.10 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 240 | HIS | Sidechain |
| 9 | I | 47 | TYR | Sidechain |
| 1 | N | 240 | HIS | Sidechain |
| 1 | N | 304 | TYR | Sidechain |

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 | 4027 | 0 | 4001 | 69 | 0 |
| 1 | N | 4027 | 0 | 4001 | 72 | 0 |
| 2 | B | 1824 | 0 | 1833 | 44 | 0 |
| 2 | O | 1824 | 0 | 1833 | 57 | 0 |
| 3 | C | 2109 | 0 | 2027 | 40 | 0 |
| 3 | P | 2109 | 0 | 2027 | 40 | 0 |
| 4 | D | 1195 | 0 | 1183 | 17 | 0 |
| 4 | Q | 1195 | 0 | 1183 | 25 | 0 |
| 5 | E | 852 | 0 | 845 | 15 | 0 |
| 5 | R | 852 | 0 | 845 | 16 | 0 |
| 6 | F | 748 | 0 | 728 | 9 | 0 |
| 6 | S | 748 | 0 | 728 | 12 | 0 |
| 7 | G | 675 | 0 | 644 | 24 | 0 |
| 7 | T | 675 | 0 | 644 | 28 | 0 |
| 8 | H | 662 | 0 | 623 | 9 | 0 |
| 8 | U | 662 | 0 | 623 | 12 | 0 |
| 9 | I | 601 | 0 | 613 | 6 | 0 |
| 9 | V | 601 | 0 | 613 | 12 | 0 |
| 10 | J | 460 | 0 | 459 | 8 | 0 |
| 10 | W | 460 | 0 | 459 | 8 | 0 |
| 11 | K | 384 | 0 | 366 | 4 | 0 |
| 11 | X | 384 | 0 | 366 | 10 | 0 |
| 12 | L | 380 | 0 | 380 | 13 | 0 |
| 12 | Y | 380 | 0 | 380 | 9 | 0 |
| 13 | M | 335 | 0 | 352 | 10 | 0 |
| 13 | Z | 335 | 0 | 352 | 8 | 0 |
| 14 | A | 1 | 0 | 0 | 0 | 0 |
| 14 | N | 1 | 0 | 0 | 0 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | N | 1 | 0 | 0 | 0 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 16 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 120 | 0 | 108 | 5 | 0 |
| 17 | N | 120 | 0 | 108 | 6 | 0 |
| 18 | A | 102 | 0 | 152 | 16 | 0 |
| 18 | C | 102 | 0 | 152 | 9 | 0 |
| 18 | N | 102 | 0 | 152 | 13 | 0 |
| 18 | P | 102 | 0 | 152 | 9 | 0 |
| 19 | B | 2 | 0 | 0 | 0 | 0 |
| 19 | O | 2 | 0 | 0 | 0 | 0 |
| 20 | B | 63 | 0 | 110 | 6 | 0 |
| 20 | D | 63 | 0 | 110 | 6 | 0 |
| 20 | L | 63 | 0 | 110 | 23 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20 | N | 126 | 0 | 220 | 19 | 0 |
| 20 | O | 63 | 0 | 110 | 7 | 0 |
| 21 | B | 52 | 0 | 80 | 23 | 0 |
| 21 | O | 52 | 0 | 80 | 21 | 0 |
| 22 | B | 29 | 0 | 39 | 1 | 0 |
| 22 | C | 58 | 0 | 77 | 1 | 0 |
| 22 | J | 29 | 0 | 39 | 2 | 0 |
| 22 | O | 29 | 0 | 39 | 0 | 0 |
| 22 | P | 58 | 0 | 78 | 2 | 0 |
| 22 | W | 29 | 0 | 39 | 4 | 0 |
| 23 | C | 16 | 0 | 23 | 9 | 0 |
| 23 | P | 16 | 0 | 23 | 8 | 0 |
| 24 | C | 33 | 0 | 37 | 5 | 0 |
| 24 | M | 33 | 0 | 37 | 1 | 0 |
| 24 | P | 33 | 0 | 37 | 5 | 0 |
| 24 | Z | 33 | 0 | 37 | 1 | 0 |
| 25 | C | 1 | 0 | 0 | 0 | 0 |
| 25 | P | 1 | 0 | 0 | 0 | 0 |
| 26 | C | 106 | 0 | 154 | 18 | 0 |
| 26 | G | 53 | 0 | 77 | 10 | 0 |
| 26 | P | 106 | 0 | 154 | 17 | 0 |
| 26 | T | 53 | 0 | 77 | 8 | 0 |
| 27 | C | 100 | 0 | 156 | 15 | 0 |
| 27 | G | 100 | 0 | 156 | 15 | 0 |
| 27 | P | 100 | 0 | 156 | 14 | 0 |
| 27 | T | 100 | 0 | 156 | 21 | 0 |
| 28 | F | 1 | 0 | 0 | 0 | 0 |
| 28 | S | 1 | 0 | 0 | 0 | 0 |
| 29 | A | 199 | 0 | 0 | 6 | 0 |
| 29 | B | 119 | 0 | 0 | 2 | 0 |
| 29 | C | 82 | 0 | 0 | 2 | 0 |
| 29 | D | 79 | 0 | 0 | 2 | 0 |
| 29 | E | 58 | 0 | 0 | 3 | 0 |
| 29 | F | 64 | 0 | 0 | 2 | 0 |
| 29 | G | 35 | 0 | 0 | 1 | 0 |
| 29 | H | 39 | 0 | 0 | 1 | 0 |
| 29 | I | 29 | 0 | 0 | 4 | 0 |
| 29 | J | 14 | 0 | 0 | 1 | 0 |
| 29 | K | 21 | 0 | 0 | 0 | 0 |
| 29 | L | 17 | 0 | 0 | 2 | 0 |
| 29 | M | 14 | 0 | 0 | 1 | 0 |
| 29 | N | 176 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29 | O | 103 | 0 | 0 | 5 | 0 |
| 29 | P | 74 | 0 | 0 | 3 | 0 |
| 29 | Q | 46 | 0 | 0 | 2 | 0 |
| 29 | R | 41 | 0 | 0 | 1 | 0 |
| 29 | S | 56 | 0 | 0 | 3 | 0 |
| 29 | T | 30 | 0 | 0 | 2 | 0 |
| 29 | U | 39 | 0 | 0 | 0 | 0 |
| 29 | V | 19 | 0 | 0 | 0 | 0 |
| 29 | W | 14 | 0 | 0 | 2 | 0 |
| 29 | X | 17 | 0 | 0 | 0 | 0 |
| 29 | Y | 13 | 0 | 0 | 0 | 0 |
| 29 | Z | 10 | 0 | 0 | 1 | 0 |
| All | All | 32170 | 0 | 31343 | 655 | 0 |

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 11.

All (655) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:33:ARG:HG2 | 22:W:101:CHD:H152 | 1.31 | 1.10 |
| 21:B:303:PSC:H343 | 21:B:303:PSC:H142 | 1.31 | 1.07 |
| 21:O:304:PSC:H142 | 21:O:304:PSC:H343 | 1.28 | 1.06 |
| 7:G:84:LYS:HD2 | 7:G:84:LYS:H | 1.22 | 1.05 |
| 12:L:20:ARG:HH12 | 20:L:101:TGL:HC61 | 1.15 | 1.05 |
| 7:T:5:LYS:HB2 | 26:T:101:PEK:H362 | 1.39 | 1.04 |
| 4:D:34:SER:H | 4:D:37:GLN:HE21 | 1.09 | 1.01 |
| 20:O:303:TGL:H281 | 20:O:303:TGL:H102 | 1.43 | 1.01 |
| 7:T:84:LYS:H | 7:T:84:LYS:HD2 | 1.27 | 0.98 |
| 7:G:5:LYS:HB2 | 26:G:102:PEK:H362 | 1.46 | 0.97 |
| 7:T:31:CYS:SG | 27:T:102:CDL:H532 | 2.04 | 0.97 |
| 20:B:302:TGL:H281 | 20:B:302:TGL:H102 | 1.45 | 0.97 |
| 3:C:63:ARG:HE | 27:C:309:CDL:HA22 | 1.31 | 0.93 |
| 27:G:101:CDL:H541 | 27:G:101:CDL:H231 | 1.54 | 0.90 |
| 20:L:101:TGL:HC62 | 20:L:101:TGL:HC22 | 1.54 | 0.90 |
| 18:A:607:PGV:H343 | 23:C:301:DCW:H41C | 1.54 | 0.89 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:H | 1.89 | 0.89 |
| 20:N:606:TGL:HC22 | 20:N:606:TGL:HC62 | 1.54 | 0.88 |
| 7:G:31:CYS:SG | 27:G:101:CDL:H532 | 2.14 | 0.88 |
| 18:N:609:PGV:H321 | 26:P:305:PEK:H361 | 1.53 | 0.87 |
| 20:O:303:TGL:C28 | 20:O:303:TGL:H102 | 2.05 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:20:ARG:NH1 | 20:L:101:TGL:HC61 | 1.91 | 0.85 |
| 3:P:63:ARG:HE | 27:P:309:CDL:HA22 | 1.38 | 0.85 |
| 27:C:309:CDL:H191 | 27:C:309:CDL:H642 | 1.59 | 0.84 |
| 20:B:302:TGL:H102 | 20:B:302:TGL:C28 | 2.07 | 0.84 |
| 26:P:305:PEK:H102 | 26:P:305:PEK:H161 | 1.60 | 0.84 |
| 2:O:224:ALA:O | 2:O:227:LEU:HG | 1.78 | 0.84 |
| 26:C:305:PEK:H161 | 26:C:305:PEK:H102 | 1.60 | 0.84 |
| 27:P:309:CDL:H642 | 27:P:309:CDL:H191 | 1.59 | 0.83 |
| 20:N:606:TGL:HC31 | 12:Y:13:PHE:HA | 1.62 | 0.82 |
| 10:J:33:ARG:HG2 | 22:J:101:CHD:H152 | 1.62 | 0.82 |
| 27:T:102:CDL:H231 | 27:T:102:CDL:H541 | 1.60 | 0.82 |
| 7:G:5:LYS:HB3 | 1:N:278:MET:SD | 2.21 | 0.80 |
| 18:A:607:PGV:H321 | 26:C:305:PEK:H361 | 1.63 | 0.79 |
| 12:L:13:PHE:HA | 20:L:101:TGL:HC31 | 1.65 | 0.79 |
| 1:N:472:ILE:HG21 | 20:N:606:TGL:HA92 | 1.64 | 0.78 |
| 5:E:82:TYR:HB3 | 5:E:83:PRO:HD3 | 1.67 | 0.77 |
| 1:A:472:ILE:HG21 | 20:L:101:TGL:HA92 | 1.67 | 0.75 |
| 7:T:5:LYS:HG3 | 26:T:101:PEK:H383 | 1.68 | 0.75 |
| 2:O:57:ASP:H | 21:O:304:PSC:H201 | 1.49 | 0.75 |
| 20:N:607:TGL:HC21 | 20:N:607:TGL:HG11 | 1.67 | 0.75 |
| 20:N:606:TGL:H202 | 20:N:606:TGL:H242 | 1.69 | 0.74 |
| 27:G:101:CDL:H622 | 18:P:308:PGV:H152 | 1.66 | 0.74 |
| 20:L:101:TGL:H242 | 20:L:101:TGL:H202 | 1.69 | 0.74 |
| 20:D:201:TGL:HG11 | 20:D:201:TGL:HC21 | 1.69 | 0.73 |
| 27:G:101:CDL:H541 | 27:G:101:CDL:C23 | 2.19 | 0.73 |
| 1:A:321:PHE:CD2 | 21:B:303:PSC:H341 | 2.23 | 0.73 |
| 7:G:84:LYS:H | 7:G:84:LYS:CD | 1.98 | 0.73 |
| 8:U:20:PHE:HE2 | 8:U:27:ARG:HG2 | 1.53 | 0.73 |
| 3:P:25:LEU:O | 3:P:29:SER:HB2 | 1.89 | 0.72 |
| 2:B:65:TRP:CZ3 | 21:B:303:PSC:H331 | 2.23 | 0.72 |
| 7:G:5:LYS:HG3 | 26:G:102:PEK:H383 | 1.71 | 0.72 |
| 21:B:303:PSC:C07 | 9:I:10:ARG:HH21 | 2.02 | 0.71 |
| 4:D:34:SER:H | 4:D:37:GLN:NE2 | 1.84 | 0.71 |
| 1:N:113:LEU:CD1 | 20:N:606:TGL:H292 | 2.21 | 0.71 |
| 21:O:304:PSC:H222 | 21:O:304:PSC:H21 | 1.71 | 0.71 |
| 21:B:303:PSC:H222 | 21:B:303:PSC:H21 | 1.73 | 0.70 |
| 13:M:42:LYS:HA | 13:M:42:LYS:HE3 | 1.73 | 0.70 |
| 29:O:500:HOH:O | 8:U:61:LYS:HE3 | 1.91 | 0.70 |
| 1:N:321:PHE:CD2 | 21:O:304:PSC:H341 | 2.27 | 0.69 |
| 9:V:63:MET:HB3 | 9:V:68:ILE:HD11 | 1.73 | 0.69 |
| 7:T:38:HIS:NE2 | 27:T:102:CDL:H111 | 2.07 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:34:TRP:HZ2 | 24:C:302:DMU:H29 | 1.57 | 0.69 |
| 21:B:303:PSC:H072 | 9:I:10:ARG:HH21 | 1.57 | 0.69 |
| 1:A:113:LEU:CD1 | 20:L:101:TGL:H292 | 2.23 | 0.69 |
| 18:C:308:PGV:H152 | 27:T:102:CDL:H622 | 1.74 | 0.69 |
| 26:P:305:PEK:H71 | 26:P:305:PEK:H32 | 1.73 | 0.69 |
| 7:T:84:LYS:H | 7:T:84:LYS:CD | 2.05 | 0.69 |
| 20:B:302:TGL:H201 | 20:B:302:TGL:H241 | 1.75 | 0.69 |
| 7:T:45:PRO:HD2 | 29:T:204:HOH:O | 1.92 | 0.68 |
| 2:O:56:MET:HA | 21:O:304:PSC:C20 | 2.24 | 0.68 |
| 1:A:379:TYR:O | 1:A:383:MET:HB2 | 1.93 | 0.68 |
| 1:N:334:TRP:CZ3 | 20:N:607:TGL:HA51 | 2.29 | 0.68 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:N | 2.61 | 0.68 |
| 1:N:1:FME:HCN | 1:N:4:ASN:H | 1.59 | 0.68 |
| 6:S:94:HIS:CG | 6:S:95:GLN:H | 2.08 | 0.67 |
| 26:C:305:PEK:H32 | 26:C:305:PEK:H71 | 1.75 | 0.67 |
| 1:N:321:PHE:CZ | 21:O:304:PSC:H171 | 2.30 | 0.67 |
| 20:O:303:TGL:H241 | 20:O:303:TGL:H201 | 1.76 | 0.66 |
| 3:C:146:TRP:CZ2 | 7:G:17:ARG:HG3 | 2.30 | 0.66 |
| 9:V:58:LYS:O | 9:V:62:GLU:HG3 | 1.95 | 0.66 |
| 27:T:102:CDL:C23 | 27:T:102:CDL:H541 | 2.24 | 0.66 |
| 1:A:113:LEU:HD12 | 20:L:101:TGL:H292 | 1.76 | 0.66 |
| 18:A:607:PGV:H343 | 23:C:301:DCW:C4 | 2.24 | 0.66 |
| 1:A:161:ALA:O | 1:A:165:ILE:HG13 | 1.95 | 0.65 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:HC32 | 1.61 | 0.65 |
| 20:O:303:TGL:HC92 | 29:O:486:HOH:O | 1.96 | 0.65 |
| 3:C:51:MET:HB3 | 27:C:309:CDL:H622 | 1.77 | 0.65 |
| 3:C:34:TRP:CZ2 | 24:C:302:DMU:H29 | 2.31 | 0.65 |
| 20:L:101:TGL:HB91 | 20:L:101:TGL:H361 | 1.79 | 0.64 |
| 1:N:417:MET:O | 1:N:421:VAL:HG22 | 1.98 | 0.64 |
| 7:G:45:PRO:HD2 | 29:G:202:HOH:O | 1.97 | 0.64 |
| 3:P:187:THR:HB | 7:T:68:THR:HG21 | 1.80 | 0.64 |
| 1:A:177:SER:H | 1:A:180:GLN:NE2 | 1.95 | 0.64 |
| 2:B:41:ILE:HD13 | 21:B:303:PSC:H342 | 1.79 | 0.64 |
| 2:O:41:ILE:CD1 | 21:O:304:PSC:H342 | 2.28 | 0.64 |
| 7:T:5:LYS:HD2 | 26:T:101:PEK:H371 | 1.78 | 0.64 |
| 27:G:101:CDL:H202 | 27:G:101:CDL:H522 | 1.80 | 0.63 |
| 26:C:306:PEK:C38 | 27:G:101:CDL:H273 | 2.28 | 0.63 |
| 18:C:307:PGV:H172 | 27:C:309:CDL:H662 | 1.78 | 0.63 |
| 5:R:89:LEU:O | 5:R:93:LEU:HG | 1.99 | 0.63 |
| 2:B:122:MET:HB2 | 2:B:208:PRO:HD2 | 1.81 | 0.63 |
| 10:W:58:LYS:HE3 | 12:Y:47:LYS:HE3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:87:ILE:O | 1:N:173:PRO:HD3 | 1.98 | 0.62 |
| 3:P:210:ILE:HG23 | 18:P:307:PGV:H102 | 1.81 | 0.62 |
| 27:T:102:CDL:H172 | 27:T:102:CDL:H511 | 1.81 | 0.62 |
| 3:C:40:MET:O | 3:C:44:MET:HG2 | 1.99 | 0.62 |
| 12:L:9:LYS:HG3 | 29:L:216:HOH:O | 1.99 | 0.62 |
| 1:N:35:LEU:HD11 | 1:N:462:LEU:HD13 | 1.82 | 0.62 |
| 3:P:34:TRP:CZ2 | 24:P:302:DMU:H29 | 2.35 | 0.62 |
| 18:C:307:PGV:H182 | 27:C:309:CDL:H673 | 1.82 | 0.61 |
| 7:G:5:LYS:HD2 | 26:G:102:PEK:H371 | 1.82 | 0.61 |
| 18:N:608:PGV:H152 | 18:N:608:PGV:H321 | 1.81 | 0.61 |
| 18:A:606:PGV:H062 | 29:M:201:HOH:O | 2.00 | 0.61 |
| 27:G:101:CDL:H172 | 27:G:101:CDL:H511 | 1.82 | 0.61 |
| 26:P:306:PEK:C38 | 27:T:102:CDL:H273 | 2.31 | 0.61 |
| 2:O:56:MET:HG2 | 21:O:304:PSC:H211 | 1.83 | 0.61 |
| 2:O:122:MET:HB2 | 2:O:208:PRO:HD2 | 1.83 | 0.61 |
| 27:T:102:CDL:H202 | 27:T:102:CDL:H522 | 1.83 | 0.61 |
| 12:L:20:ARG:HH12 | 20:L:101:TGL:CC6 | 2.03 | 0.60 |
| 1:A:383:MET:O | 1:A:387:PHE:HB2 | 2.00 | 0.60 |
| 2:B:14:SER:HB3 | 2:B:168:LEU:HD23 | 1.84 | 0.60 |
| 27:P:309:CDL:H112 | 29:P:467:HOH:O | 2.01 | 0.60 |
| 29:B:2065:HOH:O | 7:T:17:ARG:HD3 | 2.00 | 0.60 |
| 1:A:177:SER:H | 1:A:180:GLN:HE21 | 1.48 | 0.60 |
| 2:O:42:ILE:O | 2:O:46:LEU:HG | 2.02 | 0.60 |
| 3:P:146:TRP:CZ2 | 7:T:17:ARG:HG3 | 2.36 | 0.60 |
| 1:A:240:HIS:O | 1:A:243:VAL:HG22 | 2.01 | 0.60 |
| 1:A:484:THR:HB | 13:M:2:THR:OG1 | 2.02 | 0.60 |
| 3:C:210:ILE:HG23 | 18:C:307:PGV:H102 | 1.82 | 0.60 |
| 1:N:334:TRP:CH2 | 2:O:46:LEU:HD13 | 2.38 | 0.59 |
| 23:P:301:DCW:H62C | 18:P:307:PGV:H301 | 1.84 | 0.59 |
| 18:A:606:PGV:H321 | 18:A:606:PGV:H152 | 1.85 | 0.59 |
| 13:Z:10:THR:HA | 13:Z:14:GLU:OE2 | 2.03 | 0.59 |
| 3:C:246:ASP:HB2 | 29:C:467:HOH:O | 2.03 | 0.59 |
| 2:O:91:ASN:HD21 | 2:O:183:THR:HG21 | 1.68 | 0.59 |
| 10:W:33:ARG:HG2 | 22:W:101:CHD:C15 | 2.20 | 0.59 |
| 20:N:606:TGL:HB91 | 20:N:606:TGL:H361 | 1.83 | 0.58 |
| 1:A:282:PHE:HA | 7:T:4:ALA:HB3 | 1.85 | 0.58 |
| 9:V:65:LYS:O | 11:X:54:ARG:NH1 | 2.34 | 0.58 |
| 1:A:334:TRP:CZ2 | 2:B:46:LEU:HB3 | 2.39 | 0.58 |
| 1:N:290:HIS:CD2 | 1:N:291:HIS:CD2 | 2.91 | 0.58 |
| 1:N:379:TYR:O | 1:N:383:MET:HB2 | 2.03 | 0.58 |
| 2:O:56:MET:HA | 21:O:304:PSC:H202 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:56:MET:HA | 21:B:303:PSC:C20 | 2.33 | 0.58 |
| 10:J:7:GLU:HG3 | 29:J:209:HOH:O | 2.03 | 0.58 |
| 5:E:84:TYR:O | 5:E:88:GLU:HG2 | 2.04 | 0.58 |
| 18:P:307:PGV:H172 | 27:P:309:CDL:H662 | 1.86 | 0.57 |
| 10:W:40:LEU:HD12 | 22:W:101:CHD:H183 | 1.87 | 0.57 |
| 1:A:278:MET:SD | 7:T:5:LYS:HB3 | 2.44 | 0.57 |
| 26:C:306:PEK:H383 | 27:G:101:CDL:H273 | 1.86 | 0.57 |
| 18:N:609:PGV:H343 | 23:P:301:DCW:H41C | 1.86 | 0.57 |
| 5:E:67:ILE:O | 5:E:70:VAL:HG12 | 2.05 | 0.57 |
| 2:O:59:GLN:O | 2:O:59:GLN:HG3 | 2.05 | 0.57 |
| 1:A:87:ILE:O | 1:A:173:PRO:HD3 | 2.05 | 0.57 |
| 1:N:172:LYS:HD2 | 1:N:181:THR:CG2 | 2.35 | 0.57 |
| 2:O:41:ILE:HD13 | 21:O:304:PSC:H342 | 1.87 | 0.57 |
| 1:N:151:HIS:CD2 | 26:P:305:PEK:H382 | 2.40 | 0.57 |
| 2:O:65:TRP:CZ3 | 21:O:304:PSC:H331 | 2.40 | 0.57 |
| 3:P:47:LEU:O | 3:P:51:MET:HG2 | 2.05 | 0.57 |
| 1:N:397:PHE:HB3 | 1:N:398:PRO:HD3 | 1.87 | 0.56 |
| 18:N:608:PGV:H062 | 29:Z:201:HOH:O | 2.04 | 0.56 |
| 1:N:377:PHE:HA | 1:N:380:VAL:HG22 | 1.88 | 0.56 |
| 2:O:146:MET:SD | 2:O:189:PRO:HB3 | 2.45 | 0.56 |
| 3:P:149:HIS:O | 3:P:153:GLU:HG3 | 2.05 | 0.56 |
| 18:P:307:PGV:H182 | 27:P:309:CDL:H673 | 1.87 | 0.56 |
| 18:C:307:PGV:H161 | 18:C:307:PGV:H12 | 1.85 | 0.56 |
| 1:N:472:ILE:HG21 | 20:N:606:TGL:CA9 | 2.32 | 0.56 |
| 26:P:305:PEK:H102 | 26:P:305:PEK:C16 | 2.35 | 0.56 |
| 3:P:213:THR:HG23 | 27:P:309:CDL:H762 | 1.87 | 0.56 |
| 12:Y:35:ALA:HB3 | 12:Y:36:PRO:HD3 | 1.87 | 0.56 |
| 2:B:65:TRP:HZ3 | 21:B:303:PSC:H331 | 1.71 | 0.56 |
| 3:P:160:LEU:HD13 | 22:P:310:CHD:H181 | 1.88 | 0.56 |
| 2:B:56:MET:HG2 | 21:B:303:PSC:H211 | 1.86 | 0.56 |
| 27:G:101:CDL:H231 | 27:G:101:CDL:C54 | 2.33 | 0.56 |
| 3:P:168:THR:HG22 | 26:P:306:PEK:H14 | 1.86 | 0.56 |
| 1:A:472:ILE:HG21 | 20:L:101:TGL:CA9 | 2.35 | 0.56 |
| 9:V:36:LYS:HA | 9:V:40:ALA:HB3 | 1.87 | 0.56 |
| 4:D:9:GLU:HB3 | 29:D:376:HOH:O | 2.05 | 0.56 |
| 2:O:104:TRP:CG | 2:O:203:ASN:HB2 | 2.40 | 0.56 |
| 6:F:92:VAL:O | 6:F:92:VAL:HG23 | 2.04 | 0.56 |
| 12:L:24:MET:SD | 20:L:101:TGL:H162 | 2.46 | 0.56 |
| 8:U:40:GLU:HG3 | 8:U:50:VAL:CG1 | 2.36 | 0.55 |
| 6:S:93:PRO:HB3 | 29:S:240:HOH:O | 2.05 | 0.55 |
| 1:N:98:ASN:HB2 | 1:N:163:ASN:HD21 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:165:ILE:O | 1:N:169:ILE:HG12 | 2.06 | 0.55 |
| 4:Q:109:HIS:HD2 | 29:Q:207:HOH:O | 1.89 | 0.55 |
| 1:N:68:PHE:HE2 | 1:N:112:LEU:HD13 | 1.70 | 0.55 |
| 1:A:17:THR:OG1 | 20:L:101:TGL:H281 | 2.07 | 0.55 |
| 1:N:240:HIS:O | 1:N:243:VAL:HG22 | 2.07 | 0.55 |
| 3:P:151:LEU:HB2 | 3:P:159:MET:HG3 | 1.89 | 0.55 |
| 12:Y:26:THR:HG23 | 13:Z:25:SER:CB | 2.36 | 0.55 |
| 10:J:12:PHE:O | 10:J:23:LYS:HE2 | 2.07 | 0.55 |
| 1:N:106:PRO:HB2 | 1:N:107:PRO:HD3 | 1.89 | 0.55 |
| 3:P:67:PHE:HE1 | 27:P:309:CDL:H1 | 1.72 | 0.55 |
| 2:B:78:LEU:HD12 | 27:T:102:CDL:H351 | 1.89 | 0.55 |
| 18:A:607:PGV:C34 | 23:C:301:DCW:H41C | 2.33 | 0.55 |
| 7:G:50:TYR:HB3 | 7:G:52:HIS:CE1 | 2.42 | 0.55 |
| 12:L:20:ARG:NH2 | 20:L:101:TGL:HC32 | 2.22 | 0.55 |
| 5:E:105:GLY:O | 5:E:108:LYS:HG2 | 2.07 | 0.54 |
| 4:Q:58:GLU:O | 4:Q:62:LEU:HG | 2.07 | 0.54 |
| 21:O:304:PSC:H071 | 9:V:10:ARG:HE | 1.71 | 0.54 |
| 3:P:51:MET:HB3 | 27:P:309:CDL:H622 | 1.90 | 0.54 |
| 17:N:604:HEA:HBC1 | 17:N:604:HEA:HMC1 | 1.90 | 0.54 |
| 7:T:34:ASN:ND2 | 27:T:102:CDL:H151 | 2.22 | 0.54 |
| 8:H:49:ASP:O | 8:H:52:VAL:HG22 | 2.08 | 0.54 |
| 21:O:304:PSC:C07 | 9:V:10:ARG:HE | 2.21 | 0.54 |
| 2:O:67:ILE:HD11 | 29:O:488:HOH:O | 2.06 | 0.54 |
| 4:D:88:PHE:HZ | 13:M:19:LEU:HD21 | 1.73 | 0.54 |
| 2:B:57:ASP:H | 21:B:303:PSC:H201 | 1.74 | 0.53 |
| 18:P:307:PGV:H12 | 18:P:307:PGV:H161 | 1.90 | 0.53 |
| 1:A:282:PHE:HA | 7:T:4:ALA:CB | 2.38 | 0.53 |
| 1:A:334:TRP:CZ3 | 20:D:201:TGL:HA51 | 2.42 | 0.53 |
| 1:N:406:ASN:HD21 | 18:N:608:PGV:H21 | 1.72 | 0.53 |
| 1:N:98:ASN:HB2 | 1:N:163:ASN:ND2 | 2.23 | 0.53 |
| 20:N:606:TGL:H202 | 20:N:606:TGL:C24 | 2.38 | 0.53 |
| 1:A:377:PHE:HA | 1:A:380:VAL:HG22 | 1.88 | 0.53 |
| 2:B:146:MET:SD | 2:B:189:PRO:HB3 | 2.48 | 0.53 |
| 23:C:301:DCW:C10 | 26:C:305:PEK:H371 | 2.39 | 0.53 |
| 3:C:213:THR:HG23 | 27:C:309:CDL:H762 | 1.90 | 0.53 |
| 2:B:132:GLU:HB3 | 2:B:137:GLU:HG3 | 1.91 | 0.53 |
| 7:G:37:LEU:HD21 | 27:G:101:CDL:H361 | 1.91 | 0.53 |
| 11:X:54:ARG:NH2 | 11:X:54:ARG:HG3 | 2.23 | 0.53 |
| 21:B:303:PSC:H032 | 29:E:203:HOH:O | 2.09 | 0.53 |
| 8:H:60:TYR:C | 8:H:60:TYR:CD1 | 2.81 | 0.53 |
| 9:I:33:THR:HG22 | 29:I:126:HOH:O | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:P:302:DMU:H25 | 26:P:305:PEK:H322 | 1.90 | 0.53 |
| 8:U:40:GLU:HG3 | 8:U:50:VAL:HG11 | 1.91 | 0.53 |
| 3:P:34:TRP:HZ2 | 24:P:302:DMU:H29 | 1.74 | 0.53 |
| 7:G:2:SER:OG | 26:G:102:PEK:H301 | 2.09 | 0.52 |
| 1:N:383:MET:O | 1:N:387:PHE:HB2 | 2.09 | 0.52 |
| 18:N:608:PGV:H061 | 18:N:608:PGV:P | 2.49 | 0.52 |
| 7:G:17:ARG:HD2 | 29:O:401:HOH:O | 2.09 | 0.52 |
| 7:T:3:ALA:HB1 | 26:T:101:PEK:H382 | 1.91 | 0.52 |
| 11:X:54:ARG:HH21 | 11:X:54:ARG:HG3 | 1.74 | 0.52 |
| 4:D:107:ILE:HD13 | 11:K:39:GLU:HB2 | 1.91 | 0.52 |
| 2:O:82:ARG:HG2 | 2:O:86:MET:HE3 | 1.91 | 0.52 |
| 27:C:309:CDL:H642 | 27:C:309:CDL:C19 | 2.36 | 0.52 |
| 1:N:449:MET:SD | 2:O:5:MET:HG2 | 2.49 | 0.52 |
| 17:A:604:HEA:HMC1 | 17:A:604:HEA:HBC1 | 1.91 | 0.52 |
| 5:R:8:ASP:HB3 | 9:V:10:ARG:CZ | 2.39 | 0.52 |
| 4:Q:107:ILE:HD13 | 11:X:39:GLU:HB2 | 1.91 | 0.52 |
| 2:B:56:MET:HA | 21:B:303:PSC:H202 | 1.91 | 0.52 |
| 1:N:514:LYS:HE2 | 29:S:225:HOH:O | 2.10 | 0.52 |
| 20:L:101:TGL:H362 | 29:L:214:HOH:O | 2.08 | 0.52 |
| 1:N:406:ASN:HD21 | 18:N:608:PGV:C2 | 2.23 | 0.52 |
| 10:W:2:GLU:HA | 29:W:213:HOH:O | 2.10 | 0.52 |
| 1:N:175:ALA:CB | 1:N:513:LEU:HD23 | 2.40 | 0.51 |
| 3:P:187:THR:CB | 7:T:68:THR:HG21 | 2.39 | 0.51 |
| 18:N:609:PGV:C32 | 26:P:305:PEK:H361 | 2.34 | 0.51 |
| 1:A:160:GLY:HA3 | 29:A:741:HOH:O | 2.10 | 0.51 |
| 1:A:337:ALA:HB2 | 1:A:394:VAL:HG23 | 1.91 | 0.51 |
| 3:C:168:THR:HG22 | 26:C:306:PEK:H14 | 1.91 | 0.51 |
| 8:U:49:ASP:O | 8:U:52:VAL:HG22 | 2.11 | 0.51 |
| 2:B:146:MET:HA | 2:B:213:LEU:HD12 | 1.93 | 0.51 |
| 5:R:99:SER:HB2 | 5:R:104:LEU:HD21 | 1.91 | 0.51 |
| 5:R:67:ILE:O | 5:R:70:VAL:HG12 | 2.10 | 0.51 |
| 3:C:146:TRP:CE2 | 7:G:17:ARG:HG3 | 2.46 | 0.51 |
| 20:L:101:TGL:H202 | 20:L:101:TGL:C24 | 2.39 | 0.51 |
| 2:O:49:LYS:O | 4:Q:20:ARG:NH2 | 2.43 | 0.51 |
| 1:A:240:HIS:HB3 | 1:A:241:PRO:HD3 | 1.93 | 0.51 |
| 6:F:30:PRO:O | 6:F:96:LEU:HD11 | 2.11 | 0.51 |
| 7:T:3:ALA:O | 7:T:4:ALA:HB2 | 2.11 | 0.51 |
| 8:U:20:PHE:CE2 | 8:U:27:ARG:HG2 | 2.39 | 0.51 |
| 20:B:302:TGL:HC82 | 29:B:2113:HOH:O | 2.10 | 0.51 |
| 5:E:63:SER:O | 5:E:67:ILE:HG13 | 2.11 | 0.51 |
| 2:B:62:GLU:O | 2:B:66:THR:HB | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:14:SER:HB3 | 2:B:168:LEU:CD2 | 2.41 | 0.51 |
| 2:B:41:ILE:O | 2:B:45:MET:HG2 | 2.11 | 0.51 |
| 20:D:201:TGL:HG11 | 20:D:201:TGL:CC2 | 2.39 | 0.50 |
| 1:A:290:HIS:CD2 | 1:A:291:HIS:CD2 | 2.98 | 0.50 |
| 26:P:306:PEK:H383 | 27:T:102:CDL:H273 | 1.92 | 0.50 |
| 6:S:22:LEU:O | 6:S:25:ARG:HB3 | 2.11 | 0.50 |
| 2:O:145:PRO:HB2 | 2:O:148:MET:HG3 | 1.92 | 0.50 |
| 10:W:50:LEU:HD22 | 10:W:50:LEU:O | 2.12 | 0.50 |
| 2:B:196:CYS:HB2 | 2:B:207:MET:HG3 | 1.93 | 0.50 |
| 3:C:55:TYR:HE1 | 27:C:309:CDL:H521 | 1.77 | 0.50 |
| 29:A:883:HOH:O | 20:D:201:TGL:HG2 | 2.12 | 0.50 |
| 1:N:113:LEU:HD13 | 20:N:606:TGL:H292 | 1.93 | 0.50 |
| 1:N:240:HIS:HB3 | 1:N:241:PRO:HD3 | 1.93 | 0.50 |
| 26:C:306:PEK:H231 | 7:G:21:PHE:CD2 | 2.46 | 0.50 |
| 7:T:2:SER:OG | 26:T:101:PEK:H301 | 2.11 | 0.50 |
| 1:A:98:ASN:HB2 | 1:A:163:ASN:ND2 | 2.27 | 0.50 |
| 1:N:175:ALA:HB1 | 1:N:513:LEU:HD23 | 1.94 | 0.50 |
| 12:Y:2:HIS:ND1 | 12:Y:3:TYR:N | 2.60 | 0.50 |
| 26:C:305:PEK:C3 | 26:C:305:PEK:H71 | 2.42 | 0.49 |
| 4:D:127:LYS:HD2 | 29:I:108:HOH:O | 2.10 | 0.49 |
| 2:O:7:LEU:HD11 | 20:O:303:TGL:H161 | 1.92 | 0.49 |
| 8:U:7:LYS:O | 8:U:8:ILE:HG22 | 2.11 | 0.49 |
| 26:C:305:PEK:C16 | 26:C:305:PEK:H102 | 2.38 | 0.49 |
| 1:N:28:MET:CE | 17:N:604:HEA:H271 | 2.43 | 0.49 |
| 3:P:210:ILE:HG12 | 18:P:307:PGV:H132 | 1.94 | 0.49 |
| 21:B:303:PSC:H073 | 5:E:11:PHE:CG | 2.47 | 0.49 |
| 18:N:609:PGV:H262 | 18:P:307:PGV:H292 | 1.94 | 0.49 |
| 26:C:306:PEK:H383 | 27:G:101:CDL:C27 | 2.42 | 0.49 |
| 8:H:40:GLU:HG3 | 8:H:50:VAL:HG13 | 1.94 | 0.49 |
| 5:E:31:LYS:HE3 | 6:F:83:PRO:O | 2.13 | 0.49 |
| 1:N:400:PHE:HB3 | 20:N:606:TGL:H283 | 1.95 | 0.49 |
| 2:O:161:HIS:HB2 | 2:O:174:ALA:HB3 | 1.93 | 0.49 |
| 2:B:218:TYR:HE1 | 29:I:117:HOH:O | 1.95 | 0.49 |
| 2:O:1:FME:SD | 2:O:133:LEU:CD1 | 3.01 | 0.49 |
| 1:A:107:PRO:HB3 | 3:C:25:LEU:HB2 | 1.95 | 0.48 |
| 3:C:116:TRP:HA | 3:C:117:PRO:C | 2.33 | 0.48 |
| 2:O:139:ASP:OD2 | 2:O:140:ASN:N | 2.45 | 0.48 |
| 2:O:62:GLU:O | 2:O:66:THR:HB | 2.13 | 0.48 |
| 7:G:3:ALA:O | 7:G:4:ALA:HB2 | 2.12 | 0.48 |
| 1:N:347:LEU:HD13 | 1:N:383:MET:SD | 2.52 | 0.48 |
| 1:N:54:TYR:HB2 | 29:N:768:HOH:O | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:Q:127:LYS:O | 4:Q:130:PRO:HD3 | 2.13 | 0.48 |
| 2:B:102:HIS:O | 2:B:104:TRP:HA | 2.14 | 0.48 |
| 24:C:302:DMU:H25 | 26:C:305:PEK:H322 | 1.94 | 0.48 |
| 5:E:46:LYS:HG2 | 29:E:238:HOH:O | 2.13 | 0.48 |
| 3:P:187:THR:HG22 | 26:P:305:PEK:H052 | 1.94 | 0.48 |
| 29:H:138:HOH:O | 8:U:8:ILE:HG21 | 2.14 | 0.48 |
| 2:B:161:HIS:HB2 | 2:B:174:ALA:HB3 | 1.95 | 0.48 |
| 21:O:304:PSC:H62 | 21:O:304:PSC:H241 | 1.95 | 0.48 |
| 4:Q:101:HIS:HD2 | 4:Q:102:TYR:CE2 | 2.31 | 0.48 |
| 1:N:32:ALA:HB3 | 12:Y:36:PRO:HG2 | 1.95 | 0.48 |
| 2:B:82:ARG:HG2 | 2:B:86:MET:HE3 | 1.94 | 0.48 |
| 23:C:301:DCW:H62C | 18:C:307:PGV:H301 | 1.96 | 0.48 |
| 4:Q:51:LEU:HD21 | 4:Q:59:LEU:CD1 | 2.43 | 0.48 |
| 6:S:22:LEU:HD23 | 6:S:25:ARG:NH1 | 2.28 | 0.48 |
| 2:B:23:PHE:CZ | 2:B:80:SER:HB2 | 2.49 | 0.48 |
| 2:B:79:PRO:O | 2:B:83:ILE:HG13 | 2.13 | 0.48 |
| 9:I:36:LYS:HA | 9:I:40:ALA:HB3 | 1.95 | 0.48 |
| 2:O:16:ILE:HD13 | 2:O:16:ILE:HA | 1.73 | 0.48 |
| 3:P:116:TRP:HA | 3:P:117:PRO:C | 2.32 | 0.48 |
| 1:A:151:HIS:CD2 | 26:C:305:PEK:H382 | 2.49 | 0.48 |
| 20:N:607:TGL:H271 | 2:O:46:LEU:HD12 | 1.96 | 0.48 |
| 1:A:298:ASP:HB3 | 29:A:834:HOH:O | 2.13 | 0.48 |
| 3:C:16:TRP:HA | 3:C:16:TRP:CE3 | 2.48 | 0.48 |
| 1:A:1:FME:HCN | 1:A:4:ASN:H | 1.79 | 0.47 |
| 18:A:607:PGV:H262 | 18:C:307:PGV:H292 | 1.96 | 0.47 |
| 20:B:302:TGL:HC22 | 29:I:107:HOH:O | 2.12 | 0.47 |
| 27:P:309:CDL:H642 | 27:P:309:CDL:C19 | 2.36 | 0.47 |
| 1:A:2:PHE:HB3 | 29:A:890:HOH:O | 2.14 | 0.47 |
| 18:A:606:PGV:H061 | 18:A:606:PGV:P | 2.54 | 0.47 |
| 21:B:303:PSC:H241 | 21:B:303:PSC:H62 | 1.96 | 0.47 |
| 5:E:84:TYR:CZ | 5:E:88:GLU:HG3 | 2.49 | 0.47 |
| 4:Q:48:TRP:HB2 | 5:R:96:LEU:O | 2.14 | 0.47 |
| 5:R:105:GLY:O | 5:R:108:LYS:HG2 | 2.14 | 0.47 |
| 2:B:91:ASN:HD22 | 2:B:92:ASN:N | 2.12 | 0.47 |
| 18:N:608:PGV:H311 | 13:Z:16:ALA:HA | 1.97 | 0.47 |
| 27:G:101:CDL:H212 | 1:N:311:ILE:HD12 | 1.97 | 0.47 |
| 3:C:37:PHE:CD1 | 10:J:52:TRP:HZ3 | 2.33 | 0.47 |
| 1:N:177:SER:H | 1:N:180:GLN:NE2 | 2.13 | 0.47 |
| 3:P:210:ILE:HD13 | 23:P:301:DCW:H61C | 1.94 | 0.47 |
| 26:P:306:PEK:H383 | 27:T:102:CDL:C27 | 2.45 | 0.47 |
| 1:A:406:ASN:HD21 | 18:A:606:PGV:C2 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:168:THR:CG2 | 26:C:306:PEK:H14 | 2.45 | 0.47 |
| 27:C:309:CDL:H602 | 27:C:309:CDL:H632 | 1.67 | 0.47 |
| 1:N:160:GLY:HA3 | 29:N:740:HOH:O | 2.13 | 0.47 |
| 2:O:132:GLU:HB3 | 2:O:137:GLU:HG3 | 1.96 | 0.47 |
| 6:S:54:ASN:HD22 | 6:S:54:ASN:C | 2.18 | 0.47 |
| 1:A:314:ILE:HB | 1:A:315:PRO:CD | 2.45 | 0.47 |
| 5:E:37:VAL:HG11 | 5:E:70:VAL:HG21 | 1.97 | 0.47 |
| 11:K:24:PHE:O | 11:K:28:VAL:HG12 | 2.15 | 0.47 |
| 1:N:44:PRO:HG2 | 4:Q:111:PHE:CZ | 2.49 | 0.47 |
| 5:R:86:ILE:HA | 5:R:86:ILE:HD13 | 1.68 | 0.47 |
| 10:J:29:ASN:HD22 | 10:J:29:ASN:H | 1.63 | 0.47 |
| 1:A:1:FME:HCN | 1:A:4:ASN:HB2 | 1.96 | 0.47 |
| 1:A:306:THR:O | 1:A:310:MET:HG3 | 2.14 | 0.47 |
| 1:A:398:PRO:HA | 1:A:403:TYR:O | 2.15 | 0.47 |
| 6:F:85:CYS:SG | 6:F:87:THR:HG23 | 2.55 | 0.47 |
| 1:N:472:ILE:HD13 | 20:N:606:TGL:HA91 | 1.96 | 0.47 |
| 2:O:83:ILE:O | 2:O:87:MET:HG3 | 2.15 | 0.47 |
| 22:P:310:CHD:H161 | 29:P:469:HOH:O | 2.14 | 0.47 |
| 11:X:36:ILE:HG13 | 11:X:38:ILE:HG13 | 1.97 | 0.46 |
| 1:N:398:PRO:HA | 1:N:403:TYR:O | 2.15 | 0.46 |
| 1:A:35:LEU:HD11 | 1:A:462:LEU:HB2 | 1.98 | 0.46 |
| 18:C:307:PGV:H182 | 27:C:309:CDL:C67 | 2.45 | 0.46 |
| 12:L:41:ARG:HD2 | 13:M:40:TYR:CZ | 2.51 | 0.46 |
| 26:G:102:PEK:H042 | 3:P:77:LYS:NZ | 2.30 | 0.46 |
| 4:Q:131:ILE:HD12 | 4:Q:131:ILE:H | 1.81 | 0.46 |
| 3:C:146:TRP:CD2 | 3:C:162:ALA:HB2 | 2.50 | 0.46 |
| 7:G:2:SER:O | 26:G:102:PEK:H322 | 2.15 | 0.46 |
| 1:A:296:GLY:HA2 | 8:H:23:GLN:OE1 | 2.15 | 0.46 |
| 3:P:168:THR:CG2 | 26:P:306:PEK:H14 | 2.45 | 0.46 |
| 3:C:16:TRP:HE3 | 3:C:16:TRP:HA | 1.80 | 0.46 |
| 5:R:43:PRO:HB2 | 5:R:48:ILE:HD11 | 1.98 | 0.46 |
| 27:T:102:CDL:H601 | 27:T:102:CDL:H571 | 1.45 | 0.46 |
| 1:A:128:VAL:O | 1:A:128:VAL:HG12 | 2.16 | 0.46 |
| 20:N:607:TGL:H242 | 20:N:607:TGL:H212 | 1.75 | 0.46 |
| 2:B:164:ALA:O | 2:B:194:GLY:HA3 | 2.15 | 0.46 |
| 1:N:407:ASP:O | 1:N:411:LYS:HG3 | 2.15 | 0.46 |
| 2:O:215:PRO:HD3 | 9:V:60:PHE:CD2 | 2.51 | 0.46 |
| 3:P:195:SER:O | 3:P:199:VAL:HG23 | 2.16 | 0.46 |
| 4:Q:98:TRP:CD2 | 24:Z:101:DMU:H10 | 2.50 | 0.46 |
| 3:C:92:LEU:O | 3:C:95:THR:HB | 2.15 | 0.46 |
| 1:N:113:LEU:HD12 | 20:N:606:TGL:H292 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:N:607:TGL:HG11 | 20:N:607:TGL:CC2 | 2.39 | 0.46 |
| 6:F:90:LYS:HD2 | 29:F:244:HOH:O | 2.15 | 0.46 |
| 1:A:400:PHE:HB3 | 20:L:101:TGL:H283 | 1.98 | 0.46 |
| 11:X:6:ALA:HA | 11:X:7:PRO:HD2 | 1.86 | 0.46 |
| 1:A:321:PHE:CE2 | 21:B:303:PSC:H341 | 2.51 | 0.45 |
| 3:C:55:TYR:CE1 | 27:C:309:CDL:H521 | 2.51 | 0.45 |
| 1:N:440:TYR:HE2 | 2:O:204:HIS:CE1 | 2.34 | 0.45 |
| 2:O:217:LYS:HE2 | 2:O:217:LYS:HA | 1.98 | 0.45 |
| 20:O:303:TGL:HC22 | 29:Q:220:HOH:O | 2.16 | 0.45 |
| 2:O:62:GLU:HB2 | 29:O:490:HOH:O | 2.16 | 0.45 |
| 5:R:5:HIS:HB3 | 5:R:6:GLU:H | 1.63 | 0.45 |
| 1:N:242:GLU:HA | 1:N:245:ILE:HD12 | 1.99 | 0.45 |
| 2:O:92:ASN:HA | 2:O:93:PRO:HD2 | 1.79 | 0.45 |
| 21:B:303:PSC:C34 | 21:B:303:PSC:H142 | 2.23 | 0.45 |
| 10:J:40:LEU:HD12 | 22:J:101:CHD:H183 | 1.99 | 0.45 |
| 4:Q:63:LYS:HG2 | 4:Q:64:PHE:CE1 | 2.51 | 0.45 |
| 3:C:117:PRO:HG3 | 3:C:123:PRO:HG2 | 1.99 | 0.45 |
| 6:F:64:GLU:O | 6:F:65:ASP:HB2 | 2.17 | 0.45 |
| 1:N:468:MET:O | 1:N:472:ILE:HG13 | 2.16 | 0.45 |
| 1:N:310:MET:HE1 | 2:O:76:ILE:HB | 1.98 | 0.45 |
| 4:Q:23:PRO:O | 4:Q:25:PRO:HD3 | 2.16 | 0.45 |
| 21:B:303:PSC:H12 | 21:B:303:PSC:H322 | 1.99 | 0.45 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:CC4 | 2.29 | 0.45 |
| 1:A:482:VAL:HG22 | 13:M:1:ILE:HD11 | 1.98 | 0.45 |
| 13:M:42:LYS:CE | 13:M:42:LYS:HA | 2.44 | 0.45 |
| 21:O:304:PSC:H032 | 29:R:203:HOH:O | 2.17 | 0.45 |
| 2:O:68:LEU:CB | 2:O:69:PRO:HD3 | 2.47 | 0.45 |
| 3:P:112:LEU:HD13 | 3:P:118:PRO:HG3 | 1.97 | 0.45 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:CC3 | 2.28 | 0.45 |
| 18:A:606:PGV:H311 | 13:M:16:ALA:HA | 1.98 | 0.45 |
| 2:O:216:LEU:O | 2:O:219:PHE:HB3 | 2.17 | 0.45 |
| 3:P:92:LEU:O | 3:P:95:THR:HB | 2.16 | 0.45 |
| 1:A:32:ALA:HB3 | 12:L:36:PRO:HG2 | 1.98 | 0.45 |
| 2:O:164:ALA:O | 2:O:194:GLY:HA3 | 2.15 | 0.45 |
| 6:S:70:ILE:HG13 | 6:S:84:SER:HB3 | 1.98 | 0.45 |
| 1:A:165:ILE:O | 1:A:169:ILE:HG12 | 2.16 | 0.45 |
| 21:B:303:PSC:H251 | 21:B:303:PSC:H221 | 1.75 | 0.45 |
| 22:C:310:CHD:H112 | 22:C:310:CHD:H12A | 1.71 | 0.45 |
| 4:D:102:TYR:CD1 | 13:M:35:TYR:HE1 | 2.35 | 0.45 |
| 1:N:194:LEU:HD22 | 1:N:285:PHE:HE2 | 1.82 | 0.45 |
| 5:E:12:ASP:OD1 | 5:E:44:GLU:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:95:GLN:OE1 | 6:F:95:GLN:HA | 2.17 | 0.45 |
| 7:G:7:ASP:O | 1:N:169:ILE:HD12 | 2.16 | 0.45 |
| 20:N:606:TGL:H272 | 20:N:606:TGL:H231 | 1.98 | 0.45 |
| 11:X:54:ARG:HH21 | 11:X:54:ARG:CG | 2.30 | 0.45 |
| 4:D:16:TYR:CE1 | 4:D:25:PRO:HG2 | 2.52 | 0.45 |
| 1:N:265:LYS:HB2 | 1:N:490:THR:HG21 | 1.99 | 0.44 |
| 1:A:264:LYS:HE2 | 29:A:888:HOH:O | 2.15 | 0.44 |
| 23:C:301:DCW:H101 | 26:C:305:PEK:C37 | 2.47 | 0.44 |
| 1:N:334:TRP:CZ2 | 2:O:46:LEU:HB3 | 2.53 | 0.44 |
| 10:W:16:ASN:ND2 | 10:W:18:LEU:HD12 | 2.33 | 0.44 |
| 1:A:406:ASN:HD21 | 18:A:606:PGV:H21 | 1.82 | 0.44 |
| 3:C:247:VAL:HG11 | 26:T:101:PEK:H132 | 1.99 | 0.44 |
| 4:D:48:TRP:CH2 | 5:E:56:ARG:HA | 2.53 | 0.44 |
| 11:K:42:PRO:HG2 | 11:K:47:ARG:NE | 2.32 | 0.44 |
| 3:P:249:TRP:HD1 | 29:P:419:HOH:O | 1.99 | 0.44 |
| 3:P:40:MET:O | 3:P:44:MET:HG2 | 2.17 | 0.44 |
| 5:R:96:LEU:HD12 | 5:R:98:ILE:HD11 | 1.98 | 0.44 |
| 2:B:74:ILE:HD11 | 27:T:102:CDL:H452 | 1.98 | 0.44 |
| 7:T:38:HIS:CD2 | 27:T:102:CDL:HA21 | 2.52 | 0.44 |
| 6:F:8:THR:OG1 | 6:F:11:GLU:HG3 | 2.17 | 0.44 |
| 1:N:488:THR:HB | 1:N:495:LEU:HD13 | 1.99 | 0.44 |
| 1:A:472:ILE:HD13 | 20:L:101:TGL:HA91 | 2.00 | 0.44 |
| 8:H:30:TRP:CE2 | 8:H:34:LEU:HD11 | 2.51 | 0.44 |
| 7:T:6:GLY:O | 26:T:101:PEK:H311 | 2.18 | 0.44 |
| 12:Y:42:HIS:NE2 | 12:Y:46:LYS:HD2 | 2.32 | 0.44 |
| 18:N:609:PGV:H343 | 23:P:301:DCW:C4 | 2.47 | 0.44 |
| 4:Q:122:ARG:HG2 | 4:Q:126:MET:CE | 2.47 | 0.44 |
| 5:R:12:ASP:HA | 5:R:47:ILE:HD11 | 1.99 | 0.44 |
| 3:C:42:LEU:HD23 | 3:C:42:LEU:HA | 1.80 | 0.44 |
| 2:O:100:MET:HB2 | 2:O:107:SER:OG | 2.18 | 0.44 |
| 1:N:481:GLU:HB2 | 13:Z:4:LYS:HE2 | 1.97 | 0.44 |
| 1:A:377:PHE:CD1 | 17:A:605:HEA:HAD1 | 2.53 | 0.44 |
| 3:C:30:GLY:HA2 | 3:C:42:LEU:HB3 | 2.00 | 0.44 |
| 1:A:449:MET:SD | 2:B:5:MET:HG2 | 2.57 | 0.44 |
| 3:C:47:LEU:O | 3:C:51:MET:HG2 | 2.18 | 0.44 |
| 7:G:84:LYS:HD2 | 7:G:84:LYS:N | 2.07 | 0.44 |
| 2:O:196:CYS:HB2 | 2:O:207:MET:HG3 | 2.00 | 0.44 |
| 6:S:30:PRO:O | 6:S:96:LEU:HD11 | 2.18 | 0.44 |
| 12:Y:26:THR:HG23 | 13:Z:25:SER:HB3 | 2.00 | 0.44 |
| 1:A:321:PHE:CZ | 21:B:303:PSC:H171 | 2.53 | 0.43 |
| 24:C:302:DMU:H30 | 24:C:302:DMU:O1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:31:LEU:HA | 3:C:31:LEU:HD23 | 1.89 | 0.43 |
| 4:D:98:TRP:CD2 | 24:M:101:DMU:H10 | 2.53 | 0.43 |
| 5:E:97:GLY:HA2 | 29:E:258:HOH:O | 2.18 | 0.43 |
| 6:F:54:ASN:OD1 | 6:F:76:LYS:HD2 | 2.18 | 0.43 |
| 10:J:31:LEU:HA | 10:J:31:LEU:HD12 | 1.82 | 0.43 |
| 4:D:88:PHE:CZ | 13:M:19:LEU:HD21 | 2.53 | 0.43 |
| 2:O:121:TYR:O | 2:O:138:VAL:HA | 2.17 | 0.43 |
| 3:P:210:ILE:CD1 | 23:P:301:DCW:H52C | 2.48 | 0.43 |
| 5:R:53:ARG:O | 5:R:56:ARG:HB3 | 2.18 | 0.43 |
| 6:S:51:SER:HB2 | 6:S:91:LEU:HD11 | 2.00 | 0.43 |
| 23:C:301:DCW:H101 | 26:C:305:PEK:H371 | 2.01 | 0.43 |
| 8:H:9:LYS:HB2 | 8:H:9:LYS:HE2 | 1.86 | 0.43 |
| 27:T:102:CDL:HA62 | 27:T:102:CDL:H322 | 2.01 | 0.43 |
| 13:Z:35:TYR:HD2 | 13:Z:36:HIS:CE1 | 2.37 | 0.43 |
| 21:O:304:PSC:H073 | 5:R:11:PHE:CG | 2.53 | 0.43 |
| 2:O:9:PHE:HB2 | 2:O:21:LEU:HD21 | 2.00 | 0.43 |
| 2:O:134:ARG:HB2 | 4:Q:110:THR:HG21 | 1.99 | 0.43 |
| 4:Q:122:ARG:HG2 | 4:Q:126:MET:HE3 | 2.00 | 0.43 |
| 2:B:78:LEU:HA | 2:B:78:LEU:HD12 | 1.72 | 0.43 |
| 3:C:149:HIS:O | 3:C:153:GLU:HG3 | 2.19 | 0.43 |
| 1:N:513:LEU:HD22 | 1:N:513:LEU:HA | 1.81 | 0.43 |
| 2:O:74:ILE:O | 2:O:78:LEU:HD22 | 2.19 | 0.43 |
| 7:T:48:ILE:HA | 7:T:49:PRO:HD3 | 1.80 | 0.43 |
| 5:R:100:THR:HB | 5:R:101:PRO:HD2 | 2.00 | 0.43 |
| 2:O:48:THR:HB | 9:V:16:ARG:CZ | 2.48 | 0.43 |
| 4:D:82:VAL:O | 4:D:86:MET:HG3 | 2.18 | 0.43 |
| 4:D:126:MET:HA | 9:I:68:ILE:HD13 | 2.01 | 0.43 |
| 3:P:210:ILE:HD13 | 23:P:301:DCW:C6 | 2.49 | 0.43 |
| 27:P:309:CDL:H431 | 29:W:206:HOH:O | 2.19 | 0.43 |
| 1:A:468:MET:HG3 | 29:A:849:HOH:O | 2.18 | 0.43 |
| 17:A:605:HEA:HAD2 | 17:A:605:HEA:HHA | 1.85 | 0.43 |
| 10:J:50:LEU:HD22 | 10:J:50:LEU:O | 2.18 | 0.43 |
| 20:L:101:TGL:H231 | 20:L:101:TGL:H272 | 2.01 | 0.43 |
| 1:N:400:PHE:HB3 | 20:N:606:TGL:C28 | 2.49 | 0.43 |
| 2:O:1:FME:SD | 2:O:133:LEU:HD11 | 2.58 | 0.43 |
| 4:Q:86:MET:O | 11:X:25:CYS:HB2 | 2.18 | 0.43 |
| 27:T:102:CDL:C54 | 27:T:102:CDL:H231 | 2.40 | 0.43 |
| 1:A:282:PHE:HZ | 27:T:102:CDL:H761 | 1.84 | 0.43 |
| 1:A:426:PHE:HB3 | 1:A:427:PRO:HD3 | 2.01 | 0.43 |
| 17:N:604:HEA:H271 | 17:N:604:HEA:H212 | 1.84 | 0.43 |
| 21:O:304:PSC:O01 | 21:O:304:PSC:H212 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:P:309:CDL:H672 | 27:P:309:CDL:H641 | 1.87 | 0.43 |
| 4:Q:121:LYS:HG2 | 11:X:53:TRP:CD1 | 2.53 | 0.43 |
| 2:B:200:CYS:SG | 2:B:204:HIS:HA | 2.58 | 0.43 |
| 2:B:41:ILE:CD1 | 21:B:303:PSC:H342 | 2.45 | 0.43 |
| 3:C:151:LEU:HB2 | 3:C:159:MET:HG3 | 2.01 | 0.43 |
| 3:C:55:TYR:CD1 | 27:C:309:CDL:H532 | 2.54 | 0.43 |
| 4:D:69:ALA:O | 5:E:109:VAL:HG12 | 2.18 | 0.43 |
| 2:O:1:FME:SD | 2:O:133:LEU:HD13 | 2.59 | 0.43 |
| 3:P:51:MET:SD | 27:P:309:CDL:H622 | 2.59 | 0.43 |
| 4:Q:101:HIS:HD2 | 4:Q:102:TYR:CD2 | 2.37 | 0.43 |
| 7:T:2:SER:O | 26:T:101:PEK:H322 | 2.19 | 0.43 |
| 7:T:84:LYS:N | 7:T:84:LYS:HD2 | 2.10 | 0.43 |
| 8:U:57:ARG:HA | 8:U:60:TYR:CD2 | 2.53 | 0.43 |
| 1:A:98:ASN:HB2 | 1:A:163:ASN:HD21 | 1.84 | 0.42 |
| 1:A:431:LEU:HD21 | 1:A:450:TRP:HB2 | 2.01 | 0.42 |
| 7:G:34:ASN:O | 7:G:37:LEU:HB3 | 2.18 | 0.42 |
| 1:A:1:FME:HE2 | 1:A:1:FME:HA | 2.01 | 0.42 |
| 22:B:304:CHD:H231 | 22:B:304:CHD:H213 | 1.82 | 0.42 |
| 3:C:51:MET:SD | 27:C:309:CDL:H622 | 2.59 | 0.42 |
| 20:D:201:TGL:HC51 | 20:D:201:TGL:HC22 | 1.82 | 0.42 |
| 18:N:608:PGV:H012 | 29:N:860:HOH:O | 2.19 | 0.42 |
| 1:A:76:GLY:O | 1:A:80:ASN:HB2 | 2.19 | 0.42 |
| 1:N:321:PHE:HB3 | 2:O:65:TRP:CE3 | 2.54 | 0.42 |
| 27:G:101:CDL:H601 | 27:G:101:CDL:H571 | 1.42 | 0.42 |
| 26:G:102:PEK:H132 | 3:P:247:VAL:HG11 | 2.00 | 0.42 |
| 23:P:301:DCW:C10 | 26:P:305:PEK:H371 | 2.50 | 0.42 |
| 1:A:52:GLN:O | 1:A:56:VAL:HG23 | 2.20 | 0.42 |
| 18:A:607:PGV:H332 | 24:C:302:DMU:H24 | 2.01 | 0.42 |
| 2:B:7:LEU:HD11 | 20:B:302:TGL:H161 | 2.02 | 0.42 |
| 8:H:36:PHE:CD1 | 8:H:57:ARG:HB2 | 2.54 | 0.42 |
| 1:N:374:VAL:HA | 1:N:377:PHE:CE1 | 2.55 | 0.42 |
| 1:N:399:LEU:HB2 | 1:N:494:TRP:CZ3 | 2.54 | 0.42 |
| 24:P:302:DMU:H26 | 24:P:302:DMU:H18 | 1.80 | 0.42 |
| 3:P:87:ILE:O | 3:P:91:VAL:HG23 | 2.19 | 0.42 |
| 7:T:31:CYS:SG | 27:T:102:CDL:H552 | 2.60 | 0.42 |
| 4:Q:126:MET:HA | 9:V:68:ILE:HD13 | 2.01 | 0.42 |
| 2:B:134:ARG:HB2 | 4:D:110:THR:HG21 | 2.01 | 0.42 |
| 17:N:605:HEA:HAD2 | 17:N:605:HEA:HHA | 1.82 | 0.42 |
| 8:U:36:PHE:CD1 | 8:U:57:ARG:HB2 | 2.55 | 0.42 |
| 12:Y:26:THR:HG23 | 13:Z:25:SER:HB2 | 2.02 | 0.42 |
| 1:A:242:GLU:HA | 1:A:245:ILE:HD12 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:514:LYS:HE2 | 29:F:226:HOH:O | 2.18 | 0.42 |
| 18:A:606:PGV:H301 | 18:A:606:PGV:H152 | 2.02 | 0.42 |
| 3:C:241:TYR:O | 3:C:244:PHE:HB3 | 2.19 | 0.42 |
| 18:N:609:PGV:H321 | 26:P:305:PEK:C36 | 2.37 | 0.42 |
| 2:O:57:ASP:N | 21:O:304:PSC:H201 | 2.23 | 0.42 |
| 26:G:102:PEK:H132 | 3:P:247:VAL:CG1 | 2.50 | 0.42 |
| 7:G:5:LYS:CB | 26:G:102:PEK:H362 | 2.34 | 0.42 |
| 7:T:11:TPO:HG22 | 7:T:16:TRP:HE1 | 1.85 | 0.42 |
| 8:U:37:HIS:CD2 | 8:U:76:ARG:CZ | 3.03 | 0.42 |
| 18:A:607:PGV:H182 | 3:C:28:THR:HG22 | 2.00 | 0.42 |
| 3:C:64:GLU:HA | 3:C:68:GLN:HE21 | 1.84 | 0.42 |
| 20:L:101:TGL:HB61 | 20:L:101:TGL:HB31 | 1.92 | 0.42 |
| 24:P:302:DMU:H30 | 24:P:302:DMU:O1 | 2.19 | 0.42 |
| 26:P:305:PEK:C3 | 26:P:305:PEK:H71 | 2.43 | 0.42 |
| 23:P:301:DCW:H62C | 18:P:307:PGV:H281 | 2.02 | 0.42 |
| 4:Q:20:ARG:HD2 | 4:Q:72:ASN:OD1 | 2.20 | 0.42 |
| 12:L:35:ALA:HB3 | 12:L:36:PRO:HD3 | 2.01 | 0.42 |
| 21:O:304:PSC:H073 | 5:R:11:PHE:CB | 2.49 | 0.42 |
| 1:A:498:CYS:HA | 1:A:499:PRO:HA | 1.93 | 0.41 |
| 1:N:426:PHE:HB3 | 1:N:427:PRO:HD3 | 2.01 | 0.41 |
| 4:Q:130:PRO:O | 4:Q:136:ALA:HB2 | 2.20 | 0.41 |
| 4:Q:34:SER:H | 4:Q:37:GLN:HE21 | 1.68 | 0.41 |
| 6:S:92:VAL:HG23 | 6:S:92:VAL:O | 2.19 | 0.41 |
| 1:A:158:ILE:HD13 | 23:C:301:DCW:H121 | 2.01 | 0.41 |
| 2:B:122:MET:SD | 2:B:206:PHE:HB3 | 2.60 | 0.41 |
| 13:M:37:LEU:HD23 | 13:M:37:LEU:HA | 1.81 | 0.41 |
| 1:N:261:TYR:CE2 | 1:N:337:ALA:HB3 | 2.55 | 0.41 |
| 2:O:1:FME:CE | 2:O:133:LEU:HD13 | 2.51 | 0.41 |
| 2:O:224:ALA:O | 2:O:227:LEU:CG | 2.59 | 0.41 |
| 1:N:422:ASN:HB3 | 20:O:303:TGL:H242 | 2.02 | 0.41 |
| 3:P:16:TRP:HA | 3:P:16:TRP:CE3 | 2.55 | 0.41 |
| 3:P:168:THR:HG21 | 26:P:306:PEK:H12 | 2.00 | 0.41 |
| 9:V:37:PHE:HA | 9:V:41:GLU:HB2 | 2.02 | 0.41 |
| 2:O:189:PRO:HD2 | 9:V:54:TYR:OH | 2.20 | 0.41 |
| 13:Z:28:LEU:HB2 | 13:Z:29:PRO:HD3 | 2.01 | 0.41 |
| 1:A:194:LEU:HD22 | 1:A:285:PHE:HE2 | 1.84 | 0.41 |
| 2:B:78:LEU:CD1 | 27:T:102:CDL:H351 | 2.50 | 0.41 |
| 3:C:187:THR:CB | 7:G:68:THR:HG21 | 2.50 | 0.41 |
| 21:O:304:PSC:H12 | 21:O:304:PSC:H322 | 2.03 | 0.41 |
| 3:P:243:HIS:O | 3:P:247:VAL:HG23 | 2.20 | 0.41 |
| 27:P:309:CDL:H401 | 27:P:309:CDL:H371 | 1.90 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:194:LEU:HD22 | 1:A:285:PHE:CE2 | 2.55 | 0.41 |
| 17:A:604:HEA:HHC | 17:A:604:HEA:H122 | 2.03 | 0.41 |
| 18:A:606:PGV:C15 | 18:A:606:PGV:H321 | 2.50 | 0.41 |
| 27:C:309:CDL:H672 | 27:C:309:CDL:H641 | 1.90 | 0.41 |
| 1:N:171:MET:HG2 | 3:P:8:TYR:CE1 | 2.55 | 0.41 |
| 1:A:383:MET:O | 1:A:387:PHE:CB | 2.68 | 0.41 |
| 1:A:394:VAL:HG23 | 1:A:395:HIS:N | 2.35 | 0.41 |
| 2:B:151:ARG:HD3 | 2:B:181:GLN:HE21 | 1.86 | 0.41 |
| 26:C:306:PEK:H371 | 27:G:101:CDL:H261 | 2.01 | 0.41 |
| 1:N:175:ALA:HB2 | 6:S:35:ALA:HB1 | 2.03 | 0.41 |
| 1:N:390:MET:O | 1:N:394:VAL:HG13 | 2.21 | 0.41 |
| 2:O:128:LEU:HD11 | 2:O:134:ARG:HA | 2.02 | 0.41 |
| 22:W:101:CHD:H12A | 22:W:101:CHD:H112 | 1.83 | 0.41 |
| 2:B:116:LEU:HD12 | 2:B:117:SER:N | 2.36 | 0.41 |
| 5:E:52:LEU:O | 5:E:55:CYS:HB2 | 2.20 | 0.41 |
| 2:O:1:FME:HCN | 2:O:193:TYR:HB2 | 2.03 | 0.41 |
| 1:N:377:PHE:CD1 | 17:N:605:HEA:HAD1 | 2.56 | 0.41 |
| 21:O:304:PSC:H073 | 5:R:11:PHE:HB3 | 2.03 | 0.41 |
| 1:A:377:PHE:HA | 1:A:380:VAL:CG2 | 2.51 | 0.41 |
| 2:B:123:ILE:CG2 | 2:B:128:LEU:HD23 | 2.51 | 0.41 |
| 3:C:187:THR:HG22 | 26:C:305:PEK:H052 | 2.02 | 0.41 |
| 27:G:101:CDL:HA62 | 27:G:101:CDL:H322 | 2.02 | 0.41 |
| 7:G:48:ILE:HA | 7:G:49:PRO:HD3 | 1.86 | 0.41 |
| 2:O:75:LEU:HD12 | 2:O:75:LEU:HA | 1.86 | 0.41 |
| 8:H:40:GLU:HG3 | 8:H:50:VAL:CG1 | 2.51 | 0.41 |
| 8:H:64:CYS:HA | 8:H:65:PRO:HD3 | 1.97 | 0.41 |
| 2:B:215:PRO:HD3 | 9:I:60:PHE:CD2 | 2.56 | 0.41 |
| 8:U:57:ARG:HH11 | 8:U:61:LYS:HE2 | 1.86 | 0.41 |
| 1:A:1:FME:HA | 1:A:1:FME:CE | 2.51 | 0.41 |
| 1:A:229:ILE:HD11 | 2:B:175:ILE:HD13 | 2.03 | 0.41 |
| 3:C:115:CYS:HB2 | 29:C:478:HOH:O | 2.20 | 0.41 |
| 4:D:33:LEU:HD22 | 4:D:37:GLN:HB3 | 2.03 | 0.41 |
| 1:N:113:LEU:O | 1:N:117:MET:HG2 | 2.20 | 0.41 |
| 1:N:169:ILE:HD11 | 1:N:189:MET:SD | 2.61 | 0.41 |
| 1:N:172:LYS:HD2 | 1:N:181:THR:HG21 | 2.03 | 0.41 |
| 2:O:160:LEU:HD22 | 2:O:175:ILE:HG12 | 2.02 | 0.41 |
| 7:T:79:PRO:HD2 | 29:T:203:HOH:O | 2.19 | 0.41 |
| 2:B:92:ASN:HA | 2:B:93:PRO:HD2 | 1.93 | 0.40 |
| 20:D:201:TGL:HC61 | 29:D:364:HOH:O | 2.20 | 0.40 |
| 3:P:129:VAL:N | 3:P:130:PRO:CD | 2.84 | 0.40 |
| 3:P:156:ARG:HG3 | 3:P:156:ARG:HH11 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:C:301:DCW:H62C | 18:C:307:PGV:H281 | 2.02 | 0.40 |
| 3:C:29:SER:HB2 | 3:C:42:LEU:HD13 | 2.02 | 0.40 |
| 17:N:604:HEA:H122 | 17:N:604:HEA:HHC | 2.03 | 0.40 |
| 3:P:230:ASN:HB2 | 29:S:217:HOH:O | 2.21 | 0.40 |
| 27:P:309:CDL:HB21 | 27:P:309:CDL:CB3 | 2.51 | 0.40 |
| 10:W:21:HIS:O | 10:W:22:LEU:HD23 | 2.21 | 0.40 |
| 18:A:607:PGV:H91 | 3:C:50:ASN:OD1 | 2.20 | 0.40 |
| 2:B:56:MET:HA | 21:B:303:PSC:H201 | 2.04 | 0.40 |
| 3:C:51:MET:SD | 27:C:309:CDL:C62 | 3.09 | 0.40 |
| 4:D:107:ILE:HD13 | 11:K:39:GLU:CB | 2.51 | 0.40 |
| 4:Q:121:LYS:HG2 | 11:X:53:TRP:HD1 | 1.85 | 0.40 |
| 1:A:321:PHE:HB3 | 2:B:65:TRP:CE3 | 2.56 | 0.40 |
| 17:A:605:HEA:H11 | 17:A:605:HEA:HMB1 | 1.91 | 0.40 |
| 27:T:102:CDL:H251 | 27:T:102:CDL:H222 | 1.85 | 0.40 |
| 2:B:145:PRO:HA | 2:B:214:VAL:O | 2.21 | 0.40 |
| 21:B:303:PSC:H212 | 21:B:303:PSC:O01 | 2.21 | 0.40 |
| 7:G:6:GLY:O | 26:G:102:PEK:H311 | 2.21 | 0.40 |
| 1:N:459:PHE:HB3 | 4:Q:92:THR:HG23 | 2.04 | 0.40 |
| 7:T:67:HIS:HD2 | 7:T:71:HIS:CD2 | 2.39 | 0.40 |

