



Full wwPDB X-ray Structure Validation Report

Sep 16, 2014 – 06:37 AM EDT

PDB ID : 4KT0
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : 2013-05-19
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

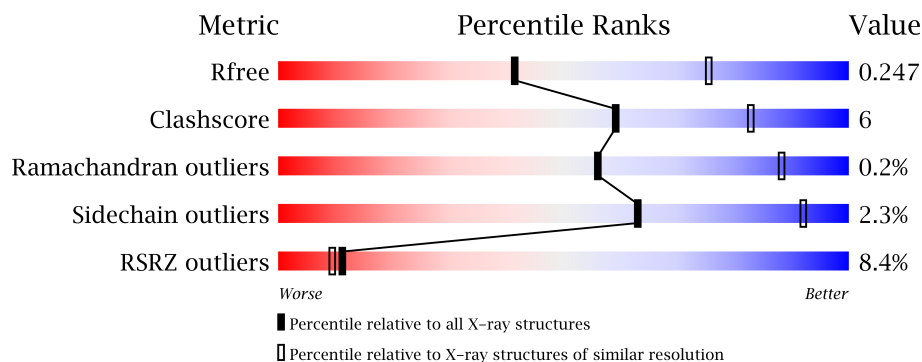
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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} | 66092 | 1799 (2.80-2.80) |
| Clashscore | 79885 | 2295 (2.80-2.80) |
| Ramachandran outliers | 78287 | 2252 (2.80-2.80) |
| Sidechain outliers | 78261 | 2254 (2.80-2.80) |
| RSRZ outliers | 66119 | 1802 (2.80-2.80) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 751 | |
| 2 | B | 731 | |
| 3 | C | 81 | |
| 4 | D | 141 | |
| 5 | E | 74 | |
| 6 | F | 165 | |
| 7 | J | 40 | |
| 8 | K | 128 | |
| 9 | M | 31 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 10 | PQN | B | 2002 | - | X |
| 11 | SF4 | A | 3001 | - | X |
| 11 | SF4 | C | 3003 | - | X |
| 12 | LHG | A | 5003 | - | X |
| 14 | BCR | A | 4002 | - | X |
| 14 | BCR | A | 4003 | - | X |
| 14 | BCR | A | 4007 | - | X |
| 14 | BCR | A | 4012 | - | X |
| 14 | BCR | B | 4006 | - | X |
| 14 | BCR | B | 4009 | - | X |
| 14 | BCR | B | 4017 | - | X |
| 14 | BCR | J | 4013 | - | X |
| 15 | CLA | A | 1106 | - | X |
| 15 | CLA | A | 1110 | - | X |
| 15 | CLA | A | 1121 | - | X |
| 15 | CLA | A | 1122 | - | X |
| 15 | CLA | A | 1801 | - | X |
| 15 | CLA | F | 1410 | - | X |
| 15 | CLA | J | 1302 | - | X |
| 15 | CLA | J | 1303 | - | X |

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22051 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 739 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5787 | 3791 | 984 | 985 | 27 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 728 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5765 | 3796 | 966 | 988 | 15 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3 | C | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 600 | 369 | 103 | 117 | 11 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1075 | 681 | 187 | 204 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|---------|-------|
| 5 | E | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 533 | 335 | 94 | 104 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1099 | 711 | 183 | 200 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | J | 40 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 319 | 215 | 47 | 54 | 3 | | | |

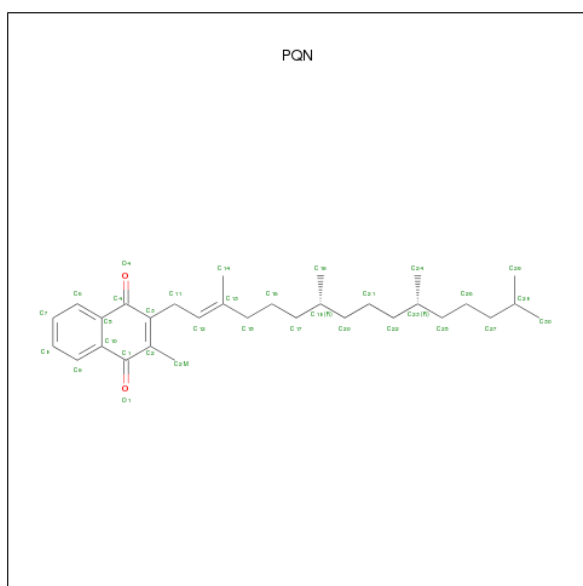
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | K | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 366 | 242 | 56 | 63 | 5 | | | |

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

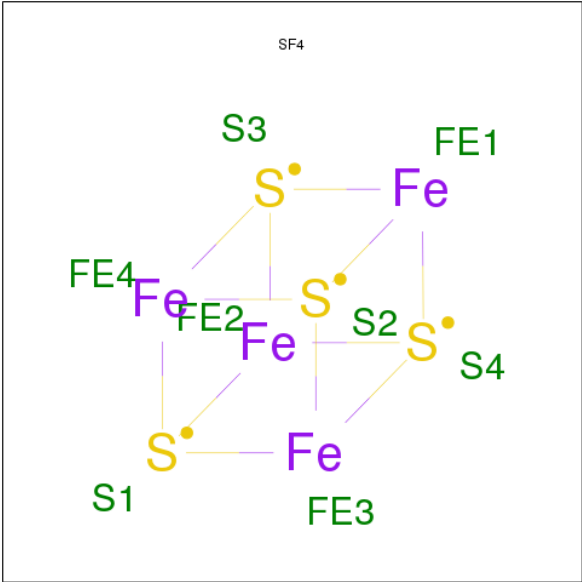
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 9 | M | 30 | Total | C | N | O | 0 | 0 | 0 |
| | | | 214 | 142 | 34 | 38 | | | |

- Molecule 10 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



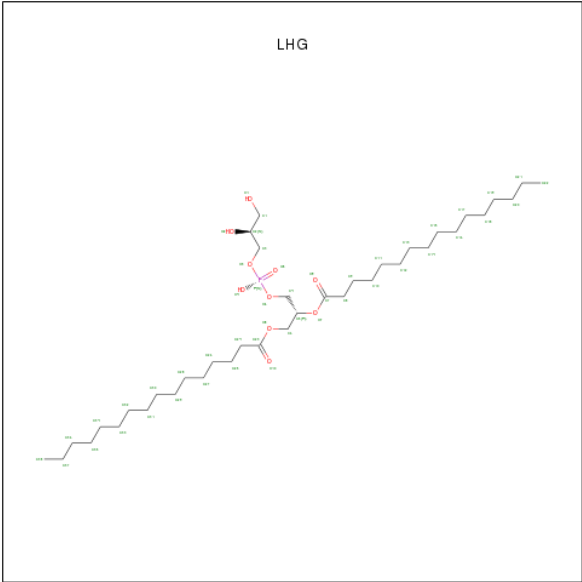
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 10 | A | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 31 | 2 | | |
| 10 | B | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 31 | 2 | | |

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



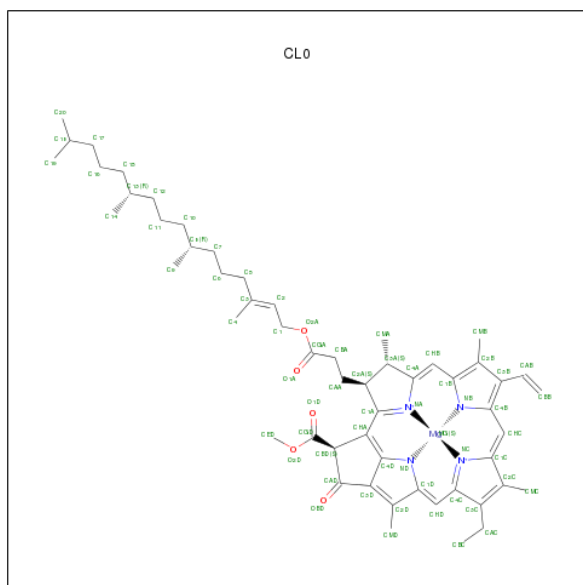
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11 | A | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 11 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 11 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



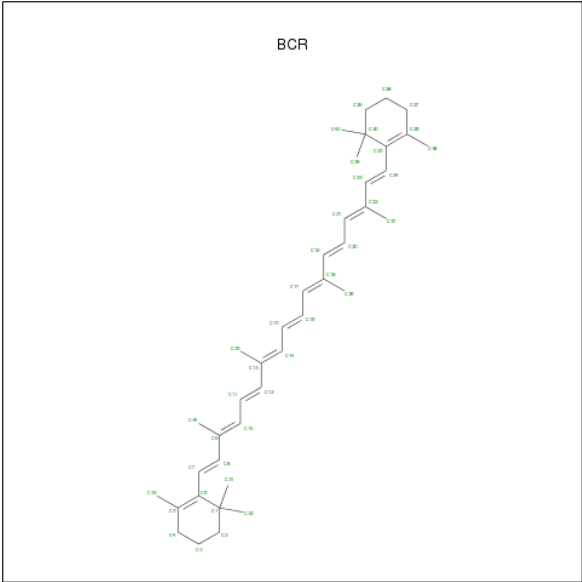
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 12 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 12 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 36 | 25 | 10 | 1 | | |
| 12 | B | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 13 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | 0 |
| 13 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | 0 |

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



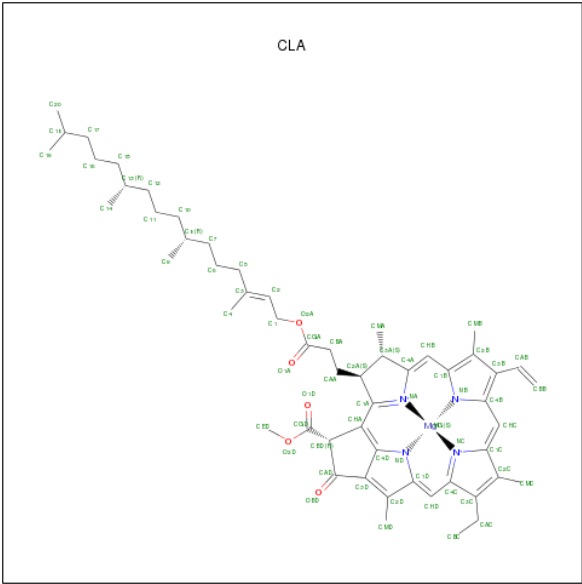
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 14 | A | 1 | Total C 40 40 | 0 | 0 |
| 14 | A | 1 | Total C 40 40 | 0 | 0 |
| 14 | A | 1 | Total C 40 40 | 0 | 0 |
| 14 | A | 1 | Total C 40 40 | 0 | 0 |
| 14 | A | 1 | Total C 40 40 | 0 | 0 |
| 14 | A | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |
| 14 | B | 1 | Total C 40 40 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 14 | F | 1 | Total C 40 40 | 0 | 0 |
| 14 | F | 1 | Total C 40 40 | 0 | 0 |
| 14 | J | 1 | Total C 40 40 | 0 | 0 |

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------------|---------|---------|
| 15 | A | 1 | Total C Mg N O 52 42 1 4 5 | 0 | 0 |
| 15 | A | 1 | Total C Mg N O 65 55 1 4 5 | 0 | 0 |
| 15 | A | 1 | Total C Mg N O 65 55 1 4 5 | 0 | 0 |
| 15 | A | 1 | Total C Mg N O 65 55 1 4 5 | 0 | 0 |
| 15 | A | 1 | Total C Mg N O 65 55 1 4 5 | 0 | 0 |
| 15 | A | 1 | Total C Mg N O 65 55 1 4 5 | 0 | 0 |
| 15 | A | 1 | Total C Mg N O 65 55 1 4 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 64 | 54 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |

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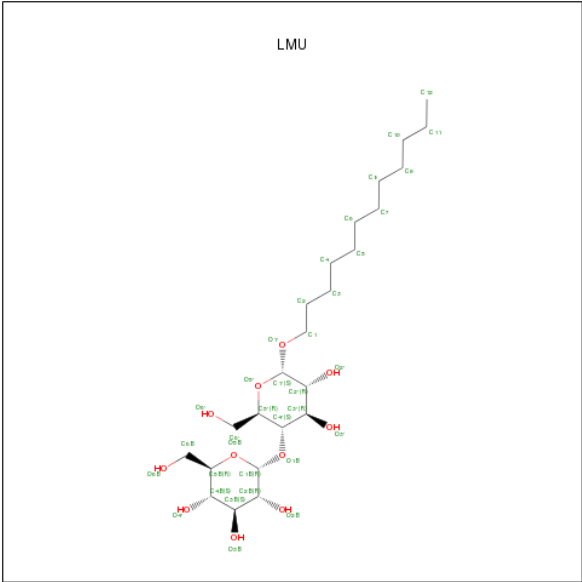
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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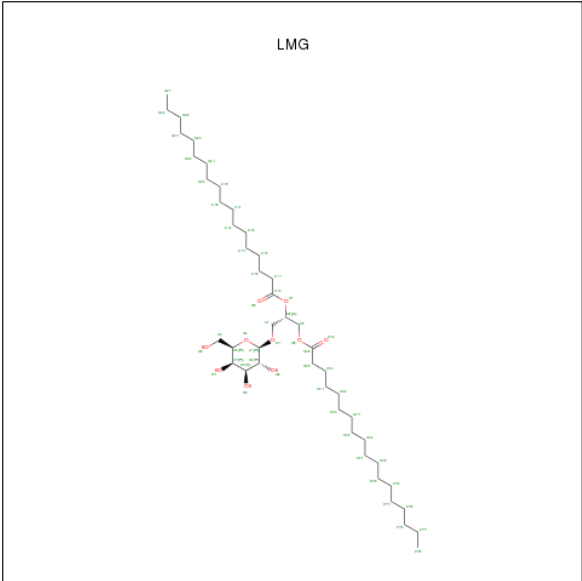
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 44 | 35 | 1 | 4 | 4 | | |
| 15 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | F | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | F | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 15 | F | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | J | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | J | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 15 | K | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 15 | K | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 16 | B | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 16 | J | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 17 | B | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 45 | 10 | | |

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 18 | B | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

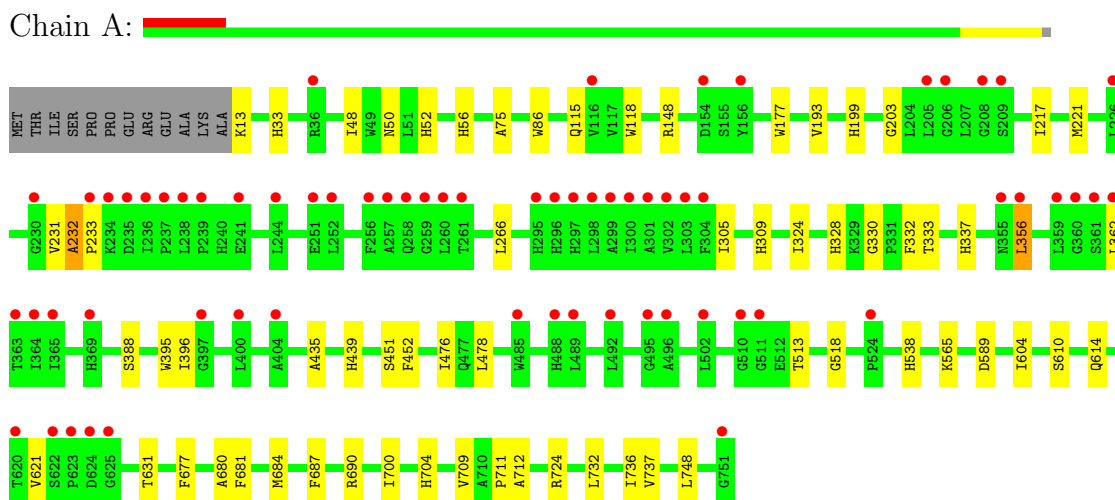
- Molecule 19 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19 | A | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 19 | B | 15 | Total | O | 0 | 0 |
| | | | 15 | 15 | | |
| 19 | C | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 19 | F | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