There are no symmetry-related clashes.

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 | 512/514 (100%) | 493 (96%) | 19 (4%) | 0 | 100 | 100 |
| 1 | N | 512/514 (100%) | 493 (96%) | 19 (4%) | 0 | 100 | 100 |
| 2 | B | 225/227 (99%) | 209 (93%) | 14 (6%) | 2 (1%) | 17 | 16 |
| 2 | O | 225/227 (99%) | 206 (92%) | 18 (8%) | 1 (0%) | 34 | 37 |
| 3 | C | 257/261 (98%) | 251 (98%) | 6 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | P | 257/261 (98%) | 251 (98%) | 6 (2%) | 0 | 100 | 100 |
| 4 | D | 142/147 (97%) | 140 (99%) | 2 (1%) | 0 | 100 | 100 |
| 4 | Q | 142/147 (97%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | E | 103/109 (94%) | 101 (98%) | 2 (2%) | 0 | 100 | 100 |
| 5 | R | 103/109 (94%) | 100 (97%) | 3 (3%) | 0 | 100 | 100 |
| 6 | F | 96/98 (98%) | 87 (91%) | 6 (6%) | 3 (3%) | 4 | 2 |
| 6 | S | 96/98 (98%) | 87 (91%) | 5 (5%) | 4 (4%) | 3 | 1 |
| 7 | G | 81/85 (95%) | 64 (79%) | 9 (11%) | 8 (10%) | 0 | 0 |
| 7 | T | 81/85 (95%) | 65 (80%) | 8 (10%) | 8 (10%) | 0 | 0 |
| 8 | H | 77/85 (91%) | 70 (91%) | 6 (8%) | 1 (1%) | 12 | 9 |
| 8 | U | 77/85 (91%) | 70 (91%) | 6 (8%) | 1 (1%) | 12 | 9 |
| 9 | I | 71/73 (97%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 9 | V | 71/73 (97%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 10 | J | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 10 | W | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | K | 47/56 (84%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | X | 47/56 (84%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 12 | L | 44/47 (94%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 12 | Y | 44/47 (94%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | M | 41/46 (89%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 13 | Z | 41/46 (89%) | 41 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3504/3614 (97%) | 3329 (95%) | 147 (4%) | 28 (1%) | 19 | 19 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 4 | ALA |
| 7 | G | 7 | ASP |
| 7 | G | 8 | HIS |
| 7 | G | 39 | SER |
| 6 | S | 94 | HIS |
| 6 | S | 95 | GLN |
| 7 | T | 4 | ALA |
| 7 | T | 7 | ASP |
| 7 | T | 8 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | T | 39 | SER |
| 2 | B | 60 | GLU |
| 6 | F | 94 | HIS |
| 6 | F | 95 | GLN |
| 7 | G | 40 | GLY |
| 8 | H | 8 | ILE |
| 2 | O | 60 | GLU |
| 7 | T | 40 | GLY |
| 7 | G | 3 | ALA |
| 6 | S | 93 | PRO |
| 7 | T | 3 | ALA |
| 8 | U | 8 | ILE |
| 7 | G | 6 | GLY |
| 6 | F | 96 | LEU |
| 6 | S | 96 | LEU |
| 7 | T | 6 | GLY |
| 2 | B | 92 | ASN |
| 7 | G | 10 | GLY |
| 7 | T | 10 | GLY |

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 | 426/426 (100%) | 416 (98%) | 10 (2%) | 50 | 63 |
| 1 | N | 426/426 (100%) | 414 (97%) | 12 (3%) | 43 | 56 |
| 2 | B | 210/210 (100%) | 201 (96%) | 9 (4%) | 29 | 36 |
| 2 | O | 210/210 (100%) | 195 (93%) | 15 (7%) | 14 | 16 |
| 3 | C | 224/226 (99%) | 217 (97%) | 7 (3%) | 40 | 51 |
| 3 | P | 224/226 (99%) | 219 (98%) | 5 (2%) | 52 | 65 |
| 4 | D | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 90 |
| 4 | Q | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 90 |
| 5 | E | 92/95 (97%) | 89 (97%) | 3 (3%) | 38 | 49 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 5 | R | 92/95 (97%) | 88 (96%) | 4 (4%) | 29 | 36 |
| 6 | F | 81/81 (100%) | 80 (99%) | 1 (1%) | 71 | 83 |
| 6 | S | 81/81 (100%) | 78 (96%) | 3 (4%) | 34 | 43 |
| 7 | G | 67/68 (98%) | 62 (92%) | 5 (8%) | 13 | 14 |
| 7 | T | 67/68 (98%) | 61 (91%) | 6 (9%) | 9 | 9 |
| 8 | H | 71/75 (95%) | 69 (97%) | 2 (3%) | 43 | 56 |
| 8 | U | 71/75 (95%) | 68 (96%) | 3 (4%) | 30 | 38 |
| 9 | I | 57/57 (100%) | 54 (95%) | 3 (5%) | 22 | 27 |
| 9 | V | 57/57 (100%) | 56 (98%) | 1 (2%) | 59 | 72 |
| 10 | J | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 39 |
| 10 | W | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 69 |
| 11 | K | 39/46 (85%) | 39 (100%) | 0 | 100 | 100 |
| 11 | X | 39/46 (85%) | 37 (95%) | 2 (5%) | 24 | 29 |
| 12 | L | 39/40 (98%) | 38 (97%) | 1 (3%) | 46 | 58 |
| 12 | Y | 39/40 (98%) | 39 (100%) | 0 | 100 | 100 |
| 13 | M | 37/38 (97%) | 29 (78%) | 8 (22%) | 1 | 1 |
| 13 | Z | 37/38 (97%) | 33 (89%) | 4 (11%) | 6 | 6 |
| All | All | 3040/3082 (99%) | 2931 (96%) | 109 (4%) | 35 | 45 |

All (109) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 38 | ARG |
| 1 | A | 109 | PHE |
| 1 | A | 115 | SER |
| 1 | A | 138 | HIS |
| 1 | A | 180 | GLN |
| 1 | A | 238 | PHE |
| 1 | A | 369 | ASP |
| 1 | A | 486 | ASP |
| 1 | A | 504 | THR |
| 1 | A | 513 | LEU |
| 2 | B | 33 | LEU |
| 2 | B | 60 | GLU |
| 2 | B | 66 | THR |
| 2 | B | 75 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 78 | LEU |
| 2 | B | 91 | ASN |
| 2 | B | 115 | ASP |
| 2 | B | 167 | SER |
| 2 | B | 171 | LYS |
| 3 | C | 13 | PRO |
| 3 | C | 17 | PRO |
| 3 | C | 110 | PRO |
| 3 | C | 159 | MET |
| 3 | C | 179 | SER |
| 3 | C | 192 | VAL |
| 3 | C | 214 | PHE |
| 4 | D | 51 | LEU |
| 5 | E | 70 | VAL |
| 5 | E | 90 | ARG |
| 5 | E | 91 | PRO |
| 6 | F | 48 | LEU |
| 7 | G | 17 | ARG |
| 7 | G | 18 | PHE |
| 7 | G | 36 | TRP |
| 7 | G | 54 | ARG |
| 7 | G | 84 | LYS |
| 8 | H | 29 | CYS |
| 8 | H | 60 | TYR |
| 9 | I | 8 | GLN |
| 9 | I | 15 | ARG |
| 9 | I | 37 | PHE |
| 10 | J | 4 | ARG |
| 10 | J | 50 | LEU |
| 12 | L | 2 | HIS |
| 13 | M | 4 | LYS |
| 13 | M | 12 | PRO |
| 13 | M | 13 | LYS |
| 13 | M | 34 | LEU |
| 13 | M | 38 | ASP |
| 13 | M | 39 | ASN |
| 13 | M | 42 | LYS |
| 13 | M | 43 | SER |
| 1 | N | 38 | ARG |
| 1 | N | 96 | ARG |
| 1 | N | 109 | PHE |
| 1 | N | 115 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 138 | HIS |
| 1 | N | 180 | GLN |
| 1 | N | 238 | PHE |
| 1 | N | 241 | PRO |
| 1 | N | 338 | MET |
| 1 | N | 369 | ASP |
| 1 | N | 484 | THR |
| 1 | N | 513 | LEU |
| 2 | O | 3 | TYR |
| 2 | O | 16 | ILE |
| 2 | O | 32 | PHE |
| 2 | O | 33 | LEU |
| 2 | O | 54 | SER |
| 2 | O | 60 | GLU |
| 2 | O | 66 | THR |
| 2 | O | 68 | LEU |
| 2 | O | 75 | LEU |
| 2 | O | 78 | LEU |
| 2 | O | 91 | ASN |
| 2 | O | 94 | SER |
| 2 | O | 115 | ASP |
| 2 | O | 148 | MET |
| 2 | O | 167 | SER |
| 3 | P | 29 | SER |
| 3 | P | 33 | MET |
| 3 | P | 159 | MET |
| 3 | P | 214 | PHE |
| 3 | P | 230 | ASN |
| 4 | Q | 121 | LYS |
| 5 | R | 5 | HIS |
| 5 | R | 70 | VAL |
| 5 | R | 77 | PRO |
| 5 | R | 90 | ARG |
| 6 | S | 37 | LYS |
| 6 | S | 53 | THR |
| 6 | S | 54 | ASN |
| 7 | T | 18 | PHE |
| 7 | T | 33 | LEU |
| 7 | T | 38 | HIS |
| 7 | T | 43 | GLU |
| 7 | T | 54 | ARG |
| 7 | T | 84 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | U | 27 | ARG |
| 8 | U | 29 | CYS |
| 8 | U | 60 | TYR |
| 9 | V | 8 | GLN |
| 10 | W | 50 | LEU |
| 11 | X | 20 | SER |
| 11 | X | 54 | ARG |
| 13 | Z | 13 | LYS |
| 13 | Z | 34 | LEU |
| 13 | Z | 38 | ASP |
| 13 | Z | 42 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 178 | GLN |
| 1 | A | 180 | GLN |
| 1 | A | 512 | ASN |
| 2 | B | 52 | HIS |
| 2 | B | 181 | GLN |
| 2 | B | 195 | GLN |
| 3 | C | 3 | HIS |
| 3 | C | 68 | GLN |
| 3 | C | 70 | HIS |
| 3 | C | 149 | HIS |
| 4 | D | 37 | GLN |
| 4 | D | 143 | ASN |
| 5 | E | 78 | HIS |
| 5 | E | 94 | ASN |
| 7 | G | 66 | ASN |
| 7 | G | 71 | HIS |
| 9 | I | 8 | GLN |
| 10 | J | 29 | ASN |
| 11 | K | 35 | GLN |
| 1 | N | 151 | HIS |
| 1 | N | 178 | GLN |
| 1 | N | 180 | GLN |
| 1 | N | 413 | HIS |
| 1 | N | 512 | ASN |
| 2 | O | 10 | GLN |
| 2 | O | 22 | HIS |
| 2 | O | 52 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | O | 91 | ASN |
| 2 | O | 181 | GLN |
| 2 | O | 195 | GLN |
| 3 | P | 50 | ASN |
| 3 | P | 68 | GLN |
| 3 | P | 149 | HIS |
| 4 | Q | 37 | GLN |
| 4 | Q | 101 | HIS |
| 5 | R | 94 | ASN |
| 6 | S | 54 | ASN |
| 6 | S | 94 | HIS |
| 7 | T | 34 | ASN |
| 7 | T | 66 | ASN |
| 7 | T | 71 | HIS |
| 9 | V | 8 | GLN |
| 10 | W | 57 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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 | $\# Z > 2$ |
| 2 | FME | O | 1 | 2 | 8,9,10 | 0.64 | 0 | 7,9,11 | 1.80 | 2 (28%) |
| 7 | TPO | G | 11 | 7 | 8,10,11 | 1.71 | 1 (12%) | 10,14,16 | 1.01 | 0 |
| 2 | FME | B | 1 | 2 | 8,9,10 | 0.95 | 0 | 7,9,11 | 1.70 | 2 (28%) |
| 9 | SAC | V | 1 | 9 | 7,8,9 | 2.93 | 2 (28%) | 8,9,11 | 2.99 | 5 (62%) |
| 1 | FME | N | 1 | 1 | 8,9,10 | 0.83 | 0 | 7,9,11 | 1.16 | 1 (14%) |
| 7 | TPO | T | 11 | 7 | 8,10,11 | 1.33 | 1 (12%) | 10,14,16 | 1.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | SAC | I | 1 | 9 | 7,8,9 | 2.53 | 2 (28%) | 8,9,11 | 2.94 | 4 (50%) |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.74 | 0 | 7,9,11 | 1.49 | 1 (14%) |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 2 | FME | O | 1 | 2 | - | 1/7/9/11 | - |
| 7 | TPO | G | 11 | 7 | - | 4/9/11/13 | - |
| 2 | FME | B | 1 | 2 | - | 1/7/9/11 | - |
| 9 | SAC | V | 1 | 9 | - | 3/7/8/10 | - |
| 1 | FME | N | 1 | 1 | - | 4/7/9/11 | - |
| 7 | TPO | T | 11 | 7 | - | 5/9/11/13 | - |
| 9 | SAC | I | 1 | 9 | - | 3/7/8/10 | - |
| 1 | FME | A | 1 | 1 | - | 3/7/9/11 | - |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 9 | V | 1 | SAC | CA-N | 5.31 | 1.53 | 1.46 |
| 9 | V | 1 | SAC | OAC-C1A | 5.19 | 1.35 | 1.23 |
| 9 | I | 1 | SAC | OAC-C1A | 5.13 | 1.34 | 1.23 |
| 9 | I | 1 | SAC | CA-N | 4.03 | 1.52 | 1.46 |
| 7 | G | 11 | TPO | CB-CA | 3.60 | 1.61 | 1.53 |
| 7 | T | 11 | TPO | CB-CA | 2.11 | 1.58 | 1.53 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 9 | I | 1 | SAC | CA-N-C1A | -6.28 | 111.56 | 123.15 |
| 9 | V | 1 | SAC | CA-N-C1A | -6.18 | 111.76 | 123.15 |
| 2 | O | 1 | FME | C-CA-N | 3.83 | 116.64 | 109.73 |
| 9 | I | 1 | SAC | CB-CA-N | 3.33 | 118.01 | 110.55 |
| 2 | B | 1 | FME | C-CA-N | 3.18 | 115.47 | 109.73 |
| 9 | I | 1 | SAC | C-CA-N | -3.05 | 104.24 | 109.73 |
| 9 | V | 1 | SAC | C-CA-N | -2.98 | 104.35 | 109.73 |
| 1 | A | 1 | FME | CA-N-CN | -2.97 | 118.25 | 122.82 |
| 9 | V | 1 | SAC | C2A-C1A-N | 2.90 | 121.00 | 116.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | B | 1 | FME | CA-N-CN | -2.76 | 118.58 | 122.82 |
| 9 | V | 1 | SAC | CB-CA-N | 2.60 | 116.39 | 110.55 |
| 9 | V | 1 | SAC | OAC-C1A-C2A | -2.51 | 117.40 | 122.06 |
| 2 | O | 1 | FME | CA-N-CN | -2.37 | 119.18 | 122.82 |
| 1 | N | 1 | FME | CA-N-CN | -2.21 | 119.43 | 122.82 |
| 9 | I | 1 | SAC | C2A-C1A-N | 2.03 | 119.53 | 116.10 |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 2 | O | 1 | FME | O1-CN-N-CA |
| 7 | G | 11 | TPO | N-CA-CB-CG2 |
| 7 | G | 11 | TPO | N-CA-CB-OG1 |
| 7 | G | 11 | TPO | C-CA-CB-CG2 |
| 2 | B | 1 | FME | O1-CN-N-CA |
| 9 | V | 1 | SAC | C2A-C1A-N-CA |
| 9 | V | 1 | SAC | OAC-C1A-N-CA |
| 9 | V | 1 | SAC | CB-CA-N-C1A |
| 1 | N | 1 | FME | O1-CN-N-CA |
| 1 | N | 1 | FME | N-CA-CB-CG |
| 1 | N | 1 | FME | C-CA-CB-CG |
| 7 | T | 11 | TPO | N-CA-CB-CG2 |
| 7 | T | 11 | TPO | N-CA-CB-OG1 |
| 7 | T | 11 | TPO | C-CA-CB-CG2 |
| 9 | I | 1 | SAC | CB-CA-N-C1A |
| 1 | A | 1 | FME | O1-CN-N-CA |
| 9 | I | 1 | SAC | C2A-C1A-N-CA |
| 9 | I | 1 | SAC | OAC-C1A-N-CA |
| 1 | A | 1 | FME | N-CA-CB-CG |
| 1 | N | 1 | FME | CA-CB-CG-SD |
| 1 | A | 1 | FME | CA-CB-CG-SD |
| 7 | G | 11 | TPO | CB-OG1-P-O2P |
| 7 | T | 11 | TPO | CB-OG1-P-O3P |
| 7 | T | 11 | TPO | O-C-CA-CB |

There are no ring outliers.

4 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | O | 1 | FME | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | N | 1 | FME | 1 | 0 |
| 7 | T | 11 | TPO | 1 | 0 |
| 1 | A | 1 | FME | 4 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 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 |
| 23 | DCW | C | 301 | 3 | 17,17,17 | 1.39 | 2 (11%) | 21,21,21 | 1.05 | 2 (9%) |
| 24 | DMU | C | 302 | - | 34,34,34 | 2.76 | 14 (41%) | 45,45,45 | 4.06 | 18 (40%) |
| 21 | PSC | B | 303 | - | 51,51,51 | 1.31 | 6 (11%) | 57,59,59 | 1.03 | 1 (1%) |
| 18 | PGV | P | 307 | - | 50,50,50 | 0.93 | 2 (4%) | 53,56,56 | 0.87 | 2 (3%) |
| 27 | CDL | G | 101 | - | 99,99,99 | 1.18 | 11 (11%) | 105,111,111 | 0.97 | 9 (8%) |
| 26 | PEK | G | 102 | - | 52,52,52 | 1.90 | 12 (23%) | 55,57,57 | 1.28 | 5 (9%) |
| 22 | CHD | W | 101 | - | 29,32,32 | 1.12 | 2 (6%) | 48,51,51 | 3.83 | 26 (54%) |
| 23 | DCW | P | 301 | 3 | 17,17,17 | 1.68 | 3 (17%) | 21,21,21 | 0.89 | 1 (4%) |
| 22 | CHD | P | 310 | - | 29,32,32 | 0.90 | 1 (3%) | 48,51,51 | 3.67 | 27 (56%) |
| 27 | CDL | T | 102 | - | 99,99,99 | 1.16 | 10 (10%) | 105,111,111 | 1.00 | 9 (8%) |
| 20 | TGL | L | 101 | - | 62,62,62 | 1.30 | 6 (9%) | 65,65,65 | 1.81 | 12 (18%) |
| 22 | CHD | P | 304 | - | 29,32,32 | 0.71 | 1 (3%) | 48,51,51 | 1.95 | 13 (27%) |
| 27 | CDL | C | 309 | - | 99,99,99 | 0.89 | 5 (5%) | 105,111,111 | 0.99 | 7 (6%) |
| 20 | TGL | N | 606 | - | 62,62,62 | 1.42 | 6 (9%) | 65,65,65 | 1.77 | 14 (21%) |
| 18 | PGV | C | 307 | - | 50,50,50 | 0.98 | 3 (6%) | 53,56,56 | 0.99 | 5 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | PEK | T | 101 | - | 52,52,52 | 2.05 | 13 (25%) | 55,57,57 | 1.29 | 6 (10%) |
| 18 | PGV | N | 608 | - | 50,50,50 | 1.20 | 4 (8%) | 53,56,56 | 1.02 | 4 (7%) |
| 19 | CUA | O | 301 | 2 | 0,1,1 | 0.00 | - | - | | |
| 18 | PGV | N | 609 | - | 50,50,50 | 1.12 | 4 (8%) | 53,56,56 | 1.12 | 5 (9%) |
| 22 | CHD | C | 310 | - | 29,32,32 | 1.01 | 2 (6%) | 48,51,51 | 3.60 | 27 (56%) |
| 20 | TGL | D | 201 | - | 62,62,62 | 0.98 | 4 (6%) | 65,65,65 | 1.42 | 11 (16%) |
| 22 | CHD | C | 304 | - | 29,32,32 | 0.93 | 2 (6%) | 48,51,51 | 2.02 | 13 (27%) |
| 17 | HEA | N | 604 | 1 | 44,67,67 | 1.39 | 5 (11%) | 37,103,103 | 1.71 | 9 (24%) |
| 26 | PEK | C | 306 | - | 52,52,52 | 1.67 | 9 (17%) | 55,57,57 | 1.11 | 5 (9%) |
| 24 | DMU | Z | 101 | - | 34,34,34 | 3.06 | 10 (29%) | 45,45,45 | 4.10 | 19 (42%) |
| 18 | PGV | A | 607 | - | 50,50,50 | 0.99 | 3 (6%) | 53,56,56 | 1.07 | 3 (5%) |
| 24 | DMU | P | 302 | - | 34,34,34 | 2.64 | 14 (41%) | 45,45,45 | 4.14 | 18 (40%) |
| 20 | TGL | B | 302 | - | 62,62,62 | 0.77 | 2 (3%) | 65,65,65 | 1.60 | 12 (18%) |
| 18 | PGV | A | 606 | - | 50,50,50 | 1.16 | 3 (6%) | 53,56,56 | 1.05 | 4 (7%) |
| 17 | HEA | N | 605 | 1 | 44,67,67 | 1.36 | 5 (11%) | 37,103,103 | 1.44 | 6 (16%) |
| 26 | PEK | P | 306 | - | 52,52,52 | 1.63 | 10 (19%) | 55,57,57 | 1.12 | 6 (10%) |
| 22 | CHD | B | 304 | - | 29,32,32 | 0.88 | 1 (3%) | 48,51,51 | 1.92 | 12 (25%) |
| 19 | CUA | B | 301 | 2 | 0,1,1 | 0.00 | - | - | | |
| 17 | HEA | A | 604 | 1 | 44,67,67 | 1.24 | 6 (13%) | 37,103,103 | 1.63 | 8 (21%) |
| 26 | PEK | C | 305 | - | 52,52,52 | 1.40 | 5 (9%) | 55,57,57 | 1.04 | 2 (3%) |
| 22 | CHD | O | 302 | - | 29,32,32 | 0.71 | 0 | 48,51,51 | 1.92 | 14 (29%) |
| 21 | PSC | O | 304 | - | 51,51,51 | 1.28 | 4 (7%) | 57,59,59 | 1.05 | 3 (5%) |
| 27 | CDL | P | 309 | - | 99,99,99 | 0.94 | 6 (6%) | 105,111,111 | 1.01 | 6 (5%) |
| 20 | TGL | O | 303 | - | 62,62,62 | 0.86 | 2 (3%) | 65,65,65 | 1.54 | 10 (15%) |
| 24 | DMU | M | 101 | - | 34,34,34 | 3.17 | 9 (26%) | 45,45,45 | 4.18 | 19 (42%) |
| 20 | TGL | N | 607 | - | 62,62,62 | 0.88 | 2 (3%) | 65,65,65 | 1.38 | 9 (13%) |
| 18 | PGV | C | 308 | - | 50,50,50 | 1.44 | 5 (10%) | 53,56,56 | 0.87 | 1 (1%) |
| 18 | PGV | P | 308 | - | 50,50,50 | 1.43 | 6 (12%) | 53,56,56 | 0.89 | 2 (3%) |
| 17 | HEA | A | 605 | 1 | 44,67,67 | 1.52 | 11 (25%) | 37,103,103 | 1.34 | 4 (10%) |
| 26 | PEK | P | 305 | - | 52,52,52 | 1.49 | 7 (13%) | 55,57,57 | 1.12 | 5 (9%) |
| 22 | CHD | J | 101 | - | 29,32,32 | 0.97 | 2 (6%) | 48,51,51 | 3.79 | 25 (52%) |

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 |
|-----|------|-------|-----|------|-----------|----------------|---------|
| 23 | DCW | C | 301 | 3 | - | 3/8/24/24 | 0/2/2/2 |
| 24 | DMU | C | 302 | - | 6/6/10/10 | 9/19/59/59 | 0/2/2/2 |
| 21 | PSC | B | 303 | - | - | 40/55/55/55 | - |
| 18 | PGV | P | 307 | - | - | 14/55/55/55 | - |
| 27 | CDL | G | 101 | - | - | 63/110/110/110 | - |
| 26 | PEK | G | 102 | - | - | 29/56/56/56 | - |
| 22 | CHD | W | 101 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |
| 23 | DCW | P | 301 | 3 | - | 2/8/24/24 | 0/2/2/2 |
| 22 | CHD | P | 310 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |
| 27 | CDL | T | 102 | - | - | 63/110/110/110 | - |
| 20 | TGL | L | 101 | - | - | 15/65/65/65 | - |
| 27 | CDL | C | 309 | - | - | 71/110/110/110 | - |
| 20 | TGL | N | 606 | - | - | 17/65/65/65 | - |
| 18 | PGV | C | 307 | - | - | 15/55/55/55 | - |
| 26 | PEK | T | 101 | - | - | 29/56/56/56 | - |
| 18 | PGV | N | 608 | - | - | 33/55/55/55 | - |
| 22 | CHD | P | 304 | - | - | 0/7/74/74 | 0/4/4/4 |
| 18 | PGV | N | 609 | - | - | 12/55/55/55 | - |
| 22 | CHD | C | 310 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |
| 17 | HEA | A | 605 | 1 | 3/3/7/16 | 2/24/76/76 | - |
| 22 | CHD | C | 304 | - | - | 0/7/74/74 | 0/4/4/4 |
| 17 | HEA | N | 604 | 1 | 3/3/7/16 | 5/24/76/76 | - |
| 26 | PEK | C | 306 | - | - | 17/56/56/56 | - |
| 24 | DMU | Z | 101 | - | 5/5/10/10 | 10/19/59/59 | 0/2/2/2 |
| 18 | PGV | A | 607 | - | - | 12/55/55/55 | - |
| 24 | DMU | P | 302 | - | 6/6/10/10 | 9/19/59/59 | 0/2/2/2 |
| 20 | TGL | B | 302 | - | - | 13/65/65/65 | - |
| 18 | PGV | A | 606 | - | - | 34/55/55/55 | - |
| 17 | HEA | N | 605 | 1 | 3/3/7/16 | 3/24/76/76 | - |
| 26 | PEK | P | 306 | - | - | 18/56/56/56 | - |
| 22 | CHD | B | 304 | - | - | 0/7/74/74 | 0/4/4/4 |
| 17 | HEA | A | 604 | 1 | 3/3/7/16 | 5/24/76/76 | - |
| 26 | PEK | C | 305 | - | - | 25/56/56/56 | - |
| 22 | CHD | O | 302 | - | - | 1/7/74/74 | 0/4/4/4 |
| 21 | PSC | O | 304 | - | - | 39/55/55/55 | - |
| 27 | CDL | P | 309 | - | - | 70/110/110/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|-------------|---------|
| 20 | TGL | O | 303 | - | - | 13/65/65/65 | - |
| 24 | DMU | M | 101 | - | 5/5/10/10 | 10/19/59/59 | 0/2/2/2 |
| 20 | TGL | N | 607 | - | - | 16/65/65/65 | - |
| 18 | PGV | C | 308 | - | - | 34/55/55/55 | - |
| 18 | PGV | P | 308 | - | - | 34/55/55/55 | - |
| 20 | TGL | D | 201 | - | - | 16/65/65/65 | - |
| 26 | PEK | P | 305 | - | - | 25/56/56/56 | - |
| 22 | CHD | J | 101 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |

All (240) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | M | 101 | DMU | O7-C3 | -7.43 | 1.24 | 1.43 |
| 24 | M | 101 | DMU | O16-C6 | -7.11 | 1.28 | 1.40 |
| 24 | Z | 101 | DMU | O7-C3 | -6.96 | 1.25 | 1.43 |
| 24 | M | 101 | DMU | O1-C9 | -6.77 | 1.27 | 1.44 |
| 24 | M | 101 | DMU | O5-C4 | -6.64 | 1.28 | 1.44 |
| 24 | Z | 101 | DMU | O16-C18 | -6.53 | 1.24 | 1.43 |
| 24 | Z | 101 | DMU | O1-C9 | -6.46 | 1.28 | 1.44 |
| 24 | Z | 101 | DMU | O16-C6 | -6.44 | 1.29 | 1.40 |
| 24 | Z | 101 | DMU | O5-C4 | -6.29 | 1.29 | 1.44 |
| 24 | P | 302 | DMU | O16-C18 | -6.28 | 1.25 | 1.43 |
| 24 | C | 302 | DMU | O16-C6 | -6.26 | 1.29 | 1.40 |
| 24 | M | 101 | DMU | O16-C18 | -6.23 | 1.25 | 1.43 |
| 24 | C | 302 | DMU | O16-C18 | -6.16 | 1.25 | 1.43 |
| 24 | M | 101 | DMU | O7-C10 | -5.98 | 1.24 | 1.41 |
| 24 | Z | 101 | DMU | O7-C10 | -5.95 | 1.25 | 1.41 |
| 24 | P | 302 | DMU | O16-C6 | -5.87 | 1.30 | 1.40 |
| 20 | N | 606 | TGL | OG2-CB1 | 5.64 | 1.50 | 1.34 |
| 20 | N | 606 | TGL | OG1-CA1 | 5.59 | 1.49 | 1.33 |
| 20 | L | 101 | TGL | OG2-CB1 | 5.34 | 1.49 | 1.34 |
| 24 | C | 302 | DMU | O1-C9 | -5.29 | 1.31 | 1.44 |
| 24 | M | 101 | DMU | O1-C10 | -5.26 | 1.28 | 1.41 |
| 18 | C | 308 | PGV | O01-C1 | 5.12 | 1.48 | 1.34 |
| 26 | T | 101 | PEK | O03-C21 | 5.09 | 1.48 | 1.33 |
| 24 | M | 101 | DMU | O5-C6 | -4.95 | 1.29 | 1.41 |
| 18 | P | 308 | PGV | O01-C1 | 4.92 | 1.48 | 1.34 |
| 26 | G | 102 | PEK | C15-C14 | 4.85 | 1.59 | 1.31 |
| 24 | Z | 101 | DMU | O1-C10 | -4.84 | 1.29 | 1.41 |
| 24 | C | 302 | DMU | O7-C3 | -4.82 | 1.31 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | P | 302 | DMU | O7-C3 | -4.80 | 1.31 | 1.43 |
| 24 | P | 302 | DMU | O1-C9 | -4.78 | 1.32 | 1.44 |
| 21 | O | 304 | PSC | C10-C9 | 4.69 | 1.59 | 1.31 |
| 26 | T | 101 | PEK | C15-C14 | 4.69 | 1.58 | 1.31 |
| 18 | P | 308 | PGV | C12-C11 | 4.67 | 1.58 | 1.31 |
| 26 | C | 305 | PEK | C15-C14 | 4.65 | 1.58 | 1.31 |
| 26 | G | 102 | PEK | C03-C02 | 4.64 | 1.64 | 1.50 |
| 24 | P | 302 | DMU | O5-C4 | -4.60 | 1.33 | 1.44 |
| 18 | C | 308 | PGV | C12-C11 | 4.60 | 1.58 | 1.31 |
| 21 | B | 303 | PSC | C10-C9 | 4.58 | 1.58 | 1.31 |
| 26 | P | 306 | PEK | C12-C11 | 4.58 | 1.58 | 1.31 |
| 26 | T | 101 | PEK | C03-C02 | 4.57 | 1.64 | 1.50 |
| 24 | C | 302 | DMU | O5-C4 | -4.55 | 1.33 | 1.44 |
| 26 | C | 306 | PEK | C12-C11 | 4.51 | 1.57 | 1.31 |
| 26 | P | 305 | PEK | C12-C11 | 4.50 | 1.57 | 1.31 |
| 26 | P | 305 | PEK | C15-C14 | 4.50 | 1.57 | 1.31 |
| 26 | C | 305 | PEK | C12-C11 | 4.48 | 1.57 | 1.31 |
| 26 | T | 101 | PEK | C01-C02 | 4.45 | 1.64 | 1.50 |
| 26 | P | 305 | PEK | C6-C5 | 4.45 | 1.57 | 1.31 |
| 24 | Z | 101 | DMU | O5-C6 | -4.40 | 1.30 | 1.41 |
| 26 | G | 102 | PEK | C6-C5 | 4.39 | 1.57 | 1.31 |
| 26 | T | 101 | PEK | C6-C5 | 4.38 | 1.57 | 1.31 |
| 26 | T | 101 | PEK | C12-C11 | 4.37 | 1.57 | 1.31 |
| 17 | N | 604 | HEA | C3B-C11 | -4.31 | 1.49 | 1.52 |
| 26 | G | 102 | PEK | C01-C02 | 4.29 | 1.63 | 1.50 |
| 26 | C | 306 | PEK | C6-C5 | 4.21 | 1.56 | 1.31 |
| 26 | P | 306 | PEK | C6-C5 | 4.20 | 1.56 | 1.31 |
| 26 | C | 306 | PEK | C9-C8 | 4.20 | 1.56 | 1.31 |
| 26 | P | 306 | PEK | C9-C8 | 4.19 | 1.56 | 1.31 |
| 26 | C | 306 | PEK | C15-C14 | 4.18 | 1.56 | 1.31 |
| 26 | P | 305 | PEK | C9-C8 | 4.10 | 1.55 | 1.31 |
| 18 | N | 608 | PGV | C12-C11 | 4.09 | 1.55 | 1.31 |
| 24 | C | 302 | DMU | O5-C6 | -4.07 | 1.31 | 1.41 |
| 18 | A | 606 | PGV | C12-C11 | 4.07 | 1.55 | 1.31 |
| 26 | G | 102 | PEK | C12-C11 | 4.03 | 1.55 | 1.31 |
| 23 | P | 301 | DCW | C8-N2 | -4.01 | 1.38 | 1.46 |
| 26 | P | 306 | PEK | C15-C14 | 3.99 | 1.54 | 1.31 |
| 21 | B | 303 | PSC | C13-C12 | 3.98 | 1.54 | 1.31 |
| 26 | C | 305 | PEK | C6-C5 | 3.98 | 1.54 | 1.31 |
| 17 | A | 605 | HEA | C3A-C2A | -3.98 | 1.34 | 1.40 |
| 24 | C | 302 | DMU | O7-C10 | -3.95 | 1.30 | 1.41 |
| 26 | G | 102 | PEK | C9-C8 | 3.95 | 1.54 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | C | 305 | PEK | C9-C8 | 3.94 | 1.54 | 1.31 |
| 26 | T | 101 | PEK | C9-C8 | 3.93 | 1.54 | 1.31 |
| 21 | O | 304 | PSC | C13-C12 | 3.90 | 1.54 | 1.31 |
| 20 | L | 101 | TGL | OG1-CA1 | 3.90 | 1.44 | 1.33 |
| 24 | P | 302 | DMU | O5-C6 | -3.82 | 1.32 | 1.41 |
| 22 | W | 101 | CHD | C13-C17 | 3.80 | 1.62 | 1.55 |
| 18 | A | 607 | PGV | C12-C11 | 3.72 | 1.53 | 1.31 |
| 17 | N | 605 | HEA | C3A-C2A | -3.71 | 1.35 | 1.40 |
| 24 | P | 302 | DMU | O7-C10 | -3.69 | 1.31 | 1.41 |
| 24 | P | 302 | DMU | C6-C1 | 3.66 | 1.63 | 1.52 |
| 17 | N | 604 | HEA | C3A-CMA | -3.65 | 1.37 | 1.46 |
| 24 | C | 302 | DMU | O1-C10 | -3.64 | 1.32 | 1.41 |
| 18 | P | 307 | PGV | C12-C11 | 3.64 | 1.52 | 1.31 |
| 18 | N | 609 | PGV | C12-C11 | 3.61 | 1.52 | 1.31 |
| 27 | T | 102 | CDL | OB6-CB5 | 3.56 | 1.44 | 1.34 |
| 26 | G | 102 | PEK | P-O11 | 3.54 | 1.73 | 1.59 |
| 18 | N | 608 | PGV | C03-C02 | 3.54 | 1.61 | 1.50 |
| 20 | N | 607 | TGL | OG1-CA1 | 3.53 | 1.43 | 1.33 |
| 24 | C | 302 | DMU | C3-C4 | 3.46 | 1.62 | 1.52 |
| 20 | D | 201 | TGL | OG1-CA1 | 3.44 | 1.43 | 1.33 |
| 24 | P | 302 | DMU | C3-C4 | 3.42 | 1.62 | 1.52 |
| 18 | C | 307 | PGV | C12-C11 | 3.41 | 1.51 | 1.31 |
| 17 | A | 604 | HEA | C3A-CMA | -3.40 | 1.38 | 1.46 |
| 27 | G | 101 | CDL | C11-CA5 | 3.39 | 1.60 | 1.50 |
| 20 | D | 201 | TGL | OG3-CC1 | 3.38 | 1.43 | 1.33 |
| 27 | G | 101 | CDL | OB6-CB5 | 3.38 | 1.43 | 1.34 |
| 18 | N | 609 | PGV | C2-C1 | 3.37 | 1.60 | 1.50 |
| 26 | G | 102 | PEK | O03-C21 | 3.36 | 1.43 | 1.33 |
| 17 | A | 604 | HEA | C3B-C11 | -3.35 | 1.50 | 1.52 |
| 24 | P | 302 | DMU | O1-C10 | -3.32 | 1.33 | 1.41 |
| 20 | L | 101 | TGL | CG1-CG2 | 3.30 | 1.60 | 1.50 |
| 26 | T | 101 | PEK | O01-C1 | 3.29 | 1.43 | 1.34 |
| 26 | T | 101 | PEK | C2-C1 | 3.26 | 1.60 | 1.50 |
| 24 | C | 302 | DMU | C6-C1 | 3.24 | 1.61 | 1.52 |
| 27 | T | 102 | CDL | CB6-CB4 | 3.23 | 1.60 | 1.50 |
| 26 | T | 101 | PEK | P-O11 | 3.22 | 1.72 | 1.59 |
| 17 | N | 604 | HEA | C1D-C2D | 3.21 | 1.49 | 1.42 |
| 20 | O | 303 | TGL | OG2-CB1 | 3.21 | 1.43 | 1.34 |
| 21 | O | 304 | PSC | C2-C1 | 3.19 | 1.60 | 1.50 |
| 22 | J | 101 | CHD | C13-C17 | 3.18 | 1.60 | 1.55 |
| 27 | G | 101 | CDL | OA6-CA5 | 3.17 | 1.43 | 1.34 |
| 27 | P | 309 | CDL | CA6-CA4 | 3.14 | 1.60 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20 | N | 606 | TGL | CG1-CG2 | 3.11 | 1.60 | 1.50 |
| 17 | A | 605 | HEA | C3C-CAC | 3.10 | 1.54 | 1.47 |
| 17 | A | 605 | HEA | C3A-CMA | -3.10 | 1.39 | 1.46 |
| 23 | P | 301 | DCW | C1-N2 | -3.09 | 1.29 | 1.35 |
| 18 | A | 606 | PGV | O03-C19 | 3.07 | 1.42 | 1.33 |
| 26 | P | 305 | PEK | C2-C1 | 3.03 | 1.59 | 1.50 |
| 20 | N | 606 | TGL | CB2-CB1 | 3.02 | 1.59 | 1.50 |
| 27 | T | 102 | CDL | C11-CA5 | 3.01 | 1.59 | 1.50 |
| 17 | N | 605 | HEA | C3A-CMA | -3.01 | 1.39 | 1.46 |
| 17 | A | 605 | HEA | C4D-ND | 2.98 | 1.42 | 1.36 |
| 18 | C | 308 | PGV | C2-C1 | 2.97 | 1.59 | 1.50 |
| 22 | C | 310 | CHD | C19-C10 | -2.93 | 1.49 | 1.54 |
| 18 | C | 307 | PGV | O03-C19 | 2.91 | 1.41 | 1.33 |
| 17 | A | 605 | HEA | C16-C15 | 2.91 | 1.57 | 1.51 |
| 22 | W | 101 | CHD | C20-C17 | 2.85 | 1.59 | 1.54 |
| 27 | C | 309 | CDL | CA6-CA4 | 2.85 | 1.59 | 1.50 |
| 18 | A | 607 | PGV | C2-C1 | 2.82 | 1.59 | 1.50 |
| 26 | C | 306 | PEK | O03-C21 | 2.81 | 1.41 | 1.33 |
| 18 | A | 606 | PGV | C03-C02 | 2.80 | 1.59 | 1.50 |
| 24 | C | 302 | DMU | C7-C5 | 2.80 | 1.59 | 1.52 |
| 22 | P | 310 | CHD | C19-C10 | -2.78 | 1.49 | 1.54 |
| 26 | C | 306 | PEK | P-O12 | 2.76 | 1.70 | 1.59 |
| 20 | N | 607 | TGL | CA2-CA1 | 2.76 | 1.58 | 1.50 |
| 17 | A | 605 | HEA | C4B-C3B | 2.76 | 1.48 | 1.42 |
| 18 | P | 308 | PGV | C2-C1 | 2.76 | 1.58 | 1.50 |
| 26 | T | 101 | PEK | C22-C21 | 2.76 | 1.58 | 1.50 |
| 26 | C | 306 | PEK | C03-C02 | 2.75 | 1.59 | 1.50 |
| 20 | L | 101 | TGL | CB2-CB1 | 2.74 | 1.58 | 1.50 |
| 24 | C | 302 | DMU | C8-C7 | 2.73 | 1.59 | 1.52 |
| 22 | C | 304 | CHD | C10-C9 | -2.73 | 1.51 | 1.56 |
| 18 | N | 609 | PGV | C20-C19 | 2.72 | 1.58 | 1.50 |
| 26 | P | 306 | PEK | O03-C21 | 2.68 | 1.41 | 1.33 |
| 20 | L | 101 | TGL | CG3-CG2 | 2.65 | 1.58 | 1.50 |
| 26 | P | 306 | PEK | C03-C02 | 2.65 | 1.58 | 1.50 |
| 18 | N | 609 | PGV | C01-C02 | 2.65 | 1.58 | 1.50 |
| 27 | G | 101 | CDL | C71-CB7 | 2.64 | 1.58 | 1.50 |
| 18 | N | 608 | PGV | O03-C19 | 2.64 | 1.41 | 1.33 |
| 26 | C | 306 | PEK | P-O11 | 2.63 | 1.69 | 1.59 |
| 23 | C | 301 | DCW | C8-N2 | -2.62 | 1.41 | 1.46 |
| 20 | B | 302 | TGL | OG2-CB1 | 2.62 | 1.41 | 1.34 |
| 26 | P | 306 | PEK | C01-C02 | 2.62 | 1.58 | 1.50 |
| 27 | P | 309 | CDL | OA8-CA7 | 2.61 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27 | G | 101 | CDL | C51-CB5 | 2.59 | 1.58 | 1.50 |
| 27 | P | 309 | CDL | CA3-CA4 | 2.59 | 1.58 | 1.50 |
| 20 | D | 201 | TGL | CA2-CA1 | 2.58 | 1.58 | 1.50 |
| 24 | P | 302 | DMU | C7-C5 | 2.58 | 1.58 | 1.52 |
| 26 | P | 305 | PEK | O03-C01 | -2.58 | 1.39 | 1.45 |
| 27 | T | 102 | CDL | C71-CB7 | 2.55 | 1.58 | 1.50 |
| 27 | G | 101 | CDL | CB6-CB4 | 2.54 | 1.58 | 1.50 |
| 26 | C | 306 | PEK | C01-C02 | 2.52 | 1.58 | 1.50 |
| 27 | T | 102 | CDL | OA6-CA5 | 2.51 | 1.41 | 1.34 |
| 27 | P | 309 | CDL | C31-CA7 | 2.51 | 1.58 | 1.50 |
| 20 | O | 303 | TGL | CG3-CG2 | 2.49 | 1.58 | 1.50 |
| 24 | C | 302 | DMU | C8-C9 | 2.47 | 1.58 | 1.53 |
| 22 | C | 304 | CHD | C13-C12 | -2.46 | 1.50 | 1.54 |
| 21 | B | 303 | PSC | C2-C1 | 2.44 | 1.57 | 1.50 |
| 18 | A | 607 | PGV | C03-C02 | 2.42 | 1.58 | 1.50 |
| 22 | B | 304 | CHD | C13-C12 | -2.42 | 1.50 | 1.54 |
| 20 | D | 201 | TGL | CB2-CB1 | 2.40 | 1.57 | 1.50 |
| 27 | T | 102 | CDL | CB2-C1 | 2.37 | 1.59 | 1.51 |
| 26 | P | 306 | PEK | P-O12 | 2.37 | 1.68 | 1.59 |
| 17 | A | 604 | HEA | C4D-ND | 2.37 | 1.41 | 1.36 |
| 21 | O | 304 | PSC | P-O12 | 2.36 | 1.68 | 1.59 |
| 27 | T | 102 | CDL | CB3-CB4 | 2.36 | 1.57 | 1.50 |
| 18 | P | 308 | PGV | C03-C02 | 2.35 | 1.57 | 1.50 |
| 27 | P | 309 | CDL | PA1-OA5 | 2.34 | 1.68 | 1.59 |
| 24 | C | 302 | DMU | C10-C5 | 2.34 | 1.59 | 1.52 |
| 27 | T | 102 | CDL | C31-CA7 | 2.33 | 1.57 | 1.50 |
| 18 | C | 308 | PGV | C03-C02 | 2.33 | 1.57 | 1.50 |
| 18 | C | 308 | PGV | C04-C05 | 2.32 | 1.59 | 1.51 |
| 24 | P | 302 | DMU | C2-C1 | 2.31 | 1.58 | 1.52 |
| 18 | C | 307 | PGV | O01-C1 | 2.31 | 1.40 | 1.34 |
| 24 | P | 302 | DMU | C10-C5 | 2.31 | 1.59 | 1.52 |
| 18 | P | 307 | PGV | C20-C19 | 2.31 | 1.57 | 1.50 |
| 21 | B | 303 | PSC | P-O12 | 2.29 | 1.68 | 1.59 |
| 27 | G | 101 | CDL | C31-CA7 | 2.28 | 1.57 | 1.50 |
| 26 | G | 102 | PEK | O01-C1 | 2.28 | 1.40 | 1.34 |
| 26 | G | 102 | PEK | C2-C1 | 2.28 | 1.57 | 1.50 |
| 18 | P | 308 | PGV | C04-C05 | 2.28 | 1.59 | 1.51 |
| 18 | N | 608 | PGV | O01-C1 | 2.27 | 1.40 | 1.34 |
| 17 | N | 605 | HEA | C3B-C11 | -2.26 | 1.51 | 1.52 |
| 27 | T | 102 | CDL | C51-CB5 | 2.26 | 1.57 | 1.50 |
| 22 | P | 304 | CHD | C8-C9 | 2.25 | 1.58 | 1.53 |
| 27 | C | 309 | CDL | C31-CA7 | 2.25 | 1.57 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | J | 101 | CHD | C20-C17 | 2.25 | 1.58 | 1.54 |
| 24 | Z | 101 | DMU | C8-C7 | 2.25 | 1.58 | 1.52 |
| 24 | Z | 101 | DMU | C8-C9 | 2.22 | 1.57 | 1.53 |
| 20 | N | 606 | TGL | CG3-CG2 | 2.20 | 1.57 | 1.50 |
| 26 | G | 102 | PEK | P-O12 | 2.20 | 1.68 | 1.59 |
| 17 | N | 605 | HEA | C17-C18 | 2.18 | 1.57 | 1.50 |
| 17 | A | 604 | HEA | C3B-C2B | -2.17 | 1.34 | 1.41 |
| 27 | C | 309 | CDL | CA3-CA4 | 2.16 | 1.57 | 1.50 |
| 27 | G | 101 | CDL | PB2-OB2 | 2.16 | 1.68 | 1.59 |
| 17 | A | 605 | HEA | C3B-C2B | -2.16 | 1.34 | 1.41 |
| 26 | P | 306 | PEK | P-O11 | 2.15 | 1.68 | 1.59 |
| 17 | A | 605 | HEA | C20-C19 | 2.15 | 1.55 | 1.51 |
| 20 | B | 302 | TGL | CG3-CG2 | 2.14 | 1.57 | 1.50 |
| 20 | L | 101 | TGL | CC2-CC1 | 2.14 | 1.57 | 1.50 |
| 17 | A | 605 | HEA | C1D-C2D | 2.14 | 1.47 | 1.42 |
| 27 | G | 101 | CDL | CB3-CB4 | 2.12 | 1.57 | 1.50 |
| 18 | P | 308 | PGV | O03-C19 | 2.12 | 1.39 | 1.33 |
| 17 | N | 604 | HEA | C3A-C2A | -2.10 | 1.37 | 1.40 |
| 22 | C | 310 | CHD | C10-C9 | -2.10 | 1.52 | 1.56 |
| 26 | T | 101 | PEK | P-O12 | 2.09 | 1.67 | 1.59 |
| 27 | C | 309 | CDL | PB2-OB2 | 2.09 | 1.67 | 1.59 |
| 23 | C | 301 | DCW | C2-N1 | -2.09 | 1.42 | 1.46 |
| 26 | C | 305 | PEK | O03-C01 | -2.08 | 1.40 | 1.45 |
| 23 | P | 301 | DCW | C9-C8 | -2.08 | 1.47 | 1.52 |
| 21 | B | 303 | PSC | O01-C1 | 2.08 | 1.40 | 1.34 |
| 26 | P | 305 | PEK | O01-C02 | -2.08 | 1.41 | 1.46 |
| 27 | P | 309 | CDL | PB2-OB2 | 2.07 | 1.67 | 1.59 |
| 20 | N | 606 | TGL | CC2-CC1 | 2.07 | 1.56 | 1.50 |
| 17 | N | 604 | HEA | C4B-C3B | 2.07 | 1.47 | 1.42 |
| 27 | C | 309 | CDL | CB2-C1 | 2.06 | 1.58 | 1.51 |
| 21 | B | 303 | PSC | C01-C02 | 2.06 | 1.57 | 1.50 |
| 26 | G | 102 | PEK | O03-C01 | 2.06 | 1.49 | 1.45 |
| 17 | A | 605 | HEA | C3C-C2C | -2.05 | 1.37 | 1.40 |
| 27 | T | 102 | CDL | PB2-OB2 | 2.05 | 1.67 | 1.59 |
| 26 | T | 101 | PEK | O03-C01 | 2.04 | 1.49 | 1.45 |
| 24 | P | 302 | DMU | C8-C7 | 2.03 | 1.57 | 1.52 |
| 27 | G | 101 | CDL | CB2-C1 | 2.03 | 1.58 | 1.51 |
| 17 | A | 604 | HEA | CAD-C3D | 2.02 | 1.55 | 1.52 |
| 17 | A | 604 | HEA | C17-C18 | 2.02 | 1.57 | 1.50 |
| 24 | M | 101 | DMU | C8-C7 | 2.01 | 1.57 | 1.52 |
| 26 | P | 306 | PEK | C05-C04 | 2.01 | 1.58 | 1.50 |
| 17 | A | 605 | HEA | C18-C19 | 2.01 | 1.37 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 17 | N | 605 | HEA | C3C-C2C | -2.00 | 1.37 | 1.40 |
| 27 | G | 101 | CDL | OB8-CB7 | 2.00 | 1.39 | 1.33 |

All (419) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | P | 302 | DMU | O16-C6-C1 | 11.21 | 125.81 | 108.30 |
| 24 | C | 302 | DMU | O16-C6-C1 | 10.91 | 125.34 | 108.30 |
| 22 | P | 310 | CHD | C17-C13-C14 | 10.80 | 110.98 | 100.09 |
| 22 | J | 101 | CHD | C17-C13-C14 | 10.57 | 110.75 | 100.09 |
| 22 | W | 101 | CHD | C17-C13-C14 | 10.50 | 110.68 | 100.09 |
| 22 | C | 310 | CHD | C17-C13-C14 | 10.45 | 110.63 | 100.09 |
| 24 | M | 101 | DMU | C10-C5-C7 | 10.16 | 131.17 | 110.00 |
| 24 | Z | 101 | DMU | C10-C5-C7 | 9.99 | 130.80 | 110.00 |
| 22 | P | 310 | CHD | C17-C13-C12 | -9.80 | 108.72 | 117.67 |
| 22 | P | 310 | CHD | C10-C9-C8 | 9.68 | 122.22 | 111.82 |
| 22 | C | 310 | CHD | C10-C9-C8 | 9.63 | 122.16 | 111.82 |
| 24 | P | 302 | DMU | C1-C2-C3 | 9.50 | 131.38 | 109.68 |
| 24 | C | 302 | DMU | C1-C2-C3 | 9.34 | 131.01 | 109.68 |
| 22 | C | 310 | CHD | C17-C13-C12 | -9.23 | 109.24 | 117.67 |
| 24 | P | 302 | DMU | O5-C4-C3 | 9.12 | 128.97 | 109.75 |
| 24 | P | 302 | DMU | O1-C9-C11 | 8.60 | 127.82 | 106.44 |
| 22 | J | 101 | CHD | C10-C9-C8 | 8.51 | 120.96 | 111.82 |
| 24 | Z | 101 | DMU | C7-C8-C9 | 8.49 | 125.38 | 110.24 |
| 22 | W | 101 | CHD | C13-C17-C20 | 8.49 | 129.63 | 119.50 |
| 24 | M | 101 | DMU | C7-C8-C9 | 8.38 | 125.18 | 110.24 |
| 22 | J | 101 | CHD | C13-C17-C20 | 8.27 | 129.37 | 119.50 |
| 24 | C | 302 | DMU | O1-C9-C11 | 8.21 | 126.86 | 106.44 |
| 24 | M | 101 | DMU | C8-C7-C5 | -8.18 | 96.55 | 110.82 |
| 24 | C | 302 | DMU | O5-C4-C3 | 8.09 | 126.82 | 109.75 |
| 22 | W | 101 | CHD | C10-C9-C8 | 8.00 | 120.41 | 111.82 |
| 24 | Z | 101 | DMU | C8-C7-C5 | -7.98 | 96.89 | 110.82 |
| 24 | M | 101 | DMU | O1-C9-C11 | 7.86 | 125.97 | 106.44 |
| 24 | Z | 101 | DMU | O1-C9-C11 | 7.83 | 125.91 | 106.44 |
| 24 | M | 101 | DMU | O5-C4-C3 | 7.44 | 125.43 | 109.75 |
| 24 | Z | 101 | DMU | O5-C4-C3 | 7.40 | 125.35 | 109.75 |
| 24 | Z | 101 | DMU | C6-O5-C4 | 6.99 | 127.41 | 113.69 |
| 24 | P | 302 | DMU | O7-C3-C4 | 6.97 | 128.56 | 109.45 |
| 24 | C | 302 | DMU | C6-O5-C4 | 6.96 | 127.36 | 113.69 |
| 22 | P | 310 | CHD | C19-C10-C9 | -6.93 | 101.63 | 111.18 |
| 22 | W | 101 | CHD | C6-C5-C10 | 6.88 | 119.97 | 112.66 |
| 22 | J | 101 | CHD | C6-C5-C10 | 6.88 | 119.96 | 112.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 310 | CHD | C19-C10-C9 | -6.87 | 101.72 | 111.18 |
| 24 | M | 101 | DMU | C6-O5-C4 | 6.87 | 127.17 | 113.69 |
| 22 | J | 101 | CHD | C11-C12-C13 | 6.68 | 118.10 | 111.24 |
| 24 | M | 101 | DMU | O16-C6-C1 | 6.65 | 118.69 | 108.30 |
| 24 | Z | 101 | DMU | O5-C4-C57 | 6.61 | 122.87 | 106.44 |
| 24 | P | 302 | DMU | C18-O16-C6 | 6.57 | 124.74 | 113.84 |
| 24 | M | 101 | DMU | C18-O16-C6 | 6.55 | 124.70 | 113.84 |
| 24 | M | 101 | DMU | O1-C9-C8 | 6.51 | 121.52 | 109.69 |
| 24 | M | 101 | DMU | O5-C4-C57 | 6.47 | 122.52 | 106.44 |
| 22 | W | 101 | CHD | C11-C12-C13 | 6.43 | 117.85 | 111.24 |
| 24 | Z | 101 | DMU | O1-C9-C8 | 6.40 | 121.32 | 109.69 |
| 24 | C | 302 | DMU | C18-O16-C6 | 6.39 | 124.44 | 113.84 |
| 24 | Z | 101 | DMU | O5-C6-O16 | 6.37 | 125.05 | 109.97 |
| 22 | W | 101 | CHD | C9-C8-C7 | 6.33 | 119.45 | 111.88 |
| 24 | M | 101 | DMU | O7-C3-C2 | 6.28 | 123.98 | 107.28 |
| 24 | C | 302 | DMU | O7-C3-C4 | 6.26 | 126.60 | 109.45 |
| 22 | C | 310 | CHD | C1-C10-C5 | 6.24 | 116.99 | 107.77 |
| 22 | W | 101 | CHD | C5-C6-C7 | 6.22 | 121.32 | 114.46 |
| 24 | Z | 101 | DMU | O16-C6-C1 | 6.21 | 118.00 | 108.30 |
| 24 | P | 302 | DMU | C6-O5-C4 | 6.12 | 125.71 | 113.69 |
| 24 | P | 302 | DMU | C8-C7-C5 | 6.02 | 121.33 | 110.82 |
| 22 | C | 304 | CHD | C10-C9-C8 | 6.00 | 118.26 | 111.82 |
| 24 | C | 302 | DMU | O7-C3-C2 | 6.00 | 123.23 | 107.28 |
| 22 | J | 101 | CHD | C9-C8-C7 | 5.97 | 119.02 | 111.88 |
| 22 | P | 310 | CHD | C1-C10-C5 | 5.94 | 116.56 | 107.77 |
| 24 | P | 302 | DMU | O7-C3-C2 | 5.93 | 123.06 | 107.28 |
| 24 | P | 302 | DMU | O1-C9-C8 | 5.89 | 120.39 | 109.69 |
| 24 | M | 101 | DMU | O5-C6-O16 | 5.87 | 123.89 | 109.97 |
| 24 | C | 302 | DMU | O1-C9-C8 | 5.87 | 120.36 | 109.69 |
| 22 | J | 101 | CHD | C5-C6-C7 | 5.75 | 120.81 | 114.46 |
| 20 | B | 302 | TGL | CG2-OG2-CB1 | 5.71 | 131.86 | 117.79 |
| 24 | Z | 101 | DMU | O7-C3-C2 | 5.69 | 122.41 | 107.28 |
| 24 | C | 302 | DMU | C8-C7-C5 | 5.68 | 120.74 | 110.82 |
| 24 | P | 302 | DMU | O5-C6-C1 | 5.53 | 122.06 | 110.35 |
| 22 | P | 310 | CHD | C9-C8-C7 | 5.53 | 118.49 | 111.88 |
| 22 | C | 310 | CHD | C19-C10-C1 | -5.53 | 99.35 | 108.26 |
| 24 | M | 101 | DMU | C10-O7-C3 | 5.52 | 131.62 | 117.96 |
| 20 | L | 101 | TGL | C12-C11-C10 | -5.51 | 86.46 | 114.42 |
| 24 | Z | 101 | DMU | C18-O16-C6 | 5.49 | 122.95 | 113.84 |
| 22 | C | 310 | CHD | C9-C8-C7 | 5.48 | 118.43 | 111.88 |
| 22 | B | 304 | CHD | C18-C13-C12 | -5.48 | 103.49 | 109.07 |
| 22 | P | 310 | CHD | C15-C14-C8 | -5.47 | 110.69 | 118.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | Z | 101 | DMU | C6-C1-C2 | 5.45 | 121.34 | 110.00 |
| 22 | W | 101 | CHD | C15-C14-C8 | -5.41 | 110.77 | 118.33 |
| 24 | C | 302 | DMU | O5-C6-C1 | 5.40 | 121.78 | 110.35 |
| 24 | M | 101 | DMU | C6-C1-C2 | 5.31 | 121.05 | 110.00 |
| 20 | N | 606 | TGL | C12-C11-C10 | -5.27 | 87.67 | 114.42 |
| 22 | J | 101 | CHD | C15-C14-C8 | -5.27 | 110.97 | 118.33 |
| 22 | C | 310 | CHD | C15-C14-C8 | -5.23 | 111.03 | 118.33 |
| 24 | C | 302 | DMU | O5-C4-C57 | 5.22 | 119.41 | 106.44 |
| 22 | J | 101 | CHD | C6-C5-C4 | 5.20 | 117.18 | 111.19 |
| 22 | W | 101 | CHD | C18-C13-C14 | -5.11 | 103.21 | 111.21 |
| 22 | W | 101 | CHD | C6-C5-C4 | 5.11 | 117.07 | 111.19 |
| 22 | W | 101 | CHD | C17-C13-C12 | -5.09 | 113.02 | 117.67 |
| 22 | W | 101 | CHD | C4-C3-C2 | 5.06 | 116.59 | 110.55 |
| 22 | P | 304 | CHD | C1-C10-C5 | 5.02 | 115.19 | 107.77 |
| 24 | Z | 101 | DMU | C10-O7-C3 | 4.98 | 130.29 | 117.96 |
| 22 | P | 304 | CHD | C10-C9-C8 | 4.98 | 117.17 | 111.82 |
| 22 | P | 310 | CHD | C19-C10-C1 | -4.96 | 100.27 | 108.26 |
| 22 | J | 101 | CHD | C17-C13-C12 | -4.85 | 113.24 | 117.67 |
| 22 | J | 101 | CHD | C4-C3-C2 | 4.81 | 116.30 | 110.55 |
| 20 | O | 303 | TGL | CG2-OG2-CB1 | 4.81 | 129.63 | 117.79 |
| 22 | J | 101 | CHD | C18-C13-C14 | -4.76 | 103.76 | 111.21 |
| 24 | P | 302 | DMU | O5-C4-C57 | 4.70 | 118.13 | 106.44 |
| 22 | O | 302 | CHD | C17-C13-C12 | 4.67 | 121.93 | 117.67 |
| 24 | C | 302 | DMU | O7-C10-C5 | 4.66 | 120.18 | 108.10 |
| 20 | N | 606 | TGL | CB9-CB8-CB7 | -4.66 | 90.79 | 114.42 |
| 20 | L | 101 | TGL | CB9-CB8-CB7 | -4.60 | 91.07 | 114.42 |
| 24 | C | 302 | DMU | C10-O1-C9 | 4.52 | 122.57 | 113.69 |
| 22 | J | 101 | CHD | C1-C10-C5 | 4.52 | 114.45 | 107.77 |
| 20 | O | 303 | TGL | CG1-OG1-CA1 | -4.49 | 100.51 | 117.12 |
| 26 | G | 102 | PEK | O03-C01-C02 | 4.40 | 121.23 | 108.43 |
| 20 | B | 302 | TGL | CG1-OG1-CA1 | -4.38 | 100.92 | 117.12 |
| 22 | O | 302 | CHD | C18-C13-C12 | -4.35 | 104.64 | 109.07 |
| 22 | W | 101 | CHD | C2-C1-C10 | 4.32 | 120.19 | 112.78 |
| 24 | P | 302 | DMU | C10-O1-C9 | 4.28 | 122.09 | 113.69 |
| 22 | W | 101 | CHD | C1-C10-C5 | 4.21 | 113.99 | 107.77 |
| 22 | C | 304 | CHD | C1-C10-C5 | 4.18 | 113.95 | 107.77 |
| 17 | A | 604 | HEA | C27-C19-C18 | -4.16 | 113.00 | 123.68 |
| 24 | P | 302 | DMU | O7-C10-C5 | 4.14 | 118.84 | 108.10 |
| 17 | N | 604 | HEA | C27-C19-C18 | -4.12 | 113.10 | 123.68 |
| 24 | P | 302 | DMU | O7-C10-O1 | 4.12 | 122.18 | 110.67 |
| 22 | J | 101 | CHD | C2-C1-C10 | 4.11 | 119.83 | 112.78 |
| 22 | P | 304 | CHD | C13-C17-C20 | 4.09 | 124.38 | 119.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | G | 102 | PEK | P-O11-C03 | 4.06 | 145.50 | 121.68 |
| 26 | T | 101 | PEK | O03-C01-C02 | 4.05 | 120.22 | 108.43 |
| 20 | L | 101 | TGL | C15-CC9-CC8 | 4.01 | 134.76 | 114.42 |
| 26 | T | 101 | PEK | P-O11-C03 | 4.00 | 145.16 | 121.68 |
| 20 | D | 201 | TGL | CG2-OG2-CB1 | 3.99 | 127.61 | 117.79 |
| 22 | W | 101 | CHD | C14-C8-C7 | 3.94 | 117.03 | 111.81 |
| 22 | B | 304 | CHD | C1-C2-C3 | 3.91 | 115.49 | 110.47 |
| 26 | T | 101 | PEK | C02-O01-C1 | 3.90 | 127.40 | 117.79 |
| 20 | N | 606 | TGL | C15-CC9-CC8 | 3.90 | 134.22 | 114.42 |
| 17 | N | 604 | HEA | C20-C19-C18 | 3.89 | 129.00 | 121.12 |
| 24 | C | 302 | DMU | O1-C10-C5 | 3.84 | 118.48 | 110.35 |
| 22 | P | 310 | CHD | C6-C5-C4 | -3.84 | 106.77 | 111.19 |
| 20 | N | 606 | TGL | C16-C15-CC9 | 3.84 | 133.90 | 114.42 |
| 22 | J | 101 | CHD | C14-C8-C7 | 3.83 | 116.88 | 111.81 |
| 20 | L | 101 | TGL | C16-C15-CC9 | 3.80 | 133.71 | 114.42 |
| 17 | N | 605 | HEA | CMC-C2C-C1C | -3.79 | 122.64 | 128.46 |
| 22 | P | 304 | CHD | C15-C14-C8 | -3.77 | 113.06 | 118.33 |
| 24 | Z | 101 | DMU | O7-C3-C4 | 3.76 | 119.77 | 109.45 |
| 22 | C | 310 | CHD | C6-C5-C4 | -3.76 | 106.86 | 111.19 |
| 27 | P | 309 | CDL | PA1-OA5-CA3 | 3.73 | 143.53 | 121.68 |
| 22 | C | 304 | CHD | C15-C14-C8 | -3.71 | 113.14 | 118.33 |
| 20 | L | 101 | TGL | CG2-OG2-CB1 | 3.70 | 126.91 | 117.79 |
| 24 | Z | 101 | DMU | O7-C10-O1 | 3.70 | 121.01 | 110.67 |
| 27 | C | 309 | CDL | PA1-OA5-CA3 | 3.69 | 143.29 | 121.68 |
| 22 | B | 304 | CHD | C18-C13-C14 | 3.67 | 116.96 | 111.21 |
| 22 | P | 304 | CHD | C14-C8-C9 | -3.67 | 104.67 | 109.71 |
| 22 | C | 304 | CHD | C14-C8-C9 | -3.64 | 104.71 | 109.71 |
| 22 | B | 304 | CHD | C17-C13-C12 | 3.64 | 120.98 | 117.67 |
| 17 | A | 605 | HEA | CMC-C2C-C1C | -3.64 | 122.88 | 128.46 |
| 24 | P | 302 | DMU | O1-C10-C5 | 3.63 | 118.04 | 110.35 |
| 22 | B | 304 | CHD | C15-C14-C8 | -3.62 | 113.27 | 118.33 |
| 22 | O | 302 | CHD | C15-C14-C8 | -3.62 | 113.27 | 118.33 |
| 26 | P | 305 | PEK | C3-C2-C1 | -3.61 | 100.49 | 113.62 |
| 24 | M | 101 | DMU | O7-C3-C4 | 3.60 | 119.32 | 109.45 |
| 18 | N | 609 | PGV | O03-C01-C02 | 3.60 | 118.92 | 108.43 |
| 26 | G | 102 | PEK | C02-O01-C1 | 3.60 | 126.65 | 117.79 |
| 22 | P | 310 | CHD | C4-C5-C10 | 3.56 | 116.44 | 112.66 |
| 22 | B | 304 | CHD | C14-C8-C9 | -3.56 | 104.83 | 109.71 |
| 22 | O | 302 | CHD | C1-C2-C3 | 3.55 | 115.03 | 110.47 |
| 20 | L | 101 | TGL | CC3-CC2-CC1 | 3.55 | 126.52 | 113.62 |
| 22 | J | 101 | CHD | C19-C10-C5 | -3.54 | 104.35 | 110.36 |
| 20 | N | 607 | TGL | CG2-OG2-CB1 | 3.54 | 126.49 | 117.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20 | N | 607 | TGL | CG3-OG3-CC1 | 3.53 | 130.20 | 117.12 |
| 22 | W | 101 | CHD | C19-C10-C5 | -3.53 | 104.38 | 110.36 |
| 21 | B | 303 | PSC | C01-O03-C19 | -3.53 | 104.06 | 117.12 |
| 20 | L | 101 | TGL | C11-C10-CB9 | 3.53 | 132.33 | 114.42 |
| 24 | M | 101 | DMU | C10-O1-C9 | 3.52 | 120.61 | 113.69 |
| 24 | P | 302 | DMU | C2-C3-C4 | -3.52 | 102.86 | 110.93 |
| 22 | C | 304 | CHD | C16-C17-C13 | -3.50 | 100.12 | 103.55 |
| 24 | C | 302 | DMU | O7-C10-O1 | 3.49 | 120.42 | 110.67 |
| 17 | A | 605 | HEA | CMC-C2C-C3C | 3.48 | 131.20 | 124.68 |
| 21 | O | 304 | PSC | C01-O03-C19 | -3.46 | 104.32 | 117.12 |
| 17 | A | 604 | HEA | C20-C19-C18 | 3.46 | 128.11 | 121.12 |
| 20 | N | 606 | TGL | CG2-OG2-CB1 | 3.45 | 126.30 | 117.79 |
| 17 | A | 604 | HEA | CMC-C2C-C3C | 3.41 | 131.06 | 124.68 |
| 22 | C | 304 | CHD | C13-C17-C20 | 3.41 | 123.56 | 119.50 |
| 20 | N | 606 | TGL | CC3-CC2-CC1 | 3.40 | 125.99 | 113.62 |
| 26 | C | 305 | PEK | C3-C2-C1 | -3.38 | 101.32 | 113.62 |
| 22 | O | 302 | CHD | C5-C6-C7 | 3.38 | 118.19 | 114.46 |
| 22 | C | 310 | CHD | C4-C5-C10 | 3.37 | 116.23 | 112.66 |
| 22 | W | 101 | CHD | C16-C15-C14 | 3.35 | 111.77 | 105.13 |
| 24 | M | 101 | DMU | O7-C10-O1 | 3.34 | 119.99 | 110.67 |
| 20 | D | 201 | TGL | CG1-OG1-CA1 | -3.32 | 104.84 | 117.12 |
| 20 | N | 606 | TGL | C11-C10-CB9 | 3.31 | 131.23 | 114.42 |
| 24 | M | 101 | DMU | O5-C6-C1 | 3.30 | 117.34 | 110.35 |
| 20 | B | 302 | TGL | CG3-CG2-CG1 | 3.29 | 119.58 | 111.79 |
| 22 | P | 310 | CHD | C14-C13-C12 | 3.27 | 110.44 | 107.40 |
| 20 | L | 101 | TGL | CC4-CC3-CC2 | 3.27 | 124.93 | 113.19 |
| 24 | C | 302 | DMU | C2-C3-C4 | -3.26 | 103.45 | 110.93 |
| 22 | C | 310 | CHD | C9-C10-C5 | 3.24 | 113.13 | 108.58 |
| 22 | W | 101 | CHD | C13-C14-C8 | 3.24 | 118.87 | 114.74 |
| 22 | C | 304 | CHD | C15-C14-C13 | -3.22 | 100.39 | 103.55 |
| 22 | P | 310 | CHD | C9-C10-C5 | 3.22 | 113.10 | 108.58 |
| 20 | N | 606 | TGL | CC4-CC3-CC2 | 3.21 | 124.73 | 113.19 |
| 17 | N | 604 | HEA | CMC-C2C-C3C | 3.20 | 130.67 | 124.68 |
| 22 | P | 310 | CHD | C1-C10-C9 | 3.19 | 116.37 | 111.35 |
| 18 | C | 307 | PGV | O01-C1-C2 | -3.18 | 104.64 | 111.50 |
| 22 | O | 302 | CHD | C5-C4-C3 | 3.18 | 117.43 | 112.76 |
| 20 | D | 201 | TGL | OG1-CG1-CG2 | 3.17 | 117.67 | 108.43 |
| 22 | C | 310 | CHD | C11-C9-C10 | 3.17 | 117.00 | 113.73 |
| 22 | C | 304 | CHD | C14-C13-C12 | -3.17 | 104.45 | 107.40 |
| 22 | P | 304 | CHD | C5-C6-C7 | 3.16 | 117.94 | 114.46 |
| 26 | C | 306 | PEK | P-O12-C04 | 3.14 | 137.07 | 121.59 |
| 26 | P | 306 | PEK | P-O12-C04 | 3.13 | 136.98 | 121.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | M | 101 | DMU | O7-C10-C5 | 3.13 | 116.20 | 108.10 |
| 22 | B | 304 | CHD | C9-C11-C12 | 3.12 | 118.42 | 114.30 |
| 22 | B | 304 | CHD | C5-C4-C3 | 3.11 | 117.33 | 112.76 |
| 24 | Z | 101 | DMU | O5-C6-C1 | 3.11 | 116.94 | 110.35 |
| 22 | C | 310 | CHD | C4-C3-C2 | 3.08 | 114.23 | 110.55 |
| 22 | J | 101 | CHD | C1-C2-C3 | 3.08 | 114.42 | 110.47 |
| 17 | N | 604 | HEA | C4B-C3B-C2B | -3.08 | 104.72 | 106.87 |
| 22 | J | 101 | CHD | C13-C14-C8 | 3.07 | 118.66 | 114.74 |
| 22 | P | 310 | CHD | C4-C3-C2 | 3.06 | 114.21 | 110.55 |
| 24 | Z | 101 | DMU | C10-O1-C9 | 3.05 | 119.67 | 113.69 |
| 22 | C | 310 | CHD | C1-C10-C9 | 3.05 | 116.14 | 111.35 |
| 22 | J | 101 | CHD | C16-C15-C14 | 3.04 | 111.17 | 105.13 |
| 26 | C | 306 | PEK | P-O11-C03 | 3.04 | 139.48 | 121.68 |
| 20 | O | 303 | TGL | CG3-CG2-CG1 | 3.02 | 118.94 | 111.79 |
| 20 | D | 201 | TGL | OG2-CG2-CG1 | 3.02 | 119.32 | 108.40 |
| 17 | N | 604 | HEA | C17-C18-C19 | -3.02 | 120.40 | 127.66 |
| 22 | O | 302 | CHD | C14-C8-C9 | -3.01 | 105.59 | 109.71 |
| 22 | J | 101 | CHD | C15-C16-C17 | 3.00 | 111.08 | 105.13 |
| 17 | N | 605 | HEA | C27-C19-C20 | 2.99 | 120.30 | 115.27 |
| 18 | A | 606 | PGV | C02-O01-C1 | 2.97 | 125.10 | 117.79 |
| 22 | P | 310 | CHD | O3-C3-C4 | -2.97 | 103.94 | 109.85 |
| 22 | O | 302 | CHD | C18-C13-C14 | 2.96 | 115.85 | 111.21 |
| 20 | N | 607 | TGL | CG1-OG1-CA1 | -2.96 | 106.16 | 117.12 |
| 18 | A | 607 | PGV | O03-C01-C02 | 2.96 | 117.05 | 108.43 |
| 22 | C | 310 | CHD | C15-C16-C17 | 2.95 | 110.98 | 105.13 |
| 17 | N | 605 | HEA | CMC-C2C-C3C | 2.94 | 130.18 | 124.68 |
| 22 | J | 101 | CHD | C5-C4-C3 | 2.94 | 117.08 | 112.76 |
| 20 | L | 101 | TGL | OG1-CG1-CG2 | 2.93 | 116.96 | 108.43 |
| 22 | P | 310 | CHD | C15-C16-C17 | 2.91 | 110.91 | 105.13 |
| 22 | W | 101 | CHD | C1-C2-C3 | 2.90 | 114.19 | 110.47 |
| 26 | C | 306 | PEK | C11-C10-C9 | 2.90 | 126.30 | 112.02 |
| 22 | W | 101 | CHD | C11-C9-C10 | 2.89 | 116.71 | 113.73 |
| 22 | W | 101 | CHD | C15-C16-C17 | 2.89 | 110.86 | 105.13 |
| 22 | C | 310 | CHD | O3-C3-C4 | -2.89 | 104.10 | 109.85 |
| 20 | D | 201 | TGL | CG3-OG3-CC1 | 2.88 | 127.78 | 117.12 |
| 22 | P | 310 | CHD | C5-C6-C7 | 2.88 | 117.63 | 114.46 |
| 22 | P | 310 | CHD | C14-C8-C9 | -2.86 | 105.78 | 109.71 |
| 22 | O | 302 | CHD | C18-C13-C17 | -2.86 | 106.74 | 111.21 |
| 20 | N | 607 | TGL | CB3-CB2-CB1 | 2.85 | 123.98 | 113.62 |
| 26 | P | 306 | PEK | C11-C10-C9 | 2.85 | 126.04 | 112.02 |
| 26 | P | 306 | PEK | P-O11-C03 | 2.84 | 138.32 | 121.68 |
| 20 | N | 606 | TGL | C13-C12-C11 | 2.83 | 128.80 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17 | N | 605 | HEA | C3C-C4C-NC | 2.82 | 112.86 | 109.21 |
| 20 | D | 201 | TGL | CB3-CB2-CB1 | 2.81 | 123.84 | 113.62 |
| 20 | N | 607 | TGL | OG1-CG1-CG2 | 2.80 | 116.60 | 108.43 |
| 27 | T | 102 | CDL | C22-C21-C20 | 2.78 | 128.55 | 114.42 |
| 22 | B | 304 | CHD | C2-C1-C10 | 2.78 | 117.55 | 112.78 |
| 24 | C | 302 | DMU | C10-O7-C3 | 2.77 | 124.83 | 117.96 |
| 22 | W | 101 | CHD | C5-C4-C3 | 2.76 | 116.80 | 112.76 |
| 22 | P | 310 | CHD | C16-C15-C14 | 2.75 | 110.58 | 105.13 |
| 22 | P | 304 | CHD | C1-C2-C3 | 2.75 | 113.99 | 110.47 |
| 18 | A | 607 | PGV | C01-O03-C19 | -2.72 | 107.04 | 117.12 |
| 22 | C | 310 | CHD | C16-C15-C14 | 2.72 | 110.52 | 105.13 |
| 22 | P | 310 | CHD | C14-C8-C7 | 2.70 | 115.38 | 111.81 |
| 22 | C | 310 | CHD | C11-C12-C13 | 2.70 | 114.01 | 111.24 |
| 22 | J | 101 | CHD | C11-C9-C10 | 2.68 | 116.49 | 113.73 |
| 27 | T | 102 | CDL | OB8-CB7-C71 | -2.68 | 103.51 | 111.91 |
| 17 | A | 604 | HEA | CMC-C2C-C1C | -2.67 | 124.35 | 128.46 |
| 27 | G | 101 | CDL | C23-C22-C21 | 2.67 | 127.98 | 114.42 |
| 22 | O | 302 | CHD | C2-C1-C10 | 2.65 | 117.33 | 112.78 |
| 24 | P | 302 | DMU | C10-O7-C3 | 2.65 | 124.52 | 117.96 |
| 22 | C | 310 | CHD | C14-C8-C7 | 2.65 | 115.31 | 111.81 |
| 18 | P | 307 | PGV | O01-C1-C2 | -2.63 | 105.83 | 111.50 |
| 18 | N | 608 | PGV | O01-C02-C03 | 2.63 | 117.93 | 108.40 |
| 18 | N | 608 | PGV | C02-O01-C1 | 2.62 | 124.24 | 117.79 |
| 20 | D | 201 | TGL | OG2-CG2-CG3 | 2.61 | 117.85 | 108.40 |
| 27 | G | 101 | CDL | C22-C21-C20 | 2.60 | 127.63 | 114.42 |
| 18 | N | 609 | PGV | C01-O03-C19 | -2.60 | 107.49 | 117.12 |
| 20 | N | 607 | TGL | OG2-CG2-CG3 | 2.60 | 117.82 | 108.40 |
| 20 | L | 101 | TGL | C20-CA9-CA8 | 2.60 | 127.61 | 114.42 |
| 18 | A | 606 | PGV | C3-C2-C1 | -2.59 | 104.21 | 113.62 |
| 27 | P | 309 | CDL | OB6-CB5-C51 | -2.58 | 105.94 | 111.50 |
| 17 | A | 604 | HEA | C21-C20-C19 | -2.57 | 104.53 | 112.98 |
| 22 | P | 310 | CHD | C11-C9-C10 | 2.56 | 116.37 | 113.73 |
| 22 | B | 304 | CHD | O3-C3-C4 | -2.55 | 104.76 | 109.85 |
| 22 | W | 101 | CHD | C9-C11-C12 | 2.55 | 117.67 | 114.30 |
| 22 | C | 310 | CHD | C6-C5-C10 | 2.55 | 115.36 | 112.66 |
| 22 | O | 302 | CHD | C9-C11-C12 | 2.55 | 117.66 | 114.30 |
| 22 | C | 310 | CHD | C1-C2-C3 | 2.54 | 113.72 | 110.47 |
| 20 | B | 302 | TGL | CA8-CA7-CA6 | -2.53 | 101.56 | 114.42 |
| 22 | C | 304 | CHD | C5-C6-C7 | 2.53 | 117.25 | 114.46 |
| 22 | P | 304 | CHD | C13-C14-C8 | -2.52 | 111.51 | 114.74 |
| 20 | O | 303 | TGL | CA8-CA7-CA6 | -2.52 | 101.61 | 114.42 |
| 22 | C | 310 | CHD | C14-C8-C9 | -2.52 | 106.25 | 109.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | P | 310 | CHD | C19-C10-C5 | -2.52 | 106.09 | 110.36 |
| 20 | O | 303 | TGL | CG3-OG3-CC1 | 2.51 | 126.43 | 117.12 |
| 22 | J | 101 | CHD | C14-C8-C9 | 2.50 | 113.15 | 109.71 |
| 22 | O | 302 | CHD | O3-C3-C4 | -2.50 | 104.87 | 109.85 |
| 20 | N | 606 | TGL | OG1-CG1-CG2 | 2.50 | 115.71 | 108.43 |
| 22 | P | 310 | CHD | C1-C2-C3 | 2.50 | 113.67 | 110.47 |
| 23 | C | 301 | DCW | C8-N2-C1 | 2.48 | 128.26 | 123.02 |
| 26 | T | 101 | PEK | C03-C02-C01 | 2.48 | 117.64 | 111.79 |
| 20 | L | 101 | TGL | C13-C12-C11 | 2.47 | 126.98 | 114.42 |
| 24 | Z | 101 | DMU | O7-C10-C5 | 2.47 | 114.50 | 108.10 |
| 22 | P | 310 | CHD | C13-C17-C20 | 2.47 | 122.44 | 119.50 |
| 22 | P | 304 | CHD | C16-C17-C13 | -2.47 | 101.13 | 103.55 |
| 27 | T | 102 | CDL | C23-C22-C21 | 2.46 | 126.93 | 114.42 |
| 27 | G | 101 | CDL | OB8-CB7-C71 | -2.46 | 104.18 | 111.91 |
| 22 | C | 310 | CHD | C5-C6-C7 | 2.46 | 117.17 | 114.46 |
| 17 | A | 605 | HEA | CBD-CAD-C3D | 2.45 | 117.01 | 112.49 |
| 20 | O | 303 | TGL | CB7-CB6-CB5 | -2.45 | 101.97 | 114.42 |
| 18 | C | 308 | PGV | C02-O01-C1 | -2.44 | 111.77 | 117.79 |
| 18 | A | 606 | PGV | O01-C02-C03 | 2.44 | 117.24 | 108.40 |
| 26 | P | 306 | PEK | C24-C23-C22 | 2.44 | 121.96 | 113.19 |
| 18 | P | 308 | PGV | C02-O01-C1 | -2.44 | 111.79 | 117.79 |
| 22 | P | 304 | CHD | C14-C13-C12 | -2.44 | 105.13 | 107.40 |
| 27 | G | 101 | CDL | C20-C19-C18 | 2.44 | 126.80 | 114.42 |
| 27 | P | 309 | CDL | CB6-OB8-CB7 | -2.43 | 108.12 | 117.12 |
| 27 | T | 102 | CDL | C83-C82-C81 | 2.43 | 126.74 | 114.42 |
| 27 | C | 309 | CDL | CB6-OB8-CB7 | -2.43 | 108.14 | 117.12 |
| 18 | N | 608 | PGV | C3-C2-C1 | -2.42 | 104.81 | 113.62 |
| 22 | C | 310 | CHD | C14-C13-C12 | 2.39 | 109.63 | 107.40 |
| 22 | O | 302 | CHD | C1-C10-C5 | 2.39 | 111.30 | 107.77 |
| 26 | P | 305 | PEK | C2-C3-C4 | 2.38 | 117.48 | 113.23 |
| 27 | C | 309 | CDL | OB6-CB5-C51 | -2.35 | 106.43 | 111.50 |
| 20 | L | 101 | TGL | CC7-CC6-CC5 | 2.35 | 126.36 | 114.42 |
| 20 | B | 302 | TGL | CB7-CB6-CB5 | -2.34 | 102.57 | 114.42 |
| 22 | J | 101 | CHD | C19-C10-C1 | -2.33 | 104.50 | 108.26 |
| 26 | C | 305 | PEK | O03-C21-C22 | -2.33 | 104.60 | 111.91 |
| 21 | O | 304 | PSC | O01-C1-C2 | -2.32 | 106.50 | 111.50 |
| 17 | N | 605 | HEA | C26-C15-C16 | 2.32 | 119.18 | 115.27 |
| 27 | T | 102 | CDL | C20-C19-C18 | 2.32 | 126.21 | 114.42 |
| 22 | C | 304 | CHD | C13-C14-C8 | -2.30 | 111.80 | 114.74 |
| 20 | B | 302 | TGL | CG3-OG3-CC1 | 2.30 | 125.63 | 117.12 |
| 17 | A | 604 | HEA | C17-C18-C19 | -2.29 | 122.14 | 127.66 |
| 27 | P | 309 | CDL | OA8-CA6-CA4 | 2.29 | 115.09 | 108.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20 | N | 606 | TGL | C20-CA9-CA8 | 2.28 | 126.01 | 114.42 |
| 22 | P | 310 | CHD | C18-C13-C14 | -2.28 | 107.64 | 111.21 |
| 27 | C | 309 | CDL | C52-C51-CB5 | -2.28 | 105.34 | 113.62 |
| 27 | T | 102 | CDL | C80-C79-C78 | 2.27 | 125.95 | 114.42 |
| 20 | O | 303 | TGL | CB9-CB8-CB7 | -2.27 | 102.91 | 114.42 |
| 20 | B | 302 | TGL | CB9-CB8-CB7 | -2.26 | 102.93 | 114.42 |
| 26 | C | 306 | PEK | C24-C23-C22 | 2.26 | 121.32 | 113.19 |
| 22 | C | 310 | CHD | C13-C17-C20 | 2.26 | 122.19 | 119.50 |
| 18 | C | 307 | PGV | O03-C01-C02 | 2.26 | 115.01 | 108.43 |
| 17 | A | 605 | HEA | C26-C15-C16 | 2.26 | 119.07 | 115.27 |
| 26 | P | 305 | PEK | C02-O01-C1 | -2.26 | 112.24 | 117.79 |
| 22 | C | 304 | CHD | C17-C13-C14 | 2.25 | 102.37 | 100.09 |
| 27 | T | 102 | CDL | C19-C18-C17 | 2.25 | 125.85 | 114.42 |
| 22 | P | 310 | CHD | C5-C4-C3 | 2.25 | 116.06 | 112.76 |
| 27 | G | 101 | CDL | C83-C82-C81 | 2.25 | 125.84 | 114.42 |
| 17 | N | 604 | HEA | C21-C20-C19 | -2.25 | 105.59 | 112.98 |
| 18 | C | 307 | PGV | O01-C1-O02 | 2.24 | 129.12 | 123.70 |
| 17 | N | 605 | HEA | C17-C18-C19 | 2.24 | 133.05 | 127.66 |
| 27 | G | 101 | CDL | C80-C79-C78 | 2.24 | 125.79 | 114.42 |
| 20 | B | 302 | TGL | C33-C19-C18 | 2.24 | 125.77 | 114.42 |
| 22 | C | 310 | CHD | C19-C10-C5 | -2.23 | 106.59 | 110.36 |
| 18 | N | 609 | PGV | C4-C3-C2 | 2.22 | 121.17 | 113.19 |
| 26 | P | 305 | PEK | C24-C23-C22 | -2.21 | 105.23 | 113.19 |
| 22 | W | 101 | CHD | C14-C8-C9 | 2.21 | 112.75 | 109.71 |
| 26 | P | 305 | PEK | O03-C21-O04 | 2.21 | 129.16 | 123.59 |
| 20 | N | 606 | TGL | C10-CB9-CB8 | 2.20 | 125.62 | 114.42 |
| 26 | G | 102 | PEK | C03-C02-C01 | 2.20 | 117.00 | 111.79 |
| 18 | C | 307 | PGV | C3-C2-C1 | -2.20 | 105.63 | 113.62 |
| 27 | P | 309 | CDL | C52-C51-CB5 | -2.20 | 105.64 | 113.62 |
| 27 | G | 101 | CDL | C19-C18-C17 | 2.19 | 125.56 | 114.42 |
| 27 | G | 101 | CDL | OB8-CB6-CB4 | 2.19 | 114.79 | 108.43 |
| 26 | P | 306 | PEK | O03-C01-C02 | 2.18 | 114.77 | 108.43 |
| 26 | T | 101 | PEK | P-O12-C04 | 2.17 | 132.29 | 121.59 |
| 18 | A | 606 | PGV | C4-C3-C2 | -2.17 | 105.38 | 113.19 |
| 22 | W | 101 | CHD | C19-C10-C1 | -2.17 | 104.76 | 108.26 |
| 22 | P | 304 | CHD | C6-C5-C10 | 2.17 | 114.96 | 112.66 |
| 20 | B | 302 | TGL | OG2-CG2-CG3 | 2.17 | 116.25 | 108.40 |
| 26 | P | 306 | PEK | C2-C3-C4 | 2.17 | 117.09 | 113.23 |
| 20 | O | 303 | TGL | CA3-CA2-CA1 | -2.16 | 105.76 | 113.62 |
| 21 | O | 304 | PSC | C07-N-C06 | -2.16 | 103.42 | 108.97 |
| 27 | T | 102 | CDL | OB8-CB6-CB4 | 2.16 | 114.72 | 108.43 |
| 22 | B | 304 | CHD | C1-C10-C5 | 2.16 | 110.96 | 107.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 301 | DCW | C2-N1-C1 | -2.15 | 118.48 | 123.02 |
| 18 | P | 308 | PGV | O03-C01-C02 | 2.15 | 114.69 | 108.43 |
| 17 | A | 604 | HEA | C27-C19-C20 | 2.14 | 118.88 | 115.27 |
| 22 | W | 101 | CHD | C9-C10-C5 | 2.14 | 111.59 | 108.58 |
| 23 | P | 301 | DCW | C8-N2-C1 | 2.13 | 127.53 | 123.02 |
| 20 | B | 302 | TGL | OG3-CG3-CG2 | 2.13 | 114.63 | 108.43 |
| 27 | C | 309 | CDL | OA8-CA6-CA4 | 2.12 | 114.62 | 108.43 |
| 26 | C | 306 | PEK | O03-C01-C02 | 2.12 | 114.60 | 108.43 |
| 18 | N | 609 | PGV | C3-C2-C1 | -2.12 | 105.93 | 113.62 |
| 27 | C | 309 | CDL | CA4-OA6-CA5 | 2.11 | 123.00 | 117.79 |
| 20 | D | 201 | TGL | CB4-CB3-CB2 | 2.11 | 120.79 | 113.19 |
| 17 | N | 604 | HEA | CMC-C2C-C1C | -2.11 | 125.22 | 128.46 |
| 20 | N | 607 | TGL | CB4-CB3-CB2 | 2.10 | 120.74 | 113.19 |
| 20 | O | 303 | TGL | C33-C19-C18 | 2.10 | 125.09 | 114.42 |
| 22 | J | 101 | CHD | C9-C11-C12 | 2.10 | 117.07 | 114.30 |
| 20 | N | 607 | TGL | CA5-CA4-CA3 | -2.10 | 103.77 | 114.42 |
| 20 | N | 606 | TGL | CC7-CC6-CC5 | 2.10 | 125.07 | 114.42 |
| 22 | C | 304 | CHD | C1-C2-C3 | 2.09 | 113.16 | 110.47 |
| 18 | N | 609 | PGV | C21-C20-C19 | 2.09 | 121.21 | 113.62 |
| 20 | B | 302 | TGL | CA3-CA2-CA1 | -2.08 | 106.04 | 113.62 |
| 18 | C | 307 | PGV | C9-C10-C11 | -2.08 | 100.51 | 112.43 |
| 20 | D | 201 | TGL | C25-C24-C23 | 2.08 | 124.99 | 114.42 |
| 22 | C | 310 | CHD | C5-C4-C3 | 2.08 | 115.81 | 112.76 |
| 20 | D | 201 | TGL | C10-CB9-CB8 | 2.07 | 124.94 | 114.42 |
| 20 | N | 607 | TGL | OG2-CG2-CG1 | 2.07 | 115.90 | 108.40 |
| 22 | P | 304 | CHD | C15-C14-C13 | -2.07 | 101.52 | 103.55 |
| 26 | T | 101 | PEK | C2-C3-C4 | 2.07 | 116.92 | 113.23 |
| 27 | T | 102 | CDL | C79-C78-C77 | 2.07 | 124.92 | 114.42 |
| 22 | C | 304 | CHD | O12-C12-C13 | -2.06 | 107.54 | 111.03 |
| 20 | B | 302 | TGL | CB6-CB5-CB4 | 2.06 | 124.90 | 114.42 |
| 22 | B | 304 | CHD | C5-C6-C7 | 2.06 | 116.73 | 114.46 |
| 18 | N | 608 | PGV | C03-C02-C01 | 2.05 | 116.64 | 111.79 |
| 27 | C | 309 | CDL | C79-C78-C77 | 2.05 | 124.84 | 114.42 |
| 18 | A | 607 | PGV | C4-C3-C2 | 2.04 | 120.54 | 113.19 |
| 22 | O | 302 | CHD | C19-C10-C9 | -2.04 | 108.37 | 111.18 |
| 22 | P | 304 | CHD | C4-C5-C10 | -2.04 | 110.49 | 112.66 |
| 20 | D | 201 | TGL | CC3-CC2-CC1 | -2.04 | 106.19 | 113.62 |
| 27 | G | 101 | CDL | C79-C78-C77 | 2.04 | 124.80 | 114.42 |
| 26 | G | 102 | PEK | P-O12-C04 | 2.04 | 131.63 | 121.59 |
| 20 | N | 606 | TGL | OG2-CB1-OB1 | 2.03 | 128.62 | 123.70 |
| 17 | N | 604 | HEA | CBD-CAD-C3D | 2.03 | 116.23 | 112.49 |
| 18 | P | 307 | PGV | C9-C10-C11 | -2.02 | 100.87 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|-------------|------|------------------------|---------------------|
| 20 | O | 303 | TGL | OG2-CG2-CG3 | 2.01 | 115.70 | 108.40 |
| 27 | P | 309 | CDL | C83-C82-C81 | 2.01 | 124.64 | 114.42 |
| 17 | N | 604 | HEA | C16-C17-C18 | 2.01 | 118.50 | 111.88 |
| 22 | P | 310 | CHD | C6-C5-C10 | 2.00 | 114.78 | 112.66 |
| 17 | A | 604 | HEA | C16-C17-C18 | 2.00 | 118.46 | 111.88 |