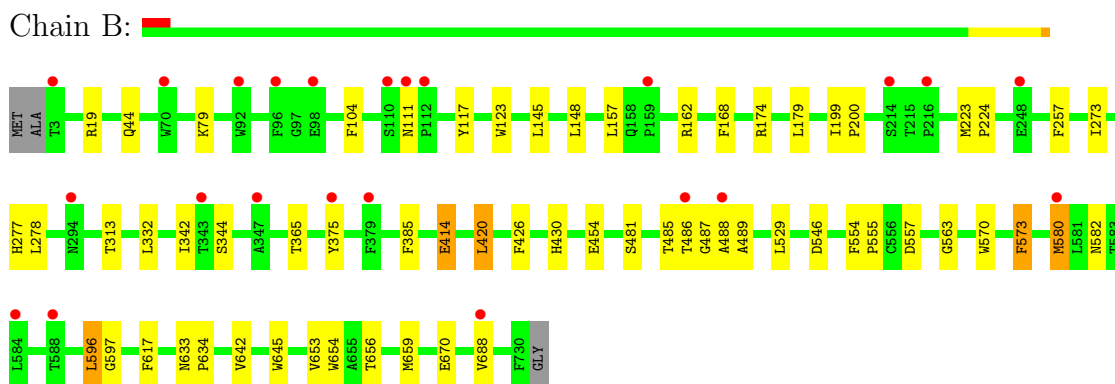
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

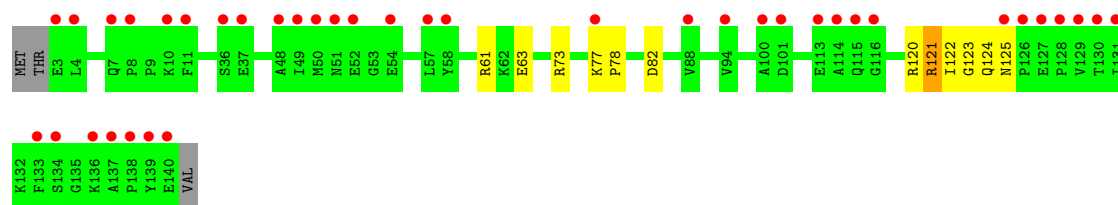


- Molecule 3: Photosystem I iron-sulfur center



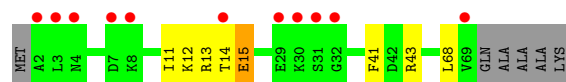
- Molecule 4: Photosystem I subunit II





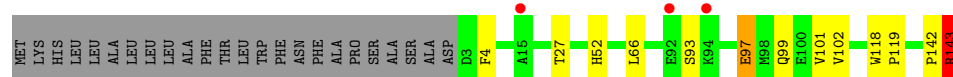
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:



- Molecule 6: Photosystem I subunit III

Chain F:



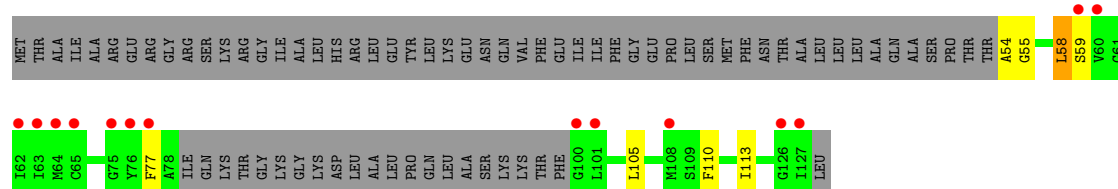
- Molecule 7: Photosystem I reaction center subunit IX

Chain J:



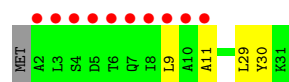
- Molecule 8: Photosystem I reaction center subunit Psak

Chain K:



- Molecule 9: Photosystem I reaction center subunit XII

Chain M:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 120.18Å 173.31Å 179.14Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.98 – 2.80 48.55 – 2.60 | Depositor EDS |
| % Data completeness (in resolution range) | 98.6 (29.98-2.80) 79.2 (48.55-2.60) | Depositor EDS |
| R_{merge} | 0.14 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.36 (at 2.61Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.4_1496) | Depositor |
| R, R_{free} | 0.198 , 0.245 0.201 , 0.247 | Depositor DCC |
| R_{free} test set | 3915 reflections (5.01%) | DCC |
| Wilson B-factor (Å ²) | 57.4 | Xtriage |
| Anisotropy | 0.546 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 64.4 | EDS |
| Estimated twinning fraction | 0.001 for -h,l,k | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 1 of 114217 reflections (0.001%) | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 22051 | wwPDB-VP |
| Average B, all atoms (Å ²) | 92.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.22 | 0/5985 | 0.38 | 0/8158 |
| 2 | B | 0.23 | 0/5976 | 0.40 | 0/8173 |
| 3 | C | 0.24 | 0/610 | 0.45 | 0/826 |
| 4 | D | 0.23 | 0/1099 | 0.40 | 0/1482 |
| 5 | E | 0.24 | 0/542 | 0.45 | 0/733 |
| 6 | F | 0.23 | 0/1129 | 0.40 | 0/1535 |
| 7 | J | 0.26 | 0/328 | 0.38 | 0/443 |
| 8 | K | 0.25 | 0/371 | 0.39 | 0/499 |
| 9 | M | 0.22 | 0/217 | 0.35 | 0/295 |
| All | All | 0.23 | 0/16257 | 0.39 | 0/22144 |

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 |
|-----|-------|---------------------|---------------------|
| 4 | D | 0 | 1 |
| 6 | F | 0 | 1 |
| All | All | 0 | 2 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 4 | D | 121 | ARG | Sidechain |
| 6 | F | 143 | ARG | Sidechain |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 5787 | 0 | 5646 | 60 | 0 |
| 2 | B | 5765 | 0 | 5544 | 56 | 0 |
| 3 | C | 600 | 0 | 581 | 4 | 0 |
| 4 | D | 1075 | 0 | 1069 | 7 | 0 |
| 5 | E | 533 | 0 | 517 | 8 | 0 |
| 6 | F | 1099 | 0 | 1096 | 7 | 0 |
| 7 | J | 319 | 0 | 328 | 4 | 0 |
| 8 | K | 366 | 0 | 376 | 7 | 0 |
| 9 | M | 214 | 0 | 213 | 2 | 0 |
| 10 | A | 33 | 0 | 46 | 1 | 0 |
| 10 | B | 33 | 0 | 46 | 3 | 0 |
| 11 | A | 8 | 0 | 0 | 0 | 0 |
| 11 | C | 16 | 0 | 0 | 0 | 0 |
| 12 | A | 134 | 0 | 190 | 18 | 0 |
| 12 | B | 49 | 0 | 74 | 2 | 0 |
| 13 | A | 110 | 0 | 105 | 12 | 0 |
| 14 | A | 240 | 0 | 294 | 17 | 0 |
| 14 | B | 320 | 0 | 390 | 26 | 0 |
| 14 | F | 80 | 0 | 97 | 8 | 0 |
| 14 | J | 40 | 0 | 49 | 3 | 0 |
| 15 | A | 2352 | 0 | 2285 | 69 | 0 |
| 15 | B | 2365 | 0 | 2272 | 58 | 0 |
| 15 | F | 175 | 0 | 177 | 3 | 0 |
| 15 | J | 91 | 0 | 66 | 2 | 0 |
| 15 | K | 92 | 0 | 66 | 2 | 0 |
| 16 | B | 35 | 0 | 46 | 0 | 0 |
| 16 | J | 35 | 0 | 46 | 2 | 0 |
| 17 | B | 55 | 0 | 86 | 2 | 0 |
| 18 | B | 1 | 0 | 0 | 0 | 0 |
| 19 | A | 10 | 0 | 0 | 5 | 0 |
| 19 | B | 15 | 0 | 0 | 6 | 0 |
| 19 | C | 3 | 0 | 0 | 0 | 0 |
| 19 | F | 1 | 0 | 0 | 1 | 0 |
| All | All | 22051 | 0 | 21705 | 267 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (267) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 13:A:1011:CL0:CMA | 19:A:9109:HOH:O | 1.91 | 1.19 |
| 13:A:1011:CL0:H6 | 19:A:9109:HOH:O | 1.48 | 1.11 |
| 14:B:4004:BCR:H403 | 14:B:4004:BCR:H23C | 1.51 | 0.92 |
| 13:A:1011:CL0:H71 | 19:A:9109:HOH:O | 1.71 | 0.88 |
| 15:A:1110:CLA:HBD | 15:A:1110:CLA:HBA1 | 1.57 | 0.86 |
| 12:A:5005:LHG:H251 | 12:A:5005:LHG:C8 | 2.11 | 0.81 |
| 1:A:395:TRP:CD1 | 15:A:1126:CLA:HAB | 2.16 | 0.80 |
| 7:J:31:ARG:NH2 | 15:J:1302:CLA:O1D | 2.15 | 0.80 |
| 14:A:4008:BCR:HC8 | 15:A:1124:CLA:HAB | 1.61 | 0.80 |
| 1:A:604:ILE:HD11 | 13:A:1011:CL0:H35 | 1.66 | 0.78 |
| 2:B:123:TRP:CZ2 | 15:B:1210:CLA:H201 | 2.18 | 0.78 |
| 12:A:5005:LHG:HC81 | 12:A:5005:LHG:H251 | 1.66 | 0.78 |
| 15:J:1302:CLA:HBB1 | 15:J:1302:CLA:HHC | 1.66 | 0.77 |
| 15:A:1113:CLA:HHC | 15:A:1113:CLA:HBB1 | 1.67 | 0.76 |
| 1:A:538:HIS:ND1 | 15:A:1135:CLA:HAB | 2.01 | 0.75 |
| 14:A:4003:BCR:H14C | 15:A:1103:CLA:H201 | 1.69 | 0.74 |
| 1:A:13:LYS:HB2 | 15:A:1110:CLA:HAA1 | 1.69 | 0.74 |
| 15:A:1128:CLA:HHC | 15:A:1128:CLA:HBB1 | 1.70 | 0.73 |
| 2:B:582:ASN:OD1 | 19:B:9102:HOH:O | 2.05 | 0.73 |
| 1:A:332:PHE:HB2 | 12:A:5003:LHG:HC41 | 1.71 | 0.73 |
| 13:A:1011:CL0:C2A | 19:A:9109:HOH:O | 2.33 | 0.72 |
| 15:A:1101:CLA:H203 | 15:A:1126:CLA:H202 | 1.73 | 0.70 |
| 14:A:4008:BCR:C8 | 15:A:1124:CLA:HAB | 2.21 | 0.70 |
| 2:B:656:THR:HA | 15:B:1023:CLA:HAB | 1.72 | 0.70 |
| 15:B:1203:CLA:HHB | 15:B:1226:CLA:HAB | 1.74 | 0.70 |
| 15:B:1227:CLA:HAB | 15:B:1236:CLA:HBB2 | 1.73 | 0.69 |
| 1:A:330:GLY:HA3 | 12:A:5003:LHG:HC32 | 1.75 | 0.69 |
| 15:A:1110:CLA:CBD | 15:A:1110:CLA:HBA1 | 2.23 | 0.69 |
| 15:A:1131:CLA:HBB1 | 15:A:1131:CLA:HHC | 1.74 | 0.69 |
| 15:A:1101:CLA:HBB1 | 15:A:1101:CLA:HHC | 1.74 | 0.69 |
| 19:B:9105:HOH:O | 14:F:4015:BCR:HC32 | 1.94 | 0.68 |
| 1:A:737:VAL:HG22 | 14:B:4011:BCR:HC21 | 1.76 | 0.68 |
| 14:A:4001:BCR:H23C | 8:K:110:PHE:HB2 | 1.75 | 0.68 |
| 5:E:13:ARG:O | 5:E:14:THR:HB | 1.93 | 0.67 |
| 1:A:476:ILE:HD12 | 12:A:5005:LHG:HC81 | 1.75 | 0.67 |
| 1:A:435:ALA:O | 1:A:439:HIS:ND1 | 2.27 | 0.66 |
| 15:A:1110:CLA:HMB3 | 15:A:1118:CLA:C3D | 2.25 | 0.66 |
| 15:A:1131:CLA:CBB | 12:A:5005:LHG:H281 | 2.26 | 0.65 |
| 15:B:1220:CLA:HMD2 | 15:B:1221:CLA:HAB | 1.76 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 14:A:4001:BCR:H24C | 15:A:1120:CLA:HMD2 | 1.78 | 0.65 |
| 15:A:1012:CLA:H42 | 14:B:4011:BCR:H362 | 1.77 | 0.65 |
| 15:A:1107:CLA:HBB1 | 15:A:1107:CLA:HHC | 1.79 | 0.64 |
| 2:B:332:LEU:HD11 | 15:B:1226:CLA:HBB1 | 1.79 | 0.64 |
| 1:A:677:PHE:CG | 14:B:4011:BCR:H363 | 2.33 | 0.64 |
| 1:A:231:VAL:O | 1:A:232:ALA:HB3 | 1.97 | 0.64 |
| 15:A:1022:CLA:H202 | 14:B:4017:BCR:H343 | 1.80 | 0.63 |
| 16:J:1304:LMU:H82 | 16:J:1304:LMU:H41 | 1.80 | 0.63 |
| 13:A:1108:CL0:H15 | 13:A:1108:CL0:H2 | 1.81 | 0.63 |
| 13:A:1011:CL0:H5 | 19:A:9109:HOH:O | 1.79 | 0.62 |
| 1:A:604:ILE:CD1 | 13:A:1011:CL0:H35 | 2.29 | 0.62 |
| 12:A:5005:LHG:HC82 | 12:A:5005:LHG:H251 | 1.82 | 0.62 |
| 12:B:5004:LHG:H202 | 14:B:4009:BCR:H353 | 1.82 | 0.62 |
| 15:B:1229:CLA:H192 | 14:F:4016:BCR:H19C | 1.81 | 0.61 |
| 1:A:680:ALA:C | 15:B:1013:CLA:HAB | 2.20 | 0.61 |
| 2:B:430:HIS:HB2 | 14:F:4015:BCR:HC22 | 1.83 | 0.61 |
| 12:A:5005:LHG:HC82 | 12:A:5005:LHG:O10 | 2.00 | 0.61 |
| 15:B:1231:CLA:HHC | 15:B:1231:CLA:HBB1 | 1.83 | 0.60 |
| 4:D:120:ARG:NH1 | 4:D:125:ASN:OD1 | 2.33 | 0.60 |
| 2:B:570:TRP:NE1 | 17:B:5002:LMG:O10 | 2.34 | 0.60 |
| 1:A:589:ASP:OD1 | 1:A:724:ARG:NH1 | 2.34 | 0.60 |
| 1:A:118:TRP:HB3 | 14:J:4013:BCR:HC21 | 1.84 | 0.60 |
| 15:B:1235:CLA:HBC2 | 14:F:4015:BCR:HC7 | 1.82 | 0.59 |
| 15:A:1110:CLA:HMB3 | 15:A:1118:CLA:CAD | 2.32 | 0.59 |
| 15:B:1227:CLA:HAB | 15:B:1236:CLA:CBB | 2.31 | 0.59 |
| 15:F:1139:CLA:HHC | 15:F:1139:CLA:HBB1 | 1.85 | 0.59 |
| 15:B:1205:CLA:CGA | 15:B:1205:CLA:C1A | 2.81 | 0.59 |
| 2:B:486:THR:N | 2:B:487:GLY:CA | 2.66 | 0.58 |
| 15:A:1102:CLA:H202 | 15:A:1105:CLA:H92 | 1.85 | 0.58 |
| 2:B:481:SER:O | 2:B:485:THR:HG23 | 2.04 | 0.58 |
| 2:B:375:TYR:CD1 | 15:B:1224:CLA:HAB | 2.39 | 0.58 |
| 15:A:1104:CLA:HBB1 | 15:A:1104:CLA:HHC | 1.86 | 0.57 |
| 15:A:1110:CLA:HHC | 15:A:1110:CLA:HBB1 | 1.86 | 0.57 |
| 14:J:4013:BCR:H23C | 14:J:4013:BCR:H392 | 1.86 | 0.57 |
| 4:D:123:GLY:HA3 | 5:E:15:GLU:HG2 | 1.87 | 0.57 |
| 4:D:121:ARG:NH1 | 4:D:124:GLN:HG3 | 2.20 | 0.57 |
| 2:B:486:THR:N | 2:B:487:GLY:HA2 | 2.19 | 0.56 |
| 14:A:4002:BCR:H342 | 15:A:1112:CLA:CHB | 2.36 | 0.56 |
| 2:B:597:GLY:HA3 | 19:B:9112:HOH:O | 2.05 | 0.55 |
| 2:B:656:THR:CA | 15:B:1023:CLA:HAB | 2.36 | 0.55 |
| 15:B:1231:CLA:C4C | 15:B:1232:CLA:HAB | 2.37 | 0.55 |
| 1:A:677:PHE:CD2 | 14:B:4011:BCR:H363 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 15:B:1218:CLA:HHC | 15:B:1218:CLA:HBB1 | 1.89 | 0.55 |
| 1:A:736:ILE:HG22 | 14:B:4011:BCR:HC31 | 1.88 | 0.55 |
| 15:A:1122:CLA:HHC | 15:A:1122:CLA:HBB1 | 1.89 | 0.54 |
| 5:E:12:LYS:O | 5:E:12:LYS:HD3 | 2.07 | 0.54 |
| 5:E:14:THR:O | 5:E:14:THR:HG22 | 2.07 | 0.54 |
| 2:B:385:PHE:CZ | 14:B:4010:BCR:H373 | 2.42 | 0.54 |
| 15:A:1106:CLA:HAB | 15:A:1126:CLA:H142 | 1.90 | 0.54 |
| 1:A:217:ILE:HA | 1:A:221:MET:HE2 | 1.90 | 0.53 |
| 9:M:9:LEU:O | 9:M:11:ALA:N | 2.37 | 0.53 |
| 15:A:1110:CLA:CHA | 15:A:1110:CLA:HBA1 | 2.39 | 0.53 |
| 15:A:1101:CLA:H203 | 15:A:1126:CLA:C20 | 2.36 | 0.53 |
| 15:B:1230:CLA:OBD | 19:B:9106:HOH:O | 2.18 | 0.53 |
| 2:B:645:TRP:CZ3 | 14:B:4017:BCR:HC41 | 2.44 | 0.53 |
| 14:A:4003:BCR:H14C | 15:A:1103:CLA:C20 | 2.38 | 0.53 |
| 2:B:385:PHE:CE2 | 14:B:4010:BCR:H373 | 2.44 | 0.53 |
| 2:B:19:ARG:HD2 | 19:B:9108:HOH:O | 2.09 | 0.53 |
| 2:B:168:PHE:O | 2:B:174:ARG:NH2 | 2.42 | 0.52 |
| 2:B:557:ASP:OD2 | 3:C:66:ARG:NH2 | 2.42 | 0.52 |
| 14:B:4014:BCR:HC41 | 15:B:1229:CLA:HBB2 | 1.91 | 0.52 |
| 15:A:1110:CLA:CBB | 15:A:1110:CLA:HHC | 2.40 | 0.52 |
| 1:A:395:TRP:NE1 | 15:A:1126:CLA:HAB | 2.23 | 0.52 |
| 1:A:395:TRP:HD1 | 15:A:1126:CLA:HAB | 1.73 | 0.52 |
| 1:A:56:HIS:CG | 15:A:1103:CLA:HAB | 2.45 | 0.52 |
| 10:B:2002:PQN:H302 | 17:B:5002:LMG:H192 | 1.92 | 0.52 |
| 4:D:61:ARG:NH2 | 4:D:63:GLU:OE1 | 2.43 | 0.52 |
| 2:B:385:PHE:HZ | 15:B:1222:CLA:HAB | 1.75 | 0.52 |
| 10:B:2002:PQN:H303 | 15:B:1239:CLA:O1A | 2.11 | 0.51 |
| 2:B:554:PHE:HB2 | 2:B:555:PRO:HD2 | 1.92 | 0.51 |
| 13:A:1108:CL0:H27 | 15:A:1110:CLA:HMD1 | 1.93 | 0.51 |
| 1:A:711:PRO:HB2 | 19:F:9301:HOH:O | 2.09 | 0.51 |
| 15:B:1229:CLA:HAB | 15:B:1230:CLA:C2B | 2.40 | 0.51 |
| 2:B:430:HIS:CG | 14:F:4015:BCR:HC42 | 2.46 | 0.51 |
| 1:A:362:LEU:CD2 | 15:A:1127:CLA:H202 | 2.41 | 0.51 |
| 2:B:44:GLN:OE1 | 2:B:162:ARG:NH1 | 2.42 | 0.51 |
| 1:A:305:ILE:HG21 | 14:A:4001:BCR:H14C | 1.93 | 0.51 |
| 15:B:1212:CLA:HAB | 15:B:1211:CLA:CMC | 2.40 | 0.51 |
| 8:K:58:LEU:N | 8:K:58:LEU:CD1 | 2.73 | 0.51 |
| 1:A:681:PHE:HA | 15:B:1013:CLA:HAB | 1.92 | 0.50 |
| 1:A:324:ILE:O | 1:A:328:HIS:ND1 | 2.36 | 0.50 |
| 1:A:231:VAL:O | 1:A:232:ALA:CB | 2.58 | 0.50 |
| 14:A:4002:BCR:HC41 | 15:A:1103:CLA:H122 | 1.94 | 0.50 |
| 2:B:426:PHE:CZ | 14:F:4015:BCR:HC41 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:B:123:TRP:CE2 | 15:B:1210:CLA:H201 | 2.46 | 0.49 |
| 13:A:1108:CL0:OBD | 15:A:1110:CLA:H71 | 2.13 | 0.49 |
| 1:A:33:His:NE2 | 15:A:1109:CLA:O1A | 2.32 | 0.49 |