All (54) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | C | 302 | DMU | C5 |
| 24 | C | 302 | DMU | C6 |
| 24 | C | 302 | DMU | C9 |
| 24 | C | 302 | DMU | C4 |
| 24 | C | 302 | DMU | C2 |
| 24 | C | 302 | DMU | C10 |
| 22 | W | 101 | CHD | C12 |
| 22 | W | 101 | CHD | C8 |
| 22 | W | 101 | CHD | C9 |
| 22 | W | 101 | CHD | C14 |
| 22 | W | 101 | CHD | C17 |
| 22 | P | 310 | CHD | C12 |
| 22 | P | 310 | CHD | C8 |
| 22 | P | 310 | CHD | C3 |
| 22 | P | 310 | CHD | C9 |
| 22 | P | 310 | CHD | C14 |
| 22 | C | 310 | CHD | C12 |
| 22 | C | 310 | CHD | C8 |
| 22 | C | 310 | CHD | C3 |
| 22 | C | 310 | CHD | C9 |
| 22 | C | 310 | CHD | C14 |
| 17 | N | 604 | HEA | ND |
| 17 | N | 604 | HEA | NA |
| 17 | N | 604 | HEA | NB |
| 24 | Z | 101 | DMU | C2 |
| 24 | Z | 101 | DMU | C4 |
| 24 | Z | 101 | DMU | C6 |
| 24 | Z | 101 | DMU | C5 |
| 24 | Z | 101 | DMU | C9 |
| 24 | P | 302 | DMU | C5 |
| 24 | P | 302 | DMU | C6 |
| 24 | P | 302 | DMU | C9 |
| 24 | P | 302 | DMU | C4 |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | P | 302 | DMU | C2 |
| 24 | P | 302 | DMU | C10 |
| 17 | N | 605 | HEA | ND |
| 17 | N | 605 | HEA | NA |
| 17 | N | 605 | HEA | NB |
| 17 | A | 604 | HEA | ND |
| 17 | A | 604 | HEA | NA |
| 17 | A | 604 | HEA | NB |
| 24 | M | 101 | DMU | C2 |
| 24 | M | 101 | DMU | C4 |
| 24 | M | 101 | DMU | C6 |
| 24 | M | 101 | DMU | C5 |
| 24 | M | 101 | DMU | C9 |
| 17 | A | 605 | HEA | ND |
| 17 | A | 605 | HEA | NA |
| 17 | A | 605 | HEA | NB |
| 22 | J | 101 | CHD | C12 |
| 22 | J | 101 | CHD | C8 |
| 22 | J | 101 | CHD | C9 |
| 22 | J | 101 | CHD | C14 |
| 22 | J | 101 | CHD | C17 |

All (850) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | C | 301 | DCW | O1-C1-N1-C2 |
| 23 | C | 301 | DCW | N2-C1-N1-C2 |
| 21 | B | 303 | PSC | C03-O11-P-O14 |
| 21 | B | 303 | PSC | C04-O12-P-O14 |
| 21 | B | 303 | PSC | O02-C1-O01-C02 |
| 27 | G | 101 | CDL | CB2-C1-CA2-OA2 |
| 27 | G | 101 | CDL | CA2-OA2-PA1-OA3 |
| 27 | G | 101 | CDL | C1-CB2-OB2-PB2 |
| 27 | G | 101 | CDL | CB3-OB5-PB2-OB3 |
| 27 | G | 101 | CDL | CB3-OB5-PB2-OB4 |
| 26 | G | 102 | PEK | C03-O11-P-O14 |
| 26 | G | 102 | PEK | O12-C04-C05-N |
| 22 | W | 101 | CHD | C16-C17-C20-C21 |
| 22 | W | 101 | CHD | C16-C17-C20-C22 |
| 23 | P | 301 | DCW | N2-C1-N1-C2 |
| 27 | T | 102 | CDL | CB2-C1-CA2-OA2 |
| 27 | T | 102 | CDL | CA2-OA2-PA1-OA3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | T | 102 | CDL | C1-CB2-OB2-PB2 |
| 27 | T | 102 | CDL | CB3-OB5-PB2-OB3 |
| 27 | T | 102 | CDL | CB3-OB5-PB2-OB4 |
| 27 | C | 309 | CDL | CA2-OA2-PA1-OA3 |
| 27 | C | 309 | CDL | CA2-OA2-PA1-OA4 |
| 27 | C | 309 | CDL | CA4-CA3-OA5-PA1 |
| 27 | C | 309 | CDL | C11-CA5-OA6-CA4 |
| 27 | C | 309 | CDL | CB2-OB2-PB2-OB3 |
| 27 | C | 309 | CDL | CB2-OB2-PB2-OB4 |
| 26 | T | 101 | PEK | C03-O11-P-O14 |
| 26 | T | 101 | PEK | O12-C04-C05-N |
| 18 | N | 608 | PGV | C04-O12-P-O11 |
| 18 | N | 608 | PGV | C04-O12-P-O13 |
| 18 | N | 608 | PGV | C04-O12-P-O14 |
| 18 | N | 608 | PGV | C02-C03-O11-P |
| 18 | N | 608 | PGV | C05-C04-O12-P |
| 18 | N | 608 | PGV | C04-C05-C06-O06 |
| 18 | N | 608 | PGV | O02-C1-O01-C02 |
| 18 | N | 608 | PGV | C20-C19-O03-C01 |
| 26 | C | 306 | PEK | C04-O12-P-O13 |
| 26 | C | 306 | PEK | C04-O12-P-O14 |
| 24 | Z | 101 | DMU | O5-C6-O16-C18 |
| 18 | A | 606 | PGV | C04-O12-P-O11 |
| 18 | A | 606 | PGV | C04-O12-P-O13 |
| 18 | A | 606 | PGV | C04-O12-P-O14 |
| 18 | A | 606 | PGV | C02-C03-O11-P |
| 18 | A | 606 | PGV | C05-C04-O12-P |
| 18 | A | 606 | PGV | C04-C05-C06-O06 |
| 18 | A | 606 | PGV | O02-C1-O01-C02 |
| 18 | A | 606 | PGV | C20-C19-O03-C01 |
| 26 | P | 306 | PEK | C03-O11-P-O13 |
| 26 | P | 306 | PEK | C04-O12-P-O13 |
| 26 | P | 306 | PEK | C04-O12-P-O14 |
| 21 | O | 304 | PSC | C03-O11-P-O14 |
| 21 | O | 304 | PSC | C04-O12-P-O14 |
| 27 | P | 309 | CDL | CA2-OA2-PA1-OA3 |
| 27 | P | 309 | CDL | CA2-OA2-PA1-OA4 |
| 27 | P | 309 | CDL | CA4-CA3-OA5-PA1 |
| 27 | P | 309 | CDL | C11-CA5-OA6-CA4 |
| 27 | P | 309 | CDL | CB2-OB2-PB2-OB3 |
| 27 | P | 309 | CDL | CB2-OB2-PB2-OB4 |
| 24 | M | 101 | DMU | O5-C6-O16-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | C | 308 | PGV | C04-O12-P-O11 |
| 18 | C | 308 | PGV | C04-O12-P-O13 |
| 18 | C | 308 | PGV | C04-O12-P-O14 |
| 18 | P | 308 | PGV | C04-O12-P-O11 |
| 18 | P | 308 | PGV | C04-O12-P-O13 |
| 18 | P | 308 | PGV | C04-O12-P-O14 |
| 17 | A | 605 | HEA | O11-C11-C12-C13 |
| 22 | J | 101 | CHD | C16-C17-C20-C21 |
| 22 | J | 101 | CHD | C16-C17-C20-C22 |
| 18 | N | 608 | PGV | O04-C19-O03-C01 |
| 18 | A | 606 | PGV | O04-C19-O03-C01 |
| 20 | D | 201 | TGL | OC1-CC1-OG3-CG3 |
| 20 | N | 607 | TGL | OC1-CC1-OG3-CG3 |
| 23 | P | 301 | DCW | O1-C1-N1-C2 |
| 20 | O | 303 | TGL | OB1-CB1-OG2-CG2 |
| 20 | B | 302 | TGL | OB1-CB1-OG2-CG2 |
| 21 | O | 304 | PSC | O02-C1-O01-C02 |
| 27 | G | 101 | CDL | C31-CA7-OA8-CA6 |
| 18 | N | 608 | PGV | C2-C1-O01-C02 |
| 18 | A | 606 | PGV | C2-C1-O01-C02 |
| 27 | G | 101 | CDL | C20-C21-C22-C23 |
| 27 | G | 101 | CDL | C57-C58-C59-C60 |
| 27 | G | 101 | CDL | C77-C78-C79-C80 |
| 27 | G | 101 | CDL | C80-C81-C82-C83 |
| 27 | T | 102 | CDL | C17-C18-C19-C20 |
| 27 | T | 102 | CDL | C20-C21-C22-C23 |
| 27 | T | 102 | CDL | C57-C58-C59-C60 |
| 27 | T | 102 | CDL | C80-C81-C82-C83 |
| 27 | C | 309 | CDL | C40-C41-C42-C43 |
| 27 | C | 309 | CDL | C60-C61-C62-C63 |
| 27 | C | 309 | CDL | C80-C81-C82-C83 |
| 20 | O | 303 | TGL | C16-C15-CC9-CC8 |
| 20 | B | 302 | TGL | C16-C15-CC9-CC8 |
| 27 | P | 309 | CDL | C40-C41-C42-C43 |
| 27 | P | 309 | CDL | C60-C61-C62-C63 |
| 27 | P | 309 | CDL | C80-C81-C82-C83 |
| 27 | T | 102 | CDL | C31-CA7-OA8-CA6 |
| 20 | D | 201 | TGL | CC2-CC1-OG3-CG3 |
| 20 | O | 303 | TGL | CA2-CA1-OG1-CG1 |
| 20 | B | 302 | TGL | CA2-CA1-OG1-CG1 |
| 20 | N | 607 | TGL | CC2-CC1-OG3-CG3 |
| 27 | G | 101 | CDL | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | G | 101 | CDL | C37-C38-C39-C40 |
| 27 | G | 101 | CDL | C40-C41-C42-C43 |
| 27 | T | 102 | CDL | C40-C41-C42-C43 |
| 27 | T | 102 | CDL | C77-C78-C79-C80 |
| 27 | C | 309 | CDL | C20-C21-C22-C23 |
| 27 | C | 309 | CDL | C57-C58-C59-C60 |
| 27 | C | 309 | CDL | C77-C78-C79-C80 |
| 27 | P | 309 | CDL | C20-C21-C22-C23 |
| 27 | P | 309 | CDL | C77-C78-C79-C80 |
| 27 | G | 101 | CDL | C60-C61-C62-C63 |
| 27 | T | 102 | CDL | C37-C38-C39-C40 |
| 27 | T | 102 | CDL | C60-C61-C62-C63 |
| 20 | L | 101 | TGL | C21-C20-CA9-CA8 |
| 20 | N | 606 | TGL | C21-C20-CA9-CA8 |
| 27 | P | 309 | CDL | C17-C18-C19-C20 |
| 27 | C | 309 | CDL | OA7-CA5-OA6-CA4 |
| 27 | P | 309 | CDL | OA7-CA5-OA6-CA4 |
| 27 | G | 101 | CDL | OA9-CA7-OA8-CA6 |
| 27 | T | 102 | CDL | OA9-CA7-OA8-CA6 |
| 20 | O | 303 | TGL | OA1-CA1-OG1-CG1 |
| 20 | B | 302 | TGL | OA1-CA1-OG1-CG1 |
| 27 | C | 309 | CDL | C17-C18-C19-C20 |
| 27 | C | 309 | CDL | C37-C38-C39-C40 |
| 27 | P | 309 | CDL | C57-C58-C59-C60 |
| 27 | P | 309 | CDL | C37-C38-C39-C40 |
| 20 | N | 607 | TGL | C21-C20-CA9-CA8 |
| 27 | G | 101 | CDL | O1-C1-CA2-OA2 |
| 27 | T | 102 | CDL | O1-C1-CA2-OA2 |
| 20 | D | 201 | TGL | C21-C20-CA9-CA8 |
| 20 | L | 101 | TGL | OA1-CA1-OG1-CG1 |
| 20 | N | 606 | TGL | OA1-CA1-OG1-CG1 |
| 24 | C | 302 | DMU | O6-C11-C9-O1 |
| 20 | O | 303 | TGL | CB2-CB1-OG2-CG2 |
| 20 | B | 302 | TGL | CB2-CB1-OG2-CG2 |
| 20 | L | 101 | TGL | C11-C10-CB9-CB8 |
| 20 | N | 606 | TGL | C16-C15-CC9-CC8 |
| 20 | B | 302 | TGL | C11-C10-CB9-CB8 |
| 20 | L | 101 | TGL | C16-C15-CC9-CC8 |
| 20 | N | 606 | TGL | C11-C10-CB9-CB8 |
| 20 | D | 201 | TGL | C11-C10-CB9-CB8 |
| 20 | D | 201 | TGL | C16-C15-CC9-CC8 |
| 20 | O | 303 | TGL | C21-C20-CA9-CA8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 20 | O | 303 | TGL | C11-C10-CB9-CB8 |
| 20 | B | 302 | TGL | C21-C20-CA9-CA8 |
| 20 | N | 607 | TGL | C11-C10-CB9-CB8 |
| 20 | N | 607 | TGL | C16-C15-CC9-CC8 |
| 24 | P | 302 | DMU | O6-C11-C9-O1 |
| 24 | Z | 101 | DMU | O6-C11-C9-C8 |
| 22 | P | 310 | CHD | C17-C20-C22-C23 |
| 22 | C | 310 | CHD | C17-C20-C22-C23 |
| 24 | M | 101 | DMU | O6-C11-C9-C8 |
| 27 | C | 309 | CDL | CA2-C1-CB2-OB2 |
| 18 | N | 608 | PGV | O12-C04-C05-C06 |
| 18 | A | 606 | PGV | O12-C04-C05-C06 |
| 27 | P | 309 | CDL | CA2-C1-CB2-OB2 |
| 21 | B | 303 | PSC | C20-C19-O03-C01 |
| 20 | L | 101 | TGL | CA2-CA1-OG1-CG1 |
| 20 | N | 606 | TGL | CA2-CA1-OG1-CG1 |
| 20 | D | 201 | TGL | CA2-CA1-OG1-CG1 |
| 21 | O | 304 | PSC | C20-C19-O03-C01 |
| 22 | W | 101 | CHD | C13-C17-C20-C22 |
| 22 | J | 101 | CHD | C13-C17-C20-C22 |
| 24 | M | 101 | DMU | O5-C4-C57-O61 |
| 24 | C | 302 | DMU | C3-C4-C57-O61 |
| 27 | G | 101 | CDL | O1-C1-CB2-OB2 |
| 27 | T | 102 | CDL | O1-C1-CB2-OB2 |
| 18 | A | 606 | PGV | O12-C04-C05-O05 |
| 22 | P | 310 | CHD | C21-C20-C22-C23 |
| 22 | C | 310 | CHD | C21-C20-C22-C23 |
| 18 | A | 606 | PGV | C19-C20-C21-C22 |
| 24 | C | 302 | DMU | C1-C6-O16-C18 |
| 24 | P | 302 | DMU | C1-C6-O16-C18 |
| 21 | O | 304 | PSC | O04-C19-O03-C01 |
| 24 | Z | 101 | DMU | O5-C4-C57-O61 |
| 21 | B | 303 | PSC | C2-C1-O01-C02 |
| 18 | N | 608 | PGV | C19-C20-C21-C22 |
| 26 | C | 305 | PEK | C1-C2-C3-C4 |
| 21 | O | 304 | PSC | C1-C2-C3-C4 |
| 21 | B | 303 | PSC | O04-C19-O03-C01 |
| 22 | W | 101 | CHD | C17-C20-C22-C23 |
| 22 | J | 101 | CHD | C17-C20-C22-C23 |
| 24 | P | 302 | DMU | C3-C4-C57-O61 |
| 20 | L | 101 | TGL | CC3-CC4-CC5-CC6 |
| 20 | N | 607 | TGL | CA2-CA1-OG1-CG1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | W | 101 | CHD | C21-C20-C22-C23 |
| 22 | J | 101 | CHD | C21-C20-C22-C23 |
| 21 | B | 303 | PSC | C1-C2-C3-C4 |
| 18 | P | 308 | PGV | O05-C05-C06-O06 |
| 26 | P | 305 | PEK | C1-C2-C3-C4 |
| 21 | B | 303 | PSC | C20-C21-C22-C23 |
| 20 | N | 606 | TGL | CC3-CC4-CC5-CC6 |
| 26 | G | 102 | PEK | C28-C29-C30-C31 |
| 21 | O | 304 | PSC | C20-C21-C22-C23 |
| 26 | T | 101 | PEK | C1-C2-C3-C4 |
| 26 | T | 101 | PEK | C28-C29-C30-C31 |
| 17 | N | 604 | HEA | C15-C16-C17-C18 |
| 20 | N | 606 | TGL | CC2-CC3-CC4-CC5 |
| 27 | C | 309 | CDL | O1-C1-CB2-OB2 |
| 18 | N | 608 | PGV | O12-C04-C05-O05 |
| 27 | P | 309 | CDL | O1-C1-CB2-OB2 |
| 18 | C | 308 | PGV | O12-C04-C05-O05 |
| 18 | P | 308 | PGV | O12-C04-C05-O05 |
| 22 | W | 101 | CHD | C13-C17-C20-C21 |
| 22 | J | 101 | CHD | C13-C17-C20-C21 |
| 20 | N | 607 | TGL | OA1-CA1-OG1-CG1 |
| 27 | C | 309 | CDL | CB7-C71-C72-C73 |
| 27 | P | 309 | CDL | CB7-C71-C72-C73 |
| 20 | L | 101 | TGL | CC2-CC3-CC4-CC5 |
| 20 | D | 201 | TGL | OA1-CA1-OG1-CG1 |
| 26 | P | 305 | PEK | O04-C21-O03-C01 |
| 21 | O | 304 | PSC | C2-C1-O01-C02 |
| 21 | B | 303 | PSC | C22-C23-C24-C25 |
| 27 | G | 101 | CDL | C73-C74-C75-C76 |
| 27 | T | 102 | CDL | C73-C74-C75-C76 |
| 27 | G | 101 | CDL | CB3-OB5-PB2-OB2 |
| 26 | G | 102 | PEK | C03-O11-P-O12 |
| 27 | T | 102 | CDL | CB3-OB5-PB2-OB2 |
| 27 | C | 309 | CDL | CA2-OA2-PA1-OA5 |
| 27 | C | 309 | CDL | CB2-OB2-PB2-OB5 |
| 26 | T | 101 | PEK | C03-O11-P-O12 |
| 26 | C | 306 | PEK | C04-O12-P-O11 |
| 26 | P | 306 | PEK | C04-O12-P-O11 |
| 27 | P | 309 | CDL | CA2-OA2-PA1-OA5 |
| 27 | P | 309 | CDL | CB2-OB2-PB2-OB5 |
| 26 | G | 102 | PEK | C1-C2-C3-C4 |
| 26 | C | 305 | PEK | C22-C21-O03-C01 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | P | 305 | PEK | C22-C21-O03-C01 |
| 27 | T | 102 | CDL | CA5-C11-C12-C13 |
| 27 | G | 101 | CDL | CA2-C1-CB2-OB2 |
| 27 | T | 102 | CDL | CA2-C1-CB2-OB2 |
| 18 | P | 308 | PGV | O12-C04-C05-C06 |
| 27 | G | 101 | CDL | OA7-CA5-OA6-CA4 |
| 27 | T | 102 | CDL | OA7-CA5-OA6-CA4 |
| 27 | G | 101 | CDL | CA5-C11-C12-C13 |
| 27 | G | 101 | CDL | C58-C59-C60-C61 |
| 18 | C | 308 | PGV | C22-C23-C24-C25 |
| 27 | G | 101 | CDL | C11-CA5-OA6-CA4 |
| 27 | T | 102 | CDL | C11-CA5-OA6-CA4 |
| 18 | C | 308 | PGV | C2-C1-O01-C02 |
| 18 | P | 308 | PGV | C2-C1-O01-C02 |
| 27 | T | 102 | CDL | C58-C59-C60-C61 |
| 27 | C | 309 | CDL | C16-C17-C18-C19 |
| 18 | C | 308 | PGV | C13-C14-C15-C16 |
| 21 | B | 303 | PSC | C29-C30-C31-C32 |
| 18 | N | 609 | PGV | C5-C6-C7-C8 |
| 26 | C | 306 | PEK | C25-C26-C27-C28 |
| 18 | A | 607 | PGV | C5-C6-C7-C8 |
| 27 | P | 309 | CDL | C59-C60-C61-C62 |
| 18 | P | 308 | PGV | C22-C23-C24-C25 |
| 18 | C | 308 | PGV | O02-C1-O01-C02 |
| 18 | P | 308 | PGV | O02-C1-O01-C02 |
| 27 | G | 101 | CDL | C13-C14-C15-C16 |
| 27 | C | 309 | CDL | C59-C60-C61-C62 |
| 18 | N | 608 | PGV | C4-C5-C6-C7 |
| 26 | P | 306 | PEK | C25-C26-C27-C28 |
| 27 | P | 309 | CDL | C16-C17-C18-C19 |
| 18 | P | 308 | PGV | C13-C14-C15-C16 |
| 21 | B | 303 | PSC | C11-C12-C13-C14 |
| 21 | O | 304 | PSC | C11-C12-C13-C14 |
| 27 | T | 102 | CDL | C13-C14-C15-C16 |
| 21 | O | 304 | PSC | C22-C23-C24-C25 |
| 21 | O | 304 | PSC | C29-C30-C31-C32 |
| 24 | M | 101 | DMU | C25-C28-C31-C34 |
| 27 | G | 101 | CDL | C72-C73-C74-C75 |
| 27 | T | 102 | CDL | C56-C57-C58-C59 |
| 24 | Z | 101 | DMU | C25-C28-C31-C34 |
| 18 | A | 606 | PGV | C4-C5-C6-C7 |
| 26 | C | 305 | PEK | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | P | 305 | PEK | C31-C32-C33-C34 |
| 26 | G | 102 | PEK | O03-C01-C02-O01 |
| 27 | T | 102 | CDL | OB6-CB4-CB6-OB8 |
| 21 | B | 303 | PSC | C2-C3-C4-C5 |
| 27 | C | 309 | CDL | C55-C56-C57-C58 |
| 27 | C | 309 | CDL | C74-C75-C76-C77 |
| 18 | A | 607 | PGV | C27-C28-C29-C30 |
| 20 | B | 302 | TGL | OC1-CC1-OG3-CG3 |
| 27 | G | 101 | CDL | C56-C57-C58-C59 |
| 26 | G | 102 | PEK | C27-C28-C29-C30 |
| 27 | T | 102 | CDL | C72-C73-C74-C75 |
| 20 | L | 101 | TGL | CB4-CB5-CB6-CB7 |
| 27 | C | 309 | CDL | C51-C52-C53-C54 |
| 26 | T | 101 | PEK | C27-C28-C29-C30 |
| 21 | O | 304 | PSC | C2-C3-C4-C5 |
| 27 | P | 309 | CDL | C51-C52-C53-C54 |
| 27 | P | 309 | CDL | C55-C56-C57-C58 |
| 27 | P | 309 | CDL | C74-C75-C76-C77 |
| 18 | P | 307 | PGV | C7-C8-C9-C10 |
| 18 | P | 307 | PGV | C24-C25-C26-C27 |
| 26 | G | 102 | PEK | C29-C30-C31-C32 |
| 18 | C | 307 | PGV | C7-C8-C9-C10 |
| 26 | T | 101 | PEK | C29-C30-C31-C32 |
| 18 | N | 608 | PGV | C22-C23-C24-C25 |
| 18 | N | 609 | PGV | C27-C28-C29-C30 |
| 24 | P | 302 | DMU | C25-C28-C31-C34 |
| 26 | C | 305 | PEK | O04-C21-O03-C01 |
| 24 | C | 302 | DMU | C25-C28-C31-C34 |
| 18 | C | 307 | PGV | C24-C25-C26-C27 |
| 20 | O | 303 | TGL | CB6-CB7-CB8-CB9 |
| 18 | C | 308 | PGV | C04-C05-C06-O06 |
| 18 | P | 308 | PGV | C04-C05-C06-O06 |
| 18 | P | 307 | PGV | C23-C24-C25-C26 |
| 20 | N | 606 | TGL | CB4-CB5-CB6-CB7 |
| 27 | P | 309 | CDL | C72-C73-C74-C75 |
| 18 | C | 308 | PGV | C24-C25-C26-C27 |
| 27 | P | 309 | CDL | CA5-C11-C12-C13 |
| 27 | C | 309 | CDL | C13-C14-C15-C16 |
| 27 | C | 309 | CDL | C71-C72-C73-C74 |
| 18 | C | 307 | PGV | C23-C24-C25-C26 |
| 18 | N | 608 | PGV | C28-C29-C30-C31 |
| 18 | A | 606 | PGV | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | A | 606 | PGV | C28-C29-C30-C31 |
| 27 | P | 309 | CDL | C13-C14-C15-C16 |
| 18 | C | 308 | PGV | C3-C4-C5-C6 |
| 18 | P | 308 | PGV | C3-C4-C5-C6 |
| 18 | P | 308 | PGV | C24-C25-C26-C27 |
| 27 | C | 309 | CDL | C72-C73-C74-C75 |
| 26 | C | 305 | PEK | C23-C24-C25-C26 |
| 27 | P | 309 | CDL | C71-C72-C73-C74 |
| 18 | P | 307 | PGV | C22-C23-C24-C25 |
| 27 | C | 309 | CDL | C73-C74-C75-C76 |
| 27 | P | 309 | CDL | C73-C74-C75-C76 |
| 27 | C | 309 | CDL | CA5-C11-C12-C13 |
| 18 | C | 307 | PGV | C22-C23-C24-C25 |
| 26 | C | 306 | PEK | C16-C17-C18-C19 |
| 26 | P | 305 | PEK | C23-C24-C25-C26 |
| 26 | T | 101 | PEK | C25-C26-C27-C28 |
| 18 | N | 609 | PGV | C6-C7-C8-C9 |
| 18 | P | 308 | PGV | C27-C28-C29-C30 |
| 26 | G | 102 | PEK | C16-C17-C18-C19 |
| 26 | G | 102 | PEK | C25-C26-C27-C28 |
| 27 | C | 309 | CDL | C36-C37-C38-C39 |
| 20 | B | 302 | TGL | CB6-CB7-CB8-CB9 |
| 27 | P | 309 | CDL | C36-C37-C38-C39 |
| 18 | C | 308 | PGV | C27-C28-C29-C30 |
| 26 | P | 306 | PEK | C31-C32-C33-C34 |
| 20 | O | 303 | TGL | OC1-CC1-OG3-CG3 |
| 27 | T | 102 | CDL | C79-C80-C81-C82 |
| 26 | C | 306 | PEK | C31-C32-C33-C34 |
| 26 | P | 306 | PEK | C16-C17-C18-C19 |
| 18 | N | 608 | PGV | O05-C05-C06-O06 |
| 18 | A | 606 | PGV | O05-C05-C06-O06 |
| 18 | C | 308 | PGV | O05-C05-C06-O06 |
| 26 | P | 305 | PEK | C27-C28-C29-C30 |
| 18 | P | 307 | PGV | C11-C10-C9-C8 |
| 18 | P | 308 | PGV | C1-C2-C3-C4 |
| 18 | A | 607 | PGV | C7-C8-C9-C10 |
| 18 | N | 609 | PGV | C7-C8-C9-C10 |
| 18 | C | 308 | PGV | C28-C29-C30-C31 |
| 18 | C | 308 | PGV | C1-C2-C3-C4 |
| 18 | C | 308 | PGV | O12-C04-C05-C06 |
| 27 | G | 101 | CDL | C82-C83-C84-C85 |
| 26 | C | 305 | PEK | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | T | 102 | CDL | C43-C44-C45-C46 |
| 27 | T | 102 | CDL | C82-C83-C84-C85 |
| 18 | A | 607 | PGV | C6-C7-C8-C9 |
| 26 | T | 101 | PEK | C16-C17-C18-C19 |
| 27 | G | 101 | CDL | C43-C44-C45-C46 |
| 27 | G | 101 | CDL | C79-C80-C81-C82 |
| 24 | Z | 101 | DMU | C22-C25-C28-C31 |
| 26 | P | 305 | PEK | C22-C23-C24-C25 |
| 27 | P | 309 | CDL | C51-CB5-OB6-CB4 |
| 27 | P | 309 | CDL | C18-C19-C20-C21 |
| 18 | P | 308 | PGV | C28-C29-C30-C31 |
| 17 | A | 604 | HEA | C21-C22-C23-C25 |
| 27 | G | 101 | CDL | C21-C22-C23-C24 |
| 26 | P | 306 | PEK | C29-C30-C31-C32 |
| 26 | C | 305 | PEK | C25-C26-C27-C28 |
| 27 | C | 309 | CDL | C18-C19-C20-C21 |
| 18 | N | 608 | PGV | C24-C25-C26-C27 |
| 18 | A | 606 | PGV | C24-C25-C26-C27 |
| 27 | P | 309 | CDL | C75-C76-C77-C78 |
| 27 | P | 309 | CDL | OB7-CB5-OB6-CB4 |
| 26 | C | 306 | PEK | C29-C30-C31-C32 |
| 26 | P | 305 | PEK | C25-C26-C27-C28 |
| 26 | P | 305 | PEK | C32-C33-C34-C35 |
| 24 | M | 101 | DMU | C22-C25-C28-C31 |
| 17 | N | 604 | HEA | C21-C22-C23-C25 |
| 27 | T | 102 | CDL | C21-C22-C23-C24 |
| 26 | C | 305 | PEK | C22-C23-C24-C25 |
| 27 | G | 101 | CDL | C33-C34-C35-C36 |
| 27 | T | 102 | CDL | C33-C34-C35-C36 |
| 27 | C | 309 | CDL | C75-C76-C77-C78 |
| 26 | C | 305 | PEK | C32-C33-C34-C35 |
| 17 | A | 604 | HEA | C15-C16-C17-C18 |
| 27 | C | 309 | CDL | C32-C33-C34-C35 |
| 27 | P | 309 | CDL | C32-C33-C34-C35 |
| 18 | C | 308 | PGV | C25-C26-C27-C28 |
| 27 | C | 309 | CDL | C51-CB5-OB6-CB4 |
| 18 | P | 308 | PGV | C25-C26-C27-C28 |
| 24 | P | 302 | DMU | O6-C11-C9-C8 |
| 26 | P | 305 | PEK | C24-C25-C26-C27 |
| 27 | G | 101 | CDL | OB6-CB4-CB6-OB8 |
| 26 | T | 101 | PEK | O03-C01-C02-O01 |
| 26 | C | 305 | PEK | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | B | 303 | PSC | C04-C05-N-C08 |
| 21 | O | 304 | PSC | C04-C05-N-C08 |
| 26 | T | 101 | PEK | C34-C35-C36-C37 |
| 26 | C | 305 | PEK | C24-C25-C26-C27 |
| 18 | C | 308 | PGV | C30-C31-C32-C33 |
| 18 | P | 308 | PGV | C30-C31-C32-C33 |
| 18 | C | 307 | PGV | C11-C10-C9-C8 |
| 18 | C | 308 | PGV | C11-C10-C9-C8 |
| 18 | P | 308 | PGV | C11-C10-C9-C8 |
| 27 | C | 309 | CDL | C42-C43-C44-C45 |
| 26 | P | 305 | PEK | C16-C17-C18-C19 |
| 26 | G | 102 | PEK | C26-C27-C28-C29 |
| 26 | G | 102 | PEK | C34-C35-C36-C37 |
| 27 | P | 309 | CDL | C61-C62-C63-C64 |
| 26 | C | 305 | PEK | C16-C17-C18-C19 |
| 20 | L | 101 | TGL | OB1-CB1-OG2-CG2 |
| 27 | C | 309 | CDL | OB7-CB5-OB6-CB4 |
| 20 | N | 606 | TGL | OB1-CB1-OG2-CG2 |
| 26 | T | 101 | PEK | C26-C27-C28-C29 |
| 20 | O | 303 | TGL | CG2-CG3-OG3-CC1 |
| 21 | B | 303 | PSC | C03-O11-P-O12 |
| 21 | B | 303 | PSC | C04-O12-P-O11 |
| 27 | G | 101 | CDL | CB2-OB2-PB2-OB5 |
| 27 | T | 102 | CDL | CB2-OB2-PB2-OB5 |
| 21 | O | 304 | PSC | C03-O11-P-O12 |
| 21 | O | 304 | PSC | C04-O12-P-O11 |
| 27 | C | 309 | CDL | C78-C79-C80-C81 |
| 27 | P | 309 | CDL | C78-C79-C80-C81 |
| 27 | T | 102 | CDL | CB7-C71-C72-C73 |
| 20 | N | 606 | TGL | CC2-CC1-OG3-CG3 |
| 20 | B | 302 | TGL | CC2-CC1-OG3-CG3 |
| 27 | C | 309 | CDL | OB5-CB3-CB4-CB6 |
| 27 | P | 309 | CDL | OB5-CB3-CB4-CB6 |
| 27 | C | 309 | CDL | C61-C62-C63-C64 |
| 26 | P | 305 | PEK | C35-C36-C37-C38 |
| 18 | P | 308 | PGV | C14-C15-C16-C17 |
| 27 | T | 102 | CDL | C53-C54-C55-C56 |
| 27 | C | 309 | CDL | C34-C35-C36-C37 |
| 20 | B | 302 | TGL | CG2-CG3-OG3-CC1 |
| 27 | T | 102 | CDL | C71-C72-C73-C74 |
| 18 | N | 609 | PGV | C23-C24-C25-C26 |
| 27 | P | 309 | CDL | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | N | 608 | PGV | C12-C13-C14-C15 |
| 18 | C | 308 | PGV | C12-C13-C14-C15 |
| 18 | P | 308 | PGV | C12-C13-C14-C15 |
| 27 | G | 101 | CDL | CB5-C51-C52-C53 |
| 27 | T | 102 | CDL | C41-C42-C43-C44 |
| 27 | P | 309 | CDL | C34-C35-C36-C37 |
| 21 | B | 303 | PSC | C24-C25-C26-C27 |
| 27 | G | 101 | CDL | C41-C42-C43-C44 |
| 21 | O | 304 | PSC | C27-C28-C29-C30 |
| 27 | G | 101 | CDL | C15-C16-C17-C18 |
| 27 | G | 101 | CDL | C53-C54-C55-C56 |
| 27 | T | 102 | CDL | C15-C16-C17-C18 |
| 26 | P | 305 | PEK | C26-C27-C28-C29 |
| 18 | C | 308 | PGV | C14-C15-C16-C17 |
| 27 | G | 101 | CDL | C31-C32-C33-C34 |
| 27 | T | 102 | CDL | C31-C32-C33-C34 |
| 26 | G | 102 | PEK | O03-C01-C02-C03 |
| 27 | T | 102 | CDL | CB3-CB4-CB6-OB8 |
| 27 | C | 309 | CDL | CB3-CB4-CB6-OB8 |
| 27 | C | 309 | CDL | C64-C65-C66-C67 |
| 26 | T | 101 | PEK | O03-C01-C02-C03 |
| 21 | O | 304 | PSC | C23-C24-C25-C26 |
| 27 | P | 309 | CDL | C38-C39-C40-C41 |
| 27 | P | 309 | CDL | CB3-CB4-CB6-OB8 |
| 27 | P | 309 | CDL | C64-C65-C66-C67 |
| 27 | C | 309 | CDL | C44-C45-C46-C47 |
| 24 | Z | 101 | DMU | C3-C4-C57-O61 |
| 27 | C | 309 | CDL | C11-C12-C13-C14 |
| 18 | N | 609 | PGV | C30-C31-C32-C33 |
| 18 | A | 607 | PGV | C30-C31-C32-C33 |
| 18 | C | 308 | PGV | C31-C32-C33-C34 |
| 27 | T | 102 | CDL | CB5-C51-C52-C53 |
| 27 | P | 309 | CDL | C44-C45-C46-C47 |
| 21 | B | 303 | PSC | C23-C24-C25-C26 |
| 27 | G | 101 | CDL | C35-C36-C37-C38 |
| 27 | G | 101 | CDL | C71-C72-C73-C74 |
| 21 | B | 303 | PSC | C13-C14-C15-C16 |
| 18 | A | 606 | PGV | C12-C13-C14-C15 |
| 21 | O | 304 | PSC | C13-C14-C15-C16 |
| 17 | A | 604 | HEA | C17-C18-C19-C27 |
| 27 | T | 102 | CDL | C35-C36-C37-C38 |
| 18 | N | 608 | PGV | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | P | 309 | CDL | C11-C12-C13-C14 |
| 27 | G | 101 | CDL | CB7-C71-C72-C73 |
| 20 | O | 303 | TGL | CC2-CC1-OG3-CG3 |
| 18 | A | 607 | PGV | C23-C24-C25-C26 |
| 18 | N | 608 | PGV | C03-C02-O01-C1 |
| 18 | A | 606 | PGV | C03-C02-O01-C1 |
| 18 | P | 307 | PGV | C15-C16-C17-C18 |
| 27 | C | 309 | CDL | C38-C39-C40-C41 |
| 27 | C | 309 | CDL | C63-C64-C65-C66 |
| 18 | C | 308 | PGV | C5-C6-C7-C8 |
| 21 | B | 303 | PSC | C27-C28-C29-C30 |
| 18 | C | 307 | PGV | C15-C16-C17-C18 |
| 27 | P | 309 | CDL | C63-C64-C65-C66 |
| 21 | O | 304 | PSC | C24-C25-C26-C27 |
| 18 | P | 308 | PGV | C31-C32-C33-C34 |
| 20 | L | 101 | TGL | CC2-CC1-OG3-CG3 |
| 18 | C | 308 | PGV | C20-C19-O03-C01 |
| 18 | P | 308 | PGV | C20-C19-O03-C01 |
| 27 | C | 309 | CDL | OA5-CA3-CA4-OA6 |
| 27 | P | 309 | CDL | OA5-CA3-CA4-OA6 |
| 26 | P | 306 | PEK | C21-C22-C23-C24 |
| 27 | G | 101 | CDL | C14-C15-C16-C17 |
| 26 | G | 102 | PEK | C30-C31-C32-C33 |
| 26 | C | 305 | PEK | C26-C27-C28-C29 |
| 18 | C | 308 | PGV | O04-C19-O03-C01 |
| 26 | T | 101 | PEK | C30-C31-C32-C33 |
| 18 | P | 308 | PGV | C5-C6-C7-C8 |
| 21 | O | 304 | PSC | O03-C01-C02-O01 |
| 18 | C | 307 | PGV | C13-C14-C15-C16 |
| 18 | P | 307 | PGV | C13-C14-C15-C16 |
| 27 | T | 102 | CDL | C14-C15-C16-C17 |
| 27 | C | 309 | CDL | C84-C85-C86-C87 |
| 18 | P | 308 | PGV | C4-C5-C6-C7 |
| 26 | C | 306 | PEK | C17-C18-C19-C20 |
| 18 | P | 308 | PGV | O04-C19-O03-C01 |
| 21 | B | 303 | PSC | C3-C4-C5-C6 |
| 27 | P | 309 | CDL | C84-C85-C86-C87 |
| 27 | T | 102 | CDL | C44-C45-C46-C47 |
| 18 | C | 308 | PGV | C4-C5-C6-C7 |
| 27 | G | 101 | CDL | C44-C45-C46-C47 |
| 26 | C | 306 | PEK | C21-C22-C23-C24 |
| 26 | P | 306 | PEK | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | O | 304 | PSC | C3-C4-C5-C6 |
| 26 | C | 305 | PEK | O12-C04-C05-N |
| 26 | P | 305 | PEK | O12-C04-C05-N |
| 20 | B | 302 | TGL | C12-C13-C14-C29 |
| 18 | C | 308 | PGV | C23-C24-C25-C26 |
| 27 | T | 102 | CDL | C19-C20-C21-C22 |
| 26 | P | 306 | PEK | C17-C18-C19-C20 |
| 26 | T | 101 | PEK | C22-C21-O03-C01 |
| 27 | G | 101 | CDL | C19-C20-C21-C22 |
| 21 | O | 304 | PSC | C14-C15-C16-C17 |
| 21 | B | 303 | PSC | O03-C01-C02-C03 |
| 27 | G | 101 | CDL | CA3-CA4-CA6-OA8 |
| 27 | T | 102 | CDL | CA3-CA4-CA6-OA8 |
| 26 | C | 305 | PEK | O03-C01-C02-C03 |
| 21 | O | 304 | PSC | O03-C01-C02-C03 |
| 26 | P | 305 | PEK | O03-C01-C02-C03 |
| 26 | C | 306 | PEK | C32-C33-C34-C35 |
| 27 | C | 309 | CDL | C52-C53-C54-C55 |
| 20 | N | 607 | TGL | CA9-C20-C21-C22 |
| 18 | C | 308 | PGV | C15-C16-C17-C18 |
| 21 | B | 303 | PSC | C14-C15-C16-C17 |
| 18 | P | 308 | PGV | C23-C24-C25-C26 |
| 26 | G | 102 | PEK | C6-C7-C8-C9 |
| 26 | T | 101 | PEK | C6-C7-C8-C9 |
| 26 | C | 306 | PEK | C11-C12-C13-C14 |
| 26 | P | 306 | PEK | C11-C12-C13-C14 |
| 26 | C | 305 | PEK | C5-C6-C7-C8 |
| 26 | C | 305 | PEK | C9-C10-C11-C12 |
| 26 | P | 305 | PEK | C5-C6-C7-C8 |
| 26 | P | 305 | PEK | C9-C10-C11-C12 |
| 18 | N | 608 | PGV | C26-C27-C28-C29 |
| 18 | N | 609 | PGV | C25-C26-C27-C28 |
| 20 | D | 201 | TGL | CA9-C20-C21-C22 |
| 18 | A | 606 | PGV | C26-C27-C28-C29 |
| 27 | P | 309 | CDL | C43-C44-C45-C46 |
| 26 | G | 102 | PEK | C22-C21-O03-C01 |
| 27 | C | 309 | CDL | C43-C44-C45-C46 |
| 24 | Z | 101 | DMU | O16-C18-C19-C22 |
| 26 | P | 305 | PEK | C17-C18-C19-C20 |
| 26 | G | 102 | PEK | C15-C16-C17-C18 |
| 17 | N | 604 | HEA | C17-C18-C19-C27 |
| 18 | A | 606 | PGV | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 20 | N | 606 | TGL | CC7-CC8-CC9-C15 |
| 21 | B | 303 | PSC | O03-C01-C02-O01 |
| 27 | P | 309 | CDL | OB6-CB4-CB6-OB8 |
| 26 | P | 305 | PEK | O03-C01-C02-O01 |
| 18 | P | 308 | PGV | C15-C16-C17-C18 |
| 27 | P | 309 | CDL | C39-C40-C41-C42 |
| 20 | D | 201 | TGL | OB1-CB1-OG2-CG2 |
| 18 | N | 609 | PGV | C26-C27-C28-C29 |
| 27 | P | 309 | CDL | C52-C53-C54-C55 |
| 26 | T | 101 | PEK | C02-C03-O11-P |
| 26 | G | 102 | PEK | O04-C21-O03-C01 |
| 26 | T | 101 | PEK | O04-C21-O03-C01 |
| 20 | L | 101 | TGL | CC7-CC8-CC9-C15 |
| 26 | C | 305 | PEK | C17-C18-C19-C20 |
| 26 | P | 305 | PEK | C29-C30-C31-C32 |
| 24 | C | 302 | DMU | C28-C31-C34-C37 |
| 27 | C | 309 | CDL | C39-C40-C41-C42 |
| 18 | A | 607 | PGV | C25-C26-C27-C28 |
| 27 | G | 101 | CDL | OA5-CA3-CA4-CA6 |
| 26 | G | 102 | PEK | C01-C02-C03-O11 |
| 27 | T | 102 | CDL | OA5-CA3-CA4-CA6 |
| 26 | T | 101 | PEK | C01-C02-C03-O11 |
| 18 | A | 606 | PGV | C01-C02-C03-O11 |
| 24 | M | 101 | DMU | C3-C4-C57-O61 |
| 24 | M | 101 | DMU | O16-C18-C19-C22 |
| 22 | P | 310 | CHD | C16-C17-C20-C22 |
| 18 | A | 606 | PGV | C5-C6-C7-C8 |
| 21 | O | 304 | PSC | C03-C02-O01-C1 |
| 26 | P | 306 | PEK | C30-C31-C32-C33 |
| 26 | G | 102 | PEK | C21-C22-C23-C24 |
| 18 | A | 607 | PGV | C26-C27-C28-C29 |
| 24 | P | 302 | DMU | O5-C6-O16-C18 |
| 18 | P | 307 | PGV | C02-C03-O11-P |
| 27 | G | 101 | CDL | CB3-CB4-CB6-OB8 |
| 26 | G | 102 | PEK | C02-C03-O11-P |
| 18 | N | 608 | PGV | O03-C01-C02-C03 |
| 18 | A | 606 | PGV | O03-C01-C02-C03 |
| 27 | C | 309 | CDL | OB5-CB3-CB4-OB6 |
| 27 | P | 309 | CDL | OB5-CB3-CB4-OB6 |
| 18 | C | 308 | PGV | O01-C02-C03-O11 |
| 18 | P | 308 | PGV | O01-C02-C03-O11 |
| 18 | P | 308 | PGV | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | P | 310 | CHD | C13-C17-C20-C21 |
| 22 | C | 310 | CHD | C13-C17-C20-C21 |
| 27 | C | 309 | CDL | C24-C25-C26-C27 |
| 26 | C | 306 | PEK | C30-C31-C32-C33 |
| 22 | P | 310 | CHD | C13-C17-C20-C22 |
| 27 | C | 309 | CDL | OB6-CB4-CB6-OB8 |
| 26 | C | 305 | PEK | O03-C01-C02-O01 |
| 22 | C | 310 | CHD | C16-C17-C20-C21 |
| 26 | C | 305 | PEK | C29-C30-C31-C32 |
| 27 | P | 309 | CDL | C24-C25-C26-C27 |
| 26 | T | 101 | PEK | C15-C16-C17-C18 |
| 22 | C | 310 | CHD | C13-C17-C20-C22 |
| 24 | C | 302 | DMU | C22-C25-C28-C31 |
| 24 | P | 302 | DMU | C28-C31-C34-C37 |
| 17 | N | 605 | HEA | O11-C11-C12-C13 |
| 26 | T | 101 | PEK | C21-C22-C23-C24 |
| 27 | G | 101 | CDL | C24-C25-C26-C27 |
| 24 | P | 302 | DMU | C22-C25-C28-C31 |
| 22 | C | 310 | CHD | C16-C17-C20-C22 |
| 27 | G | 101 | CDL | CB4-CB3-OB5-PB2 |
| 27 | T | 102 | CDL | CB4-CB3-OB5-PB2 |
| 18 | C | 307 | PGV | C02-C03-O11-P |
| 22 | P | 310 | CHD | C16-C17-C20-C21 |
| 27 | T | 102 | CDL | C54-C55-C56-C57 |
| 21 | B | 303 | PSC | C03-O11-P-O13 |
| 21 | B | 303 | PSC | C04-O12-P-O13 |
| 21 | B | 303 | PSC | C04-C05-N-C07 |
| 26 | G | 102 | PEK | C03-O11-P-O13 |
| 26 | T | 101 | PEK | C03-O11-P-O13 |
| 26 | C | 306 | PEK | C03-O11-P-O13 |
| 17 | N | 605 | HEA | C3B-C11-C12-C13 |
| 26 | P | 306 | PEK | C03-O11-P-O14 |
| 21 | O | 304 | PSC | C03-O11-P-O13 |
| 21 | O | 304 | PSC | C04-O12-P-O13 |
| 21 | O | 304 | PSC | C04-C05-N-C07 |
| 17 | A | 605 | HEA | C3B-C11-C12-C13 |
| 27 | G | 101 | CDL | CA7-C31-C32-C33 |
| 24 | C | 302 | DMU | O5-C6-O16-C18 |
| 18 | N | 608 | PGV | C01-C02-C03-O11 |
| 18 | C | 308 | PGV | C01-C02-C03-O11 |
| 18 | P | 307 | PGV | C1-C2-C3-C4 |
| 27 | T | 102 | CDL | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | G | 101 | CDL | C22-C23-C24-C25 |
| 18 | N | 608 | PGV | C5-C6-C7-C8 |
| 26 | P | 306 | PEK | C35-C36-C37-C38 |
| 27 | T | 102 | CDL | CA7-C31-C32-C33 |
| 18 | C | 307 | PGV | C1-C2-C3-C4 |
| 26 | G | 102 | PEK | C32-C33-C34-C35 |
| 27 | T | 102 | CDL | C12-C13-C14-C15 |
| 21 | O | 304 | PSC | C04-C05-N-C06 |
| 17 | N | 605 | HEA | C2D-C3D-CAD-CBD |
| 27 | G | 101 | CDL | OA6-CA4-CA6-OA8 |
| 27 | T | 102 | CDL | OA6-CA4-CA6-OA8 |
| 18 | N | 608 | PGV | O03-C01-C02-O01 |
| 20 | D | 201 | TGL | OG2-CG2-CG3-OG3 |
| 18 | A | 606 | PGV | O03-C01-C02-O01 |
| 20 | O | 303 | TGL | C12-C13-C14-C29 |
| 26 | C | 306 | PEK | C35-C36-C37-C38 |
| 18 | A | 606 | PGV | C21-C22-C23-C24 |
| 27 | G | 101 | CDL | C54-C55-C56-C57 |
| 26 | G | 102 | PEK | C31-C32-C33-C34 |
| 18 | N | 608 | PGV | C21-C22-C23-C24 |
| 27 | P | 309 | CDL | C23-C24-C25-C26 |
| 27 | C | 309 | CDL | C23-C24-C25-C26 |
| 21 | O | 304 | PSC | C31-C32-C33-C34 |
| 26 | T | 101 | PEK | C31-C32-C33-C34 |
| 26 | G | 102 | PEK | C2-C3-C4-C5 |
| 21 | B | 303 | PSC | C04-C05-N-C06 |
| 27 | T | 102 | CDL | C22-C23-C24-C25 |
| 18 | C | 307 | PGV | O04-C19-O03-C01 |
| 26 | T | 101 | PEK | C32-C33-C34-C35 |
| 21 | B | 303 | PSC | C03-C02-O01-C1 |
| 18 | P | 308 | PGV | C01-C02-C03-O11 |
| 18 | C | 308 | PGV | C26-C27-C28-C29 |
| 27 | G | 101 | CDL | C12-C13-C14-C15 |
| 20 | L | 101 | TGL | CB5-CB6-CB7-CB8 |
| 18 | A | 606 | PGV | C25-C26-C27-C28 |
| 18 | C | 307 | PGV | C05-C04-O12-P |
| 26 | G | 102 | PEK | O01-C02-C03-O11 |
| 26 | T | 101 | PEK | O01-C02-C03-O11 |
| 20 | N | 607 | TGL | OB1-CB1-OG2-CG2 |
| 27 | G | 101 | CDL | C64-C65-C66-C67 |
| 27 | T | 102 | CDL | C64-C65-C66-C67 |
| 27 | G | 101 | CDL | CA2-OA2-PA1-OA5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | C | 309 | CDL | CA3-OA5-PA1-OA2 |
| 18 | N | 608 | PGV | C03-O11-P-O12 |
| 18 | A | 606 | PGV | C03-O11-P-O12 |
| 27 | P | 309 | CDL | CA3-OA5-PA1-OA2 |
| 17 | A | 604 | HEA | C21-C22-C23-C24 |
| 18 | N | 609 | PGV | C9-C10-C11-C12 |
| 17 | A | 604 | HEA | C12-C13-C14-C15 |
| 26 | P | 306 | PEK | C34-C35-C36-C37 |
| 26 | P | 305 | PEK | C30-C31-C32-C33 |
| 27 | C | 309 | CDL | C1-CA2-OA2-PA1 |
| 27 | P | 309 | CDL | C1-CA2-OA2-PA1 |
| 18 | P | 308 | PGV | C02-C03-O11-P |
| 27 | G | 101 | CDL | C36-C37-C38-C39 |
| 18 | A | 607 | PGV | C9-C10-C11-C12 |
| 26 | C | 305 | PEK | C3-C4-C5-C6 |
| 27 | T | 102 | CDL | C36-C37-C38-C39 |
| 26 | P | 305 | PEK | C3-C4-C5-C6 |
| 20 | N | 606 | TGL | CC5-CC6-CC7-CC8 |
| 21 | B | 303 | PSC | C31-C32-C33-C34 |
| 18 | C | 308 | PGV | C02-C03-O11-P |
| 27 | T | 102 | CDL | C11-C12-C13-C14 |
| 26 | T | 101 | PEK | C2-C3-C4-C5 |
| 20 | D | 201 | TGL | C21-C22-C23-C24 |
| 20 | O | 303 | TGL | C13-C14-C29-C30 |
| 27 | P | 309 | CDL | C15-C16-C17-C18 |
| 27 | P | 309 | CDL | CA3-CA4-CA6-OA8 |
| 26 | C | 306 | PEK | C34-C35-C36-C37 |
| 27 | G | 101 | CDL | C11-C12-C13-C14 |
| 27 | C | 309 | CDL | C76-C77-C78-C79 |
| 26 | C | 305 | PEK | C30-C31-C32-C33 |
| 20 | N | 607 | TGL | CG1-CG2-OG2-CB1 |
| 26 | P | 306 | PEK | C3-C4-C5-C6 |
| 21 | B | 303 | PSC | C4-C5-C6-C7 |
| 21 | B | 303 | PSC | C9-C10-C11-C12 |
| 21 | O | 304 | PSC | C9-C10-C11-C12 |
| 21 | O | 304 | PSC | C4-C5-C6-C7 |
| 17 | N | 604 | HEA | C21-C22-C23-C24 |
| 27 | G | 101 | CDL | C38-C39-C40-C41 |
| 27 | P | 309 | CDL | C76-C77-C78-C79 |
| 18 | P | 307 | PGV | C05-C04-O12-P |
| 23 | C | 301 | DCW | C3-C2-N1-C1 |
| 22 | O | 302 | CHD | C17-C20-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | P | 307 | PGV | C21-C22-C23-C24 |
| 18 | P | 308 | PGV | C7-C8-C9-C10 |
| 27 | C | 309 | CDL | C15-C16-C17-C18 |
| 18 | P | 308 | PGV | O03-C01-C02-O01 |
| 26 | C | 306 | PEK | C3-C4-C5-C6 |
| 17 | N | 604 | HEA | C12-C13-C14-C15 |
| 27 | G | 101 | CDL | C78-C79-C80-C81 |
| 26 | C | 305 | PEK | C02-C03-O11-P |
| 27 | P | 309 | CDL | C22-C23-C24-C25 |
| 20 | N | 606 | TGL | CB5-CB6-CB7-CB8 |
| 20 | L | 101 | TGL | OG2-CB1-CB2-CB3 |
| 27 | C | 309 | CDL | CA3-CA4-CA6-OA8 |
| 20 | N | 606 | TGL | OG2-CB1-CB2-CB3 |
| 27 | T | 102 | CDL | C38-C39-C40-C41 |
| 20 | L | 101 | TGL | CC5-CC6-CC7-CC8 |
| 26 | T | 101 | PEK | C33-C34-C35-C36 |
| 18 | N | 608 | PGV | C25-C26-C27-C28 |
| 27 | G | 101 | CDL | C52-C53-C54-C55 |
| 27 | C | 309 | CDL | OA5-CA3-CA4-CA6 |
| 27 | P | 309 | CDL | OA5-CA3-CA4-CA6 |
| 24 | C | 302 | DMU | O6-C11-C9-C8 |
| 26 | T | 101 | PEK | C3-C4-C5-C6 |
| 20 | L | 101 | TGL | OG3-CC1-CC2-CC3 |
| 27 | C | 309 | CDL | CB2-C1-CA2-OA2 |
| 27 | C | 309 | CDL | C56-C57-C58-C59 |
| 20 | N | 607 | TGL | OG2-CG2-CG3-OG3 |
| 18 | C | 308 | PGV | O03-C01-C02-O01 |
| 18 | P | 307 | PGV | C14-C15-C16-C17 |
| 27 | C | 309 | CDL | C52-C51-CB5-OB6 |
| 21 | O | 304 | PSC | O03-C19-C20-C21 |
| 18 | C | 307 | PGV | C21-C22-C23-C24 |
| 18 | P | 307 | PGV | C9-C10-C11-C12 |
| 26 | G | 102 | PEK | C3-C4-C5-C6 |
| 21 | O | 304 | PSC | C7-C8-C9-C10 |
| 21 | B | 303 | PSC | O03-C19-C20-C21 |
| 27 | T | 102 | CDL | CA2-OA2-PA1-OA5 |
| 18 | N | 608 | PGV | O01-C1-C2-C3 |
| 18 | A | 606 | PGV | O01-C1-C2-C3 |
| 20 | N | 607 | TGL | C21-C22-C23-C24 |
| 20 | N | 606 | TGL | OG3-CC1-CC2-CC3 |
| 27 | P | 309 | CDL | C32-C31-CA7-OA8 |
| 26 | P | 305 | PEK | O01-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | B | 303 | PSC | C7-C8-C9-C10 |
| 18 | P | 307 | PGV | C11-C12-C13-C14 |
| 18 | C | 307 | PGV | C11-C12-C13-C14 |
| 27 | C | 309 | CDL | C22-C23-C24-C25 |
| 27 | C | 309 | CDL | C32-C31-CA7-OA8 |
| 27 | P | 309 | CDL | C52-C51-CB5-OB6 |
| 20 | N | 606 | TGL | OC1-CC1-OG3-CG3 |
| 24 | Z | 101 | DMU | O6-C11-C9-O1 |
| 18 | A | 607 | PGV | C11-C12-C13-C14 |
| 24 | P | 302 | DMU | C31-C34-C37-C40 |
| 26 | C | 305 | PEK | O01-C1-C2-C3 |
| 21 | O | 304 | PSC | O01-C1-C2-C3 |
| 24 | Z | 101 | DMU | C34-C37-C40-C43 |
| 20 | N | 607 | TGL | OG2-CB1-CB2-CB3 |
| 18 | N | 609 | PGV | C11-C12-C13-C14 |
| 18 | A | 606 | PGV | C11-C10-C9-C8 |
| 21 | B | 303 | PSC | C01-C02-C03-O11 |
| 21 | O | 304 | PSC | C01-C02-C03-O11 |
| 20 | D | 201 | TGL | OG2-CB1-CB2-CB3 |
| 27 | P | 309 | CDL | C56-C57-C58-C59 |
| 18 | C | 308 | PGV | C7-C8-C9-C10 |
| 21 | B | 303 | PSC | C12-C13-C14-C15 |
| 26 | G | 102 | PEK | C14-C15-C16-C17 |
| 18 | C | 307 | PGV | C9-C10-C11-C12 |
| 24 | M | 101 | DMU | C19-C22-C25-C28 |
| 18 | A | 606 | PGV | C9-C10-C11-C12 |
| 21 | O | 304 | PSC | C12-C13-C14-C15 |
| 21 | B | 303 | PSC | O01-C1-C2-C3 |
| 27 | T | 102 | CDL | C52-C53-C54-C55 |
| 21 | B | 303 | PSC | O04-C19-C20-C21 |
| 20 | N | 607 | TGL | OC1-CC1-CC2-CC3 |
| 27 | T | 102 | CDL | C78-C79-C80-C81 |
| 27 | C | 309 | CDL | C54-C55-C56-C57 |
| 27 | T | 102 | CDL | C39-C40-C41-C42 |
| 27 | P | 309 | CDL | C12-C11-CA5-OA6 |
| 26 | P | 305 | PEK | C28-C29-C30-C31 |
| 18 | A | 606 | PGV | O02-C1-C2-C3 |
| 21 | O | 304 | PSC | O04-C19-C20-C21 |
| 26 | P | 305 | PEK | O02-C1-C2-C3 |
| 21 | B | 303 | PSC | C15-C16-C17-C18 |
| 21 | B | 303 | PSC | O02-C1-C2-C3 |
| 20 | N | 606 | TGL | CB2-CB1-OG2-CG2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | C | 309 | CDL | C32-C31-CA7-OA9 |
| 20 | D | 201 | TGL | OC1-CC1-CC2-CC3 |
| 26 | C | 305 | PEK | O02-C1-C2-C3 |
| 27 | P | 309 | CDL | C32-C31-CA7-OA9 |
| 26 | P | 306 | PEK | C03-O11-P-O12 |
| 20 | N | 607 | TGL | CB2-CB3-CB4-CB5 |
| 26 | G | 102 | PEK | C33-C34-C35-C36 |
| 18 | C | 307 | PGV | C14-C15-C16-C17 |
| 21 | O | 304 | PSC | O02-C1-C2-C3 |
| 20 | D | 201 | TGL | CB2-CB3-CB4-CB5 |
| 18 | N | 608 | PGV | C03-O11-P-O13 |
| 18 | N | 609 | PGV | C04-O12-P-O13 |
| 26 | C | 306 | PEK | C03-O11-P-O14 |
| 18 | A | 607 | PGV | C04-O12-P-O13 |
| 18 | A | 606 | PGV | C03-O11-P-O13 |
| 24 | M | 101 | DMU | O6-C11-C9-O1 |
| 27 | C | 309 | CDL | C12-C11-CA5-OA6 |
| 18 | N | 608 | PGV | C9-C10-C11-C12 |
| 27 | P | 309 | CDL | C41-C42-C43-C44 |
| 21 | B | 303 | PSC | C05-C04-O12-P |
| 20 | D | 201 | TGL | CG1-CG2-OG2-CB1 |
| 21 | O | 304 | PSC | C05-C04-O12-P |
| 18 | N | 608 | PGV | O02-C1-C2-C3 |
| 26 | T | 101 | PEK | C14-C15-C16-C17 |
| 27 | C | 309 | CDL | C41-C42-C43-C44 |
| 18 | A | 607 | PGV | O03-C19-C20-C21 |
| 20 | B | 302 | TGL | C13-C14-C29-C30 |
| 24 | M | 101 | DMU | C34-C37-C40-C43 |
| 24 | C | 302 | DMU | C31-C34-C37-C40 |
| 24 | Z | 101 | DMU | C19-C18-O16-C6 |
| 18 | N | 609 | PGV | O03-C19-C20-C21 |
| 27 | P | 309 | CDL | C54-C55-C56-C57 |
| 27 | G | 101 | CDL | C39-C40-C41-C42 |
| 20 | N | 607 | TGL | C12-C13-C14-C29 |
| 20 | D | 201 | TGL | OG3-CC1-CC2-CC3 |