| 2:B:454:GLU:OE2 | 6:F:52:His:ND1 | 2.41 | 0.49 |
| 2:B:642:VAL:HG22 | 15:B:1206:CLA:HHD | 1.95 | 0.49 |
| 8:K:58:LEU:HD13 | 8:K:58:LEU:H | 1.78 | 0.48 |
| 1:A:75:ALA:HB1 | 15:A:1103:CLA:HBB1 | 1.95 | 0.48 |
| 14:A:4007:BCR:H15C | 14:A:4007:BCR:H351 | 1.70 | 0.48 |
| 1:A:333:THR:OG1 | 12:A:5003:LHG:HC2 | 2.13 | 0.48 |
| 12:A:5005:LHG:HC82 | 12:A:5005:LHG:C23 | 2.43 | 0.48 |
| 1:A:684:MET:HE2 | 10:A:2001:PQN:H2M3 | 1.95 | 0.48 |
| 2:B:420:LEU:HD22 | 2:B:529:LEU:HB2 | 1.94 | 0.48 |
| 15:B:1235:CLA:H122 | 14:F:4016:BCR:H23C | 1.95 | 0.48 |
| 15:A:1133:CLA:HHC | 15:A:1133:CLA:HBB1 | 1.95 | 0.48 |
| 1:A:396:ILE:HD12 | 15:A:1127:CLA:HAB | 1.94 | 0.48 |
| 14:A:4008:BCR:H371 | 14:A:4008:BCR:H24C | 1.73 | 0.47 |
| 14:B:4006:BCR:H403 | 14:B:4006:BCR:C23 | 2.44 | 0.47 |
| 1:A:690:ARG:NH1 | 2:B:563:GLY:O | 2.46 | 0.47 |
| 5:E:11:ILE:N | 5:E:11:ILE:HD12 | 2.30 | 0.47 |
| 1:A:330:GLY:CA | 12:A:5003:LHG:HC32 | 2.44 | 0.47 |
| 12:A:5005:LHG:H262 | 12:A:5005:LHG:H112 | 1.95 | 0.47 |
| 2:B:179:LEU:CD2 | 15:B:1216:CLA:HAB | 2.44 | 0.47 |
| 1:A:610:SER:OG | 1:A:614:GLN:NE2 | 2.47 | 0.47 |
| 15:A:1022:CLA:CAD | 15:B:1021:CLA:HMB3 | 2.44 | 0.47 |
| 15:B:1215:CLA:H3A | 15:B:1215:CLA:CGA | 2.44 | 0.47 |
| 15:B:1235:CLA:C1A | 15:B:1235:CLA:CGA | 2.93 | 0.47 |
| 2:B:633:ASN:HB2 | 2:B:634:PRO:CD | 2.44 | 0.47 |
| 15:A:1119:CLA:HMB2 | 15:A:1123:CLA:HMA3 | 1.97 | 0.47 |
| 15:B:1224:CLA:H3A | 15:B:1224:CLA:CGA | 2.45 | 0.47 |
| 2:B:486:THR:OG1 | 2:B:487:GLY:HA2 | 2.13 | 0.47 |
| 13:A:1011:CL0:H13 | 15:A:1012:CLA:HMD1 | 1.97 | 0.47 |
| 1:A:687:PHE:HB2 | 15:B:1013:CLA:HBC2 | 1.97 | 0.47 |
| 8:K:58:LEU:HD13 | 8:K:58:LEU:N | 2.29 | 0.47 |
| 15:B:1013:CLA:CGA | 15:B:1013:CLA:H3A | 2.46 | 0.46 |
| 14:B:4010:BCR:H351 | 14:B:4010:BCR:H15C | 1.69 | 0.46 |
| 14:A:4003:BCR:H24C | 15:A:1127:CLA:H2 | 1.97 | 0.46 |
| 1:A:712:ALA:HB1 | 6:F:97:GLU:OE1 | 2.15 | 0.46 |
| 8:K:54:ALA:O | 8:K:58:LEU:HD22 | 2.14 | 0.46 |
| 1:A:199:His:O | 1:A:203:GLY:N | 2.48 | 0.46 |
| 2:B:111:ASN:N | 2:B:111:ASN:OD1 | 2.49 | 0.46 |
| 15:A:1137:CLA:HAB | 15:A:1129:CLA:CBB | 2.45 | 0.46 |
| 1:A:86:TRP:HA | 15:A:1105:CLA:HBB2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:B:273:ILE:O | 2:B:277:HIS:ND1 | 2.43 | 0.46 |
| 14:J:4013:BCR:H15C | 14:J:4013:BCR:H351 | 1.67 | 0.46 |
| 15:A:1022:CLA:H171 | 14:B:4017:BCR:H343 | 1.96 | 0.46 |
| 15:B:1203:CLA:OBD | 15:B:1201:CLA:HHC | 2.16 | 0.46 |
| 14:B:4017:BCR:H15C | 14:B:4017:BCR:H351 | 1.68 | 0.46 |
| 1:A:681:PHE:N | 15:B:1013:CLA:HAB | 2.30 | 0.45 |
| 15:B:1215:CLA:HBB2 | 15:B:1221:CLA:H201 | 1.99 | 0.45 |
| 2:B:199:ILE:HB | 2:B:200:PRO:HD3 | 1.99 | 0.45 |
| 1:A:362:LEU:HD22 | 15:A:1127:CLA:H202 | 1.97 | 0.45 |
| 15:A:1114:CLA:HBB1 | 15:A:1114:CLA:HHC | 1.97 | 0.45 |
| 2:B:546:ASP:OD2 | 3:C:66:ARG:NH1 | 2.48 | 0.45 |
| 2:B:688:VAL:HG11 | 15:B:1237:CLA:HAB | 1.99 | 0.45 |
| 15:A:1110:CLA:C3C | 15:A:1111:CLA:HBB2 | 2.47 | 0.45 |
| 1:A:305:ILE:O | 1:A:309:HIS:ND1 | 2.45 | 0.45 |
| 15:B:1236:CLA:HHC | 15:B:1236:CLA:HBB1 | 1.99 | 0.45 |
| 14:B:4010:BCR:C23 | 14:B:4010:BCR:H403 | 2.46 | 0.45 |
| 1:A:565:LYS:NZ | 2:B:670:GLU:OE2 | 2.44 | 0.45 |
| 1:A:476:ILE:CD1 | 12:A:5005:LHG:HC81 | 2.45 | 0.45 |
| 14:B:4010:BCR:H14C | 15:B:1222:CLA:HMA1 | 1.99 | 0.45 |
| 5:E:13:ARG:O | 5:E:14:THR:CB | 2.59 | 0.45 |
| 2:B:573:PHE:CE2 | 15:B:1226:CLA:HMD2 | 2.52 | 0.45 |
| 2:B:104:PHE:CZ | 2:B:642:VAL:HG23 | 2.52 | 0.44 |
| 14:B:4005:BCR:H351 | 14:B:4005:BCR:H15C | 1.74 | 0.44 |
| 2:B:656:THR:N | 15:B:1023:CLA:HAB | 2.32 | 0.44 |
| 15:B:1212:CLA:HAB | 15:B:1211:CLA:HMC3 | 1.99 | 0.44 |
| 15:A:1110:CLA:CGA | 15:A:1110:CLA:C1A | 2.95 | 0.44 |
| 14:A:4008:BCR:H15C | 14:A:4008:BCR:H351 | 1.63 | 0.44 |
| 14:A:4012:BCR:C8 | 14:A:4012:BCR:H331 | 2.45 | 0.44 |
| 1:A:700:ILE:O | 1:A:704:HIS:ND1 | 2.46 | 0.44 |
| 1:A:193:VAL:CG1 | 15:A:1123:CLA:HHD | 2.48 | 0.44 |
| 8:K:54:ALA:HB3 | 15:K:1402:CLA:C1 | 2.48 | 0.44 |
| 1:A:680:ALA:O | 15:B:1013:CLA:HAB | 2.17 | 0.44 |
| 16:J:1304:LMU:H101 | 16:J:1304:LMU:H71 | 1.82 | 0.44 |
| 14:A:4002:BCR:H24C | 14:A:4002:BCR:H371 | 1.72 | 0.44 |
| 14:B:4011:BCR:H392 | 14:B:4011:BCR:H23C | 2.00 | 0.44 |
| 15:A:1106:CLA:H43 | 15:A:1126:CLA:HMD2 | 2.00 | 0.43 |
| 15:A:1801:CLA:HAB | 15:A:1122:CLA:HHB | 2.00 | 0.43 |
| 1:A:337:HIS:CE1 | 12:A:5003:LHG:HC12 | 2.53 | 0.43 |
| 15:B:1215:CLA:HBB1 | 15:B:1215:CLA:HHC | 2.00 | 0.43 |
| 15:A:1122:CLA:HBB1 | 15:A:1129:CLA:HMD2 | 2.00 | 0.43 |
| 2:B:117:TYR:HA | 2:B:365:THR:HG22 | 2.01 | 0.43 |
| 2:B:426:PHE:CE1 | 14:F:4015:BCR:HC41 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:B:645:TRP:CE3 | 14:B:4017:BCR:HC41 | 2.54 | 0.43 |
| 5:E:11:ILE:HD11 | 5:E:41:PHE:HE1 | 1.82 | 0.43 |
| 14:A:4008:BCR:HC8 | 15:A:1124:CLA:CAB | 2.42 | 0.43 |
| 5:E:14:THR:O | 6:F:142:PRO:HG3 | 2.19 | 0.43 |
| 2:B:278:LEU:HG | 15:B:1213:CLA:HAB | 2.01 | 0.43 |
| 14:B:4014:BCR:HC8 | 15:B:1229:CLA:HBB1 | 2.01 | 0.43 |
| 15:A:1114:CLA:HHC | 15:A:1114:CLA:CBB | 2.49 | 0.42 |
| 15:A:1110:CLA:HMB3 | 15:A:1118:CLA:C4D | 2.48 | 0.42 |
| 4:D:77:LYS:HB2 | 4:D:78:PRO:HD3 | 2.01 | 0.42 |
| 15:B:1222:CLA:H3A | 15:B:1222:CLA:HBA2 | 1.88 | 0.42 |
| 15:B:1215:CLA:HHC | 15:B:1215:CLA:CBB | 2.49 | 0.42 |
| 14:A:4012:BCR:HC7 | 7:J:26:LEU:HD13 | 2.01 | 0.42 |
| 12:A:5003:LHG:H282 | 15:A:1122:CLA:H202 | 2.02 | 0.42 |
| 1:A:681:PHE:HA | 15:B:1013:CLA:CAB | 2.49 | 0.42 |
| 2:B:654:TRP:CE3 | 15:B:1021:CLA:HMA1 | 2.55 | 0.42 |
| 2:B:596:LEU:HD12 | 2:B:596:LEU:HA | 1.81 | 0.42 |
| 1:A:177:TRP:HB2 | 15:A:1109:CLA:HMC3 | 2.01 | 0.42 |
| 1:A:356:LEU:HD11 | 15:A:1128:CLA:CBB | 2.50 | 0.42 |
| 1:A:48:ILE:O | 1:A:52:HIS:ND1 | 2.51 | 0.42 |
| 15:B:1235:CLA:HAB | 19:B:9105:HOH:O | 2.19 | 0.42 |
| 2:B:223:MET:N | 2:B:224:PRO:CD | 2.83 | 0.42 |
| 14:B:4004:BCR:H351 | 14:B:4004:BCR:H15C | 1.67 | 0.42 |
| 6:F:93:SER:OG | 6:F:99:GLN:NE2 | 2.53 | 0.42 |
| 1:A:518:GLY:O | 1:A:621:VAL:N | 2.52 | 0.42 |
| 1:A:737:VAL:HG22 | 14:B:4011:BCR:H323 | 2.01 | 0.42 |
| 2:B:488:ALA:O | 2:B:489:ALA:HB3 | 2.19 | 0.42 |
| 15:A:1138:CLA:H203 | 15:F:1139:CLA:H62 | 2.02 | 0.41 |
| 1:A:337:HIS:HE1 | 12:A:5003:LHG:HC12 | 1.83 | 0.41 |
| 2:B:313:THR:OG1 | 12:B:5004:LHG:HC11 | 2.19 | 0.41 |
| 6:F:118:TRP:N | 6:F:119:PRO:CD | 2.83 | 0.41 |
| 1:A:50:ASN:ND2 | 12:A:5001:LHG:HC12 | 2.35 | 0.41 |
| 15:A:1121:CLA:HHC | 15:A:1121:CLA:CBB | 2.50 | 0.41 |
| 3:C:62:PHE:HD2 | 4:D:122:ILE:HG21 | 1.85 | 0.41 |
| 15:F:1139:CLA:H41 | 7:J:18:LEU:HD22 | 2.02 | 0.41 |
| 1:A:604:ILE:HD11 | 13:A:1011:CL0:C4 | 2.45 | 0.41 |
| 2:B:385:PHE:CZ | 15:B:1222:CLA:HAB | 2.53 | 0.41 |
| 6:F:27:THR:HG21 | 7:J:34:PRO:HG3 | 2.03 | 0.41 |
| 15:K:1401:CLA:HHC | 15:K:1401:CLA:CBB | 2.51 | 0.41 |
| 2:B:342:ILE:HG21 | 15:B:1221:CLA:H41 | 2.02 | 0.41 |
| 15:B:1216:CLA:HMB2 | 15:B:1221:CLA:HMA3 | 2.03 | 0.41 |
| 14:B:4017:BCR:H24C | 14:B:4017:BCR:H371 | 1.78 | 0.41 |
| 2:B:580:MET:HB3 | 2:B:580:MET:HE2 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 2:B:414:GLU:OE2 | 6:F:143:ARG:NH2 | 2.54 | 0.41 |
| 15:A:1121:CLA:HBB1 | 15:A:1121:CLA:HHC | 2.02 | 0.41 |
| 2:B:157:LEU:HD11 | 9:M:29:LEU:HD12 | 2.03 | 0.41 |
| 4:D:120:ARG:HG2 | 4:D:124:GLN:HB2 | 2.01 | 0.41 |
| 1:A:451:SER:OG | 1:A:452:PHE:N | 2.54 | 0.41 |
| 2:B:653:VAL:HG22 | 15:B:1239:CLA:HMB3 | 2.03 | 0.41 |
| 3:C:54:CYS:SG | 3:C:55:GLU:N | 2.94 | 0.41 |
| 8:K:55:GLY:O | 8:K:59:SER:OG | 2.30 | 0.41 |
| 15:A:1102:CLA:HMA2 | 15:A:1109:CLA:HMD2 | 2.02 | 0.40 |
| 15:B:1231:CLA:CBB | 15:B:1231:CLA:HHC | 2.51 | 0.40 |
| 15:A:1133:CLA:HHC | 15:A:1133:CLA:CBB | 2.51 | 0.40 |
| 1:A:681:PHE:CA | 15:B:1013:CLA:HAB | 2.50 | 0.40 |
| 2:B:659:MET:HE2 | 10:B:2002:PQN:H2M3 | 2.02 | 0.40 |
| 15:A:1102:CLA:HMB1 | 15:A:1102:CLA:HBB1 | 2.04 | 0.40 |
| 12:A:5005:LHG:HC2 | 12:A:5005:LHG:O4 | 2.22 | 0.40 |
| 14:B:4004:BCR:H321 | 14:B:4004:BCR:HC8 | 2.03 | 0.40 |
| 1:A:388:SER:HB3 | 15:A:1126:CLA:HMA1 | 2.04 | 0.40 |
| 15:B:1218:CLA:CBB | 15:B:1218:CLA:HHC | 2.50 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | A | 737/751 (98%) | 694 (94%) | 40 (5%) | 3 (0%) | 43 | 80 |
| 2 | B | 726/731 (99%) | 695 (96%) | 31 (4%) | 0 | 100 | 100 |
| 3 | C | 78/81 (96%) | 74 (95%) | 4 (5%) | 0 | 100 | 100 |
| 4 | D | 136/141 (96%) | 123 (90%) | 13 (10%) | 0 | 100 | 100 |
| 5 | E | 66/74 (89%) | 57 (86%) | 9 (14%) | 0 | 100 | 100 |
| 6 | F | 139/165 (84%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 7 | J | 38/40 (95%) | 38 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 8 | K | 49/128 (38%) | 46 (94%) | 3 (6%) | 0 | 100 | 100 |
| 9 | M | 28/31 (90%) | 25 (89%) | 3 (11%) | 0 | 100 | 100 |
| All | All | 1997/2142 (93%) | 1887 (94%) | 107 (5%) | 3 (0%) | 56 | 88 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 115 | GLN |
| 1 | A | 232 | ALA |
| 1 | A | 233 | PRO |