There are no ring outliers.

41 monomers are involved in 284 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | C | 301 | DCW | 9 | 0 |
| 24 | C | 302 | DMU | 5 | 0 |

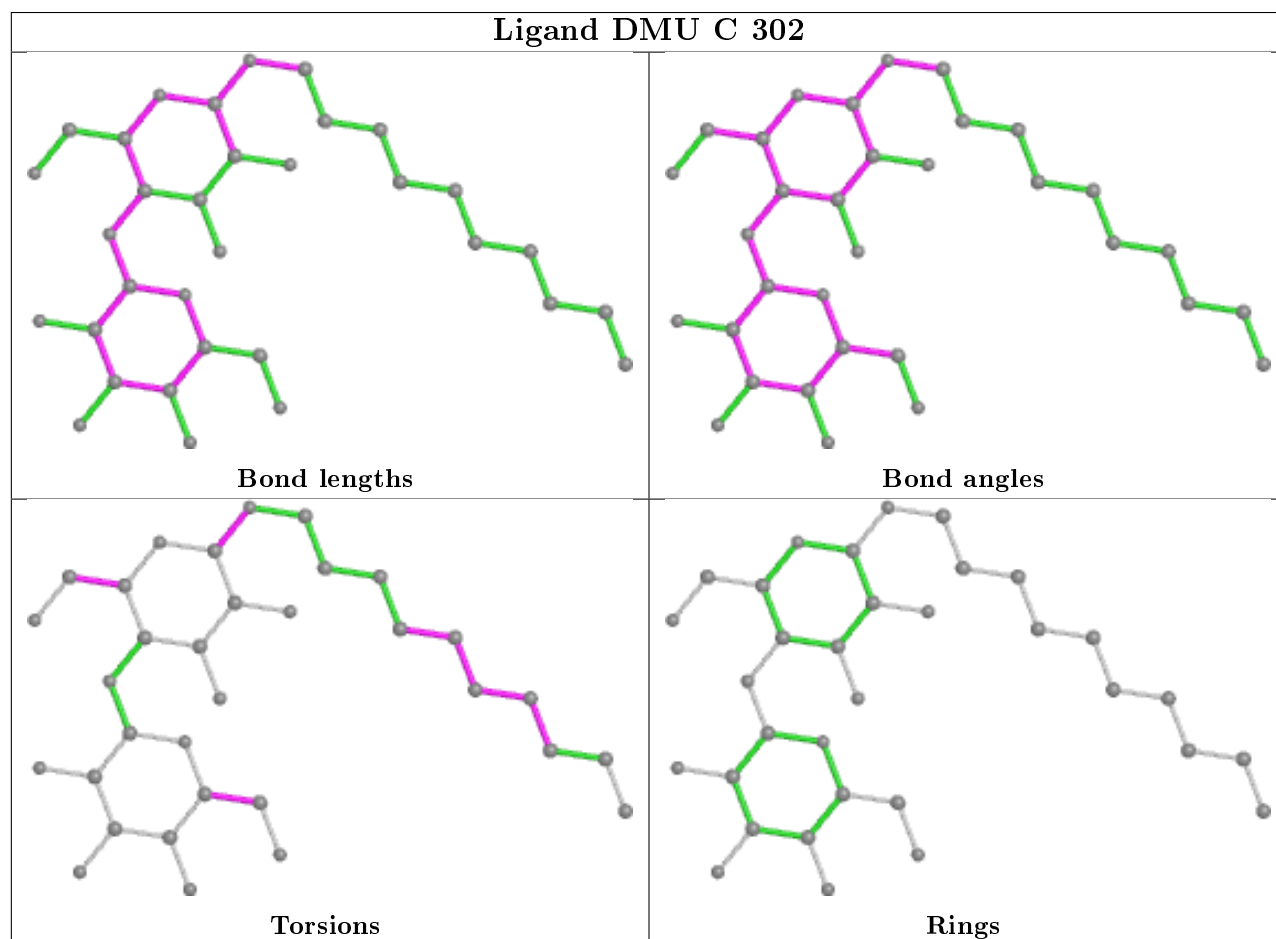
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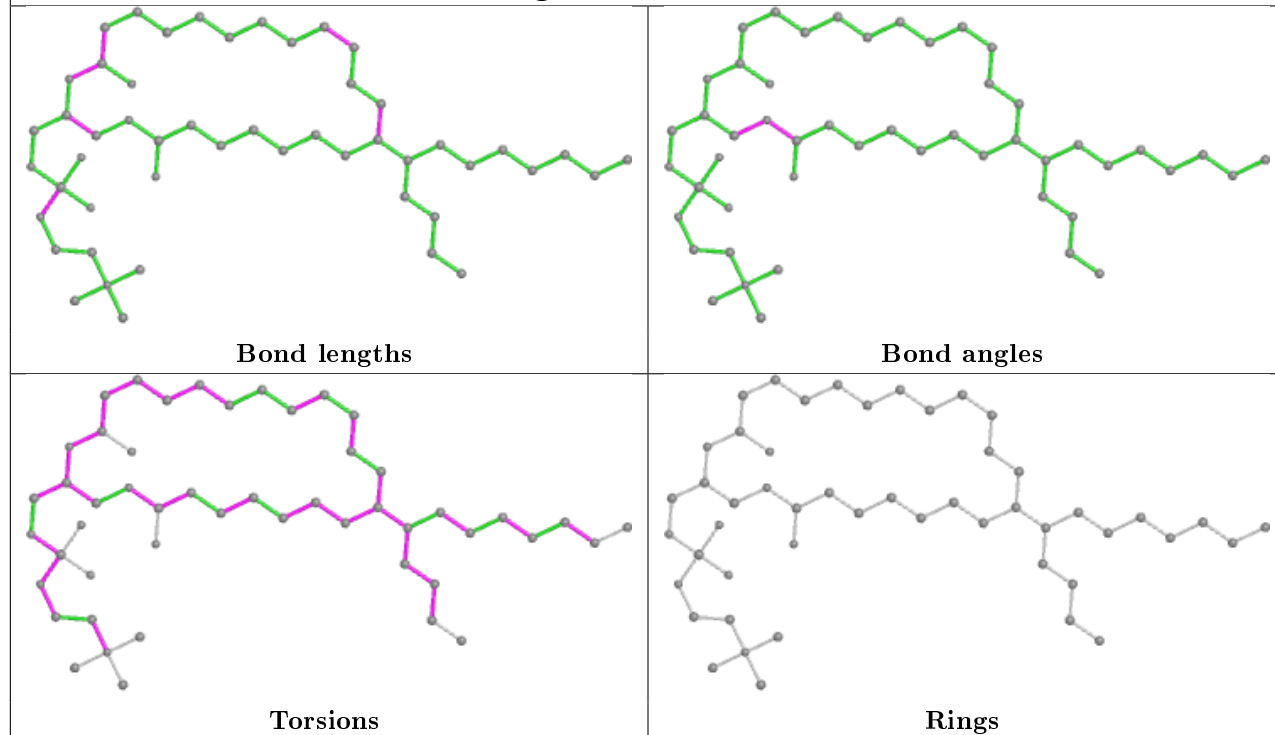
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21 | B | 303 | PSC | 23 | 0 |
| 18 | P | 307 | PGV | 8 | 0 |
| 27 | G | 101 | CDL | 15 | 0 |
| 26 | G | 102 | PEK | 10 | 0 |
| 22 | W | 101 | CHD | 4 | 0 |
| 23 | P | 301 | DCW | 8 | 0 |
| 22 | P | 310 | CHD | 2 | 0 |
| 27 | T | 102 | CDL | 21 | 0 |
| 20 | L | 101 | TGL | 23 | 0 |
| 27 | C | 309 | CDL | 15 | 0 |
| 20 | N | 606 | TGL | 14 | 0 |
| 18 | C | 307 | PGV | 8 | 0 |
| 26 | T | 101 | PEK | 8 | 0 |
| 18 | N | 608 | PGV | 7 | 0 |
| 18 | N | 609 | PGV | 6 | 0 |
| 22 | C | 310 | CHD | 1 | 0 |
| 20 | D | 201 | TGL | 6 | 0 |
| 17 | N | 604 | HEA | 4 | 0 |
| 26 | C | 306 | PEK | 7 | 0 |
| 24 | Z | 101 | DMU | 1 | 0 |
| 18 | A | 607 | PGV | 8 | 0 |
| 24 | P | 302 | DMU | 5 | 0 |
| 20 | B | 302 | TGL | 6 | 0 |
| 18 | A | 606 | PGV | 8 | 0 |
| 17 | N | 605 | HEA | 2 | 0 |
| 26 | P | 306 | PEK | 6 | 0 |
| 22 | B | 304 | CHD | 1 | 0 |
| 17 | A | 604 | HEA | 2 | 0 |
| 26 | C | 305 | PEK | 11 | 0 |
| 21 | O | 304 | PSC | 21 | 0 |
| 27 | P | 309 | CDL | 14 | 0 |
| 20 | O | 303 | TGL | 7 | 0 |
| 24 | M | 101 | DMU | 1 | 0 |
| 20 | N | 607 | TGL | 5 | 0 |
| 18 | C | 308 | PGV | 1 | 0 |
| 18 | P | 308 | PGV | 1 | 0 |
| 17 | A | 605 | HEA | 3 | 0 |
| 26 | P | 305 | PEK | 11 | 0 |
| 22 | J | 101 | CHD | 2 | 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

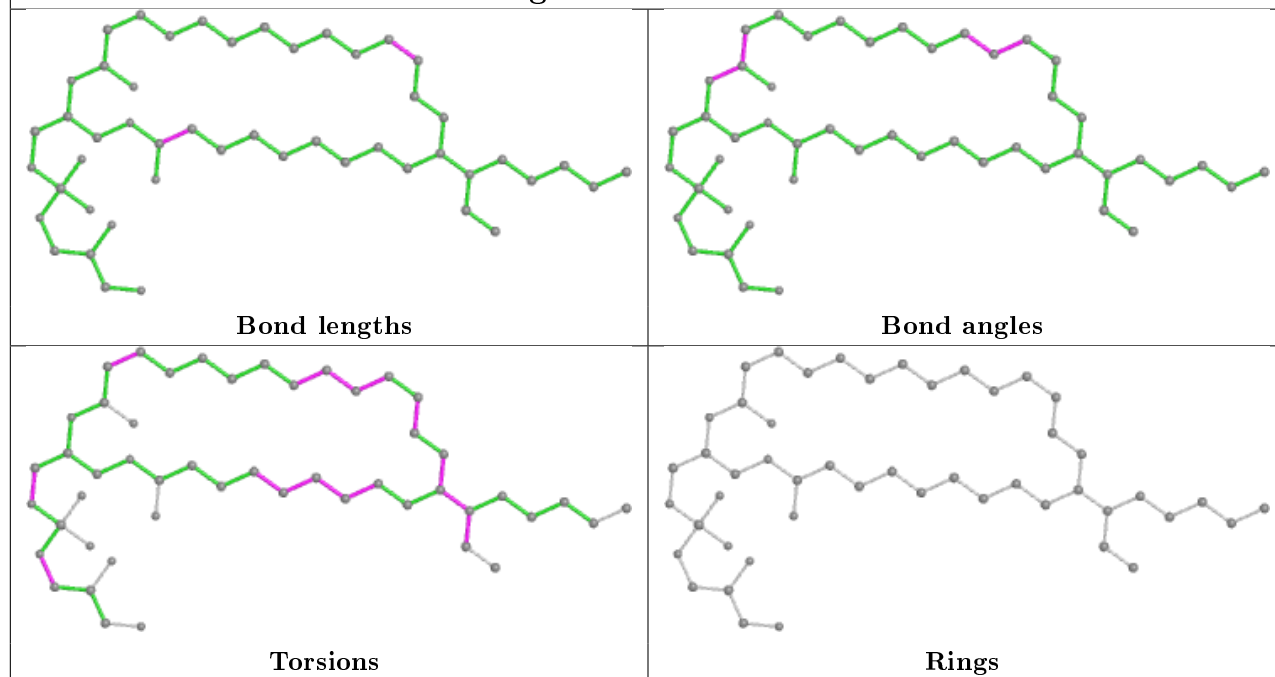
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

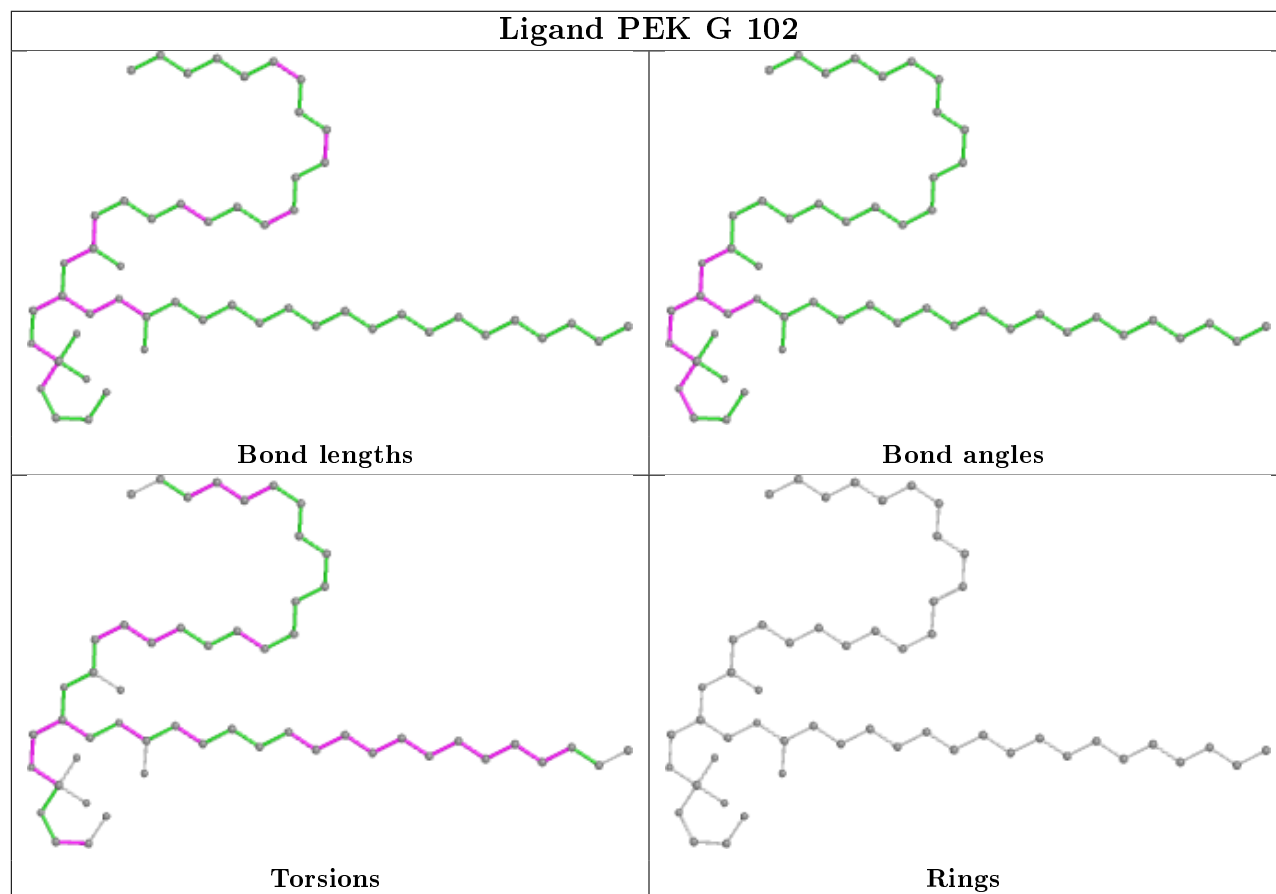
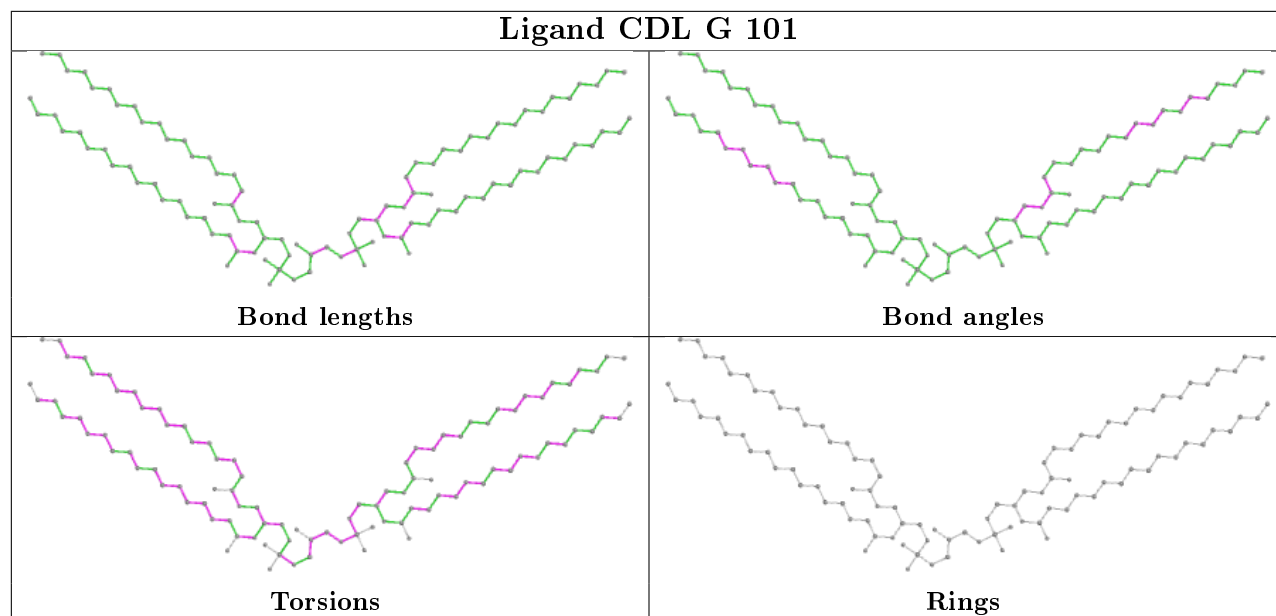


Ligand PSC B 303

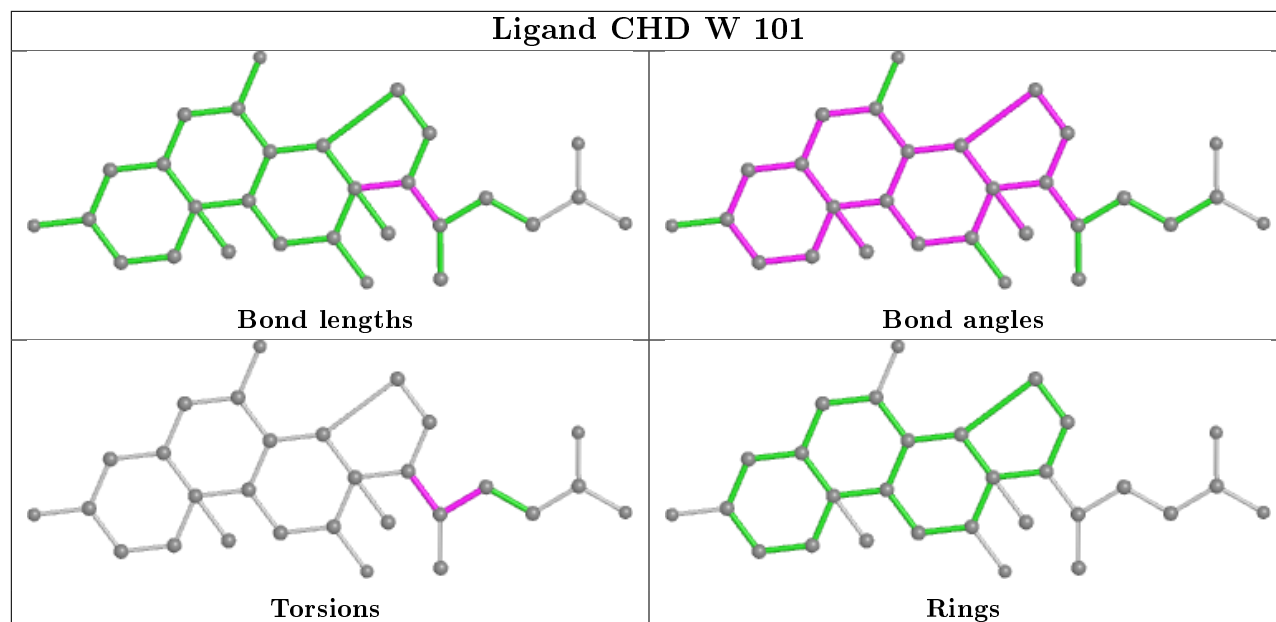


Ligand PGV P 307

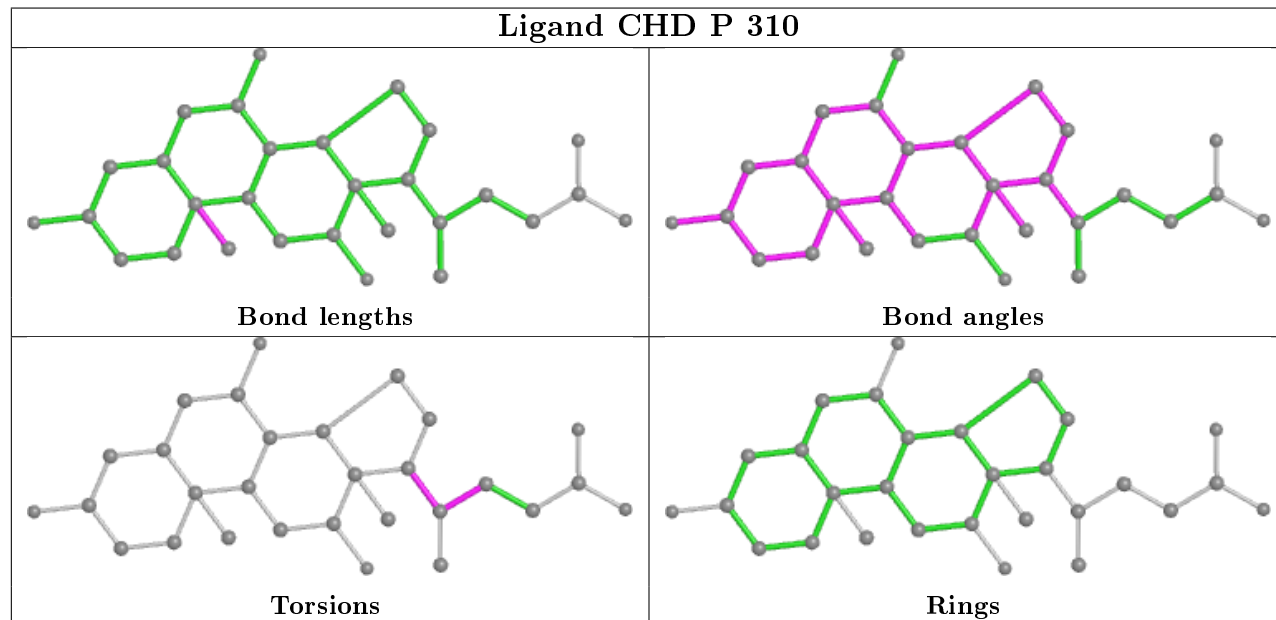


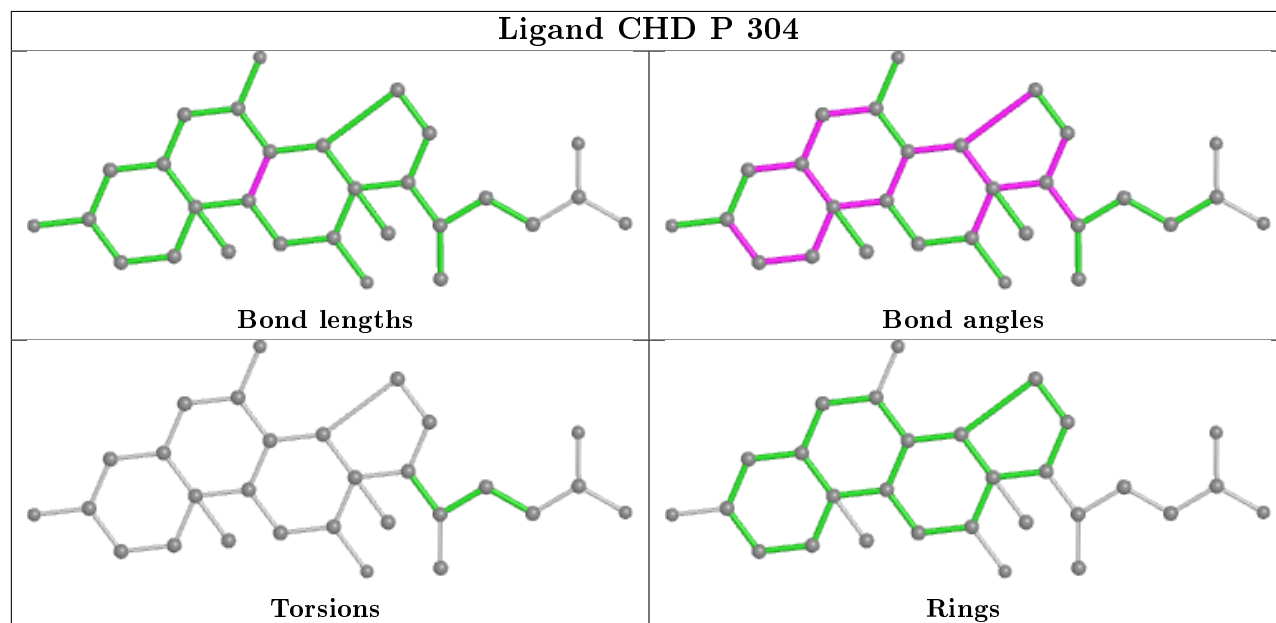
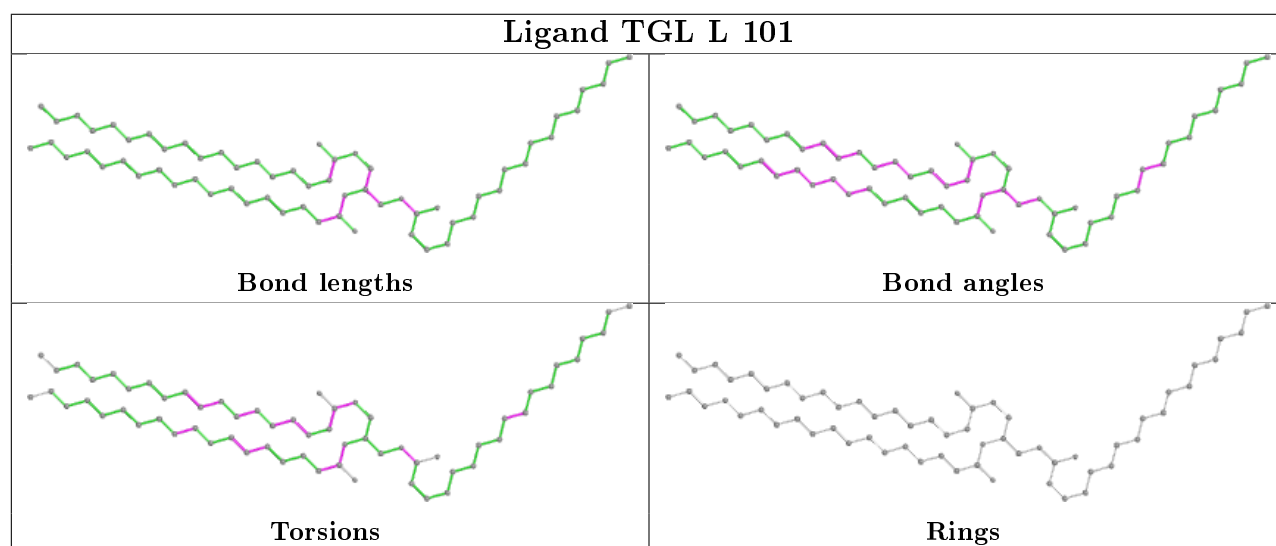
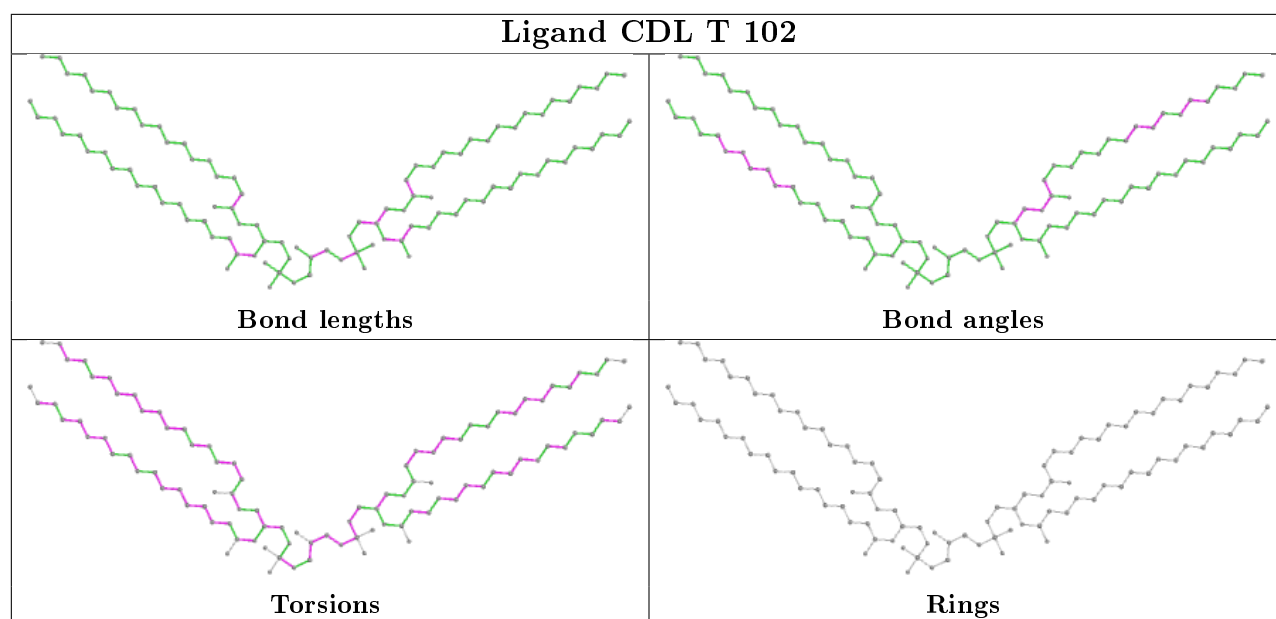


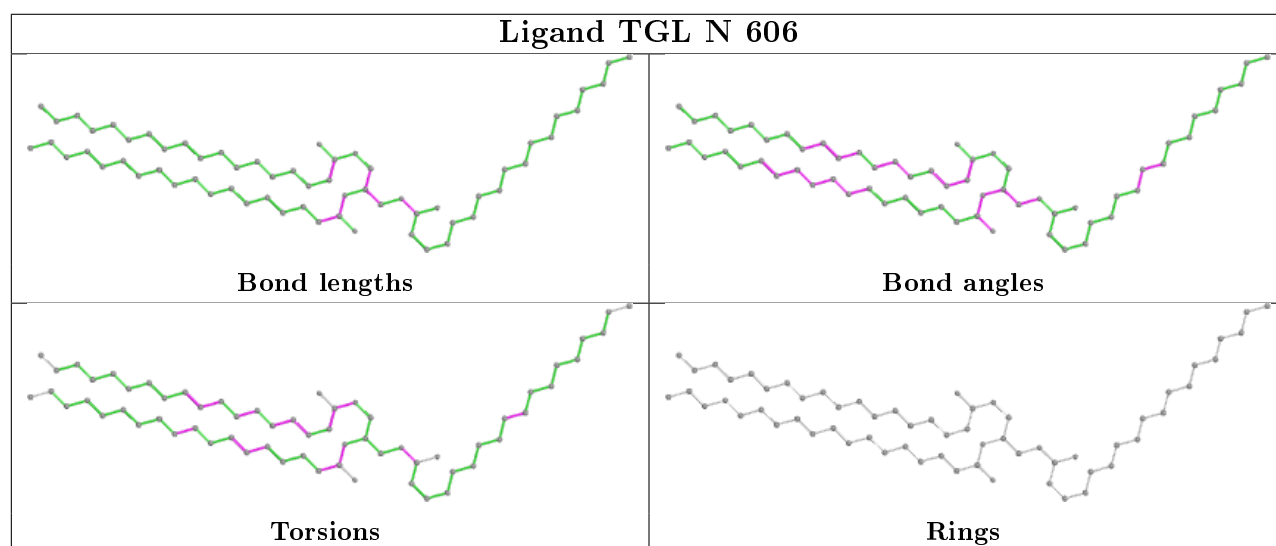
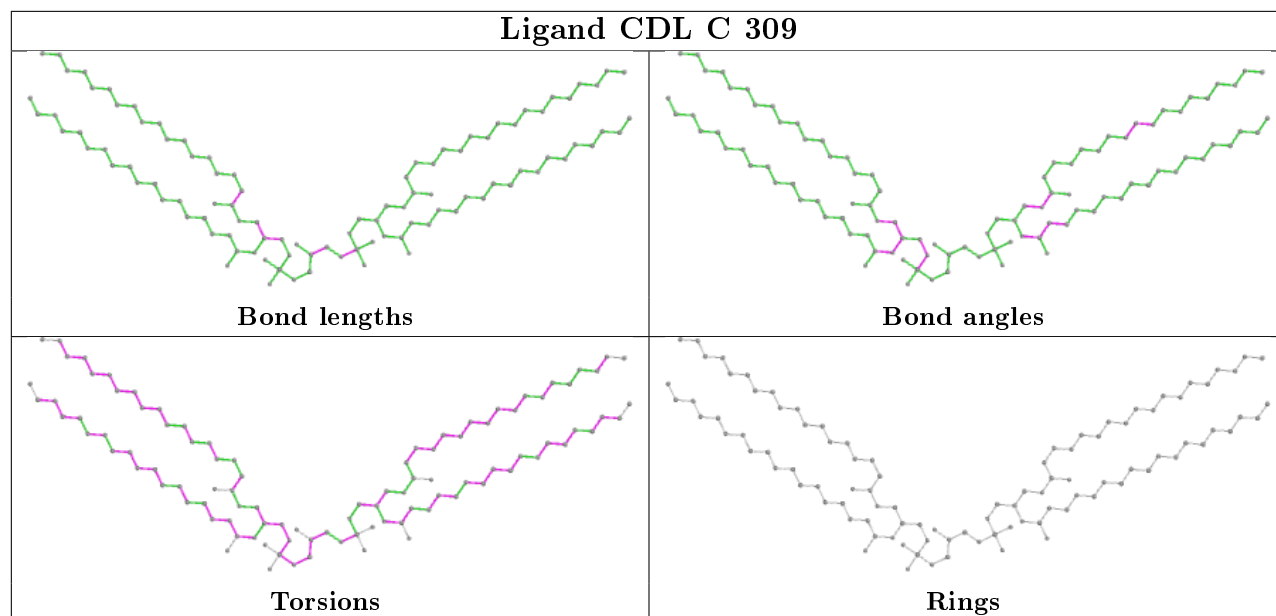
Ligand CHD W 101

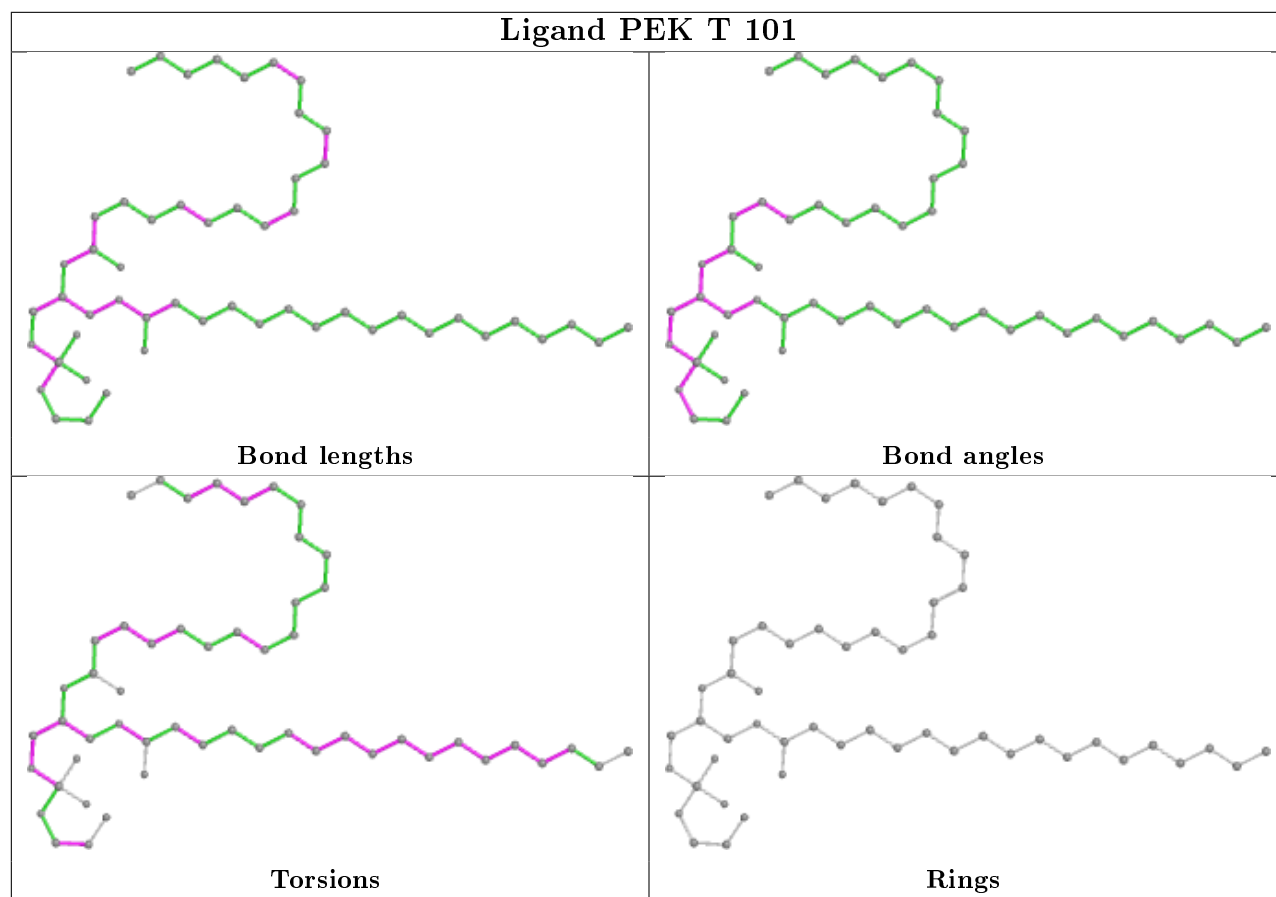
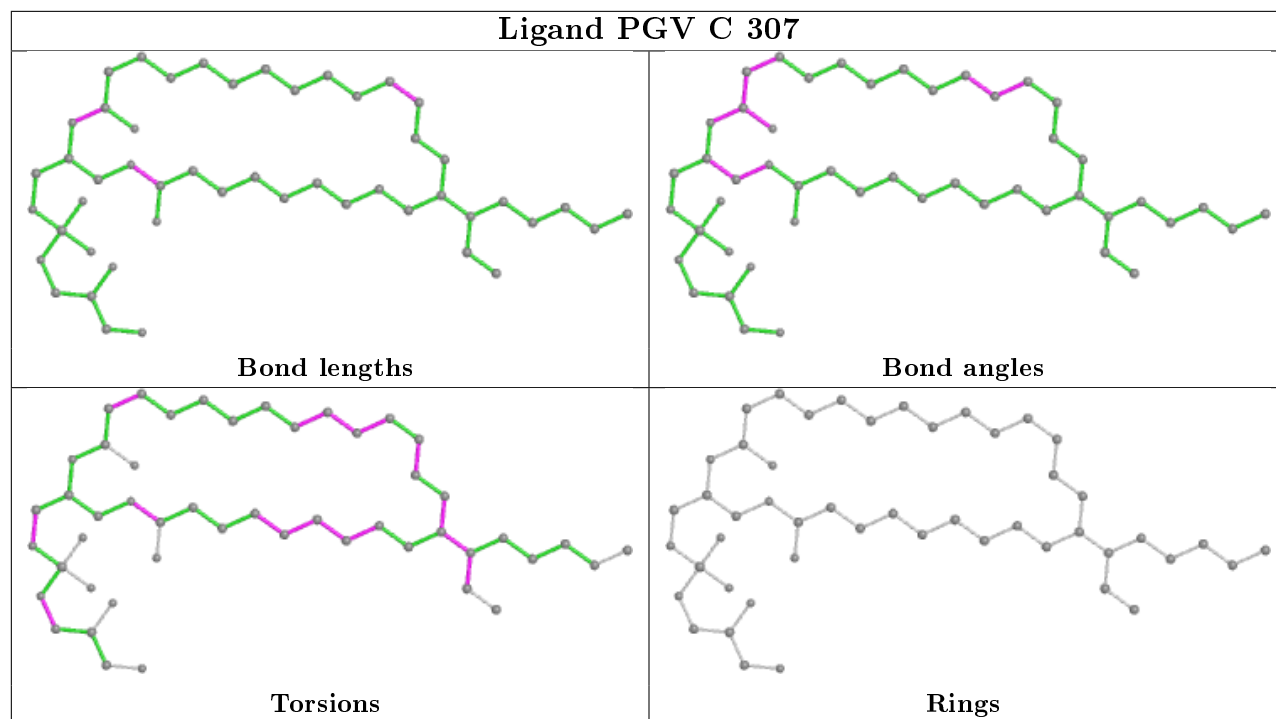


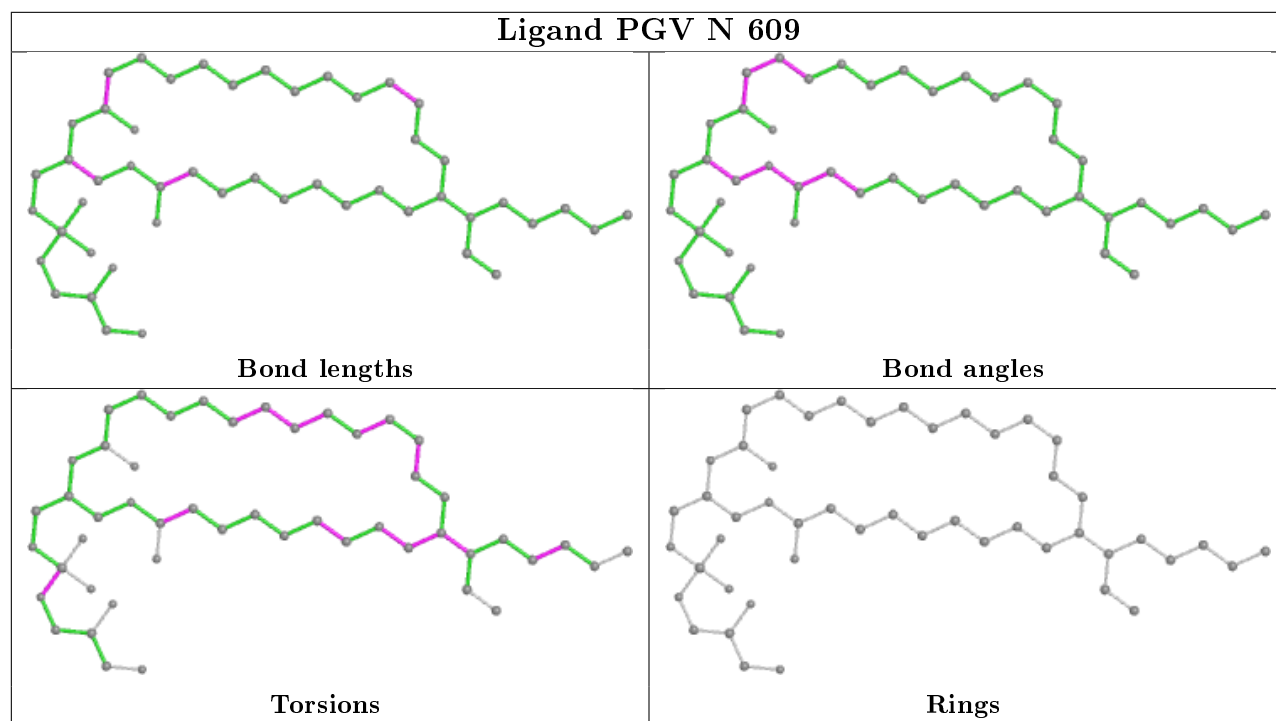
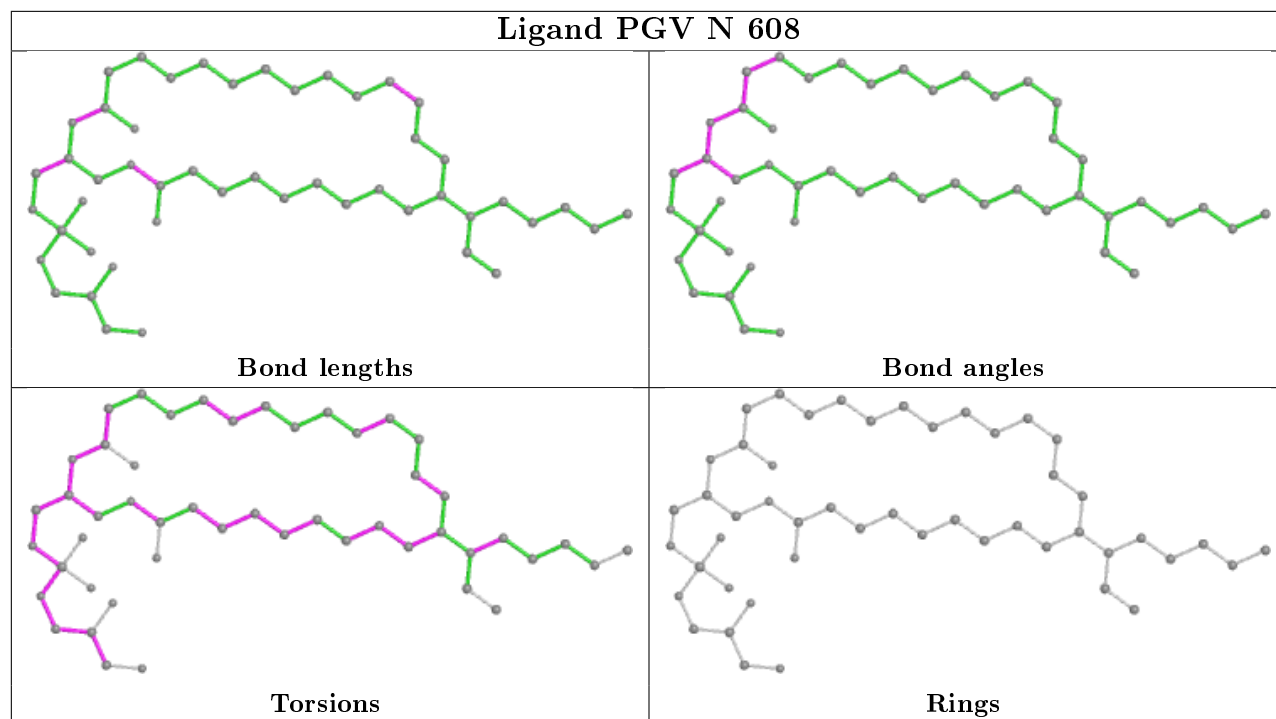
Ligand CHD P 310