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 | 593/603 (98%) | 584 (98%) | 9 (2%) | 76 | 96 |
| 2 | B | 582/583 (100%) | 571 (98%) | 11 (2%) | 69 | 94 |
| 3 | C | 68/69 (99%) | 67 (98%) | 1 (2%) | 76 | 96 |
| 4 | D | 112/116 (97%) | 110 (98%) | 2 (2%) | 71 | 94 |
| 5 | E | 57/60 (95%) | 54 (95%) | 3 (5%) | 32 | 67 |
| 6 | F | 118/137 (86%) | 112 (95%) | 6 (5%) | 33 | 69 |
| 7 | J | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 8 | K | 37/100 (37%) | 33 (89%) | 4 (11%) | 9 | 26 |
| 9 | M | 19/25 (76%) | 18 (95%) | 1 (5%) | 32 | 67 |
| All | All | 1621/1728 (94%) | 1584 (98%) | 37 (2%) | 63 | 92 |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 148 | ARG |
| 1 | A | 266 | LEU |
| 1 | A | 356 | LEU |
| 1 | A | 478 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 513 | THR |
| 1 | A | 631 | THR |
| 1 | A | 709 | VAL |
| 1 | A | 732 | LEU |
| 1 | A | 748 | LEU |
| 2 | B | 79 | LYS |
| 2 | B | 145 | LEU |
| 2 | B | 148 | LEU |
| 2 | B | 257 | PHE |
| 2 | B | 344 | SER |
| 2 | B | 414 | GLU |
| 2 | B | 420 | LEU |
| 2 | B | 573 | PHE |
| 2 | B | 580 | MET |
| 2 | B | 596 | LEU |
| 2 | B | 617 | PHE |
| 3 | C | 66 | ARG |
| 4 | D | 73 | ARG |
| 4 | D | 82 | ASP |
| 5 | E | 15 | GLU |
| 5 | E | 43 | ARG |
| 5 | E | 68 | LEU |
| 6 | F | 4 | PHE |
| 6 | F | 66 | LEU |
| 6 | F | 97 | GLU |
| 6 | F | 101 | VAL |
| 6 | F | 102 | VAL |
| 6 | F | 143 | ARG |
| 8 | K | 58 | LEU |
| 8 | K | 77 | PHE |
| 8 | K | 105 | LEU |
| 8 | K | 113 | ILE |
| 9 | M | 30 | TYR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 138 | GLN |
| 1 | A | 441 | ASN |
| 1 | A | 538 | HIS |
| 1 | A | 614 | GLN |
| 2 | B | 34 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 114 | ASN |
| 4 | D | 81 | GLN |
| 4 | D | 95 | GLN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 122 ligands modelled in this entry, 1 is monoatomic - leaving 121 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 | $\# Z > 2$ |
| 13 | CL0 | A | 1011 | - | 73,73,73 | 2.18 | 19 (26%) | 96,113,113 | 2.32 | 24 (25%) |
| 15 | CLA | A | 1012 | 19 | 73,73,73 | 2.21 | 21 (28%) | 96,113,113 | 2.37 | 28 (29%) |
| 15 | CLA | A | 1022 | 19 | 73,73,73 | 2.21 | 20 (27%) | 96,113,113 | 2.33 | 23 (23%) |
| 15 | CLA | A | 1101 | - | 73,73,73 | 2.22 | 20 (27%) | 96,113,113 | 2.40 | 27 (28%) |
| 15 | CLA | A | 1102 | 15 | 73,73,73 | 2.23 | 20 (27%) | 96,113,113 | 2.32 | 25 (26%) |
| 15 | CLA | A | 1103 | - | 73,73,73 | 2.21 | 19 (26%) | 96,113,113 | 2.24 | 27 (28%) |
| 15 | CLA | A | 1104 | - | 73,73,73 | 2.19 | 20 (27%) | 96,113,113 | 2.33 | 26 (27%) |
| 15 | CLA | A | 1105 | - | 73,73,73 | 2.18 | 20 (27%) | 96,113,113 | 2.40 | 24 (25%) |
| 15 | CLA | A | 1106 | 1 | 73,73,73 | 2.22 | 20 (27%) | 96,113,113 | 2.37 | 29 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 15 | CLA | A | 1107 | 1 | 58,58,73 | 2.50 | 23 (39%) | 76,95,113 | 2.60 | 27 (35%) |
| 13 | CL0 | A | 1108 | - | 51,53,73 | 2.62 | 20 (39%) | 69,89,113 | 2.44 | 22 (31%) |
| 15 | CLA | A | 1109 | 15 | 73,73,73 | 2.23 | 20 (27%) | 96,113,113 | 2.38 | 28 (29%) |
| 15 | CLA | A | 1110 | - | 62,62,73 | 2.36 | 22 (35%) | 81,99,113 | 2.53 | 24 (29%) |
| 15 | CLA | A | 1111 | - | 67,68,73 | 2.29 | 20 (29%) | 88,107,113 | 2.38 | 26 (29%) |
| 15 | CLA | A | 1112 | - | 51,53,73 | 2.61 | 21 (41%) | 69,89,113 | 2.45 | 23 (33%) |
| 15 | CLA | A | 1113 | - | 51,53,73 | 2.61 | 20 (39%) | 69,89,113 | 2.44 | 21 (30%) |
| 15 | CLA | A | 1114 | - | 56,57,73 | 2.53 | 20 (35%) | 74,93,113 | 2.53 | 23 (31%) |
| 15 | CLA | A | 1115 | - | 53,54,73 | 2.52 | 19 (35%) | 72,90,113 | 2.47 | 20 (27%) |
| 15 | CLA | A | 1116 | - | 62,62,73 | 2.39 | 20 (32%) | 81,99,113 | 2.51 | 26 (32%) |
| 15 | CLA | A | 1117 | - | 73,73,73 | 2.21 | 20 (27%) | 96,113,113 | 2.26 | 25 (26%) |
| 15 | CLA | A | 1118 | - | 53,54,73 | 2.49 | 18 (33%) | 72,90,113 | 2.51 | 20 (27%) |
| 15 | CLA | A | 1119 | - | 71,72,73 | 2.29 | 22 (30%) | 91,111,113 | 2.32 | 24 (26%) |
| 15 | CLA | A | 1120 | - | 56,57,73 | 2.53 | 21 (37%) | 74,93,113 | 2.55 | 25 (33%) |
| 15 | CLA | A | 1121 | - | 53,54,73 | 2.52 | 19 (35%) | 72,90,113 | 2.52 | 20 (27%) |
| 15 | CLA | A | 1122 | - | 73,73,73 | 2.23 | 20 (27%) | 96,113,113 | 2.31 | 25 (26%) |
| 15 | CLA | A | 1123 | - | 73,73,73 | 2.19 | 20 (27%) | 96,113,113 | 2.30 | 28 (29%) |
| 15 | CLA | A | 1124 | - | 62,63,73 | 2.39 | 20 (32%) | 82,101,113 | 2.50 | 24 (29%) |
| 15 | CLA | A | 1125 | - | 60,60,73 | 2.52 | 20 (33%) | 80,97,113 | 2.60 | 30 (37%) |
| 15 | CLA | A | 1126 | - | 73,73,73 | 2.22 | 21 (28%) | 96,113,113 | 2.36 | 29 (30%) |
| 15 | CLA | A | 1127 | - | 73,73,73 | 2.20 | 19 (26%) | 96,113,113 | 2.29 | 28 (29%) |
| 15 | CLA | A | 1128 | - | 73,73,73 | 2.19 | 20 (27%) | 96,113,113 | 2.27 | 26 (27%) |
| 15 | CLA | A | 1129 | - | 53,54,73 | 2.50 | 19 (35%) | 72,90,113 | 2.56 | 24 (33%) |
| 15 | CLA | A | 1130 | - | 62,63,73 | 2.40 | 21 (33%) | 82,101,113 | 2.48 | 25 (30%) |
| 15 | CLA | A | 1131 | - | 62,63,73 | 2.43 | 21 (33%) | 82,101,113 | 2.50 | 25 (30%) |
| 15 | CLA | A | 1132 | - | 70,70,73 | 2.33 | 20 (28%) | 92,109,113 | 2.37 | 25 (27%) |
| 15 | CLA | A | 1133 | - | 53,54,73 | 2.50 | 19 (35%) | 72,90,113 | 2.50 | 25 (34%) |
| 15 | CLA | A | 1134 | 1 | 53,54,73 | 2.52 | 19 (35%) | 72,90,113 | 2.51 | 22 (30%) |
| 15 | CLA | A | 1135 | - | 62,63,73 | 2.38 | 20 (32%) | 82,101,113 | 2.52 | 26 (31%) |
| 15 | CLA | A | 1136 | - | 73,73,73 | 2.19 | 20 (27%) | 96,113,113 | 2.29 | 23 (23%) |
| 15 | CLA | A | 1137 | - | 58,58,73 | 2.48 | 21 (36%) | 76,95,113 | 2.53 | 25 (32%) |
| 15 | CLA | A | 1138 | - | 73,73,73 | 2.25 | 20 (27%) | 96,113,113 | 2.29 | 27 (28%) |
| 15 | CLA | A | 1140 | - | 73,73,73 | 2.21 | 20 (27%) | 96,113,113 | 2.22 | 24 (25%) |
| 15 | CLA | A | 1801 | 12 | 60,60,73 | 2.55 | 23 (38%) | 80,97,113 | 2.53 | 28 (35%) |
| 10 | PQN | A | 2001 | - | 34,34,34 | 1.38 | 2 (5%) | 45,45,45 | 1.00 | 4 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 11 | SF4 | A | 3001 | 1,2 | 12,12,12 | 6.48 | 12 (100%) | 0,24,24 | 0.00 | - |
| 14 | BCR | A | 4001 | - | 41,41,41 | 2.75 | 6 (14%) | 56,56,56 | 6.05 | 25 (44%) |
| 14 | BCR | A | 4002 | - | 41,41,41 | 2.74 | 6 (14%) | 56,56,56 | 6.25 | 25 (44%) |
| 14 | BCR | A | 4003 | - | 41,41,41 | 2.72 | 6 (14%) | 56,56,56 | 6.28 | 25 (44%) |
| 14 | BCR | A | 4007 | - | 41,41,41 | 2.71 | 6 (14%) | 56,56,56 | 6.49 | 24 (42%) |
| 14 | BCR | A | 4008 | - | 41,41,41 | 2.72 | 7 (17%) | 56,56,56 | 6.56 | 24 (42%) |
| 14 | BCR | A | 4012 | - | 41,41,41 | 2.79 | 6 (14%) | 56,56,56 | 5.98 | 22 (39%) |
| 12 | LHG | A | 5001 | - | 48,48,48 | 0.89 | 2 (4%) | 54,54,54 | 1.05 | 3 (5%) |
| 12 | LHG | A | 5003 | 15 | 48,48,48 | 0.90 | 2 (4%) | 54,54,54 | 1.08 | 3 (5%) |
| 12 | LHG | A | 5005 | - | 35,35,48 | 1.74 | 4 (11%) | 41,41,54 | 1.11 | 3 (7%) |
| 15 | CLA | B | 1013 | - | 73,73,73 | 2.20 | 20 (27%) | 96,113,113 | 2.42 | 27 (28%) |
| 15 | CLA | B | 1021 | - | 73,73,73 | 2.20 | 21 (28%) | 96,113,113 | 2.28 | 27 (28%) |
| 15 | CLA | B | 1023 | - | 73,73,73 | 2.17 | 22 (30%) | 96,113,113 | 2.27 | 25 (26%) |
| 15 | CLA | B | 1201 | - | 53,54,73 | 2.51 | 19 (35%) | 72,90,113 | 2.54 | 23 (31%) |
| 15 | CLA | B | 1202 | - | 73,73,73 | 2.21 | 20 (27%) | 96,113,113 | 2.32 | 26 (27%) |
| 15 | CLA | B | 1203 | - | 73,73,73 | 2.19 | 20 (27%) | 96,113,113 | 2.29 | 25 (26%) |
| 15 | CLA | B | 1204 | - | 53,54,73 | 2.50 | 19 (35%) | 72,90,113 | 2.57 | 23 (31%) |
| 15 | CLA | B | 1205 | - | 62,63,73 | 2.37 | 19 (30%) | 82,101,113 | 2.45 | 23 (28%) |
| 15 | CLA | B | 1206 | 2 | 53,54,73 | 2.52 | 19 (35%) | 72,90,113 | 2.54 | 24 (33%) |
| 15 | CLA | B | 1207 | - | 53,54,73 | 2.52 | 19 (35%) | 72,90,113 | 2.54 | 21 (29%) |
| 15 | CLA | B | 1208 | - | 51,53,73 | 2.61 | 20 (39%) | 69,89,113 | 2.43 | 18 (26%) |
| 15 | CLA | B | 1209 | - | 51,53,73 | 2.57 | 20 (39%) | 69,89,113 | 2.48 | 25 (36%) |
| 15 | CLA | B | 1210 | - | 73,73,73 | 2.20 | 20 (27%) | 96,113,113 | 2.29 | 27 (28%) |
| 15 | CLA | B | 1211 | - | 53,54,73 | 2.50 | 19 (35%) | 72,90,113 | 2.48 | 22 (30%) |
| 15 | CLA | B | 1212 | - | 51,53,73 | 2.60 | 20 (39%) | 69,89,113 | 2.44 | 20 (28%) |
| 15 | CLA | B | 1213 | - | 58,58,73 | 2.52 | 22 (37%) | 76,95,113 | 2.51 | 24 (31%) |
| 15 | CLA | B | 1214 | - | 73,73,73 | 2.21 | 20 (27%) | 96,113,113 | 2.35 | 26 (27%) |
| 15 | CLA | B | 1215 | - | 73,73,73 | 2.21 | 20 (27%) | 96,113,113 | 2.43 | 27 (28%) |
| 15 | CLA | B | 1216 | - | 73,73,73 | 2.20 | 20 (27%) | 96,113,113 | 2.23 | 25 (26%) |
| 15 | CLA | B | 1217 | - | 54,55,73 | 2.88 | 21 (38%) | 73,91,113 | 2.58 | 25 (34%) |
| 15 | CLA | B | 1218 | - | 59,59,73 | 2.55 | 21 (35%) | 78,96,113 | 2.56 | 27 (34%) |
| 15 | CLA | B | 1219 | - | 62,63,73 | 2.43 | 21 (33%) | 82,101,113 | 2.56 | 27 (32%) |
| 15 | CLA | B | 1220 | - | 64,64,73 | 2.50 | 22 (34%) | 84,102,113 | 2.43 | 25 (29%) |
| 15 | CLA | B | 1221 | - | 73,73,73 | 2.19 | 21 (28%) | 96,113,113 | 2.31 | 24 (25%) |
| 15 | CLA | B | 1222 | - | 64,64,73 | 2.45 | 20 (31%) | 84,102,113 | 2.48 | 25 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 15 | CLA | B | 1223 | - | 73,73,73 | 2.19 | 20 (27%) | 96,113,113 | 2.33 | 27 (28%) |
| 15 | CLA | B | 1224 | - | 73,73,73 | 2.19 | 19 (26%) | 96,113,113 | 2.32 | 25 (26%) |
| 15 | CLA | B | 1225 | - | 73,73,73 | 2.18 | 20 (27%) | 96,113,113 | 2.33 | 25 (26%) |
| 15 | CLA | B | 1226 | - | 73,73,73 | 2.18 | 19 (26%) | 96,113,113 | 2.29 | 24 (25%) |
| 15 | CLA | B | 1227 | - | 51,53,73 | 2.56 | 21 (41%) | 69,89,113 | 2.49 | 19 (27%) |
| 15 | CLA | B | 1228 | - | 73,73,73 | 2.23 | 22 (30%) | 96,113,113 | 2.25 | 24 (25%) |
| 15 | CLA | B | 1229 | - | 73,73,73 | 2.18 | 20 (27%) | 96,113,113 | 2.29 | 24 (25%) |
| 15 | CLA | B | 1230 | - | 73,73,73 | 2.20 | 21 (28%) | 96,113,113 | 2.41 | 30 (31%) |
| 15 | CLA | B | 1231 | - | 73,73,73 | 2.22 | 20 (27%) | 96,113,113 | 2.33 | 27 (28%) |
| 15 | CLA | B | 1232 | - | 51,53,73 | 2.55 | 20 (39%) | 69,89,113 | 2.40 | 21 (30%) |
| 15 | CLA | B | 1234 | - | 73,73,73 | 2.20 | 20 (27%) | 96,113,113 | 2.32 | 27 (28%) |
| 15 | CLA | B | 1235 | - | 73,73,73 | 2.20 | 20 (27%) | 96,113,113 | 2.28 | 26 (27%) |
| 15 | CLA | B | 1236 | - | 58,58,73 | 2.49 | 21 (36%) | 76,95,113 | 2.59 | 26 (34%) |
| 15 | CLA | B | 1237 | 19 | 62,63,73 | 2.39 | 20 (32%) | 82,101,113 | 2.47 | 28 (34%) |
| 15 | CLA | B | 1238 | 19 | 52,52,73 | 3.40 | 20 (38%) | 68,87,113 | 2.41 | 20 (29%) |
| 15 | CLA | B | 1239 | - | 53,54,73 | 2.52 | 20 (37%) | 72,90,113 | 2.55 | 22 (30%) |
| 15 | CLA | B | 1240 | 12 | 51,53,73 | 2.61 | 21 (41%) | 69,89,113 | 2.43 | 21 (30%) |
| 16 | LMU | B | 1301 | - | 36,36,36 | 0.44 | 0 | 47,47,47 | 0.92 | 4 (8%) |
| 10 | PQN | B | 2002 | - | 34,34,34 | 1.38 | 2 (5%) | 45,45,45 | 1.10 | 4 (8%) |
| 14 | BCR | B | 4004 | - | 41,41,41 | 2.74 | 6 (14%) | 56,56,56 | 6.13 | 28 (50%) |
| 14 | BCR | B | 4005 | - | 41,41,41 | 2.73 | 6 (14%) | 56,56,56 | 6.20 | 23 (41%) |
| 14 | BCR | B | 4006 | - | 41,41,41 | 2.82 | 6 (14%) | 56,56,56 | 6.46 | 24 (42%) |
| 14 | BCR | B | 4009 | - | 41,41,41 | 2.73 | 7 (17%) | 56,56,56 | 6.55 | 24 (42%) |
| 14 | BCR | B | 4010 | - | 41,41,41 | 2.71 | 6 (14%) | 56,56,56 | 6.42 | 23 (41%) |
| 14 | BCR | B | 4011 | - | 41,41,41 | 2.75 | 6 (14%) | 56,56,56 | 6.51 | 25 (44%) |
| 14 | BCR | B | 4014 | - | 41,41,41 | 2.73 | 6 (14%) | 56,56,56 | 6.44 | 21 (37%) |
| 14 | BCR | B | 4017 | - | 41,41,41 | 2.71 | 6 (14%) | 56,56,56 | 6.35 | 24 (42%) |
| 17 | LMG | B | 5002 | - | 55,55,55 | 0.88 | 2 (3%) | 63,63,63 | 0.98 | 2 (3%) |
| 12 | LHG | B | 5004 | 15 | 48,48,48 | 0.90 | 2 (4%) | 54,54,54 | 1.13 | 3 (5%) |
| 11 | SF4 | C | 3002 | 3 | 12,12,12 | 6.40 | 12 (100%) | 0,24,24 | 0.00 | - |
| 11 | SF4 | C | 3003 | 3 | 12,12,12 | 6.54 | 12 (100%) | 0,24,24 | 0.00 | - |
| 15 | CLA | F | 1139 | 19 | 73,73,73 | 2.22 | 21 (28%) | 96,113,113 | 2.23 | 22 (22%) |
| 15 | CLA | F | 1301 | - | 51,53,73 | 2.59 | 20 (39%) | 69,89,113 | 2.43 | 20 (28%) |
| 15 | CLA | F | 1410 | 6 | 73,73,73 | 2.20 | 20 (27%) | 96,113,113 | 2.38 | 28 (29%) |
| 14 | BCR | F | 4015 | - | 41,41,41 | 2.73 | 7 (17%) | 56,56,56 | 6.41 | 26 (46%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | BCR | F | 4016 | - | 41,41,41 | 2.72 | 6 (14%) | 56,56,56 | 6.50 | 24 (42%) |
| 15 | CLA | J | 1302 | 7 | 51,53,73 | 2.61 | 20 (39%) | 69,89,113 | 2.42 | 18 (26%) |
| 15 | CLA | J | 1303 | - | 53,54,73 | 2.53 | 20 (37%) | 72,90,113 | 2.53 | 21 (29%) |
| 16 | LMU | J | 1304 | - | 36,36,36 | 0.41 | 0 | 47,47,47 | 0.64 | 1 (2%) |
| 14 | BCR | J | 4013 | - | 41,41,41 | 2.71 | 6 (14%) | 56,56,56 | 6.40 | 28 (50%) |
| 15 | CLA | K | 1401 | - | 53,54,73 | 2.51 | 19 (35%) | 72,90,113 | 2.59 | 24 (33%) |
| 15 | CLA | K | 1402 | - | 53,54,73 | 2.51 | 19 (35%) | 72,90,113 | 2.51 | 21 (29%) |