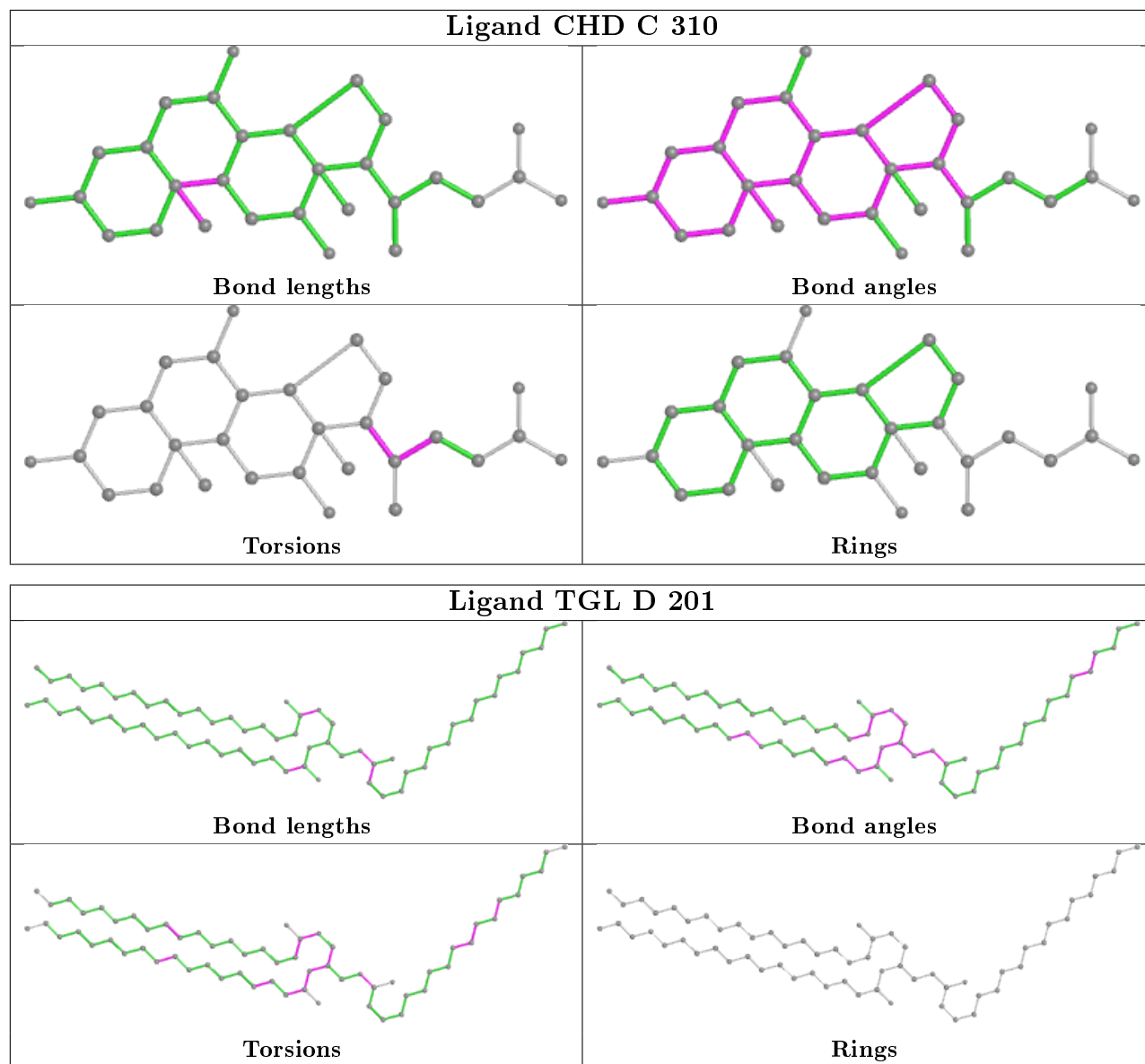


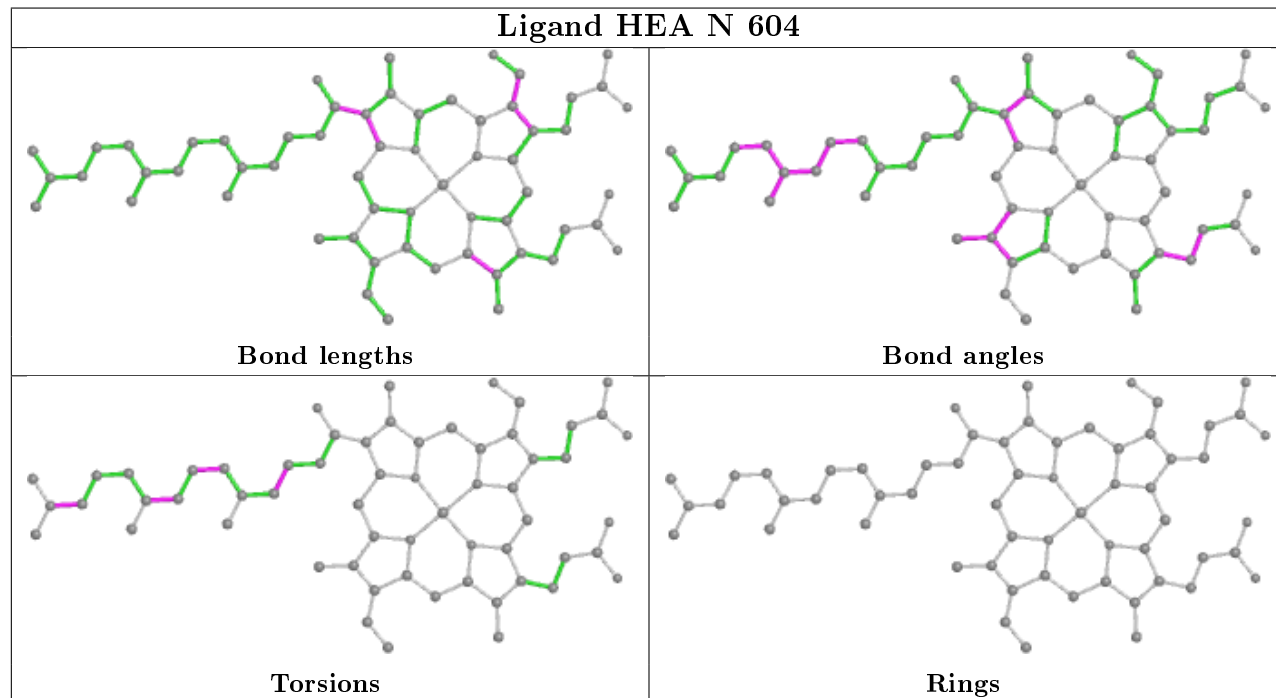
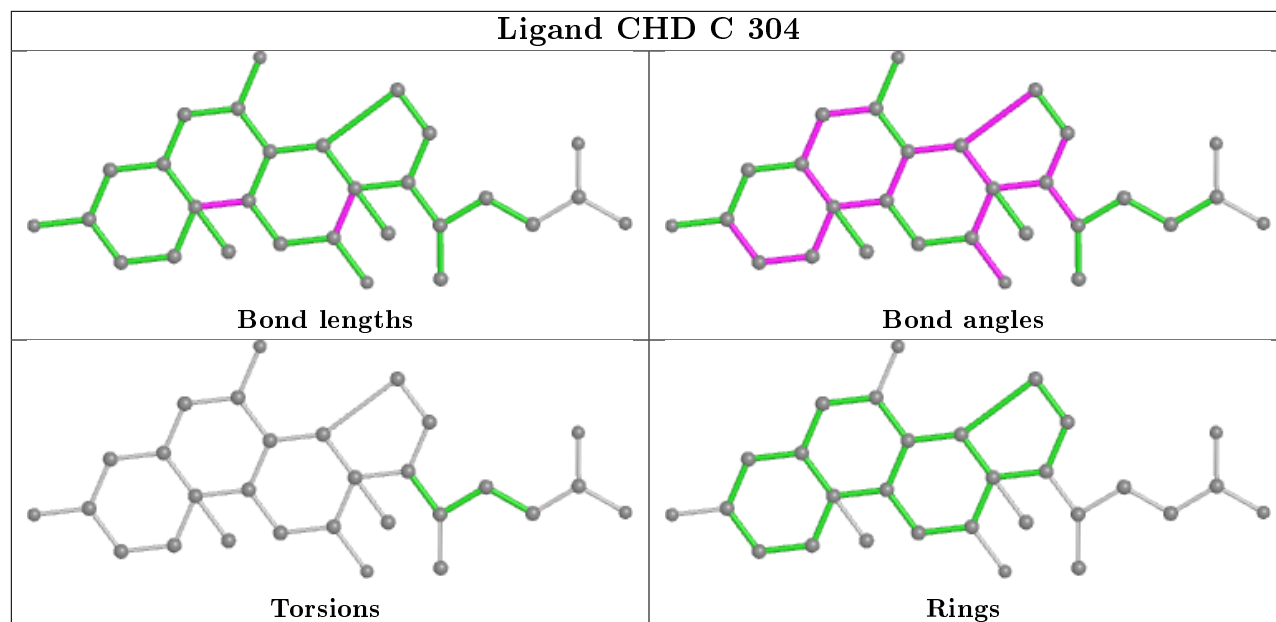


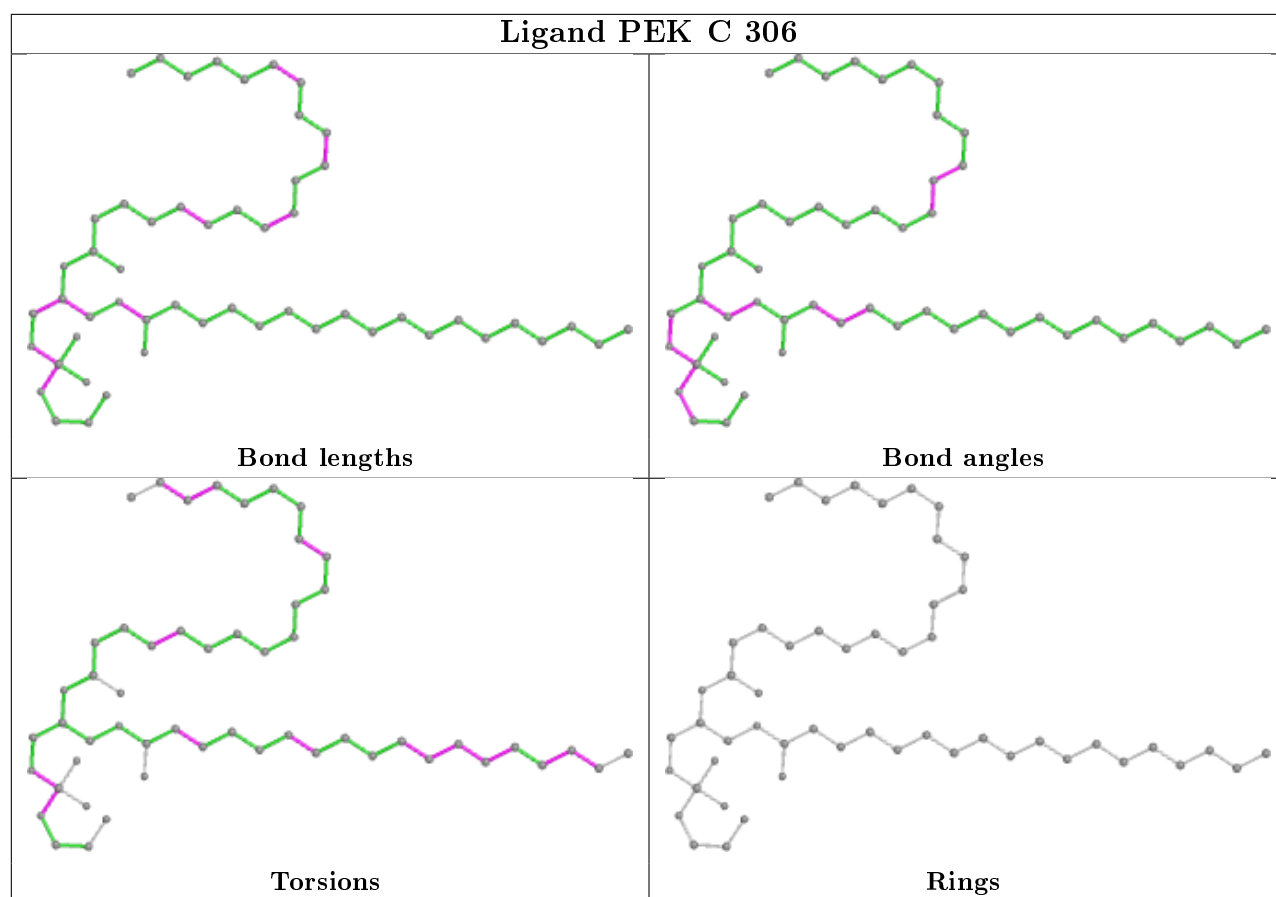


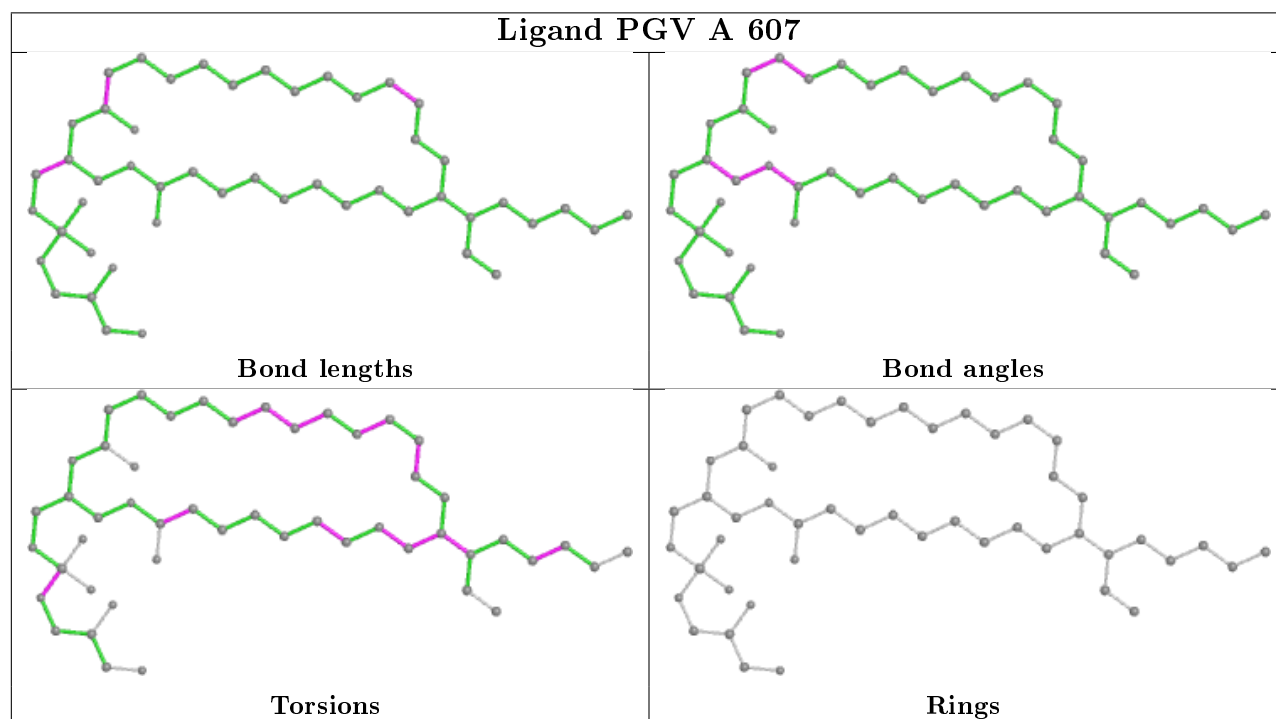
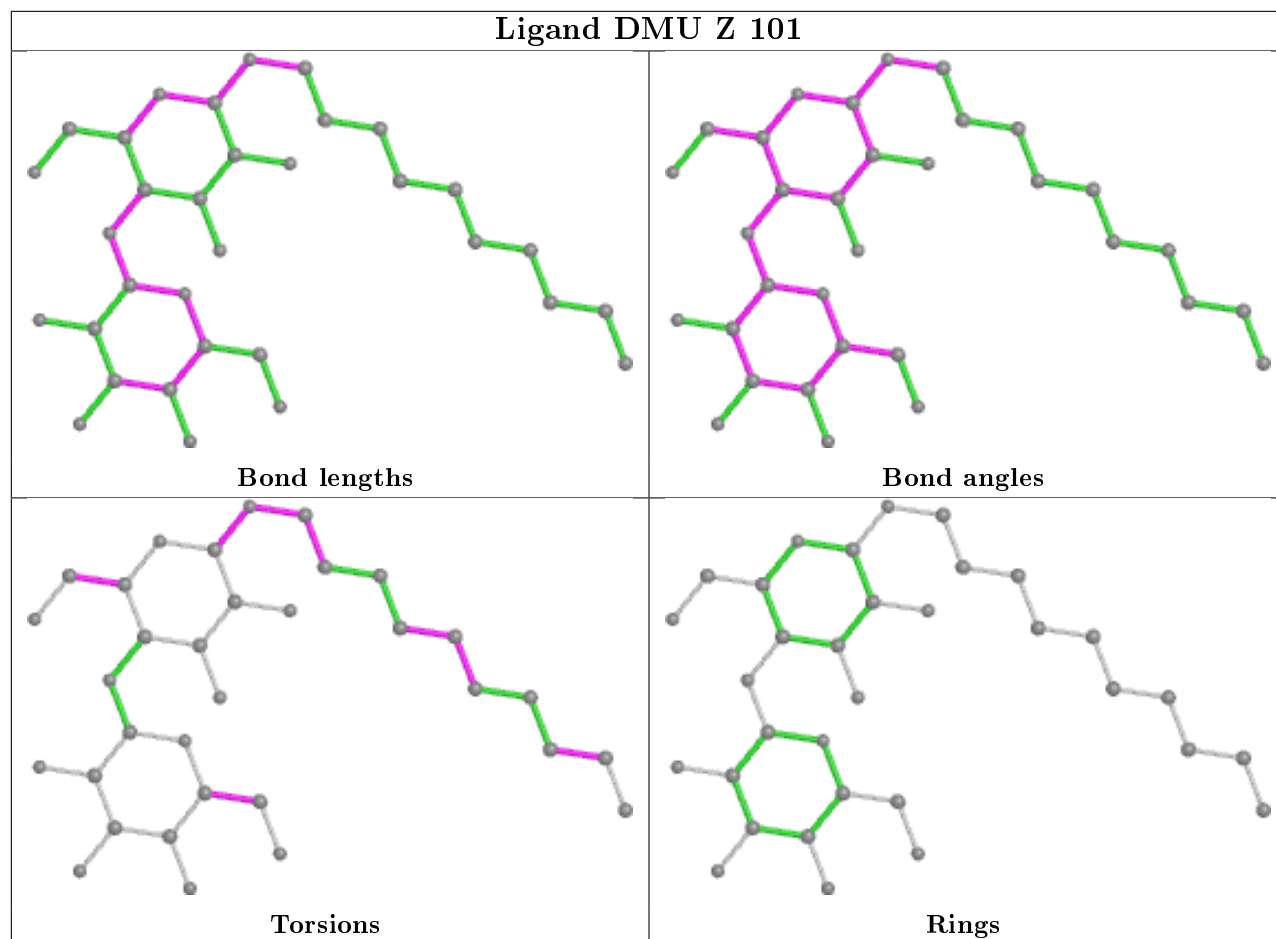


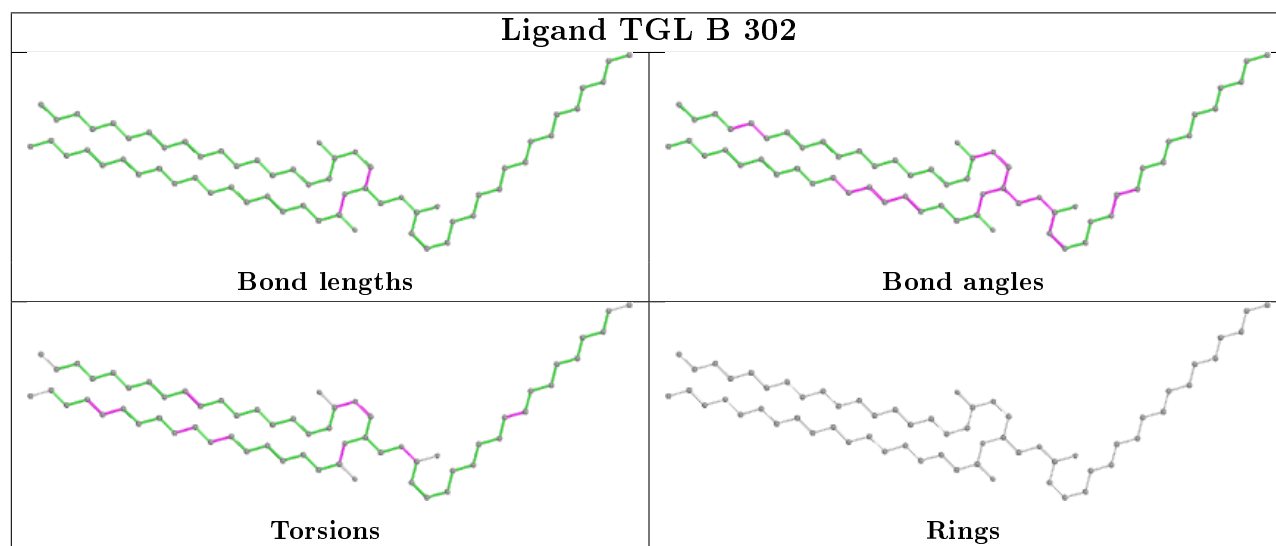
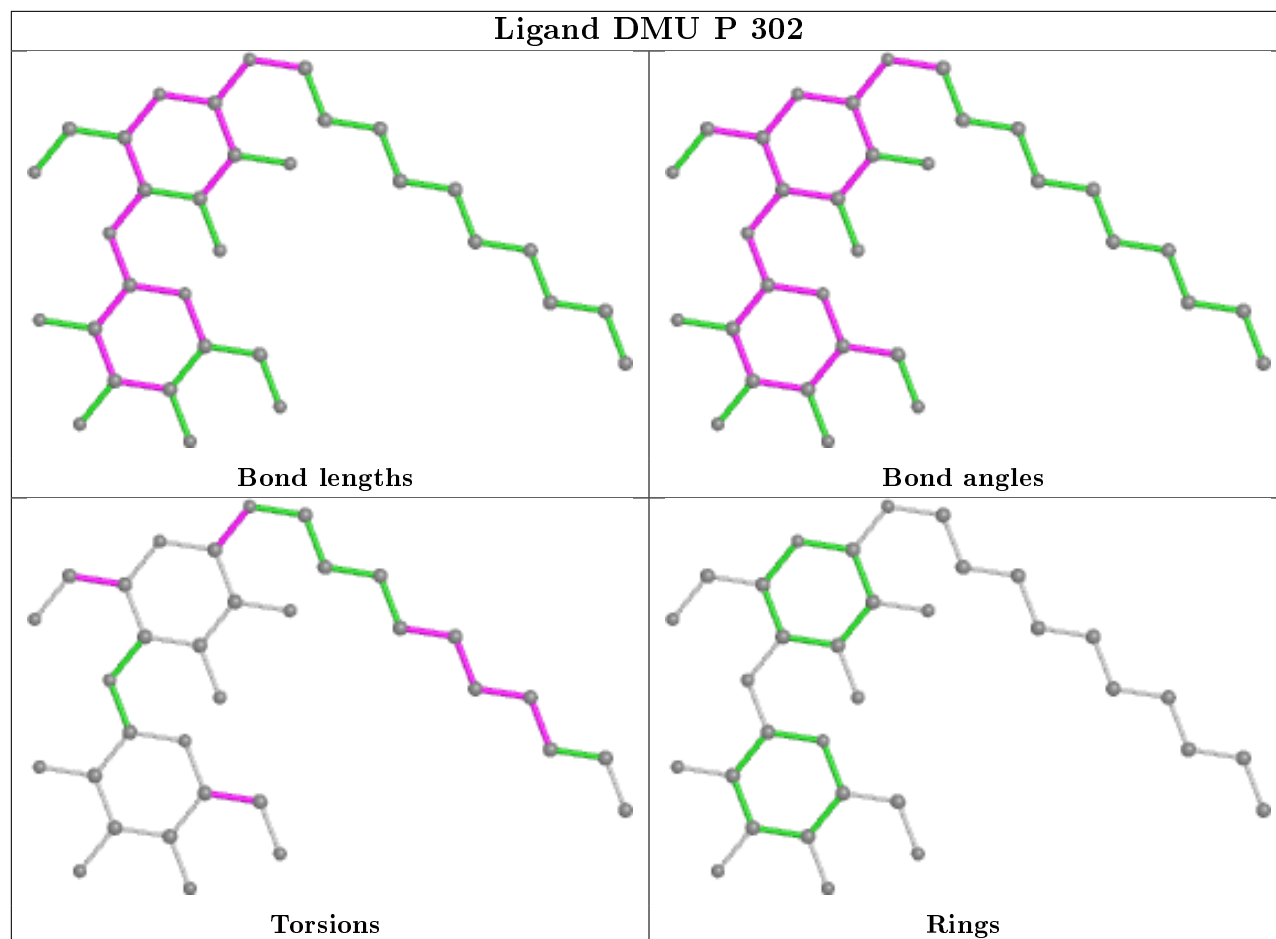


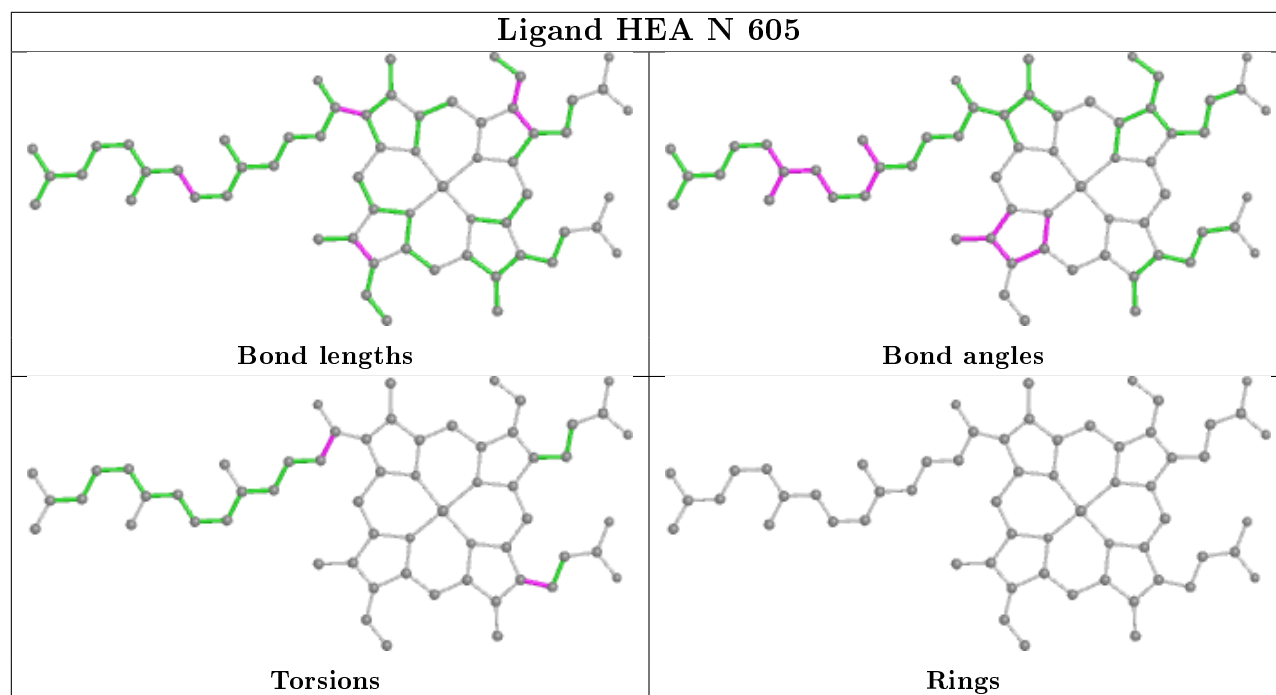
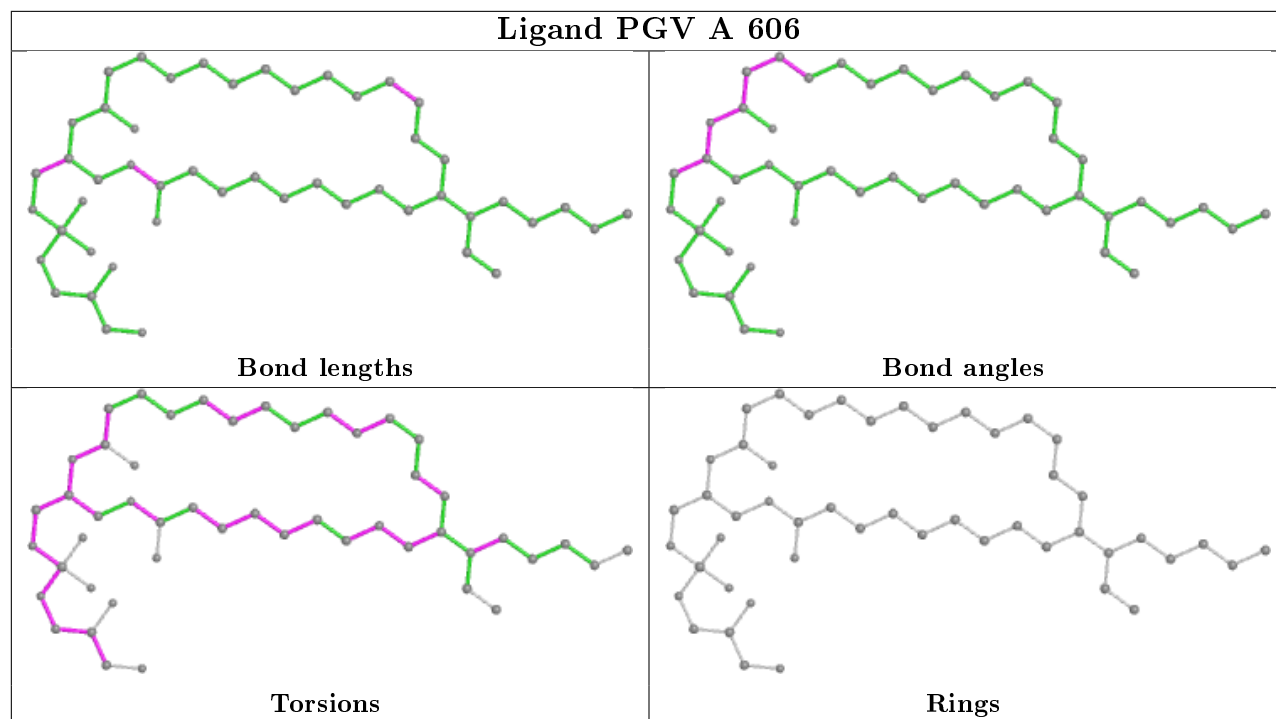




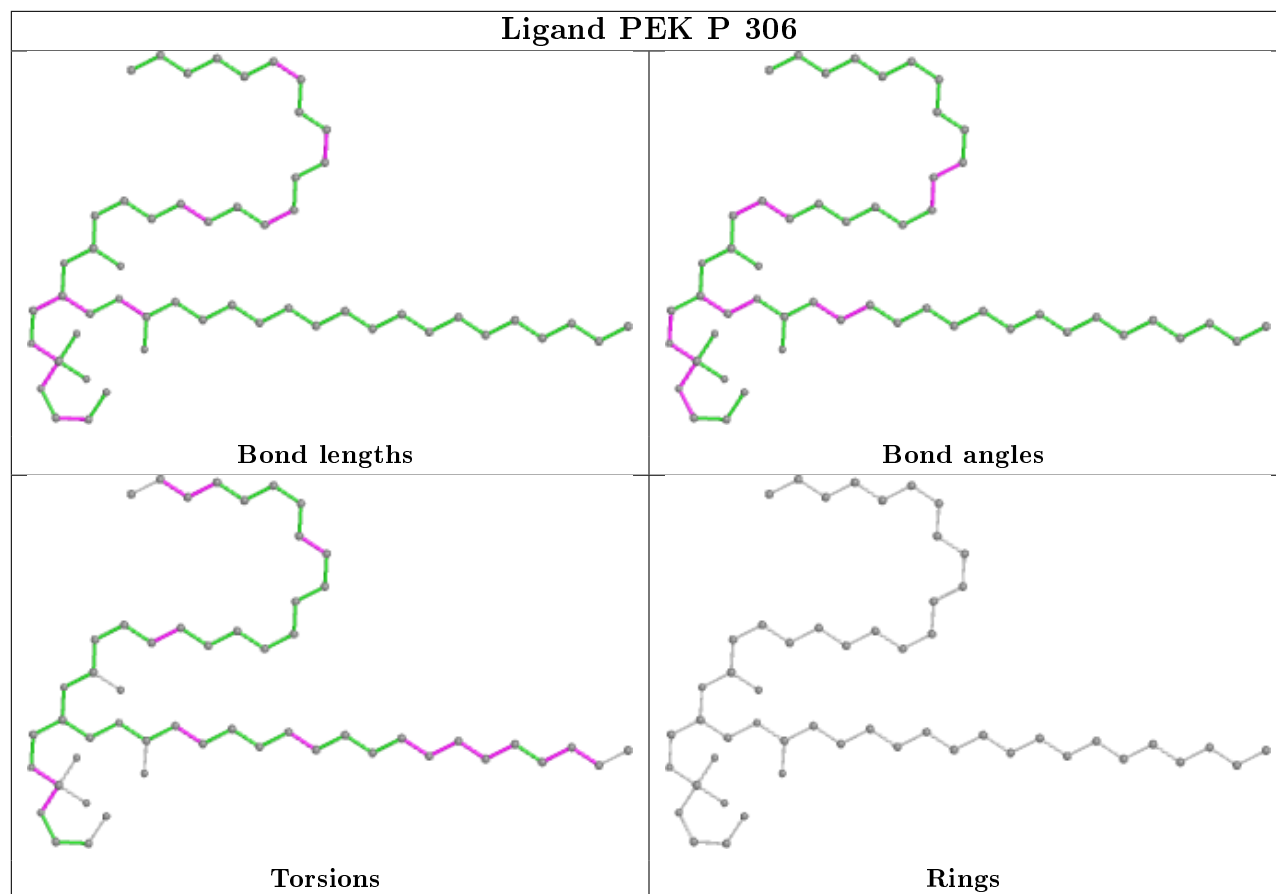




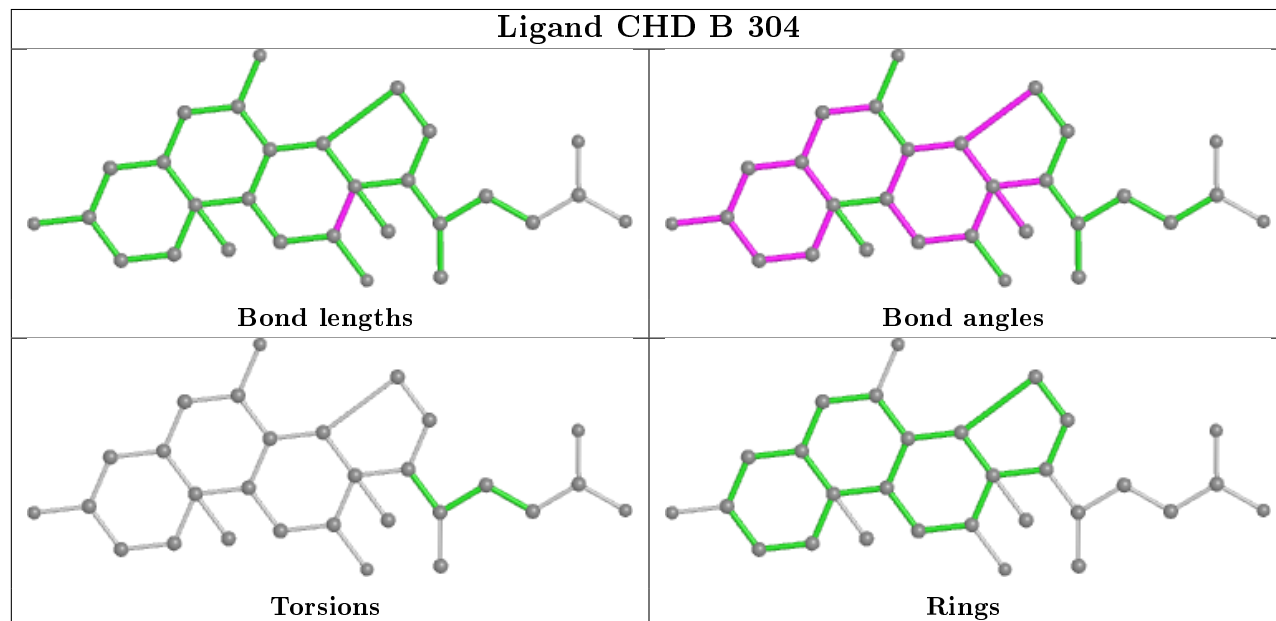


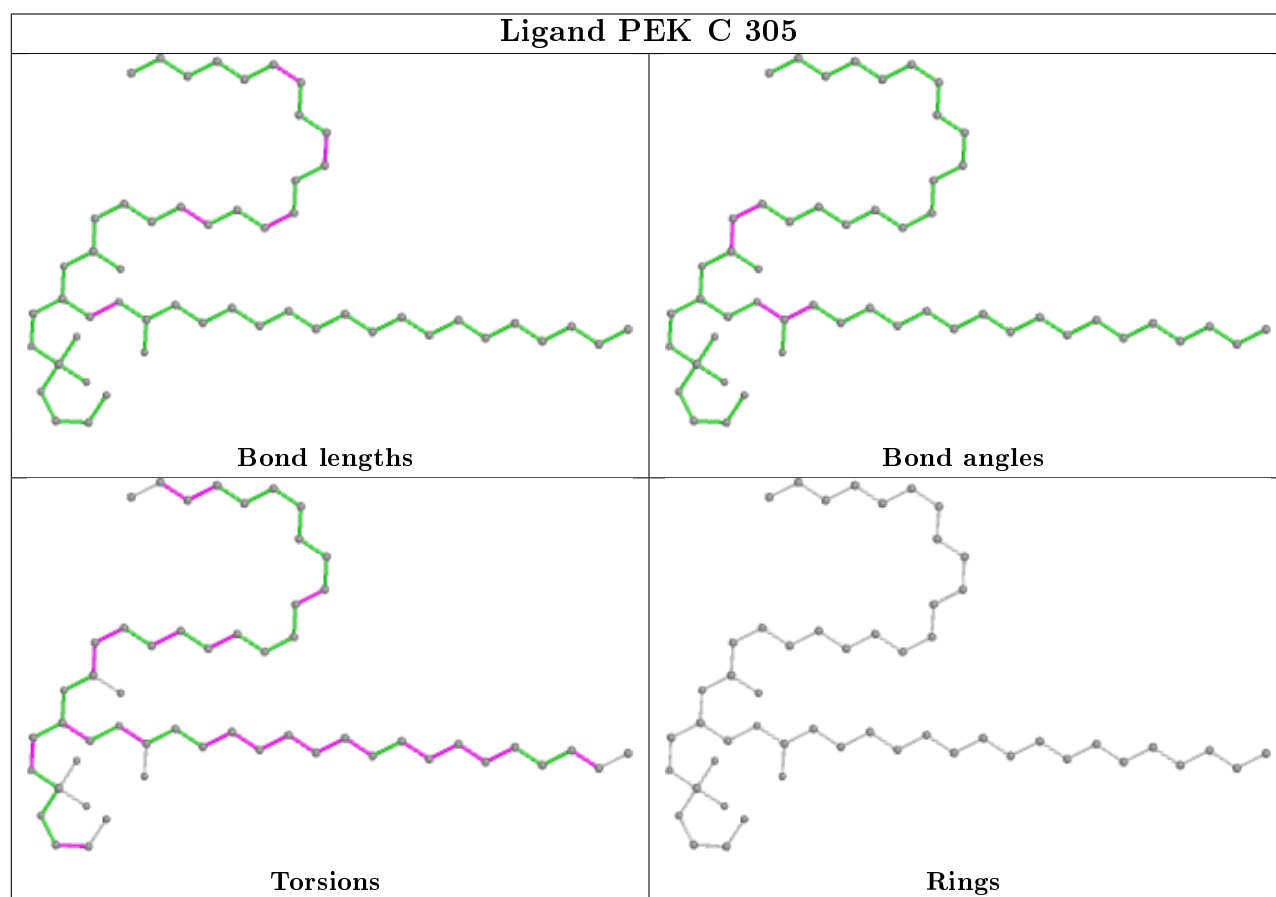
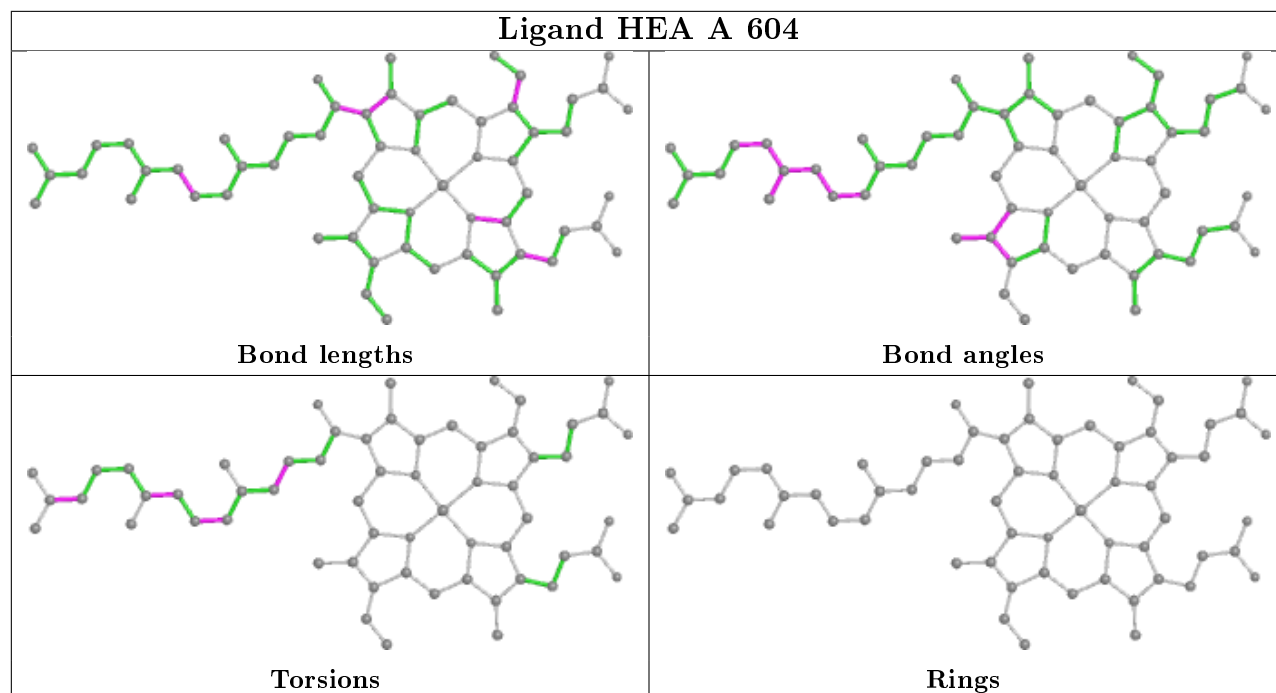


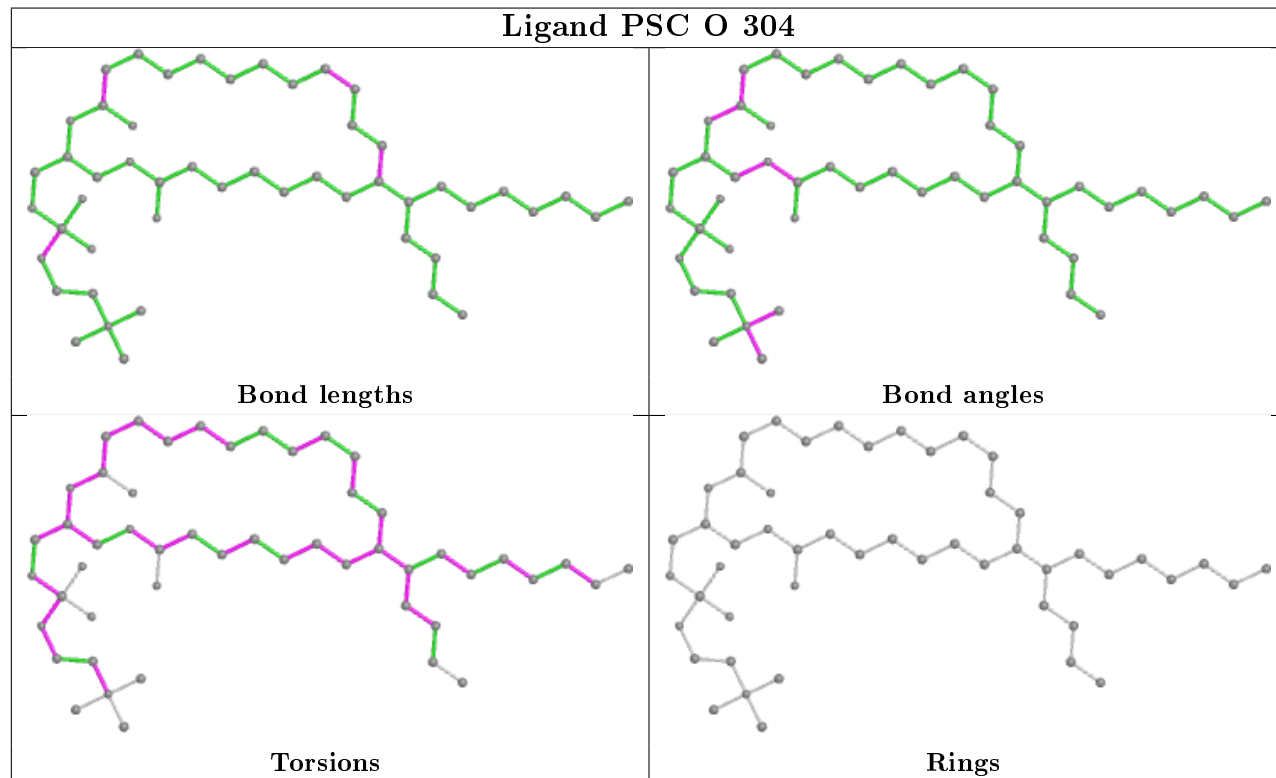
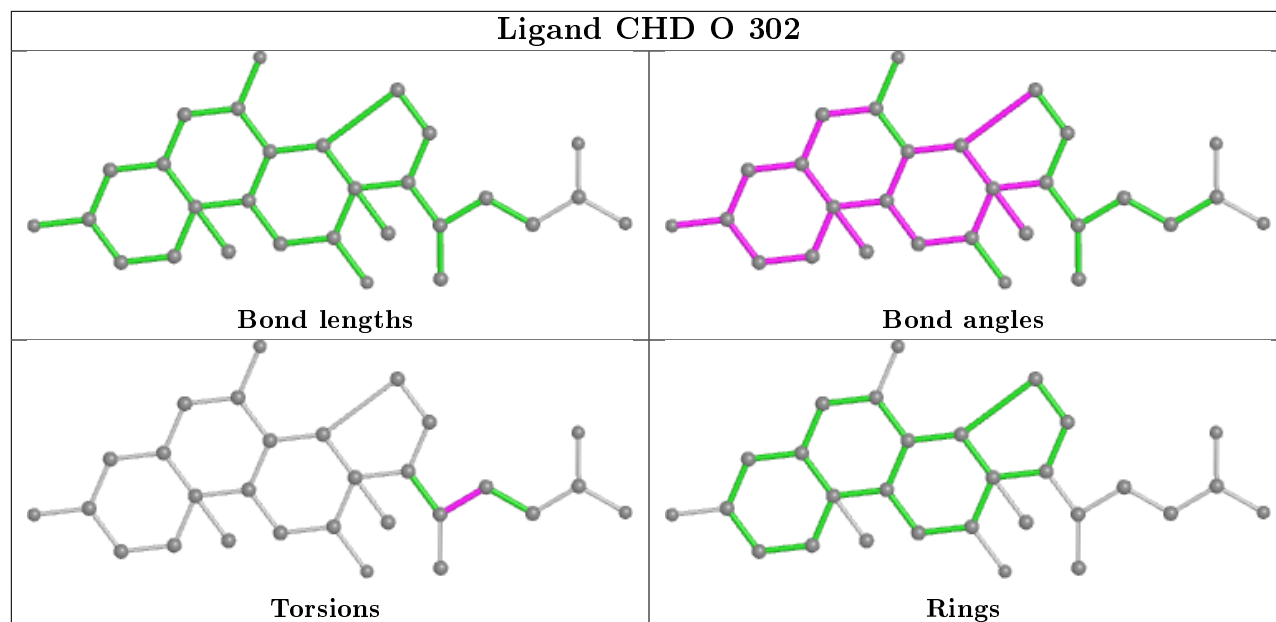
Ligand PEK P 306

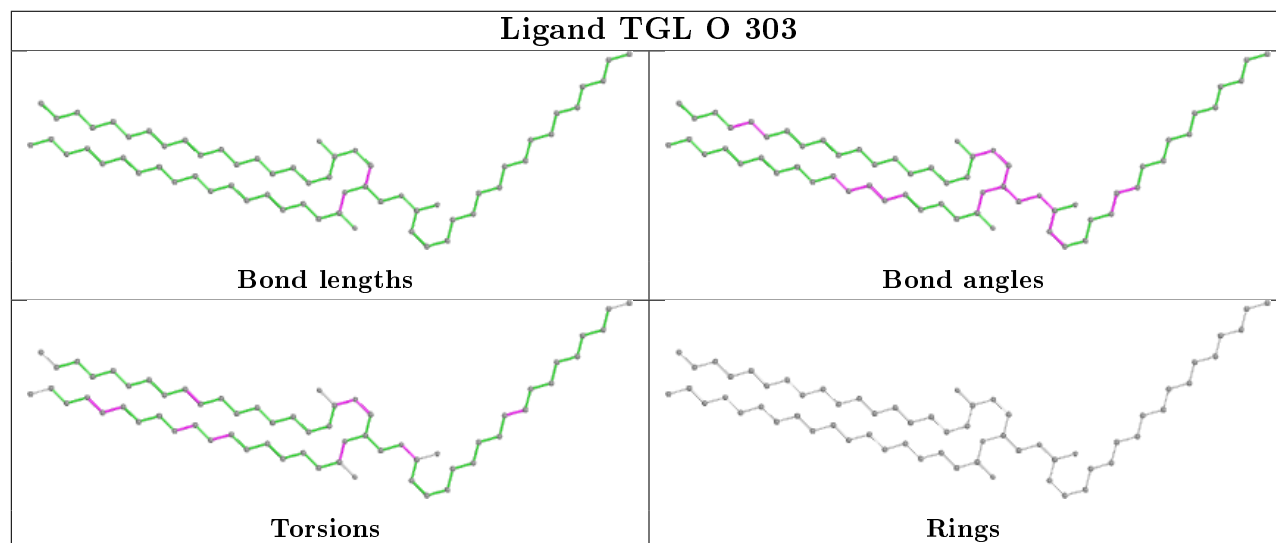
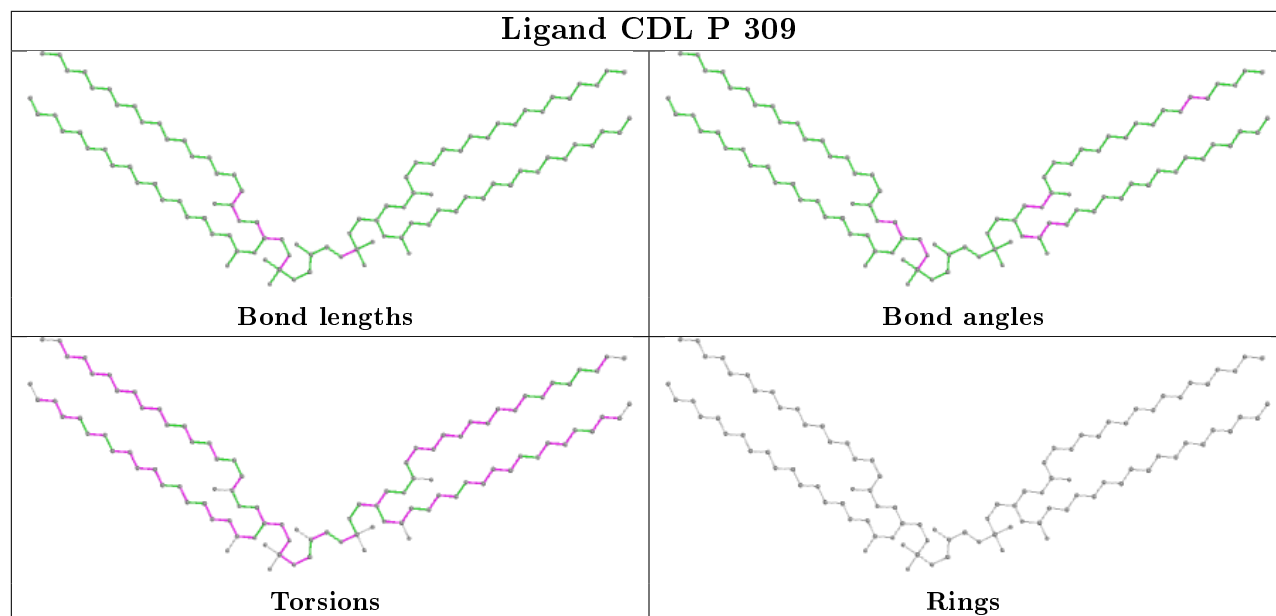