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 |
|-----|------|-------|------|------|---------|--------------|---------|
| 13 | CL0 | A | 1011 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1012 | 19 | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1022 | 19 | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1101 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1102 | 15 | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1103 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1104 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1105 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1106 | 1 | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1107 | 1 | - | 0/19/117/135 | 0/0/9/9 |
| 13 | CL0 | A | 1108 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | A | 1109 | 15 | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1110 | - | - | 0/23/122/135 | 0/0/9/9 |
| 15 | CLA | A | 1111 | - | - | 0/31/129/135 | 0/0/9/9 |
| 15 | CLA | A | 1112 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | A | 1113 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | A | 1114 | - | - | 0/17/116/135 | 0/0/9/9 |
| 15 | CLA | A | 1115 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | A | 1116 | - | - | 0/23/122/135 | 0/0/9/9 |
| 15 | CLA | A | 1117 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1118 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | A | 1119 | - | - | 0/33/133/135 | 0/0/9/9 |
| 15 | CLA | A | 1120 | - | - | 0/17/116/135 | 0/0/9/9 |
| 15 | CLA | A | 1121 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | A | 1122 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1123 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1124 | - | - | 0/25/123/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 15 | CLA | A | 1125 | - | - | 0/22/120/135 | 0/0/9/9 |
| 15 | CLA | A | 1126 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1127 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1128 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1129 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | A | 1130 | - | - | 0/25/123/135 | 0/0/9/9 |
| 15 | CLA | A | 1131 | - | - | 0/25/123/135 | 0/0/9/9 |
| 15 | CLA | A | 1132 | - | - | 0/34/132/135 | 0/0/9/9 |
| 15 | CLA | A | 1133 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | A | 1134 | 1 | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | A | 1135 | - | - | 0/25/123/135 | 0/0/9/9 |
| 15 | CLA | A | 1136 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1137 | - | - | 0/19/117/135 | 0/0/9/9 |
| 15 | CLA | A | 1138 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1140 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | A | 1801 | 12 | - | 0/22/120/135 | 0/0/9/9 |
| 10 | PQN | A | 2001 | - | - | 0/23/43/43 | 0/2/2/2 |
| 11 | SF4 | A | 3001 | 1,2 | - | 0/0/48/48 | 0/6/5/5 |
| 14 | BCR | A | 4001 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | A | 4002 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | A | 4003 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | A | 4007 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | A | 4008 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | A | 4012 | - | - | 0/29/63/63 | 0/2/2/2 |
| 12 | LHG | A | 5001 | - | - | 0/53/53/53 | 0/0/0/0 |
| 12 | LHG | A | 5003 | 15 | - | 0/53/53/53 | 0/0/0/0 |
| 12 | LHG | A | 5005 | - | - | 0/40/40/53 | 0/0/0/0 |
| 15 | CLA | B | 1013 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1021 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1023 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1201 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | B | 1202 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1203 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1204 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | B | 1205 | - | - | 0/25/123/135 | 0/0/9/9 |
| 15 | CLA | B | 1206 | 2 | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | B | 1207 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | B | 1208 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | B | 1209 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | B | 1210 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1211 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | B | 1212 | - | - | 0/11/111/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 15 | CLA | B | 1213 | - | - | 0/19/117/135 | 0/0/9/9 |
| 15 | CLA | B | 1214 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1215 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1216 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1217 | - | - | 0/16/114/135 | 0/0/9/9 |
| 15 | CLA | B | 1218 | - | - | 0/21/119/135 | 0/0/9/9 |
| 15 | CLA | B | 1219 | - | - | 0/25/123/135 | 0/0/9/9 |
| 15 | CLA | B | 1220 | - | - | 0/27/125/135 | 0/0/9/9 |
| 15 | CLA | B | 1221 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1222 | - | - | 0/27/125/135 | 0/0/9/9 |
| 15 | CLA | B | 1223 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1224 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1225 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1226 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1227 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | B | 1228 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1229 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1230 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1231 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1232 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | B | 1234 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1235 | - | - | 0/37/135/135 | 0/0/9/9 |
| 15 | CLA | B | 1236 | - | - | 0/19/117/135 | 0/0/9/9 |
| 15 | CLA | B | 1237 | 19 | - | 0/25/123/135 | 0/0/9/9 |
| 15 | CLA | B | 1238 | 19 | - | 0/11/110/135 | 0/0/9/9 |
| 15 | CLA | B | 1239 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | B | 1240 | 12 | - | 0/11/111/135 | 0/0/9/9 |
| 16 | LMU | B | 1301 | - | - | 0/21/61/61 | 0/2/2/2 |
| 10 | PQN | B | 2002 | - | - | 0/23/43/43 | 0/2/2/2 |
| 14 | BCR | B | 4004 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4005 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4006 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4009 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4010 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4011 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4014 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | B | 4017 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | LMG | B | 5002 | - | - | 0/50/70/70 | 0/1/1/1 |
| 12 | LHG | B | 5004 | 15 | - | 0/53/53/53 | 0/0/0/0 |
| 11 | SF4 | C | 3002 | 3 | - | 0/0/48/48 | 0/6/5/5 |
| 11 | SF4 | C | 3003 | 3 | - | 0/0/48/48 | 0/6/5/5 |
| 15 | CLA | F | 1139 | 19 | - | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 15 | CLA | F | 1301 | - | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | F | 1410 | 6 | - | 0/37/135/135 | 0/0/9/9 |
| 14 | BCR | F | 4015 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | BCR | F | 4016 | - | - | 0/29/63/63 | 0/2/2/2 |
| 15 | CLA | J | 1302 | 7 | - | 0/11/111/135 | 0/0/9/9 |
| 15 | CLA | J | 1303 | - | - | 0/15/113/135 | 0/0/9/9 |
| 16 | LMU | J | 1304 | - | - | 0/21/61/61 | 0/2/2/2 |
| 14 | BCR | J | 4013 | - | - | 0/29/63/63 | 0/2/2/2 |
| 15 | CLA | K | 1401 | - | - | 0/15/113/135 | 0/0/9/9 |
| 15 | CLA | K | 1402 | - | - | 0/15/113/135 | 0/0/9/9 |