Ligand CHD B 304

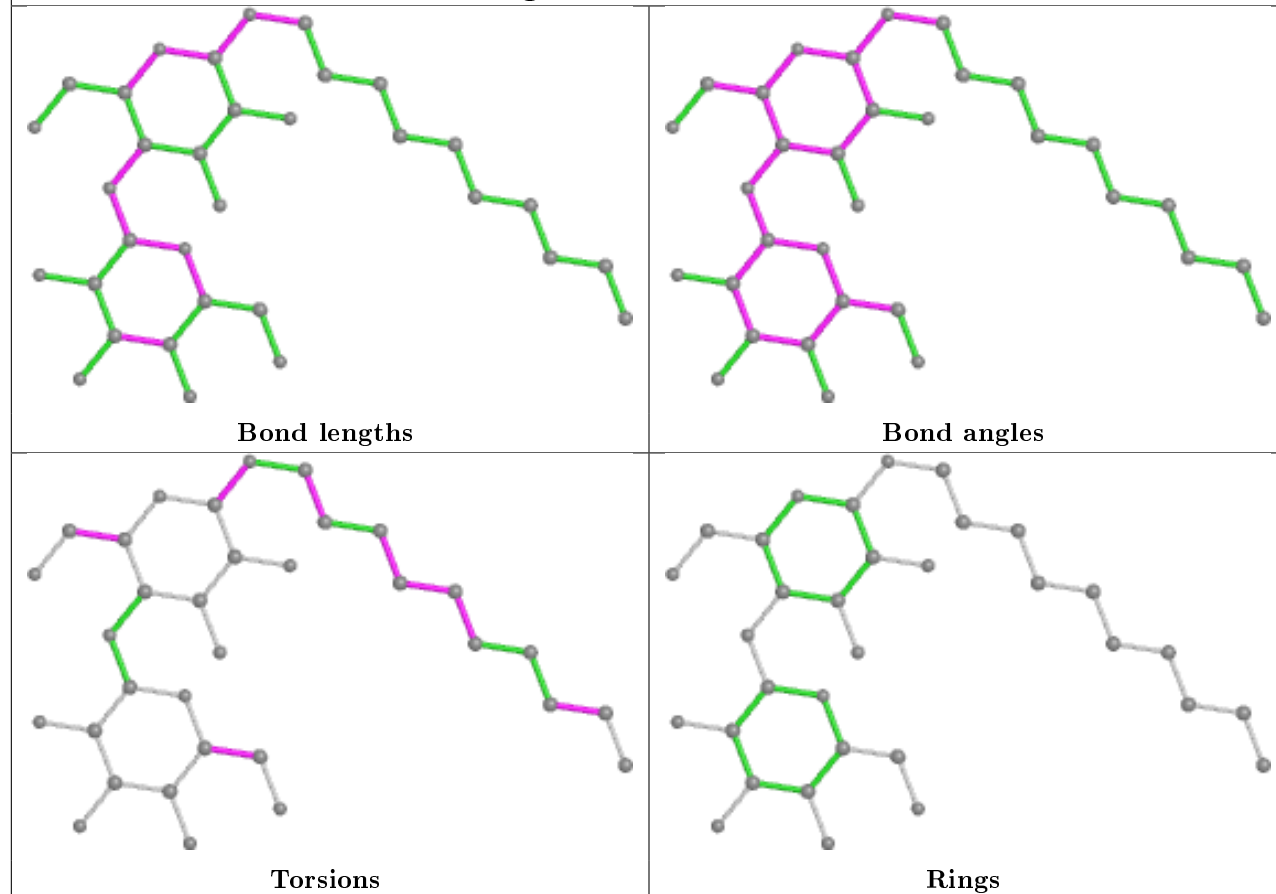




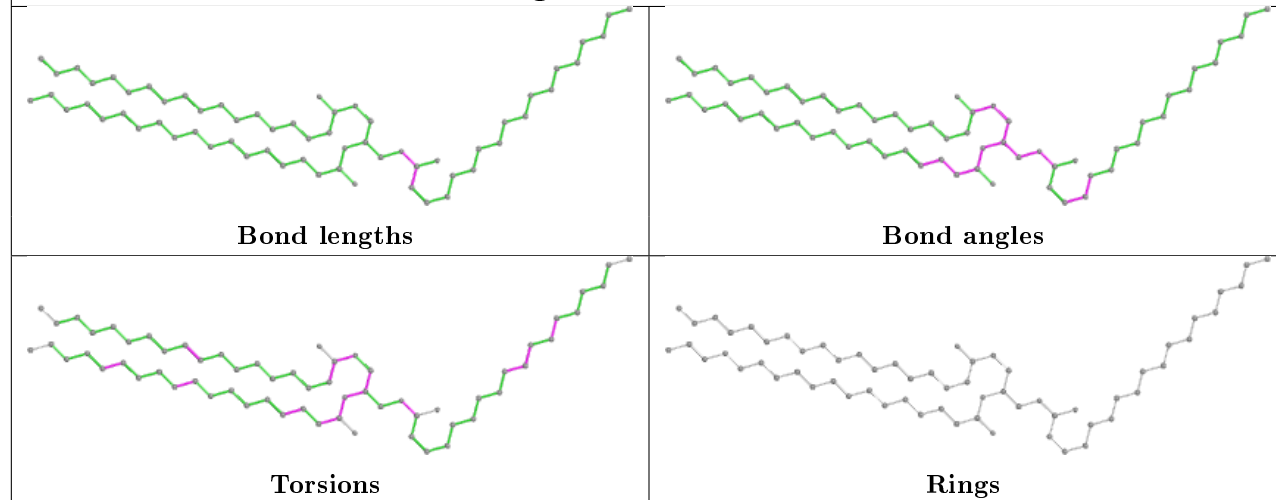


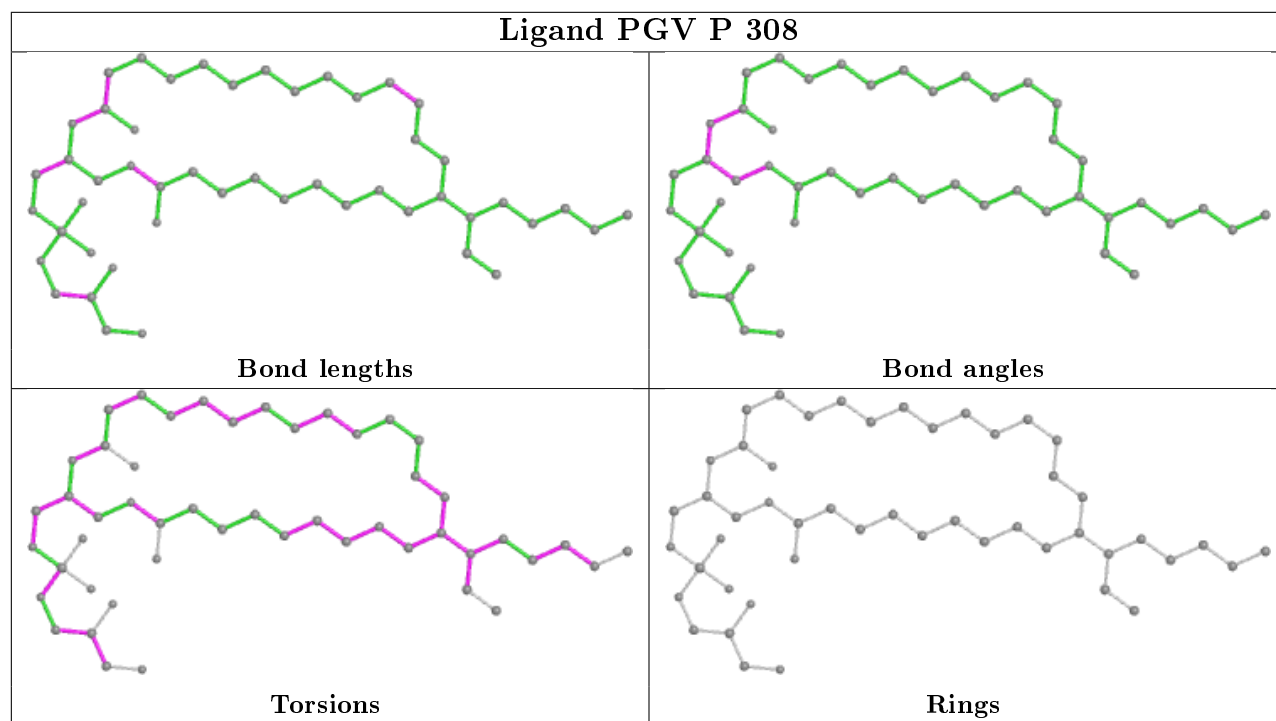
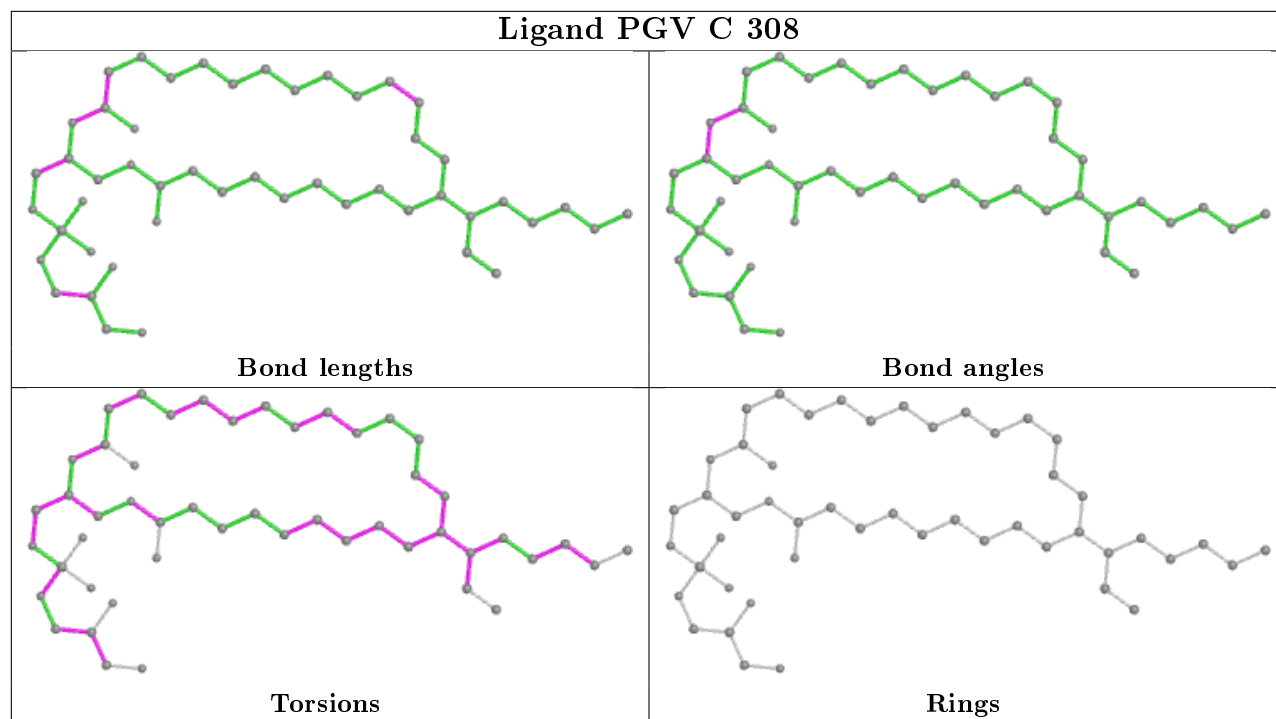


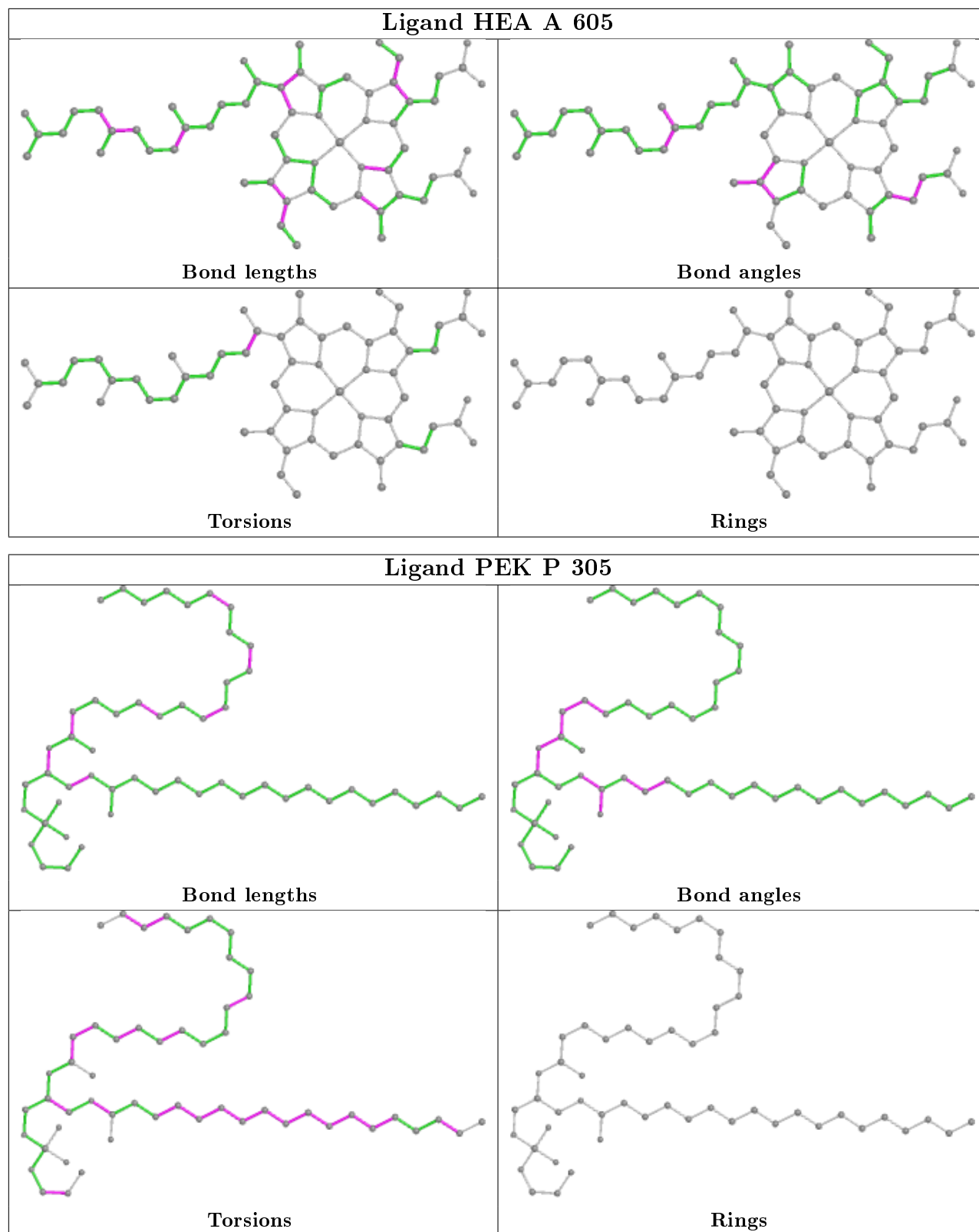
Ligand DMU M 101

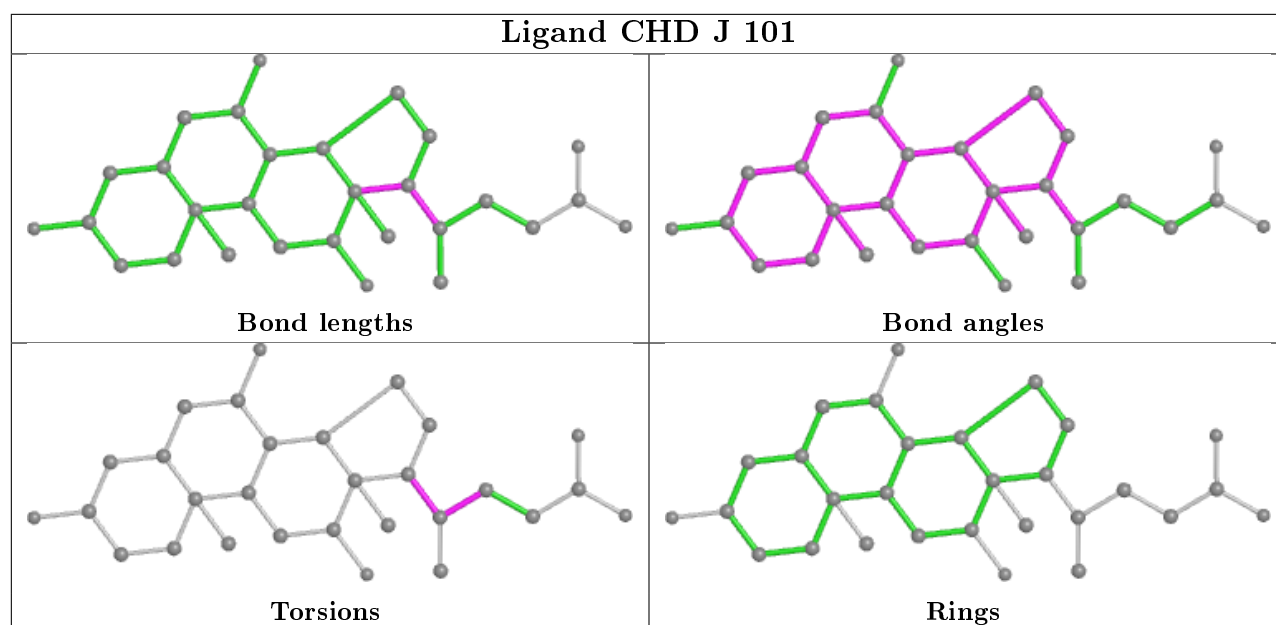


Ligand TGL N 607









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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1 | A | 513/514 (99%) | -0.14 | 1 (0%) 95 94 | 16, 25, 36, 67 | 0 |
| 1 | N | 513/514 (99%) | -0.22 | 2 (0%) 92 91 | 20, 32, 45, 70 | 0 |
| 2 | B | 226/227 (99%) | -0.57 | 1 (0%) 92 91 | 16, 31, 65, 95 | 0 |
| 2 | O | 226/227 (99%) | -0.48 | 3 (1%) 77 75 | 27, 41, 71, 96 | 0 |
| 3 | C | 259/261 (99%) | -0.59 | 0 100 100 | 20, 30, 50, 83 | 0 |
| 3 | P | 259/261 (99%) | -0.60 | 1 (0%) 92 91 | 23, 33, 56, 89 | 0 |
| 4 | D | 144/147 (97%) | -0.46 | 5 (3%) 44 42 | 24, 36, 63, 90 | 0 |
| 4 | Q | 144/147 (97%) | 0.73 | 17 (11%) 4 4 | 35, 53, 78, 108 | 0 |
| 5 | E | 105/109 (96%) | -0.15 | 2 (1%) 66 65 | 26, 36, 68, 109 | 0 |
| 5 | R | 105/109 (96%) | 0.33 | 6 (5%) 23 22 | 32, 45, 70, 111 | 0 |
| 6 | F | 98/98 (100%) | 0.16 | 8 (8%) 11 10 | 22, 37, 100, 118 | 0 |
| 6 | S | 98/98 (100%) | 0.42 | 9 (9%) 9 7 | 26, 43, 103, 115 | 0 |
| 7 | G | 83/85 (97%) | 0.64 | 16 (19%) 1 1 | 23, 39, 103, 112 | 0 |
| 7 | T | 83/85 (97%) | 0.71 | 17 (20%) 1 1 | 26, 45, 103, 113 | 0 |
| 8 | H | 79/85 (92%) | 0.11 | 9 (11%) 5 4 | 25, 41, 99, 105 | 0 |
| 8 | U | 79/85 (92%) | 0.62 | 13 (16%) 1 1 | 32, 48, 99, 109 | 0 |
| 9 | I | 72/73 (98%) | 0.10 | 1 (1%) 75 73 | 27, 45, 74, 83 | 0 |
| 9 | V | 72/73 (98%) | 0.43 | 7 (9%) 7 6 | 34, 56, 80, 97 | 0 |
| 10 | J | 58/59 (98%) | 0.09 | 6 (10%) 6 5 | 27, 41, 79, 106 | 0 |
| 10 | W | 58/59 (98%) | 0.34 | 4 (6%) 16 15 | 34, 49, 87, 110 | 0 |
| 11 | K | 49/56 (87%) | -0.33 | 0 100 100 | 29, 41, 57, 74 | 0 |
| 11 | X | 49/56 (87%) | 0.60 | 5 (10%) 6 6 | 44, 56, 74, 88 | 0 |
| 12 | L | 46/47 (97%) | -0.49 | 0 100 100 | 21, 32, 55, 92 | 0 |
| 12 | Y | 46/47 (97%) | -0.34 | 2 (4%) 35 33 | 34, 43, 69, 98 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | M | 43/46 (93%) | -0.19 | 3 (6%) 16 15 | 23, 32, 97, 108 | 0 |
| 13 | Z | 43/46 (93%) | 0.28 | 7 (16%) 1 1 | 39, 47, 101, 112 | 0 |
| All | All | 3550/3614 (98%) | -0.11 | 145 (4%) 37 35 | 16, 35, 74, 118 | 0 |

All (145) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | Q | 5 | VAL | 18.0 |
| 4 | Q | 6 | VAL | 15.0 |
| 6 | S | 97 | ALA | 14.6 |
| 6 | S | 96 | LEU | 14.5 |
| 4 | Q | 8 | SER | 10.8 |
| 6 | F | 98 | HIS | 10.1 |
| 6 | F | 97 | ALA | 8.9 |
| 4 | Q | 7 | LYS | 8.7 |
| 6 | F | 96 | LEU | 8.7 |
| 6 | S | 94 | HIS | 8.4 |
| 13 | Z | 43 | SER | 8.4 |
| 5 | R | 5 | HIS | 8.4 |
| 6 | S | 2 | SER | 8.3 |
| 6 | F | 1 | ALA | 8.2 |
| 8 | U | 8 | ILE | 8.1 |
| 8 | U | 7 | LYS | 8.1 |
| 6 | F | 95 | GLN | 7.7 |
| 6 | F | 2 | SER | 7.2 |
| 10 | W | 58 | LYS | 7.2 |
| 4 | Q | 35 | ALA | 7.1 |
| 7 | T | 2 | SER | 6.9 |
| 7 | T | 3 | ALA | 6.8 |
| 5 | E | 5 | HIS | 6.7 |
| 6 | S | 98 | HIS | 6.6 |
| 7 | G | 1 | ALA | 6.5 |
| 4 | Q | 4 | SER | 6.5 |
| 9 | V | 2 | THR | 6.3 |
| 7 | T | 42 | ARG | 6.2 |
| 6 | S | 1 | ALA | 6.1 |
| 10 | J | 58 | LYS | 6.1 |
| 7 | G | 40 | GLY | 6.1 |
| 7 | G | 42 | ARG | 6.0 |
| 8 | H | 45 | ALA | 5.8 |
| 7 | T | 39 | SER | 5.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7 | G | 2 | SER | 5.7 |
| 7 | G | 5 | LYS | 5.6 |
| 8 | H | 44 | THR | 5.5 |
| 7 | T | 36 | TRP | 5.4 |
| 8 | U | 44 | THR | 5.4 |
| 7 | T | 5 | LYS | 5.2 |
| 8 | H | 46 | LYS | 5.1 |
| 5 | R | 109 | VAL | 4.9 |
| 7 | T | 4 | ALA | 4.8 |
| 8 | H | 7 | LYS | 4.8 |
| 7 | G | 4 | ALA | 4.7 |
| 7 | G | 9 | GLY | 4.7 |
| 4 | Q | 147 | LYS | 4.6 |
| 8 | U | 9 | LYS | 4.6 |
| 9 | I | 37 | PHE | 4.6 |
| 3 | P | 3 | HIS | 4.6 |
| 2 | O | 113 | TYR | 4.6 |
| 8 | H | 47 | GLY | 4.5 |
| 7 | G | 3 | ALA | 4.5 |
| 8 | U | 45 | ALA | 4.4 |
| 7 | T | 8 | HIS | 4.4 |
| 7 | G | 8 | HIS | 4.4 |
| 6 | S | 93 | PRO | 4.2 |
| 7 | T | 84 | LYS | 4.2 |
| 13 | Z | 39 | ASN | 4.2 |
| 6 | F | 94 | HIS | 4.1 |
| 11 | X | 6 | ALA | 4.1 |
| 6 | S | 95 | GLN | 4.0 |
| 10 | J | 1 | PHE | 4.0 |
| 7 | T | 41 | HIS | 4.0 |
| 2 | O | 227 | LEU | 3.9 |
| 4 | Q | 39 | ALA | 3.9 |
| 13 | M | 40 | TYR | 3.9 |
| 13 | Z | 41 | LYS | 3.9 |
| 8 | U | 47 | GLY | 3.9 |
| 13 | Z | 37 | LEU | 3.9 |
| 9 | V | 3 | ALA | 3.8 |
| 11 | X | 13 | TYR | 3.8 |
| 13 | Z | 40 | TYR | 3.6 |
| 4 | Q | 51 | LEU | 3.6 |
| 10 | W | 48 | TYR | 3.5 |
| 7 | T | 40 | GLY | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8 | H | 48 | GLY | 3.4 |
| 7 | T | 1 | ALA | 3.3 |
| 1 | N | 513 | LEU | 3.3 |
| 8 | H | 43 | MET | 3.2 |
| 7 | G | 41 | HIS | 3.1 |
| 13 | M | 43 | SER | 3.1 |
| 10 | J | 52 | TRP | 3.1 |
| 10 | J | 57 | HIS | 3.0 |
| 12 | Y | 47 | LYS | 3.0 |
| 5 | R | 79 | LYS | 3.0 |
| 9 | V | 36 | LYS | 2.9 |
| 10 | W | 52 | TRP | 2.9 |
| 4 | D | 5 | VAL | 2.9 |
| 7 | T | 9 | GLY | 2.9 |
| 8 | U | 48 | GLY | 2.8 |
| 7 | G | 6 | GLY | 2.8 |
| 4 | Q | 62 | LEU | 2.8 |
| 4 | Q | 142 | LYS | 2.8 |
| 6 | F | 3 | GLY | 2.7 |
| 9 | V | 25 | PHE | 2.7 |
| 7 | G | 84 | LYS | 2.7 |
| 8 | U | 50 | VAL | 2.7 |
| 4 | D | 6 | VAL | 2.7 |
| 2 | O | 226 | MET | 2.7 |
| 4 | Q | 58 | GLU | 2.6 |
| 7 | T | 7 | ASP | 2.6 |
| 2 | B | 59 | GLN | 2.6 |
| 5 | R | 52 | LEU | 2.6 |
| 9 | V | 37 | PHE | 2.6 |
| 7 | G | 36 | TRP | 2.6 |
| 10 | J | 2 | GLU | 2.6 |
| 11 | X | 9 | PHE | 2.5 |
| 8 | U | 85 | ILE | 2.5 |
| 10 | W | 4 | ARG | 2.5 |
| 8 | H | 8 | ILE | 2.5 |
| 4 | Q | 102 | TYR | 2.5 |
| 6 | S | 3 | GLY | 2.5 |
| 8 | U | 43 | MET | 2.4 |
| 12 | Y | 20 | ARG | 2.4 |
| 7 | G | 43 | GLU | 2.3 |
| 8 | U | 51 | SER | 2.3 |
| 7 | T | 10 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | V | 34 | PHE | 2.3 |
| 7 | G | 7 | ASP | 2.3 |
| 4 | D | 147 | LYS | 2.3 |
| 1 | N | 48 | LEU | 2.3 |
| 13 | M | 39 | ASN | 2.3 |
| 5 | R | 96 | LEU | 2.2 |
| 4 | Q | 55 | GLU | 2.2 |
| 4 | D | 7 | LYS | 2.2 |
| 4 | Q | 136 | ALA | 2.2 |
| 4 | Q | 48 | TRP | 2.2 |
| 5 | E | 109 | VAL | 2.1 |
| 4 | D | 8 | SER | 2.1 |
| 11 | X | 7 | PRO | 2.1 |
| 13 | Z | 42 | LYS | 2.1 |
| 5 | R | 16 | VAL | 2.1 |
| 11 | X | 34 | THR | 2.1 |
| 7 | G | 45 | PRO | 2.1 |
| 8 | U | 10 | ASN | 2.1 |
| 1 | A | 241 | PRO | 2.1 |
| 7 | T | 6 | GLY | 2.0 |
| 8 | U | 49 | ASP | 2.0 |
| 4 | Q | 73 | ARG | 2.0 |
| 13 | Z | 35 | TYR | 2.0 |
| 9 | V | 4 | LEU | 2.0 |
| 8 | H | 49 | ASP | 2.0 |
| 10 | J | 4 | ARG | 2.0 |
| 7 | T | 38 | HIS | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 7 | TPO | T | 11 | 11/12 | 0.48 | 0.29 | 87,93,112,113 | 0 |
| 9 | SAC | V | 1 | 9/10 | 0.49 | 0.64 | 101,107,109,110 | 0 |
| 7 | TPO | G | 11 | 11/12 | 0.55 | 0.32 | 89,96,117,119 | 0 |
| 9 | SAC | I | 1 | 9/10 | 0.80 | 0.27 | 89,93,96,97 | 0 |
| 1 | FME | A | 1 | 10/11 | 0.87 | 0.14 | 50,60,76,86 | 0 |
| 1 | FME | N | 1 | 10/11 | 0.92 | 0.21 | 57,61,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | FME | B | 1 | 10/11 | 0.95 | 0.13 | 25,33,44,53 | 0 |
| 2 | FME | O | 1 | 10/11 | 0.95 | 0.14 | 40,42,47,54 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|---------|------|------|-----------------------------|-------|
| 26 | PEK | T | 101 | 53/53 | 0.47 | 0.46 | 50,90,115,120 | 0 |
| 26 | PEK | G | 102 | 53/53 | 0.54 | 0.41 | 50,89,115,120 | 0 |
| 26 | PEK | C | 306 | 53/53 | 0.55 | 0.30 | 46,91,115,120 | 0 |
| 21 | PSC | B | 303 | 52/52 | 0.57 | 0.35 | 47,90,120,120 | 0 |
| 27 | CDL | T | 102 | 100/100 | 0.62 | 0.35 | 47,86,112,120 | 0 |
| 27 | CDL | G | 101 | 100/100 | 0.64 | 0.34 | 55,88,111,120 | 0 |
| 24 | DMU | P | 302 | 33/33 | 0.64 | 0.41 | 91,116,120,120 | 0 |
| 21 | PSC | O | 304 | 52/52 | 0.64 | 0.39 | 48,88,120,120 | 0 |
| 24 | DMU | C | 302 | 33/33 | 0.65 | 0.41 | 88,116,120,120 | 0 |
| 26 | PEK | P | 306 | 53/53 | 0.66 | 0.35 | 40,89,110,114 | 0 |
| 25 | UNX | P | 303 | 1/1 | 0.67 | 0.26 | 50,50,50,50 | 0 |
| 20 | TGL | N | 606 | 63/63 | 0.68 | 0.34 | 39,68,86,88 | 0 |
| 18 | PGV | P | 308 | 51/51 | 0.68 | 0.39 | 66,90,112,116 | 0 |
| 18 | PGV | C | 308 | 51/51 | 0.69 | 0.39 | 61,87,113,116 | 0 |
| 20 | TGL | N | 607 | 63/63 | 0.73 | 0.22 | 48,69,85,92 | 0 |
| 20 | TGL | D | 201 | 63/63 | 0.74 | 0.25 | 45,70,82,87 | 0 |
| 27 | CDL | P | 309 | 100/100 | 0.74 | 0.39 | 37,90,108,118 | 0 |
| 18 | PGV | A | 606 | 51/51 | 0.75 | 0.30 | 32,75,113,120 | 0 |
| 27 | CDL | C | 309 | 100/100 | 0.75 | 0.36 | 43,92,103,109 | 0 |
| 22 | CHD | W | 101 | 29/29 | 0.75 | 0.34 | 89,100,103,108 | 0 |
| 25 | UNX | C | 303 | 1/1 | 0.75 | 0.39 | 45,45,45,45 | 0 |
| 20 | TGL | O | 303 | 63/63 | 0.76 | 0.26 | 46,70,91,96 | 0 |
| 20 | TGL | L | 101 | 63/63 | 0.76 | 0.29 | 36,67,81,84 | 0 |
| 16 | NA | A | 603 | 1/1 | 0.78 | 0.20 | 44,44,44,44 | 0 |
| 18 | PGV | N | 608 | 51/51 | 0.79 | 0.36 | 38,80,114,119 | 0 |
| 16 | NA | N | 603 | 1/1 | 0.81 | 0.19 | 50,50,50,50 | 0 |

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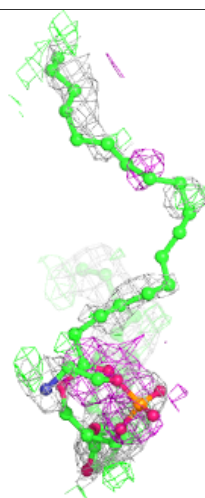
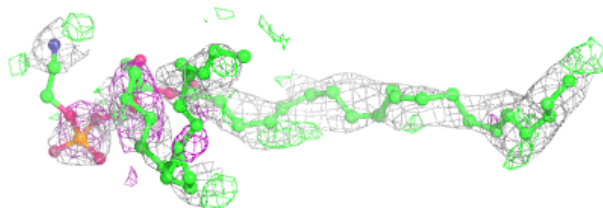
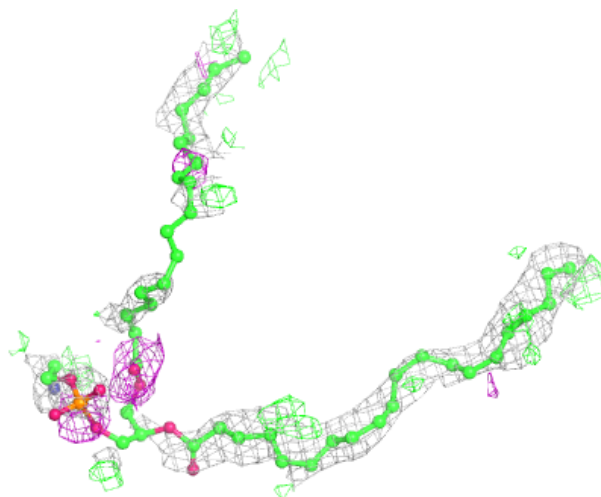
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22 | CHD | J | 101 | 29/29 | 0.81 | 0.37 | 91,99,104,107 | 0 |
| 24 | DMU | Z | 101 | 33/33 | 0.82 | 0.33 | 50,72,86,92 | 0 |
| 20 | TGL | B | 302 | 63/63 | 0.82 | 0.22 | 41,67,89,94 | 0 |
| 22 | CHD | C | 310 | 29/29 | 0.84 | 0.26 | 75,92,97,101 | 0 |
| 24 | DMU | M | 101 | 33/33 | 0.85 | 0.20 | 45,63,80,87 | 0 |
| 22 | CHD | P | 310 | 29/29 | 0.85 | 0.24 | 78,91,94,99 | 0 |
| 23 | DCW | C | 301 | 16/16 | 0.90 | 0.17 | 46,50,53,54 | 0 |
| 23 | DCW | P | 301 | 16/16 | 0.93 | 0.15 | 52,59,70,70 | 0 |
| 26 | PEK | P | 305 | 53/53 | 0.94 | 0.14 | 24,46,73,77 | 0 |
| 15 | MG | N | 602 | 1/1 | 0.94 | 0.16 | 35,35,35,35 | 0 |
| 26 | PEK | C | 305 | 53/53 | 0.95 | 0.13 | 17,43,71,73 | 0 |
| 15 | MG | A | 602 | 1/1 | 0.95 | 0.17 | 23,23,23,23 | 0 |
| 18 | PGV | P | 307 | 51/51 | 0.96 | 0.13 | 23,36,68,73 | 0 |
| 22 | CHD | P | 304 | 29/29 | 0.96 | 0.12 | 25,32,40,46 | 0 |
| 18 | PGV | C | 307 | 51/51 | 0.96 | 0.12 | 22,33,65,72 | 0 |
| 22 | CHD | B | 304 | 29/29 | 0.97 | 0.08 | 20,27,34,38 | 0 |
| 18 | PGV | A | 607 | 51/51 | 0.97 | 0.15 | 22,41,66,76 | 0 |
| 22 | CHD | O | 302 | 29/29 | 0.97 | 0.10 | 17,29,37,40 | 0 |
| 18 | PGV | N | 609 | 51/51 | 0.97 | 0.14 | 25,43,64,77 | 0 |
| 22 | CHD | C | 304 | 29/29 | 0.97 | 0.12 | 25,31,37,39 | 0 |
| 19 | CUA | O | 301 | 2/2 | 0.98 | 0.10 | 36,36,36,36 | 0 |
| 17 | HEA | A | 605 | 60/60 | 0.98 | 0.16 | 10,24,31,33 | 0 |
| 17 | HEA | N | 605 | 60/60 | 0.98 | 0.17 | 16,27,34,36 | 0 |
| 17 | HEA | N | 604 | 60/60 | 0.98 | 0.17 | 20,32,50,55 | 0 |
| 17 | HEA | A | 604 | 60/60 | 0.99 | 0.17 | 16,25,49,54 | 0 |
| 28 | ZN | F | 101 | 1/1 | 0.99 | 0.09 | 32,32,32,32 | 0 |
| 28 | ZN | S | 101 | 1/1 | 0.99 | 0.06 | 34,34,34,34 | 0 |
| 14 | CU | A | 601 | 1/1 | 0.99 | 0.12 | 23,23,23,23 | 0 |
| 19 | CUA | B | 301 | 2/2 | 0.99 | 0.14 | 24,24,24,27 | 0 |
| 14 | CU | N | 601 | 1/1 | 0.99 | 0.15 | 28,28,28,28 | 0 |

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.

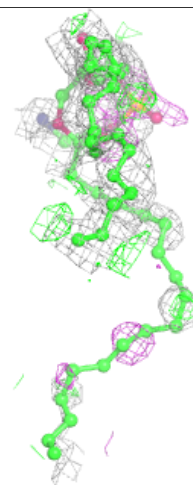
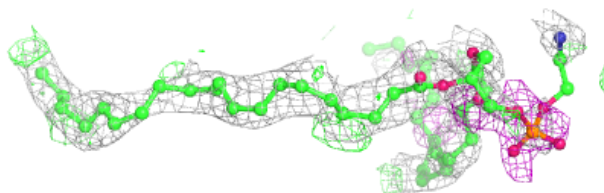
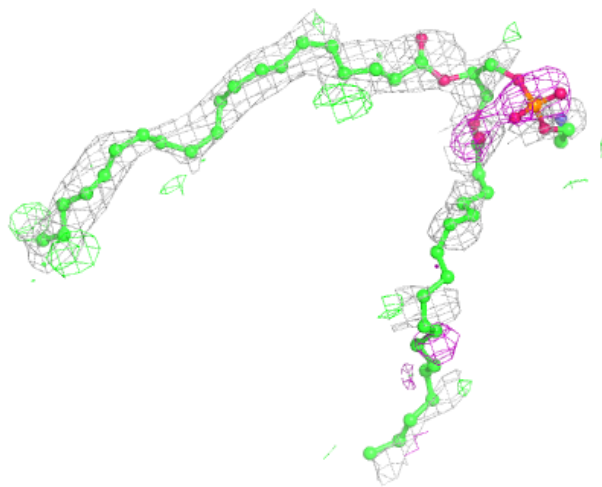
Electron density around PEK T 101:

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



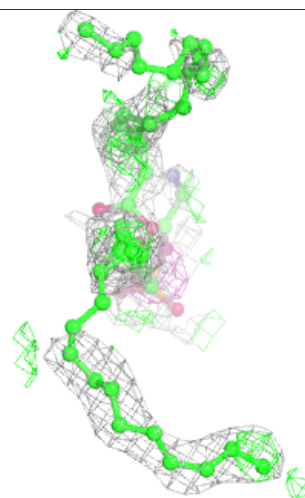
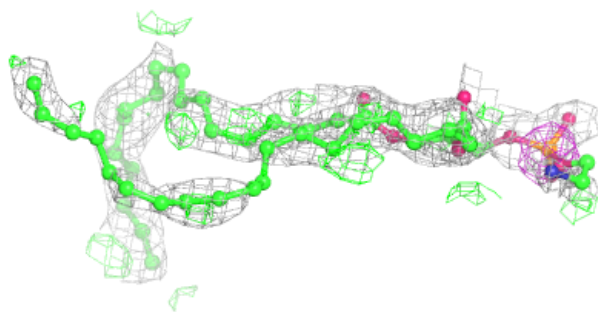
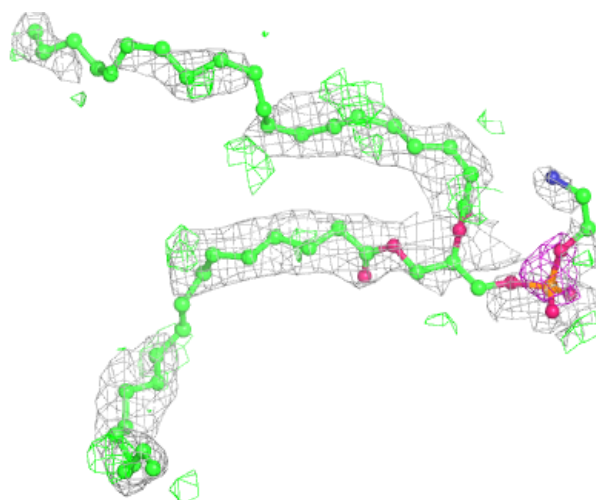
Electron density around PEK G 102:

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



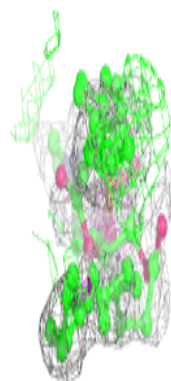
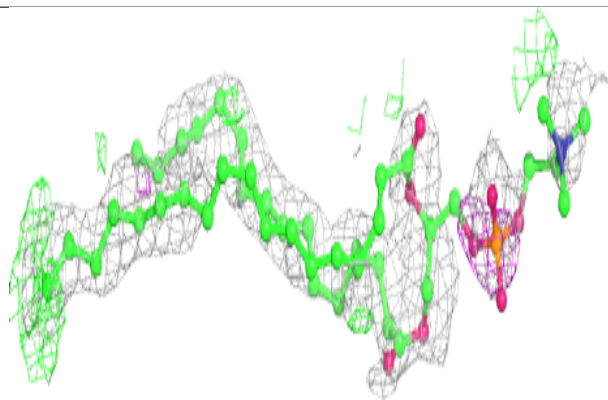
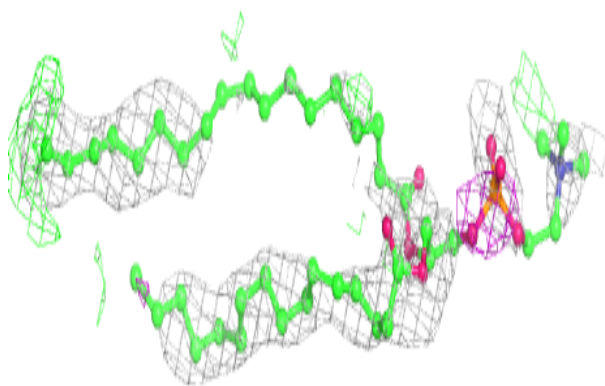
Electron density around PEK C 306:

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

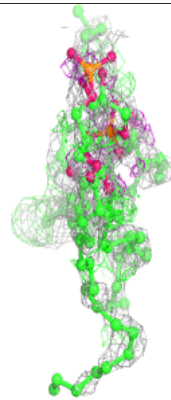
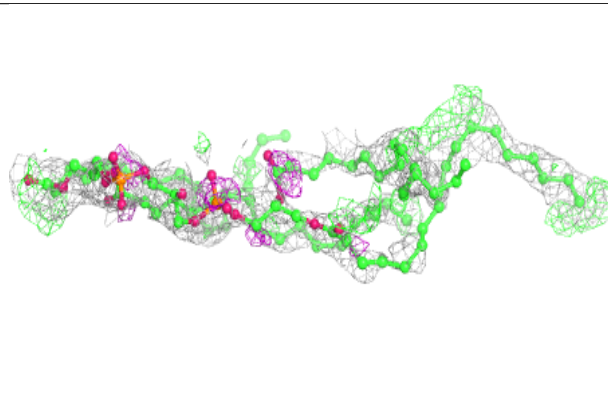
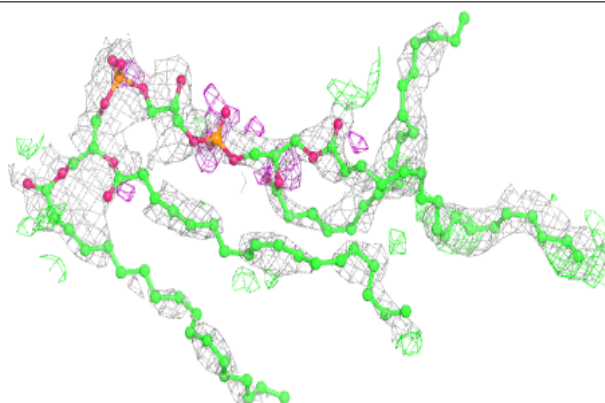


Electron density around PSC B 303:

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

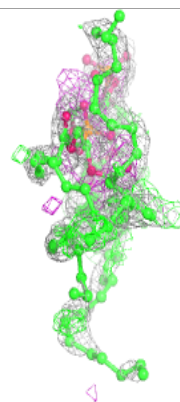
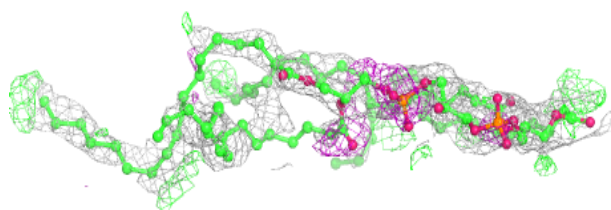
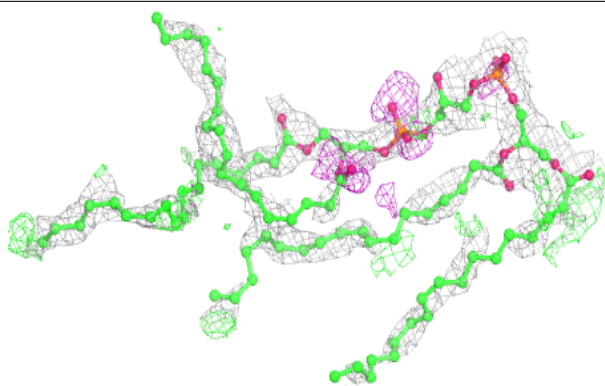
**Electron density around CDL T 102:**

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

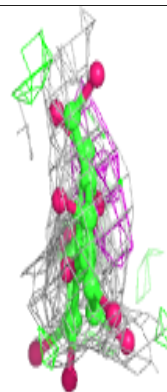
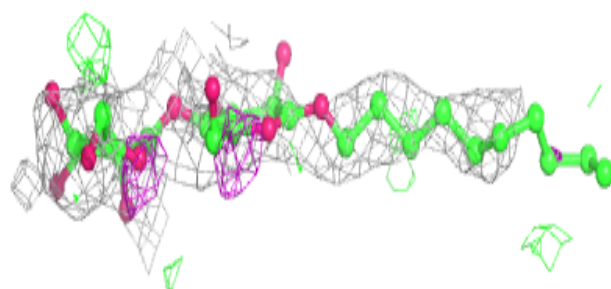
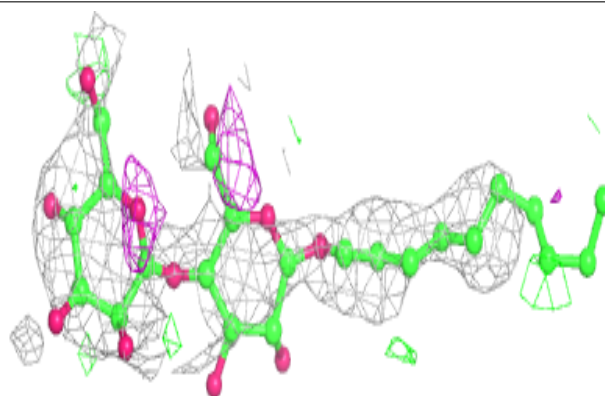


Electron density around CDL G 101:

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

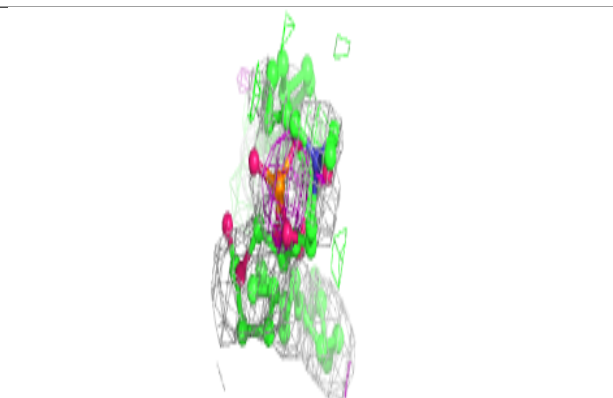
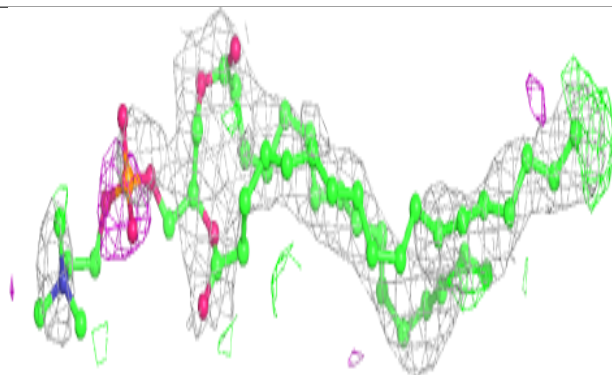
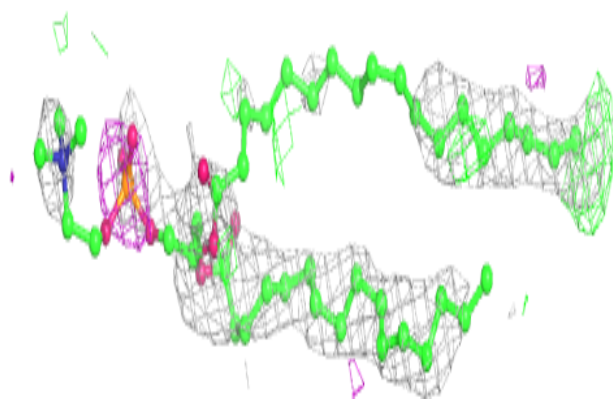
**Electron density around DMU P 302:**

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

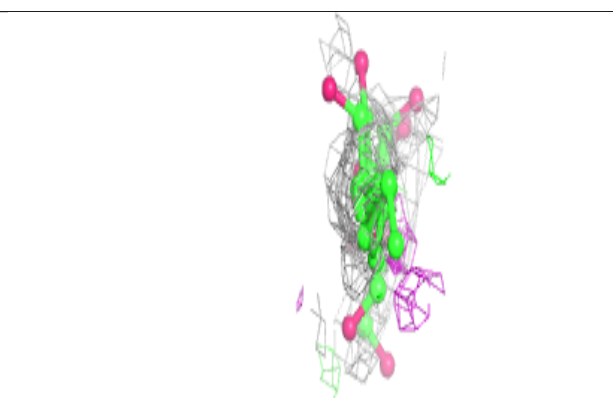
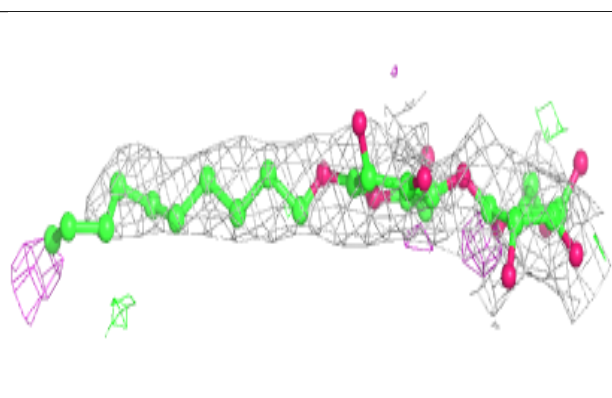
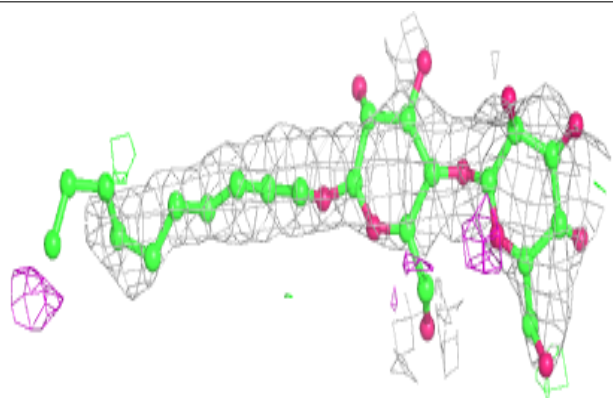


Electron density around PSC O 304:

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

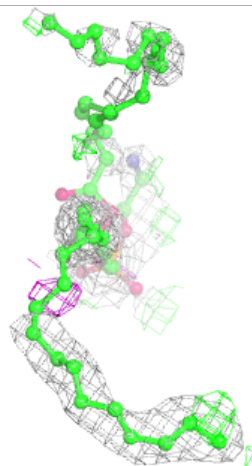
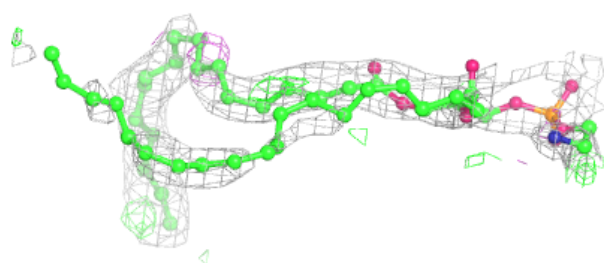
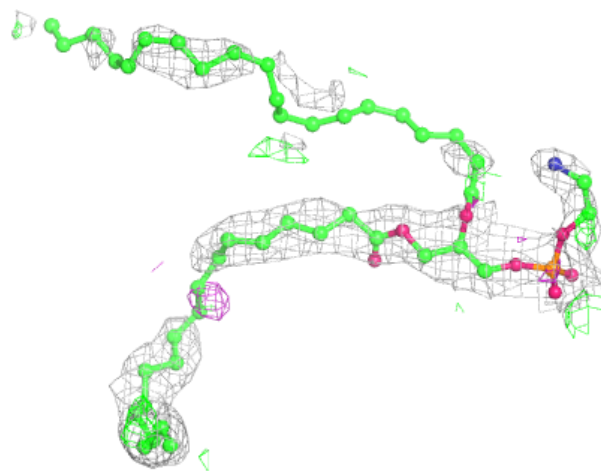
**Electron density around DMU C 302:**