All (2012) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1238 | CLA | O1A-CGA | 16.37 | 1.22 | 1.11 |
| 15 | B | 1217 | CLA | O2A-C1 | 10.62 | 1.60 | 1.45 |
| 14 | A | 4012 | BCR | C11-C10 | -8.24 | 1.18 | 1.43 |
| 14 | B | 4006 | BCR | C11-C10 | -8.22 | 1.18 | 1.43 |
| 14 | F | 4016 | BCR | C11-C10 | -8.12 | 1.18 | 1.43 |
| 14 | B | 4004 | BCR | C11-C10 | -8.08 | 1.18 | 1.43 |
| 14 | B | 4010 | BCR | C11-C10 | -8.05 | 1.18 | 1.43 |
| 14 | B | 4011 | BCR | C11-C10 | -8.03 | 1.18 | 1.43 |
| 14 | B | 4006 | BCR | C10-C9 | -8.01 | 1.25 | 1.35 |
| 14 | B | 4009 | BCR | C8-C9 | -8.00 | 1.28 | 1.45 |
| 14 | A | 4002 | BCR | C11-C10 | -8.00 | 1.18 | 1.43 |
| 14 | B | 4014 | BCR | C11-C10 | -7.98 | 1.18 | 1.43 |
| 14 | B | 4009 | BCR | C11-C10 | -7.98 | 1.18 | 1.43 |
| 14 | B | 4005 | BCR | C11-C10 | -7.96 | 1.18 | 1.43 |
| 14 | F | 4015 | BCR | C8-C9 | -7.95 | 1.28 | 1.45 |
| 14 | F | 4015 | BCR | C11-C10 | -7.95 | 1.19 | 1.43 |
| 14 | B | 4017 | BCR | C11-C10 | -7.94 | 1.19 | 1.43 |
| 14 | B | 4014 | BCR | C8-C9 | -7.93 | 1.28 | 1.45 |
| 14 | F | 4016 | BCR | C8-C9 | -7.93 | 1.28 | 1.45 |
| 14 | A | 4003 | BCR | C11-C10 | -7.93 | 1.19 | 1.43 |
| 14 | A | 4007 | BCR | C11-C10 | -7.91 | 1.19 | 1.43 |
| 14 | A | 4001 | BCR | C11-C10 | -7.91 | 1.19 | 1.43 |
| 14 | A | 4012 | BCR | C8-C9 | -7.90 | 1.28 | 1.45 |
| 14 | B | 4005 | BCR | C8-C9 | -7.89 | 1.28 | 1.45 |
| 14 | J | 4013 | BCR | C8-C9 | -7.88 | 1.28 | 1.45 |
| 14 | A | 4008 | BCR | C11-C10 | -7.87 | 1.19 | 1.43 |
| 14 | J | 4013 | BCR | C11-C10 | -7.86 | 1.19 | 1.43 |
| 14 | B | 4006 | BCR | C8-C9 | -7.83 | 1.28 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 4003 | BCR | C8-C9 | -7.83 | 1.28 | 1.45 |
| 14 | B | 4011 | BCR | C8-C9 | -7.78 | 1.28 | 1.45 |
| 14 | A | 4008 | BCR | C8-C9 | -7.77 | 1.28 | 1.45 |
| 14 | A | 4001 | BCR | C8-C9 | -7.77 | 1.28 | 1.45 |
| 14 | A | 4001 | BCR | C10-C9 | -7.73 | 1.25 | 1.35 |
| 14 | A | 4002 | BCR | C8-C9 | -7.72 | 1.28 | 1.45 |
| 14 | B | 4004 | BCR | C8-C9 | -7.70 | 1.28 | 1.45 |
| 14 | A | 4007 | BCR | C8-C9 | -7.68 | 1.28 | 1.45 |
| 14 | B | 4017 | BCR | C8-C9 | -7.68 | 1.28 | 1.45 |
| 14 | B | 4010 | BCR | C8-C9 | -7.64 | 1.29 | 1.45 |
| 15 | A | 1123 | CLA | MG-NA | 7.43 | 2.29 | 2.07 |
| 14 | A | 4012 | BCR | C10-C9 | -7.41 | 1.26 | 1.35 |
| 14 | B | 4017 | BCR | C20-C21 | -7.41 | 1.20 | 1.43 |
| 14 | B | 4011 | BCR | C20-C21 | -7.40 | 1.20 | 1.43 |
| 13 | A | 1108 | CL0 | MG-NA | 7.40 | 2.29 | 2.07 |
| 14 | B | 4004 | BCR | C10-C9 | -7.39 | 1.26 | 1.35 |
| 15 | B | 1220 | CLA | MG-NA | 7.39 | 2.29 | 2.07 |
| 14 | A | 4002 | BCR | C20-C21 | -7.37 | 1.20 | 1.43 |
| 15 | A | 1138 | CLA | MG-NA | 7.37 | 2.29 | 2.07 |
| 14 | A | 4012 | BCR | C20-C21 | -7.37 | 1.20 | 1.43 |
| 15 | B | 1221 | CLA | MG-NA | 7.36 | 2.29 | 2.07 |
| 14 | A | 4008 | BCR | C20-C21 | -7.36 | 1.20 | 1.43 |
| 14 | B | 4006 | BCR | C20-C21 | -7.36 | 1.20 | 1.43 |
| 15 | B | 1240 | CLA | MG-NA | 7.35 | 2.29 | 2.07 |
| 15 | A | 1120 | CLA | MG-NA | 7.35 | 2.29 | 2.07 |
| 15 | A | 1801 | CLA | MG-NA | 7.35 | 2.29 | 2.07 |
| 14 | A | 4012 | BCR | C16-C17 | -7.34 | 1.20 | 1.43 |
| 15 | A | 1135 | CLA | MG-NA | 7.34 | 2.29 | 2.07 |
| 14 | F | 4015 | BCR | C20-C21 | -7.32 | 1.20 | 1.43 |
| 14 | B | 4006 | BCR | C16-C17 | -7.32 | 1.20 | 1.43 |
| 15 | J | 1303 | CLA | MG-NA | 7.31 | 2.28 | 2.07 |
| 15 | A | 1125 | CLA | MG-NA | 7.31 | 2.28 | 2.07 |
| 15 | B | 1236 | CLA | MG-NA | 7.31 | 2.28 | 2.07 |
| 15 | B | 1238 | CLA | MG-NA | 7.30 | 2.28 | 2.07 |
| 14 | A | 4002 | BCR | C10-C9 | -7.31 | 1.26 | 1.35 |
| 15 | A | 1117 | CLA | MG-NA | 7.30 | 2.28 | 2.07 |
| 15 | B | 1223 | CLA | MG-NA | 7.30 | 2.28 | 2.07 |
| 15 | J | 1302 | CLA | MG-NA | 7.30 | 2.28 | 2.07 |
| 14 | B | 4009 | BCR | C20-C21 | -7.30 | 1.21 | 1.43 |
| 15 | B | 1206 | CLA | MG-NA | 7.29 | 2.28 | 2.07 |
| 15 | A | 1112 | CLA | MG-NA | 7.29 | 2.28 | 2.07 |
| 15 | B | 1237 | CLA | MG-NA | 7.29 | 2.28 | 2.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1134 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 14 | B | 4005 | BCR | C20-C21 | -7.28 | 1.21 | 1.43 |
| 15 | A | 1101 | CLA | C3B-C4B | 7.28 | 1.50 | 1.41 |
| 15 | B | 1209 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 14 | A | 4001 | BCR | C20-C21 | -7.28 | 1.21 | 1.43 |
| 15 | A | 1131 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 15 | F | 1410 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 14 | A | 4007 | BCR | C20-C21 | -7.28 | 1.21 | 1.43 |
| 15 | A | 1101 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 14 | J | 4013 | BCR | C20-C21 | -7.27 | 1.21 | 1.43 |
| 15 | A | 1113 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 15 | B | 1229 | CLA | MG-NA | 7.28 | 2.28 | 2.07 |
| 15 | A | 1130 | CLA | MG-NA | 7.27 | 2.28 | 2.07 |
| 14 | F | 4016 | BCR | C20-C21 | -7.27 | 1.21 | 1.43 |
| 15 | A | 1119 | CLA | MG-NA | 7.27 | 2.28 | 2.07 |
| 15 | A | 1124 | CLA | MG-NA | 7.27 | 2.28 | 2.07 |
| 15 | A | 1114 | CLA | MG-NA | 7.27 | 2.28 | 2.07 |
| 15 | A | 1137 | CLA | MG-NA | 7.27 | 2.28 | 2.07 |
| 15 | A | 1121 | CLA | MG-NA | 7.26 | 2.28 | 2.07 |
| 14 | B | 4010 | BCR | C10-C9 | -7.27 | 1.26 | 1.35 |
| 14 | A | 4008 | BCR | C16-C17 | -7.26 | 1.21 | 1.43 |
| 15 | B | 1212 | CLA | MG-NA | 7.26 | 2.28 | 2.07 |
| 14 | A | 4003 | BCR | C20-C21 | -7.26 | 1.21 | 1.43 |
| 15 | B | 1021 | CLA | MG-NA | 7.26 | 2.28 | 2.07 |
| 15 | B | 1239 | CLA | MG-NA | 7.26 | 2.28 | 2.07 |
| 14 | A | 4002 | BCR | C16-C17 | -7.26 | 1.21 | 1.43 |
| 15 | A | 1012 | CLA | MG-NA | 7.26 | 2.28 | 2.07 |
| 15 | B | 1217 | CLA | MG-NA | 7.26 | 2.28 | 2.07 |
| 14 | B | 4009 | BCR | C16-C17 | -7.26 | 1.21 | 1.43 |
| 14 | A | 4001 | BCR | C16-C17 | -7.25 | 1.21 | 1.43 |
| 14 | B | 4004 | BCR | C20-C21 | -7.25 | 1.21 | 1.43 |
| 15 | B | 1210 | CLA | MG-NA | 7.24 | 2.28 | 2.07 |
| 15 | B | 1213 | CLA | MG-NA | 7.24 | 2.28 | 2.07 |
| 15 | B | 1232 | CLA | MG-NA | 7.24 | 2.28 | 2.07 |
| 14 | B | 4011 | BCR | C16-C17 | -7.24 | 1.21 | 1.43 |
| 15 | B | 1215 | CLA | MG-NA | 7.24 | 2.28 | 2.07 |
| 15 | F | 1301 | CLA | MG-NA | 7.23 | 2.28 | 2.07 |
| 15 | A | 1110 | CLA | MG-NA | 7.23 | 2.28 | 2.07 |
| 14 | A | 4003 | BCR | C16-C17 | -7.23 | 1.21 | 1.43 |
| 11 | A | 3001 | SF4 | S3-FE4 | -7.23 | 2.28 | 2.33 |
| 15 | K | 1402 | CLA | MG-NA | 7.23 | 2.28 | 2.07 |
| 14 | B | 4005 | BCR | C10-C9 | -7.23 | 1.26 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 4005 | BCR | C16-C17 | -7.23 | 1.21 | 1.43 |
| 14 | B | 4014 | BCR | C10-C9 | -7.23 | 1.26 | 1.35 |
| 15 | A | 1122 | CLA | MG-NA | 7.23 | 2.28 | 2.07 |
| 14 | B | 4011 | BCR | C10-C9 | -7.22 | 1.26 | 1.35 |
| 14 | B | 4014 | BCR | C20-C21 | -7.22 | 1.21 | 1.43 |
| 15 | F | 1139 | CLA | MG-NA | 7.22 | 2.28 | 2.07 |
| 15 | A | 1105 | CLA | MG-NA | 7.22 | 2.28 | 2.07 |
| 15 | A | 1132 | CLA | MG-NA | 7.22 | 2.28 | 2.07 |
| 15 | B | 1214 | CLA | MG-NA | 7.22 | 2.28 | 2.07 |
| 14 | B | 4010 | BCR | C20-C21 | -7.22 | 1.21 | 1.43 |
| 15 | B | 1207 | CLA | MG-NA | 7.22 | 2.28 | 2.07 |
| 15 | B | 1205 | CLA | MG-NA | 7.21 | 2.28 | 2.07 |
| 15 | B | 1234 | CLA | MG-NA | 7.21 | 2.28 | 2.07 |
| 15 | A | 1138 | CLA | C3B-C4B | 7.21 | 1.49 | 1.41 |
| 14 | F | 4015 | BCR | C16-C17 | -7.21 | 1.21 | 1.43 |
| 15 | A | 1116 | CLA | MG-NA | 7.21 | 2.28 | 2.07 |
| 15 | B | 1216 | CLA | MG-NA | 7.21 | 2.28 | 2.07 |
| 15 | B | 1204 | CLA | MG-NA | 7.20 | 2.28 | 2.07 |
| 15 | A | 1133 | CLA | MG-NA | 7.20 | 2.28 | 2.07 |
| 15 | A | 1140 | CLA | MG-NA | 7.20 | 2.28 | 2.07 |
| 14 | B | 4004 | BCR | C16-C17 | -7.20 | 1.21 | 1.43 |
| 15 | B | 1225 | CLA | MG-NA | 7.19 | 2.28 | 2.07 |
| 14 | B | 4017 | BCR | C16-C17 | -7.19 | 1.21 | 1.43 |
| 15 | B | 1226 | CLA | MG-NA | 7.19 | 2.28 | 2.07 |
| 15 | B | 1201 | CLA | MG-NA | 7.19 | 2.28 | 2.07 |
| 15 | K | 1401 | CLA | MG-NA | 7.19 | 2.28 | 2.07 |
| 15 | A | 1022 | CLA | MG-NA | 7.18 | 2.28 | 2.07 |
| 15 | A | 1127 | CLA | MG-NA | 7.18 | 2.28 | 2.07 |
| 14 | J | 4013 | BCR | C16-C17 | -7.18 | 1.21 | 1.43 |
| 15 | B | 1203 | CLA | MG-NA | 7.18 | 2.28 | 2.07 |
| 15 | B | 1224 | CLA | MG-NA | 7.18 | 2.28 | 2.07 |
| 14 | B | 4014 | BCR | C16-C17 | -7.18 | 1.21 | 1.43 |
| 15 | A | 1126 | CLA | MG-NA | 7.18 | 2.28 | 2.07 |
| 15 | B | 1211 | CLA | MG-NA | 7.17 | 2.28 | 2.07 |
| 11 | A | 3001 | SF4 | S3-FE1 | -7.17 | 2.28 | 2.33 |
| 14 | A | 4007 | BCR | C10-C9 | -7.17 | 1.26 | 1.35 |
| 15 | A | 1129 | CLA | MG-NA | 7.17 | 2.28 | 2.07 |
| 15 | A | 1102 | CLA | MG-NA | 7.16 | 2.28 | 2.07 |
| 14 | A | 4003 | BCR | C10-C9 | -7.16 | 1.26 | 1.35 |
| 15 | B | 1218 | CLA | MG-NA | 7.16 | 2.28 | 2.07 |
| 14 | F | 4015 | BCR | C10-C9 | -7.16 | 1.26 | 1.35 |
| 14 | F | 4016 | BCR | C16-C17 | -7.15 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1115 | CLA | MG-NA | 7.14 | 2.28 | 2.07 |
| 15 | A | 1111 | CLA | MG-NA | 7.14 | 2.28 | 2.07 |
| 14 | A | 4007 | BCR | C16-C17 | -7.14 | 1.21 | 1.43 |
| 15 | B | 1231 | CLA | MG-NA | 7.14 | 2.28 | 2.07 |
| 15 | A | 1103 | CLA | MG-NA | 7.14 | 2.28 | 2.07 |
| 15 | B | 1219 | CLA | MG-NA | 7.14 | 2.28 | 2.07 |
| 13 | A | 1011 | CL0 | MG-NA | 7.13 | 2.28 | 2.07 |
| 15 | A | 1122 | CLA | C3B-C4B | 7.13 | 1.49 | 1.41 |
| 15 | A | 1118 | CLA | MG-NA | 7.13 | 2.28 | 2.07 |
| 15 | A | 1104 | CLA | MG-NA | 7.13 | 2.28 | 2.07 |
| 15 | B | 1208 | CLA | MG-NA | 7.13 | 2.28 | 2.07 |
| 15 | B | 1202 | CLA | MG-NA | 7.13 | 2.28 | 2.07 |
| 15 | B | 1228 | CLA | MG-NA | 7.12 | 2.28 | 2.07 |
| 15 | A | 1106 | CLA | MG-NA | 7.12 | 2.28 | 2.07 |
| 11 | C | 3003 | SF4 | S3-FE4 | -7.10 | 2.28 | 2.33 |
| 15 | B | 1227 | CLA | MG-NA | 7.10 | 2.28 | 2.07 |
| 15 | A | 1136 | CLA | MG-NA | 7.10 | 2.28 | 2.07 |
| 15 | A | 1109 | CLA | MG-NA | 7.10 | 2.28 | 2.07 |
| 15 | B | 1023 | CLA | MG-NA | 7.09 | 2.28 | 2.07 |
| 15 | B | 1222 | CLA | MG-NA | 7.08 | 2.28 | 2.07 |
| 14 | B | 4010 | BCR | C16-C17 | -7.08 | 1.21 | 1.43 |
| 15 | A | 1128 | CLA | MG-NA | 7.07 | 2.28 | 2.07 |
| 14 | J | 4013 | BCR | C10-C9 | -7.07 | 1.26 | 1.35 |
| 15 | B | 1235 | CLA | MG-NA | 7.07 | 2.28 | 2.07 |
| 15 | A | 1107 | CLA | MG-NA | 7.06 | 2.28 | 2.07 |
| 15 | A | 1107 | CLA | C3B-C4B | 7.06 | 1.49 | 1.41 |
| 15 | B | 1230 | CLA | MG-NA | 7.05 | 2.28 | 2.07 |
| 14 | B | 4017 | BCR | C10-C9 | -7.02 | 1.26 | 1.35 |
| 14 | B | 4009 | BCR | C10-C9 | -7.02 | 1.26 | 1.35 |
| 14 | A | 4008 | BCR | C10-C9 | -6.96 | 1.26 | 1.35 |
| 15 | B | 1013 | CLA | MG-NA | 6.96 | 2.27 | 2.07 |
| 15 | A | 1126 | CLA | C3B-C4B | 6.95 | 1.49 | 1.41 |
| 15 | B | 1236 | CLA | C3B-C4B | 6.94 | 1.49 | 1.41 |
| 15 | A | 1113 | CLA | C3B-C4B | 6.93 | 1.49 | 1.41 |
| 14 | F | 4016 | BCR | C10-C9 | -6.93 | 1.26 | 1.35 |
| 11 | C | 3003 | SF4 | S4-FE3 | -6.89 | 2.28 | 2.33 |
| 11 | C | 3003 | SF4 | S3-FE1 | -6.86 | 2.28 | 2.33 |
| 15 | A | 1128 | CLA | C3B-C4B | 6.85 | 1.49 | 1.41 |
| 11 | C | 3003 | SF4 | S3-FE2 | -6.85 | 2.28 | 2.33 |