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



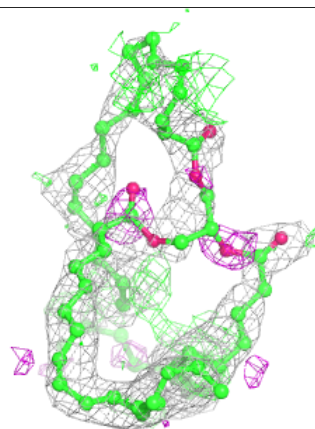
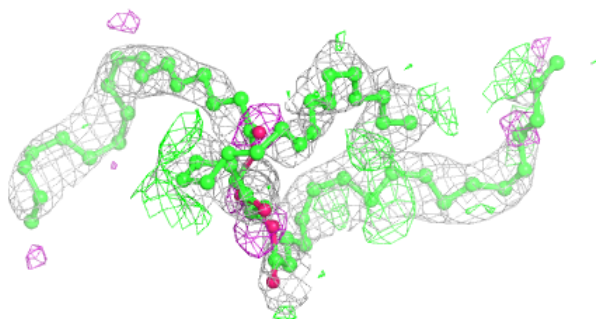
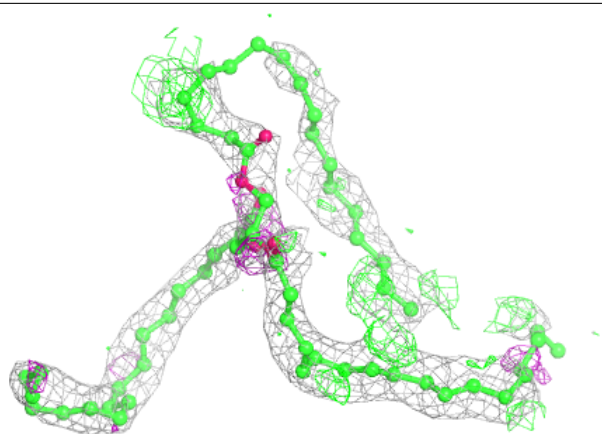
Electron density around PEK P 306:

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

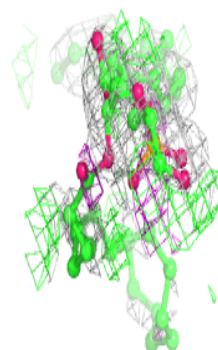
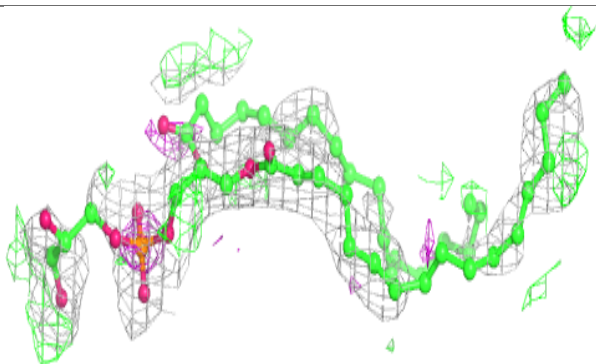
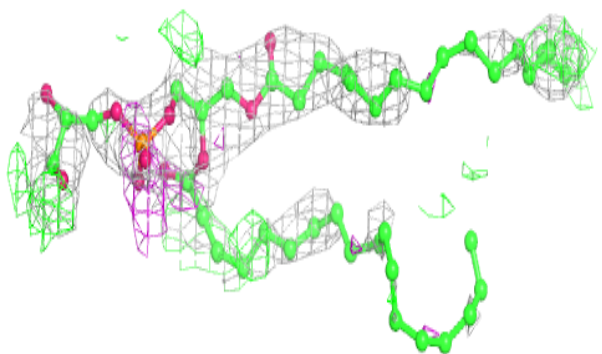


Electron density around TGL N 606:

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

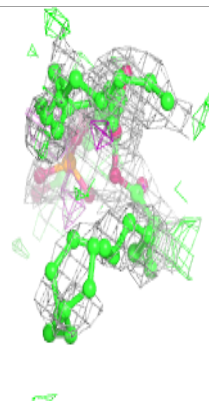
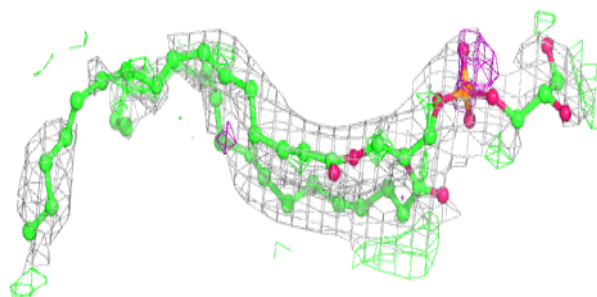
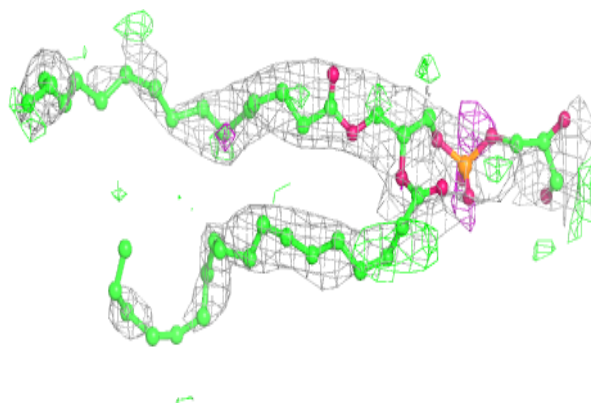
**Electron density around PGV P 308:**

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

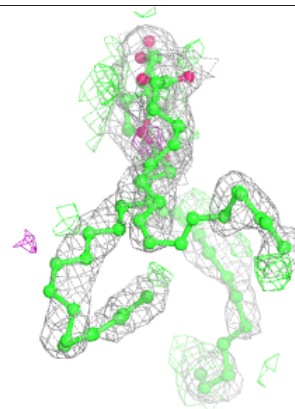
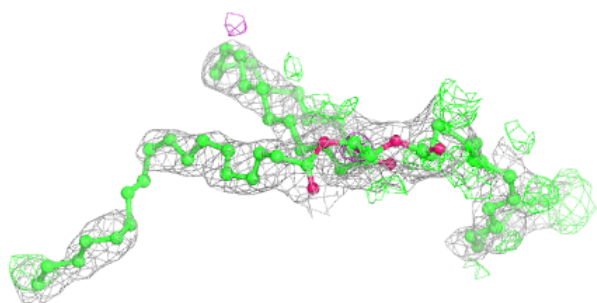
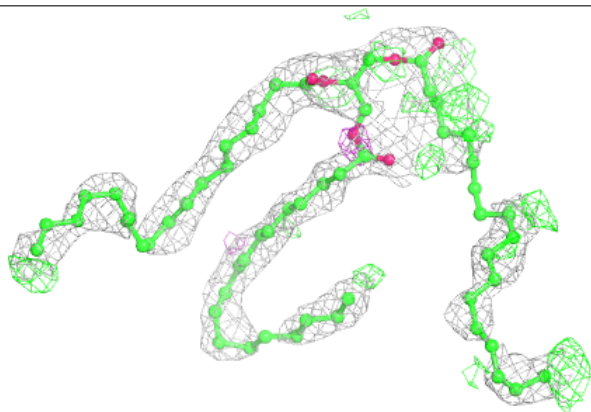


Electron density around PGV C 308:

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

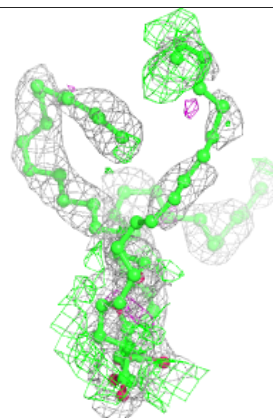
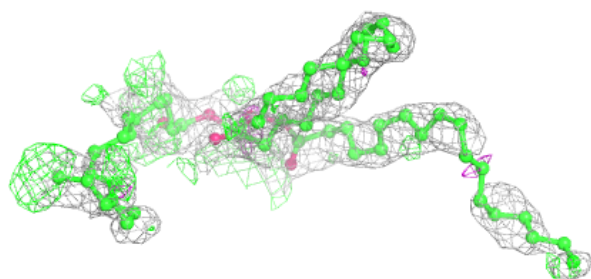
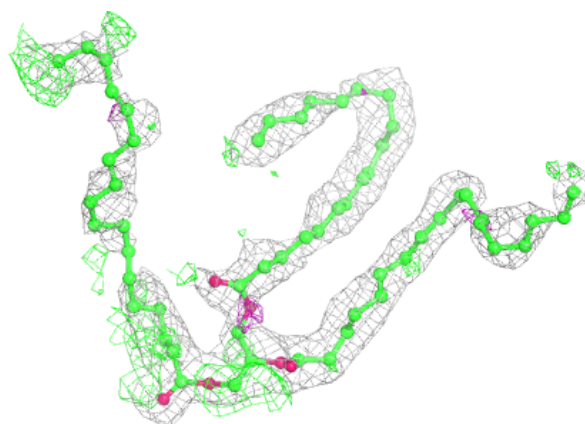
**Electron density around TGL N 607:**

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



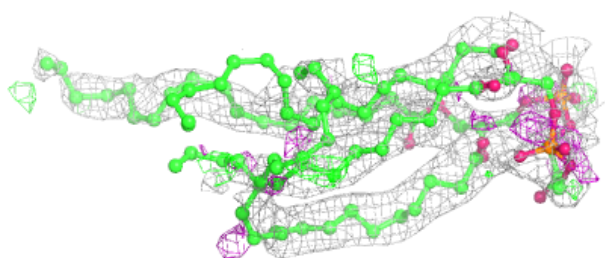
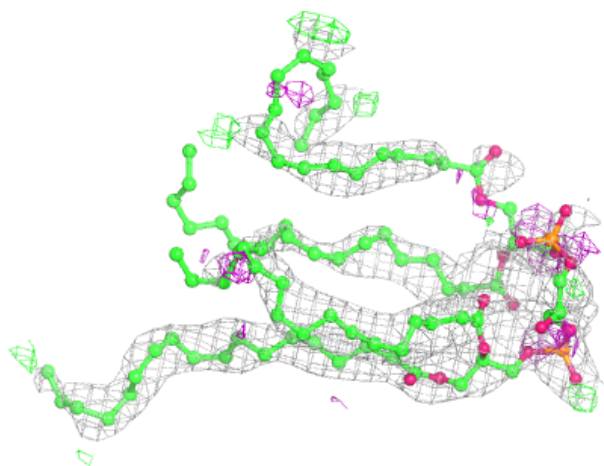
Electron density around TGL D 201:

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



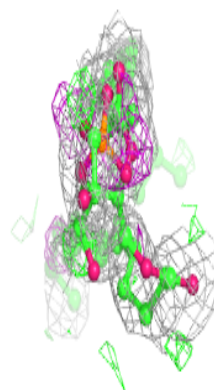
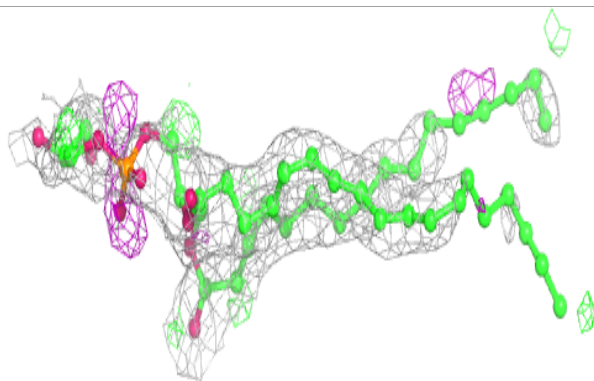
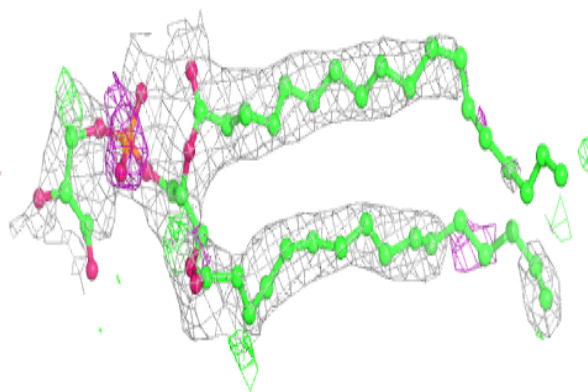
Electron density around CDL P 309:

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



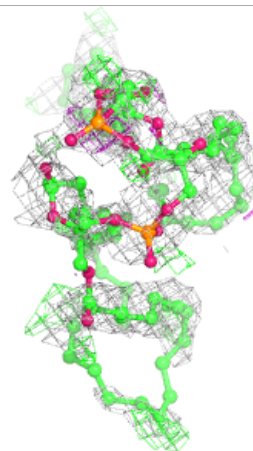
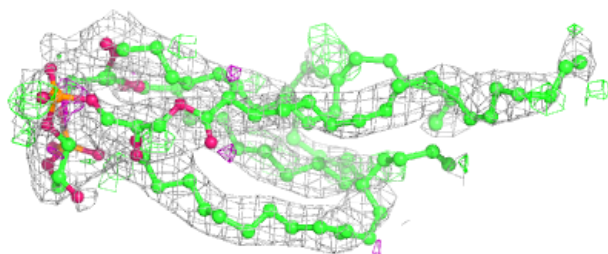
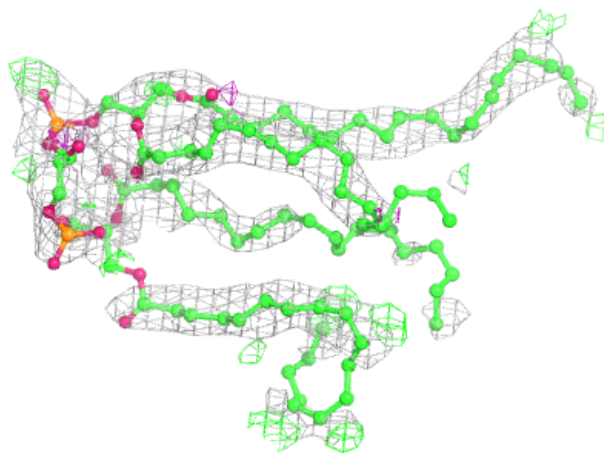
Electron density around PGV A 606:

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



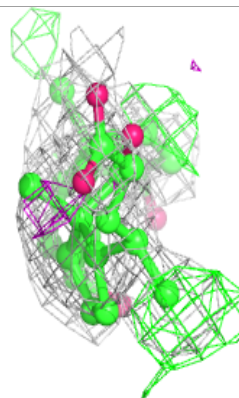
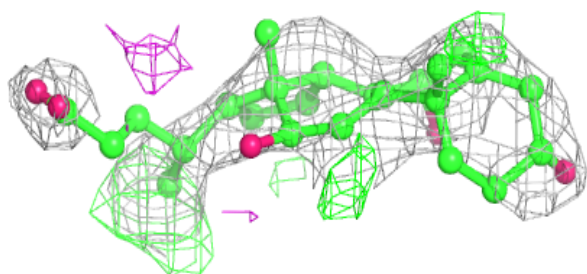
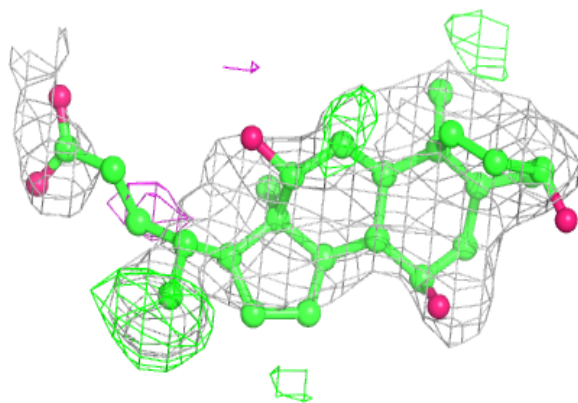
Electron density around CDL C 309:

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

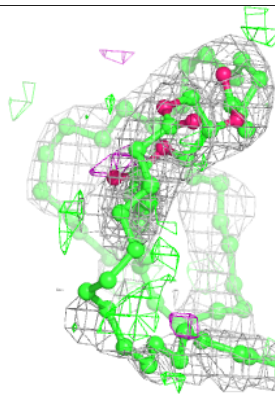
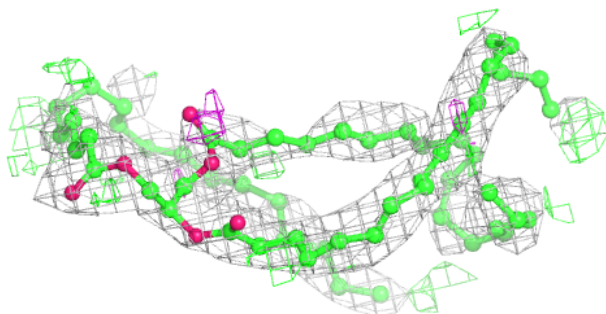
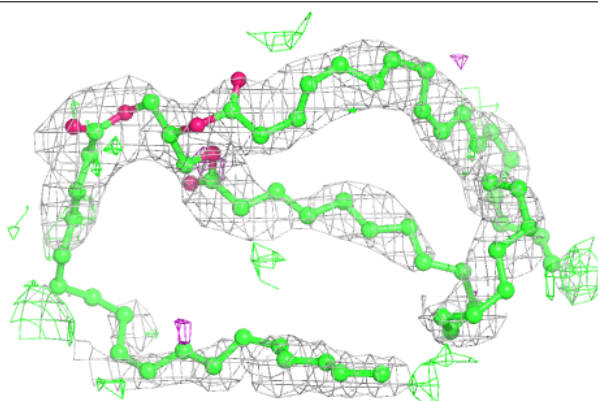


Electron density around CHD W 101:

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

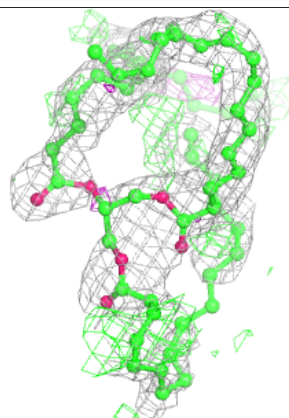
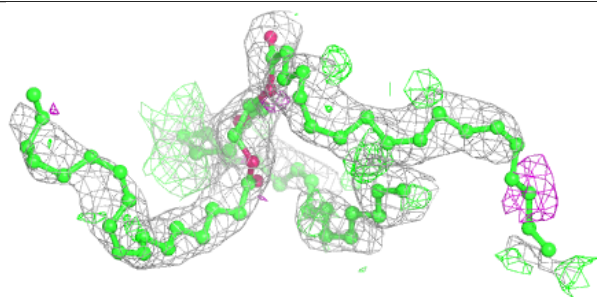
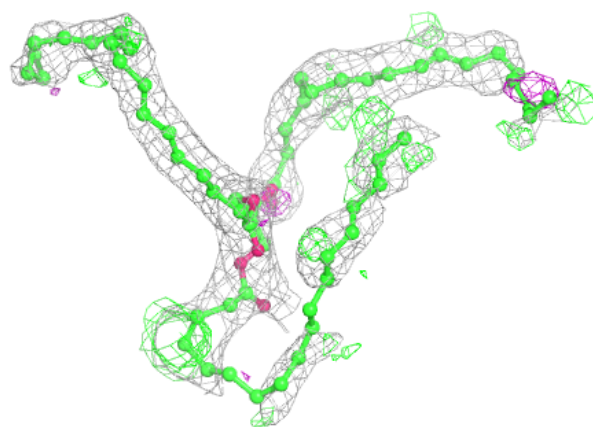
**Electron density around TGL O 303:**

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

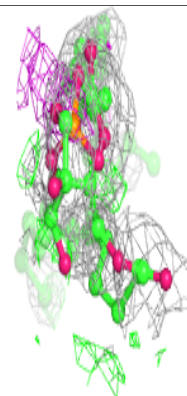
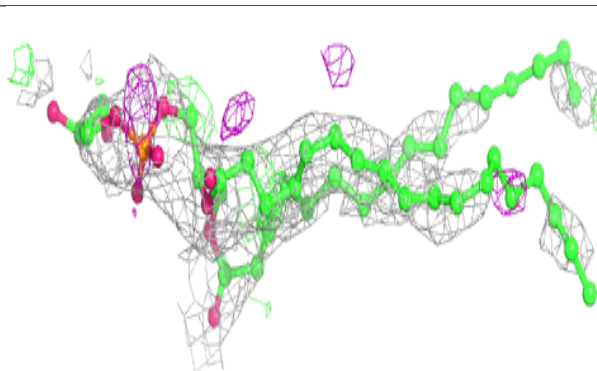
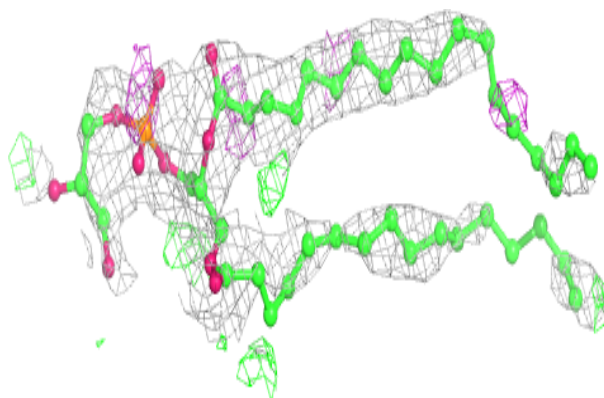


Electron density around TGL L 101:

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

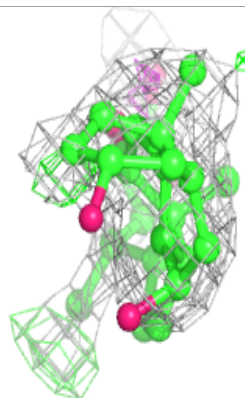
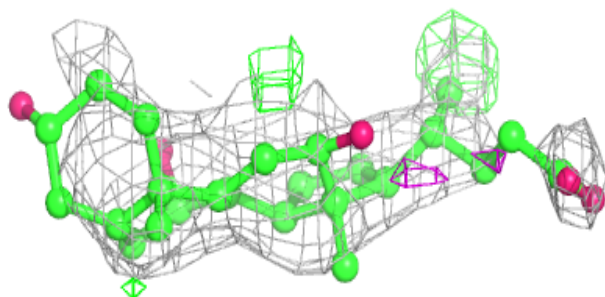
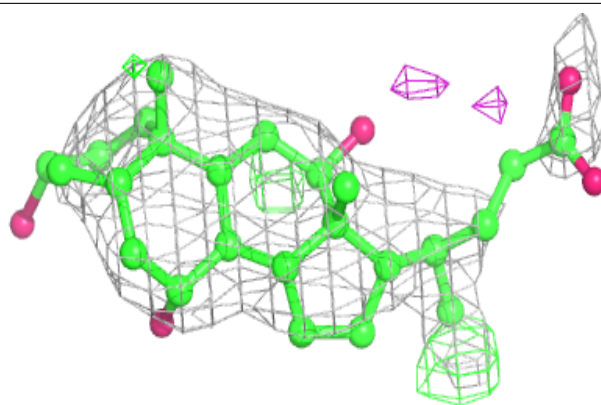
**Electron density around PGV N 608:**

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

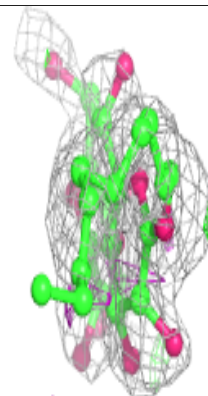
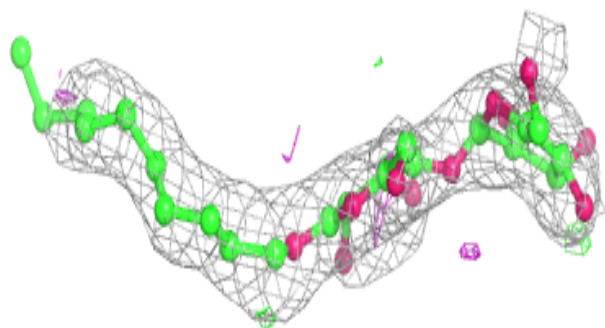
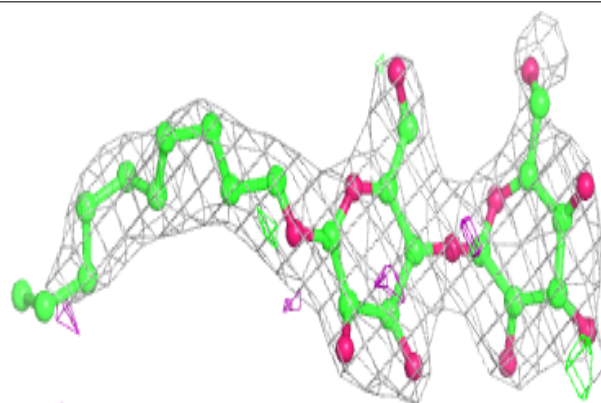


Electron density around CHD J 101:

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

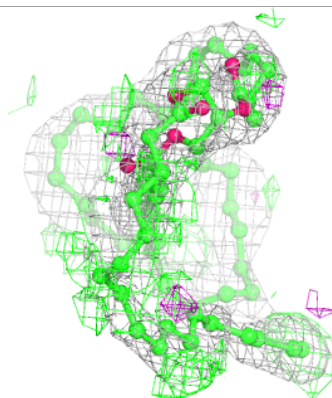
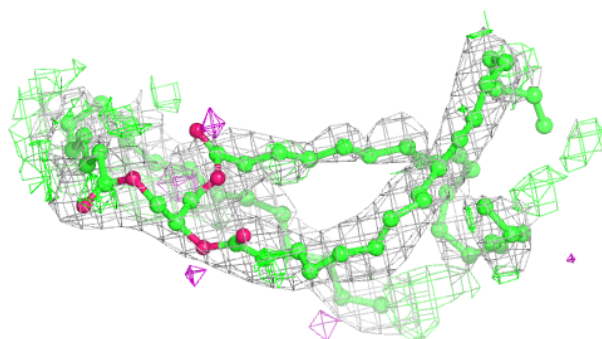
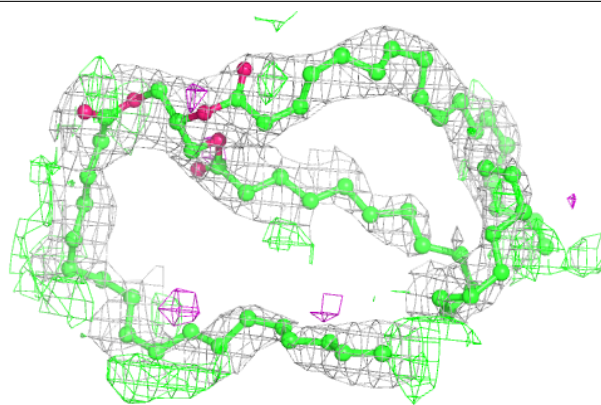
**Electron density around DMU Z 101:**

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

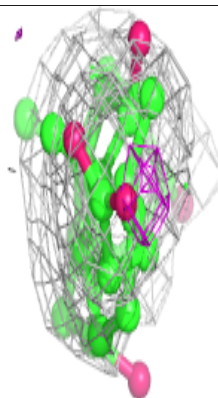
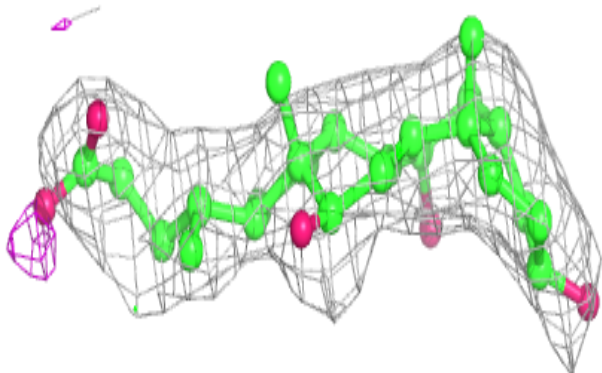
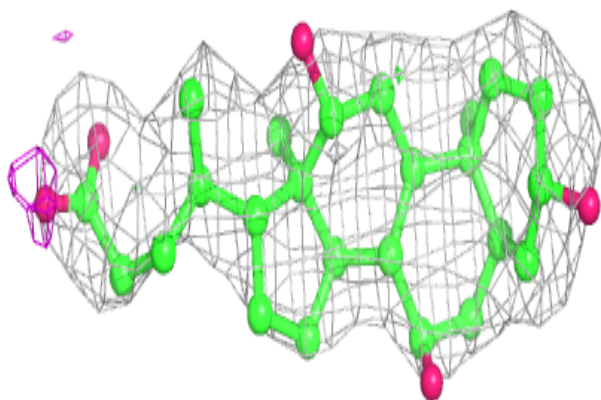


Electron density around TGL B 302:

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

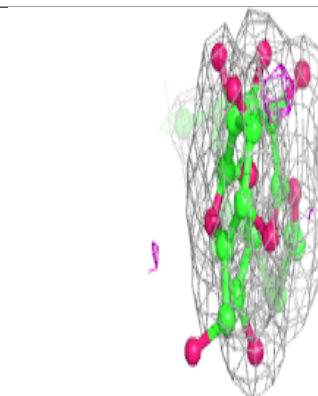
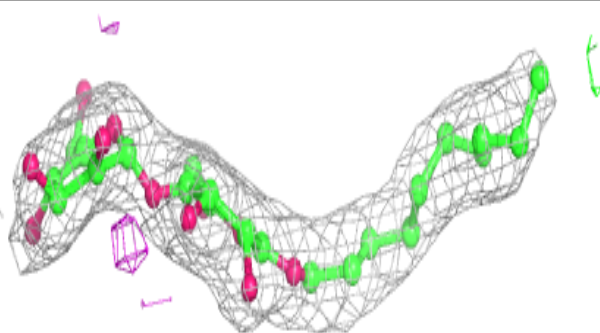
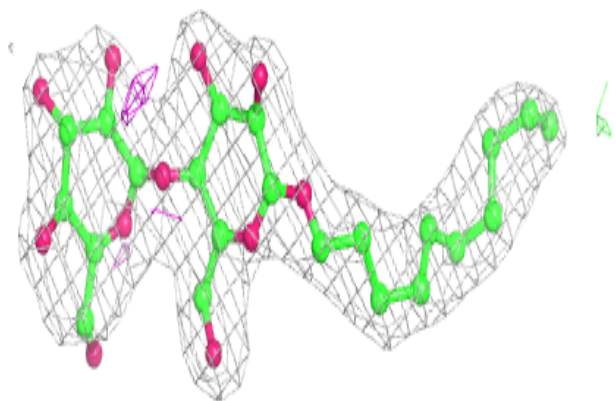
**Electron density around CHD C 310:**

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

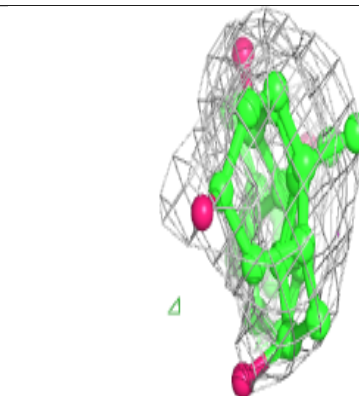
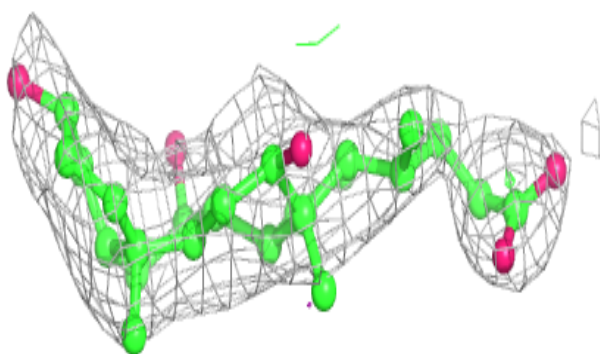
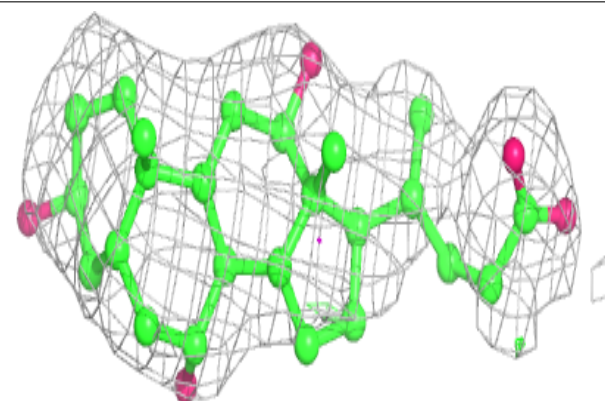


Electron density around DMU M 101:

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

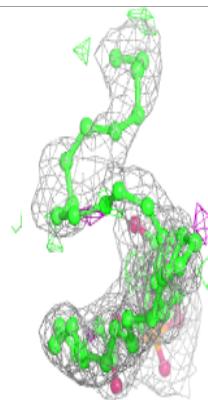
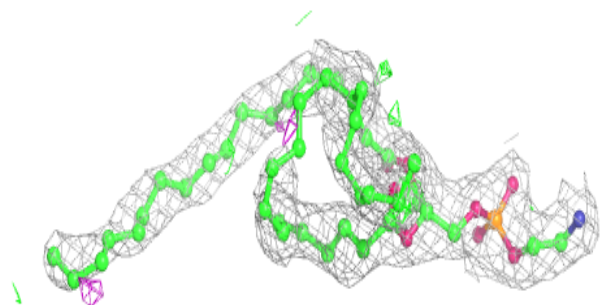
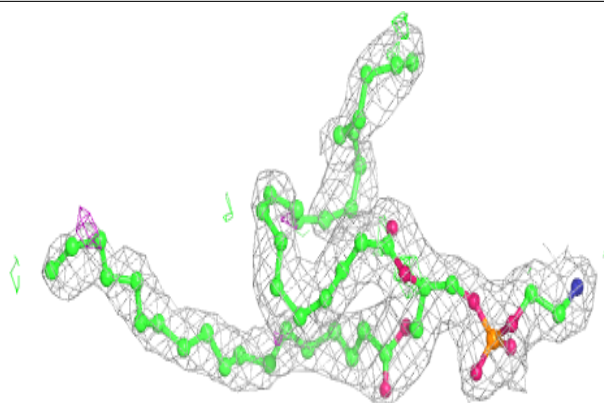
**Electron density around CHD P 310:**

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

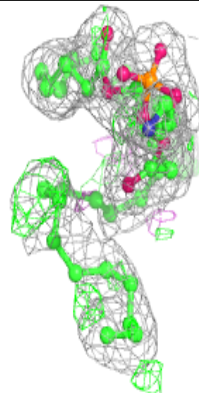
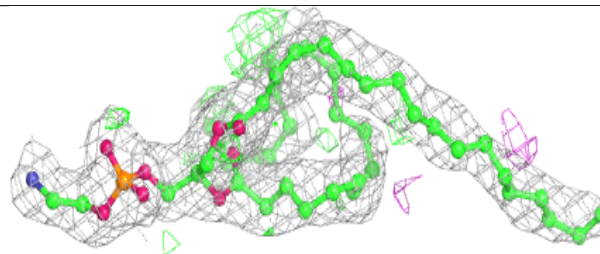
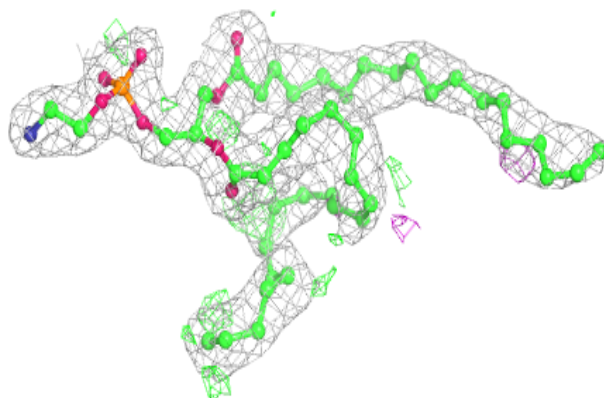


Electron density around PEK P 305:

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

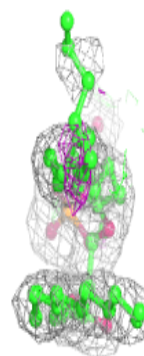
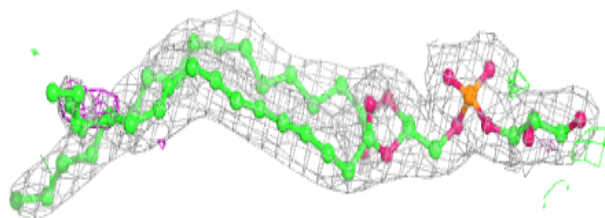
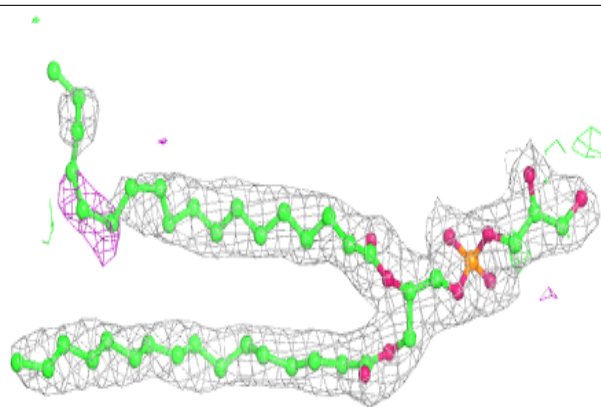
**Electron density around PEK C 305:**

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

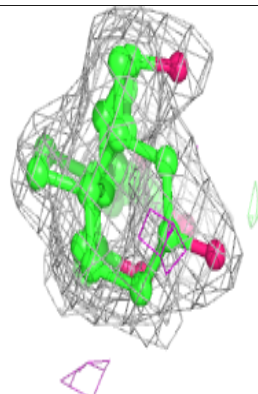
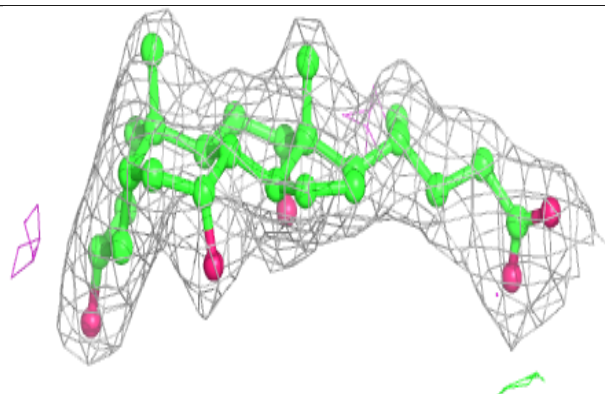
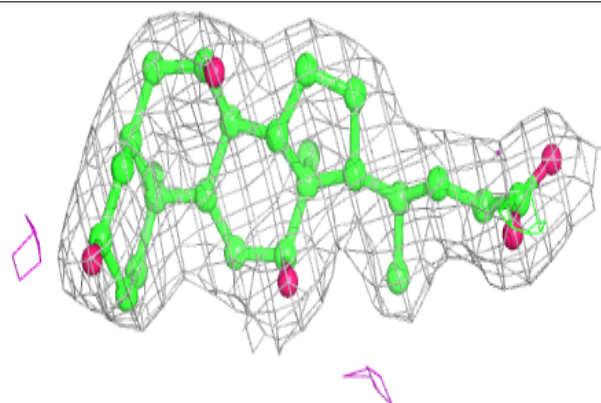


Electron density around PGV P 307:

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

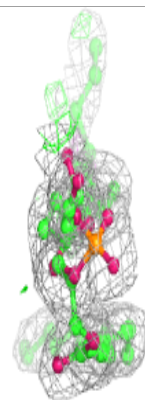
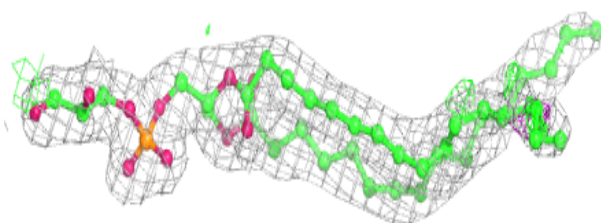
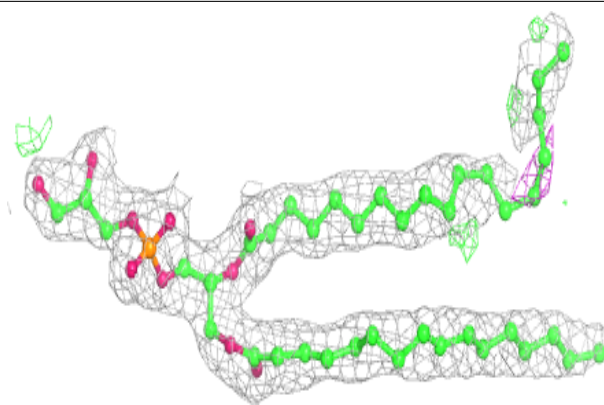
**Electron density around CHD P 304:**

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

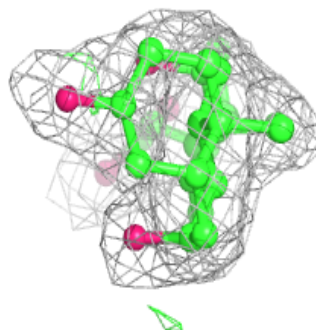
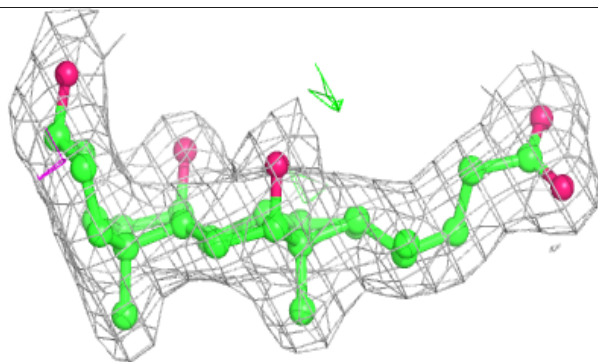
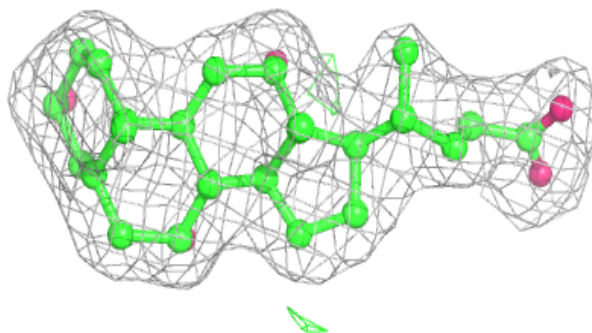


Electron density around PGV C 307:

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

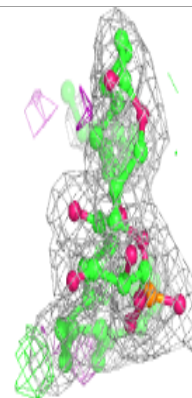
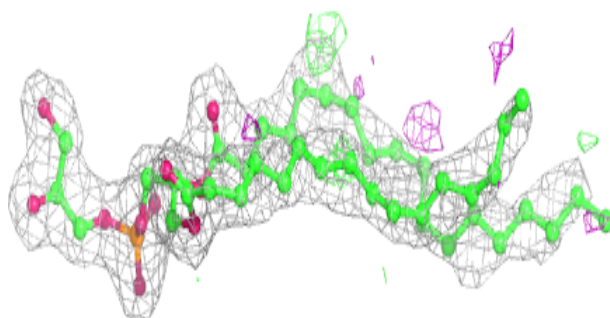
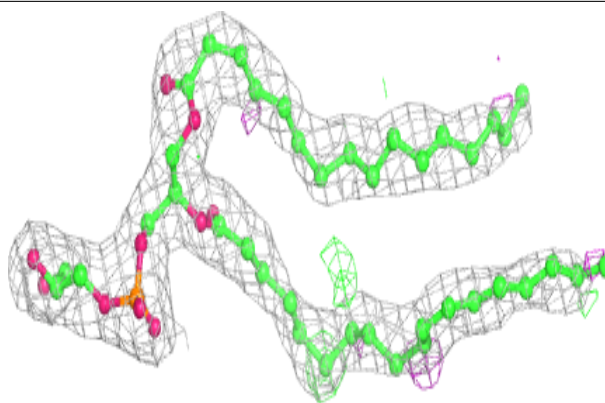
**Electron density around CHD B 304:**

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

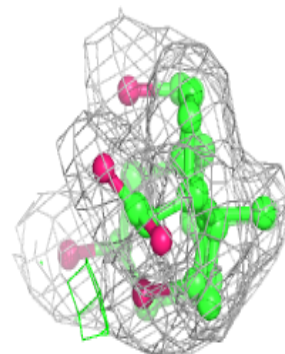
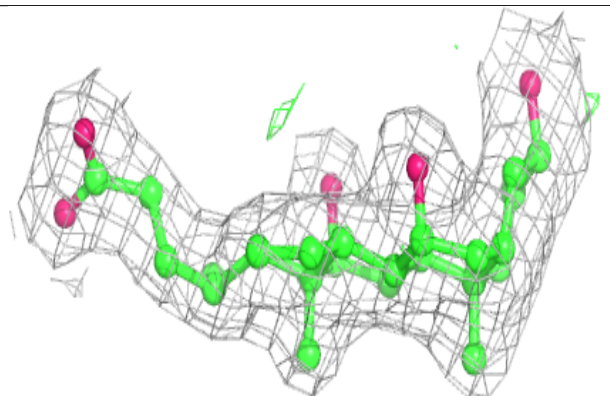
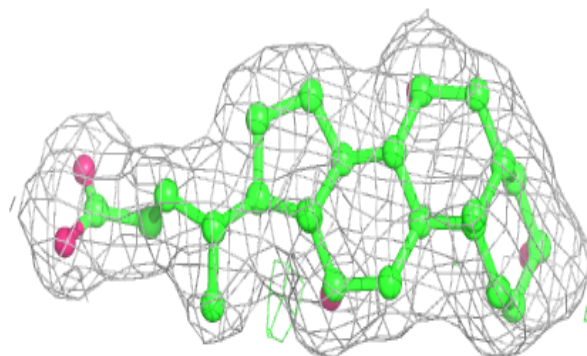


Electron density around PGV A 607:

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

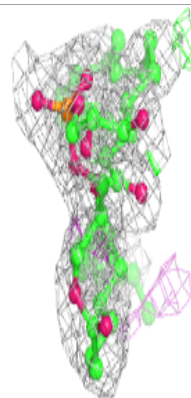
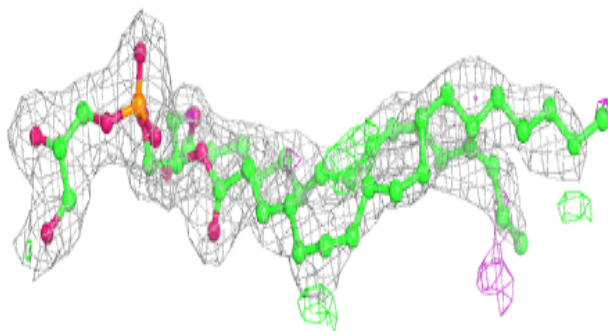
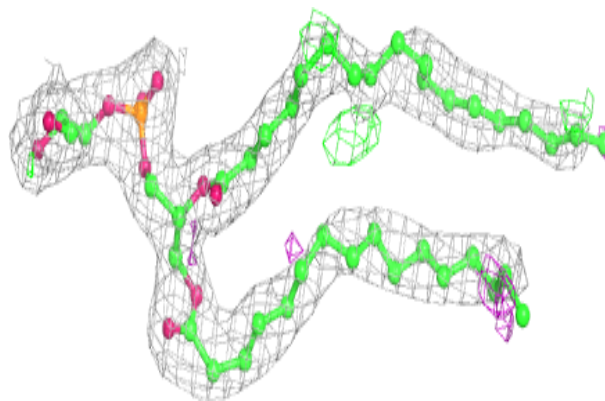
**Electron density around CHD O 302:**

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

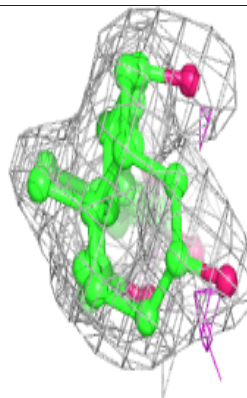
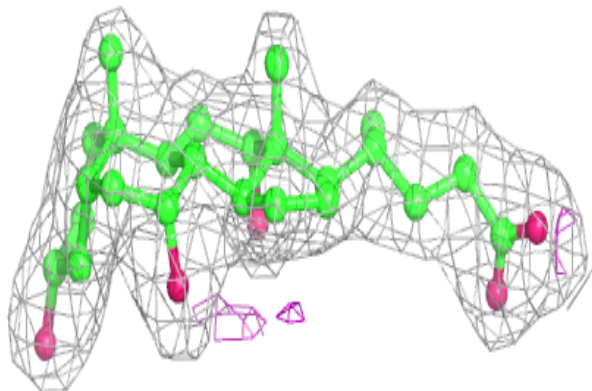
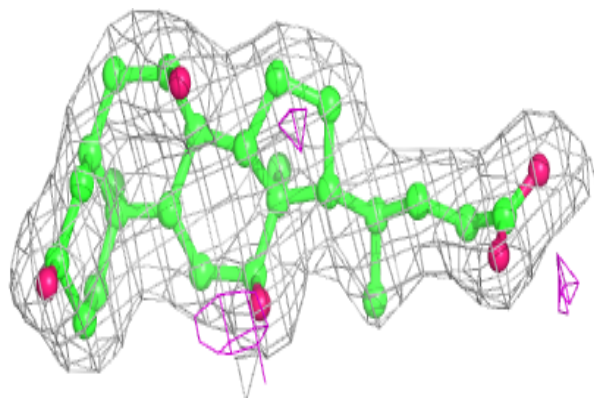


Electron density around PGV N 609:

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

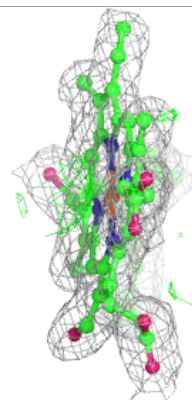
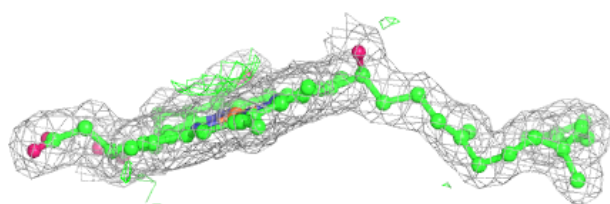
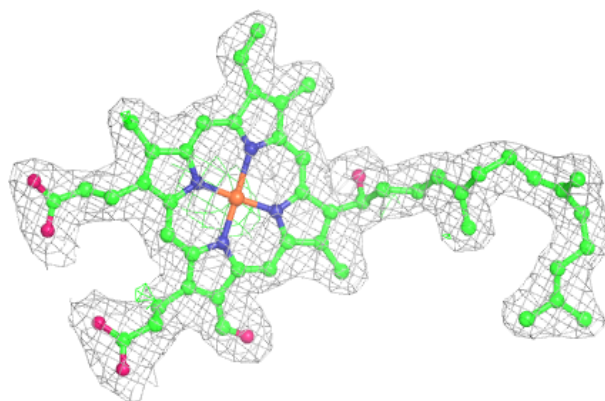
**Electron density around CHD C 304:**

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

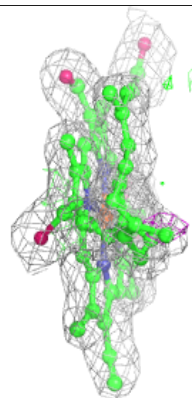
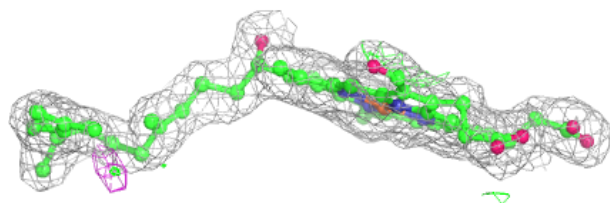
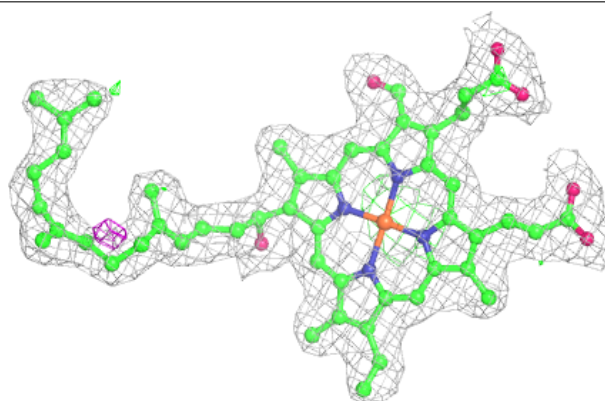


Electron density around HEA A 605:

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

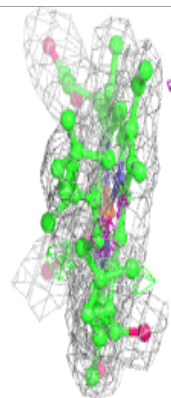
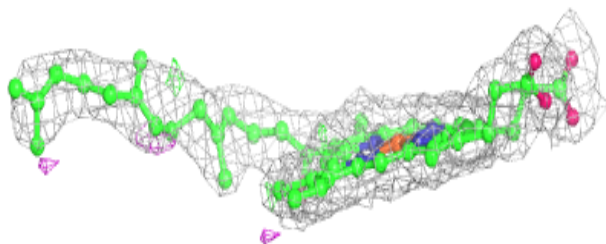
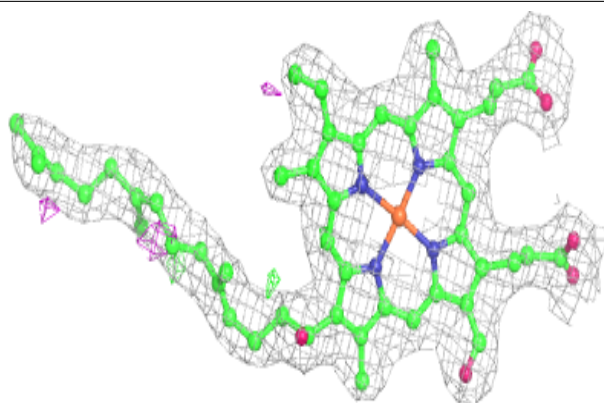
**Electron density around HEA N 605:**

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

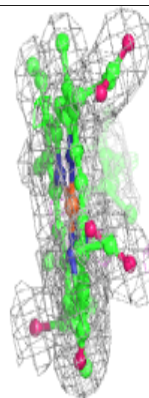
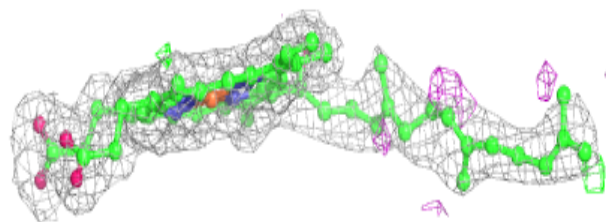
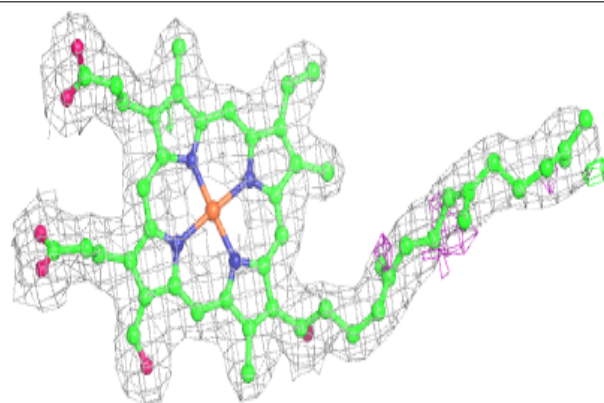


Electron density around HEA N 604:

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

**Electron density around HEA A 604:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.