| 15 | F | 1139 | CLA | C3B-C4B | 6.83 | 1.49 | 1.41 |
| 11 | C | 3002 | SF4 | S4-FE3 | -6.82 | 2.28 | 2.33 |
| 11 | A | 3001 | SF4 | S2-FE4 | -6.78 | 2.28 | 2.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11 | C | 3003 | SF4 | S4-FE2 | -6.76 | 2.28 | 2.33 |
| 15 | J | 1302 | CLA | C3B-C4B | 6.74 | 1.49 | 1.41 |
| 15 | A | 1125 | CLA | C3B-C4B | 6.73 | 1.49 | 1.41 |
| 15 | A | 1112 | CLA | C3B-C4B | 6.72 | 1.49 | 1.41 |
| 13 | A | 1108 | CL0 | C3B-C4B | 6.71 | 1.49 | 1.41 |
| 15 | A | 1131 | CLA | C3B-C4B | 6.71 | 1.49 | 1.41 |
| 11 | C | 3002 | SF4 | S3-FE4 | -6.70 | 2.28 | 2.33 |
| 15 | A | 1130 | CLA | C3B-C4B | 6.68 | 1.49 | 1.41 |
| 15 | A | 1104 | CLA | C3B-C4B | 6.67 | 1.49 | 1.41 |
| 11 | A | 3001 | SF4 | S3-FE2 | -6.64 | 2.28 | 2.33 |
| 11 | C | 3002 | SF4 | S3-FE1 | -6.63 | 2.28 | 2.33 |
| 15 | B | 1235 | CLA | C3B-C4B | 6.63 | 1.49 | 1.41 |
| 15 | B | 1228 | CLA | C3B-C4B | 6.62 | 1.49 | 1.41 |
| 11 | C | 3003 | SF4 | S2-FE1 | -6.61 | 2.28 | 2.33 |
| 11 | A | 3001 | SF4 | S1-FE2 | -6.61 | 2.28 | 2.33 |
| 15 | B | 1231 | CLA | C3B-C4B | 6.60 | 1.49 | 1.41 |
| 15 | A | 1117 | CLA | C3B-C4B | 6.58 | 1.49 | 1.41 |
| 15 | B | 1214 | CLA | C3B-C4B | 6.56 | 1.49 | 1.41 |
| 15 | A | 1102 | CLA | C3B-C4B | 6.56 | 1.49 | 1.41 |
| 11 | C | 3002 | SF4 | S4-FE2 | -6.56 | 2.28 | 2.33 |
| 15 | A | 1119 | CLA | C3B-C4B | 6.55 | 1.49 | 1.41 |
| 15 | B | 1021 | CLA | C3B-C4B | 6.54 | 1.49 | 1.41 |
| 11 | C | 3002 | SF4 | S1-FE4 | -6.54 | 2.28 | 2.33 |
| 15 | A | 1140 | CLA | C3B-C4B | 6.54 | 1.49 | 1.41 |
| 15 | A | 1134 | CLA | C3B-C4B | 6.52 | 1.49 | 1.41 |
| 11 | A | 3001 | SF4 | S1-FE3 | -6.52 | 2.28 | 2.33 |
| 15 | B | 1223 | CLA | C3B-C4B | 6.51 | 1.49 | 1.41 |
| 15 | A | 1115 | CLA | C3B-C4B | 6.51 | 1.49 | 1.41 |
| 15 | B | 1218 | CLA | C3B-C4B | 6.50 | 1.49 | 1.41 |
| 15 | A | 1109 | CLA | C3B-C4B | 6.49 | 1.49 | 1.41 |
| 15 | B | 1013 | CLA | C3B-C4B | 6.49 | 1.49 | 1.41 |
| 15 | B | 1240 | CLA | C3B-C4B | 6.49 | 1.49 | 1.41 |
| 15 | B | 1213 | CLA | C3B-C4B | 6.47 | 1.49 | 1.41 |
| 15 | B | 1220 | CLA | C3B-C4B | 6.47 | 1.49 | 1.41 |
| 15 | A | 1103 | CLA | C3B-C4B | 6.45 | 1.49 | 1.41 |
| 15 | A | 1012 | CLA | C3B-C4B | 6.45 | 1.49 | 1.41 |
| 11 | C | 3002 | SF4 | S1-FE2 | -6.44 | 2.28 | 2.33 |
| 11 | A | 3001 | SF4 | S2-FE1 | -6.44 | 2.28 | 2.33 |
| 11 | C | 3002 | SF4 | S4-FE1 | -6.43 | 2.28 | 2.33 |
| 15 | F | 1301 | CLA | C3B-C4B | 6.42 | 1.48 | 1.41 |
| 15 | J | 1303 | CLA | C3B-C4B | 6.41 | 1.48 | 1.41 |
| 15 | A | 1106 | CLA | C3B-C4B | 6.40 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11 | A | 3001 | SF4 | S4-FE3 | -6.40 | 2.29 | 2.33 |
| 15 | B | 1237 | CLA | C3B-C4B | 6.39 | 1.48 | 1.41 |
| 15 | A | 1111 | CLA | C3B-C4B | 6.38 | 1.48 | 1.41 |
| 15 | B | 1217 | CLA | C3B-C4B | 6.37 | 1.48 | 1.41 |
| 15 | B | 1201 | CLA | C3B-C4B | 6.37 | 1.48 | 1.41 |
| 11 | C | 3003 | SF4 | S4-FE1 | -6.37 | 2.29 | 2.33 |
| 15 | B | 1238 | CLA | C3B-C4B | 6.36 | 1.48 | 1.41 |
| 15 | B | 1202 | CLA | C3B-C4B | 6.36 | 1.48 | 1.41 |
| 15 | B | 1210 | CLA | C3B-C4B | 6.36 | 1.48 | 1.41 |
| 15 | A | 1124 | CLA | C3B-C4B | 6.36 | 1.48 | 1.41 |
| 15 | B | 1230 | CLA | C3B-C4B | 6.36 | 1.48 | 1.41 |
| 15 | B | 1206 | CLA | C3B-C4B | 6.36 | 1.48 | 1.41 |
| 15 | F | 1410 | CLA | C3B-C4B | 6.35 | 1.48 | 1.41 |
| 15 | A | 1114 | CLA | C3B-C4B | 6.35 | 1.48 | 1.41 |
| 15 | K | 1401 | CLA | C3B-C4B | 6.34 | 1.48 | 1.41 |
| 15 | A | 1022 | CLA | C3B-C4B | 6.34 | 1.48 | 1.41 |
| 15 | B | 1207 | CLA | C3B-C4B | 6.34 | 1.48 | 1.41 |
| 15 | A | 1121 | CLA | C3B-C4B | 6.34 | 1.48 | 1.41 |
| 11 | C | 3003 | SF4 | S1-FE3 | -6.33 | 2.29 | 2.33 |
| 15 | B | 1212 | CLA | C3B-C4B | 6.31 | 1.48 | 1.41 |
| 11 | C | 3002 | SF4 | S1-FE3 | -6.30 | 2.29 | 2.33 |
| 11 | C | 3003 | SF4 | S1-FE2 | -6.30 | 2.29 | 2.33 |
| 13 | A | 1011 | CL0 | C3B-C4B | 6.29 | 1.48 | 1.41 |
| 15 | B | 1219 | CLA | C3B-C4B | 6.29 | 1.48 | 1.41 |
| 15 | A | 1133 | CLA | C3B-C4B | 6.29 | 1.48 | 1.41 |
| 11 | C | 3002 | SF4 | S3-FE2 | -6.28 | 2.29 | 2.33 |
| 15 | B | 1225 | CLA | C3B-C4B | 6.26 | 1.48 | 1.41 |
| 11 | A | 3001 | SF4 | S4-FE2 | -6.26 | 2.29 | 2.33 |
| 15 | B | 1208 | CLA | C3B-C4B | 6.24 | 1.48 | 1.41 |
| 15 | B | 1215 | CLA | C3B-C4B | 6.22 | 1.48 | 1.41 |
| 15 | A | 1801 | CLA | C3B-C4B | 6.21 | 1.48 | 1.41 |
| 11 | C | 3003 | SF4 | S2-FE3 | -6.19 | 2.29 | 2.33 |
| 15 | A | 1129 | CLA | C3B-C4B | 6.19 | 1.48 | 1.41 |
| 15 | A | 1120 | CLA | C3B-C4B | 6.19 | 1.48 | 1.41 |
| 15 | B | 1216 | CLA | C3B-C4B | 6.18 | 1.48 | 1.41 |
| 15 | B | 1209 | CLA | C3B-C4B | 6.18 | 1.48 | 1.41 |
| 15 | B | 1229 | CLA | C3B-C4B | 6.17 | 1.48 | 1.41 |
| 15 | B | 1221 | CLA | C3B-C4B | 6.17 | 1.48 | 1.41 |
| 15 | B | 1226 | CLA | C3B-C4B | 6.16 | 1.48 | 1.41 |
| 15 | A | 1127 | CLA | C3B-C4B | 6.15 | 1.48 | 1.41 |
| 15 | B | 1204 | CLA | C3B-C4B | 6.15 | 1.48 | 1.41 |
| 15 | B | 1023 | CLA | C3B-C4B | 6.13 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | K | 1402 | CLA | C3B-C4B | 6.12 | 1.48 | 1.41 |
| 15 | A | 1118 | CLA | C3B-C4B | 6.12 | 1.48 | 1.41 |
| 15 | B | 1227 | CLA | C3B-C4B | 6.11 | 1.48 | 1.41 |
| 11 | A | 3001 | SF4 | S2-FE3 | -6.10 | 2.29 | 2.33 |
| 15 | A | 1110 | CLA | C3B-C4B | 6.10 | 1.48 | 1.41 |
| 11 | C | 3002 | SF4 | S2-FE1 | -6.09 | 2.29 | 2.33 |
| 15 | B | 1224 | CLA | C3B-C4B | 6.09 | 1.48 | 1.41 |
| 15 | B | 1232 | CLA | C3B-C4B | 6.08 | 1.48 | 1.41 |
| 15 | B | 1203 | CLA | C3B-C4B | 6.07 | 1.48 | 1.41 |
| 11 | C | 3002 | SF4 | S2-FE4 | -6.07 | 2.29 | 2.33 |
| 11 | C | 3003 | SF4 | S2-FE4 | -6.06 | 2.29 | 2.33 |
| 15 | A | 1116 | CLA | C3B-C4B | 6.05 | 1.48 | 1.41 |
| 15 | A | 1123 | CLA | C3B-C4B | 6.03 | 1.48 | 1.41 |
| 15 | B | 1205 | CLA | C3B-C4B | 6.03 | 1.48 | 1.41 |
| 12 | A | 5005 | LHG | C16-C15 | -6.00 | 1.52 | 1.55 |
| 15 | A | 1137 | CLA | C3B-C4B | 6.00 | 1.48 | 1.41 |
| 15 | B | 1219 | CLA | C3B-C2B | 6.00 | 1.47 | 1.40 |
| 15 | B | 1211 | CLA | C3B-C4B | 5.99 | 1.48 | 1.41 |
| 11 | C | 3003 | SF4 | S1-FE4 | -5.99 | 2.29 | 2.33 |
| 15 | B | 1222 | CLA | C3B-C4B | 5.97 | 1.48 | 1.41 |
| 15 | A | 1132 | CLA | C3B-C4B | 5.97 | 1.48 | 1.41 |
| 15 | B | 1239 | CLA | C3B-C4B | 5.96 | 1.48 | 1.41 |
| 15 | B | 1234 | CLA | C3B-C4B | 5.95 | 1.48 | 1.41 |
| 15 | A | 1135 | CLA | C3B-C4B | 5.94 | 1.48 | 1.41 |
| 10 | A | 2001 | PQN | C3-C2 | 5.93 | 1.49 | 1.35 |
| 11 | C | 3002 | SF4 | S2-FE3 | -5.92 | 2.29 | 2.33 |
| 10 | B | 2002 | PQN | C3-C2 | 5.88 | 1.49 | 1.35 |
| 15 | B | 1222 | CLA | C11-C10 | -5.87 | 1.52 | 1.55 |
| 12 | A | 5005 | LHG | C31-C30 | -5.80 | 1.52 | 1.55 |
| 15 | A | 1801 | CLA | C7-C6 | -5.80 | 1.52 | 1.55 |
| 15 | A | 1132 | CLA | C17-C16 | -5.77 | 1.52 | 1.55 |
| 15 | A | 1136 | CLA | C3B-C4B | 5.76 | 1.48 | 1.41 |
| 11 | A | 3001 | SF4 | S4-FE1 | -5.75 | 2.29 | 2.33 |
| 11 | A | 3001 | SF4 | S1-FE4 | -5.68 | 2.29 | 2.33 |
| 15 | B | 1228 | CLA | C3B-C2B | 5.64 | 1.47 | 1.40 |
| 15 | A | 1105 | CLA | C3B-C4B | 5.63 | 1.48 | 1.41 |
| 15 | B | 1220 | CLA | C11-C10 | -5.62 | 1.52 | 1.55 |
| 15 | B | 1208 | CLA | C3B-C2B | 5.59 | 1.47 | 1.40 |
| 15 | B | 1220 | CLA | C3B-C2B | 5.53 | 1.47 | 1.40 |
| 15 | A | 1125 | CLA | C7-C6 | -5.51 | 1.53 | 1.55 |
| 15 | A | 1102 | CLA | C3B-C2B | 5.44 | 1.47 | 1.40 |
| 15 | A | 1115 | CLA | C3B-C2B | 5.42 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1210 | CLA | C3B-C2B | 5.37 | 1.47 | 1.40 |
| 15 | A | 1137 | CLA | C3B-C2B | 5.35 | 1.47 | 1.40 |
| 15 | A | 1127 | CLA | C3B-C2B | 5.32 | 1.47 | 1.40 |
| 15 | A | 1131 | CLA | C3B-C2B | 5.31 | 1.47 | 1.40 |
| 13 | A | 1108 | CL0 | C3B-C2B | 5.27 | 1.47 | 1.40 |
| 15 | B | 1212 | CLA | C3B-C2B | 5.26 | 1.47 | 1.40 |
| 15 | B | 1221 | CLA | C3B-C2B | 5.26 | 1.47 | 1.40 |
| 15 | A | 1136 | CLA | C3B-C2B | 5.25 | 1.46 | 1.40 |
| 15 | B | 1234 | CLA | C3B-C2B | 5.25 | 1.46 | 1.40 |
| 15 | B | 1218 | CLA | C6-C5 | -5.25 | 1.53 | 1.55 |
| 15 | B | 1213 | CLA | C3B-C2B | 5.24 | 1.46 | 1.40 |
| 15 | B | 1230 | CLA | C3B-C2B | 5.22 | 1.46 | 1.40 |
| 15 | B | 1202 | CLA | C3B-C2B | 5.21 | 1.46 | 1.40 |
| 15 | A | 1140 | CLA | C3B-C2B | 5.21 | 1.46 | 1.40 |
| 15 | J | 1302 | CLA | C3B-C2B | 5.20 | 1.46 | 1.40 |
| 15 | B | 1201 | CLA | C3B-C2B | 5.19 | 1.46 | 1.40 |
| 15 | A | 1113 | CLA | C3B-C2B | 5.19 | 1.46 | 1.40 |
| 15 | B | 1211 | CLA | C3B-C2B | 5.18 | 1.46 | 1.40 |
| 15 | B | 1238 | CLA | C3B-C2B | 5.18 | 1.46 | 1.40 |
| 15 | B | 1231 | CLA | C3B-C2B | 5.17 | 1.46 | 1.40 |
| 15 | A | 1134 | CLA | C3B-C2B | 5.17 | 1.46 | 1.40 |
| 15 | B | 1237 | CLA | C3B-C2B | 5.16 | 1.46 | 1.40 |
| 15 | A | 1135 | CLA | C3B-C2B | 5.15 | 1.46 | 1.40 |
| 15 | A | 1103 | CLA | C3B-C2B | 5.14 | 1.46 | 1.40 |
| 15 | B | 1225 | CLA | C3B-C2B | 5.14 | 1.46 | 1.40 |
| 15 | A | 1123 | CLA | C3B-C2B | 5.14 | 1.46 | 1.40 |
| 15 | A | 1111 | CLA | C3B-C2B | 5.12 | 1.46 | 1.40 |
| 15 | A | 1114 | CLA | C3B-C2B | 5.12 | 1.46 | 1.40 |
| 15 | B | 1224 | CLA | C3B-C2B | 5.12 | 1.46 | 1.40 |
| 15 | F | 1139 | CLA | C3B-C2B | 5.11 | 1.46 | 1.40 |
| 15 | A | 1120 | CLA | C3B-C2B | 5.08 | 1.46 | 1.40 |
| 15 | J | 1303 | CLA | C3B-C2B | 5.08 | 1.46 | 1.40 |
| 15 | B | 1207 | CLA | C3B-C2B | 5.08 | 1.46 | 1.40 |
| 15 | K | 1402 | CLA | C3B-C2B | 5.08 | 1.46 | 1.40 |
| 15 | B | 1222 | CLA | C3B-C2B | 5.07 | 1.46 | 1.40 |
| 15 | A | 1118 | CLA | C3B-C2B | 5.07 | 1.46 | 1.40 |
| 15 | K | 1401 | CLA | C3B-C2B | 5.07 | 1.46 | 1.40 |
| 15 | B | 1206 | CLA | C3B-C2B | 5.07 | 1.46 | 1.40 |
| 15 | F | 1301 | CLA | C3B-C2B | 5.07 | 1.46 | 1.40 |
| 15 | B | 1209 | CLA | C3B-C2B | 5.06 | 1.46 | 1.40 |
| 15 | B | 1218 | CLA | C3B-C2B | 5.06 | 1.46 | 1.40 |
| 15 | B | 1215 | CLA | C3B-C2B | 5.06 | 1.46 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1216 | CLA | C3B-C2B | 5.06 | 1.46 | 1.40 |
| 15 | A | 1109 | CLA | C3B-C2B | 5.06 | 1.46 | 1.40 |
| 15 | B | 1239 | CLA | C3B-C2B | 5.05 | 1.46 | 1.40 |
| 15 | A | 1801 | CLA | C3B-C2B | 5.05 | 1.46 | 1.40 |
| 15 | B | 1223 | CLA | C3B-C2B | 5.05 | 1.46 | 1.40 |
| 15 | B | 1240 | CLA | C3B-C2B | 5.04 | 1.46 | 1.40 |
| 15 | A | 1107 | CLA | C3B-C2B | 5.02 | 1.46 | 1.40 |
| 15 | B | 1013 | CLA | O2D-CGD | 5.01 | 1.46 | 1.33 |
| 15 | A | 1121 | CLA | C3B-C2B | 5.01 | 1.46 | 1.40 |
| 15 | A | 1132 | CLA | C3B-C2B | 5.01 | 1.46 | 1.40 |
| 15 | A | 1101 | CLA | C3B-C2B | 5.00 | 1.46 | 1.40 |
| 15 | A | 1138 | CLA | O2D-CGD | 5.00 | 1.46 | 1.33 |
| 15 | B | 1217 | CLA | C3B-C2B | 4.99 | 1.46 | 1.40 |
| 15 | B | 1013 | CLA | C3B-C2B | 4.98 | 1.46 | 1.40 |
| 15 | F | 1139 | CLA | O2D-CGD | 4.98 | 1.46 | 1.33 |
| 15 | A | 1119 | CLA | O2D-CGD | 4.98 | 1.46 | 1.33 |
| 15 | A | 1012 | CLA | O2D-CGD | 4.98 | 1.46 | 1.33 |
| 15 | K | 1401 | CLA | O2D-CGD | 4.98 | 1.46 | 1.33 |
| 15 | A | 1103 | CLA | O2D-CGD | 4.97 | 1.46 | 1.33 |
| 15 | A | 1129 | CLA | C3B-C2B | 4.97 | 1.46 | 1.40 |
| 15 | B | 1235 | CLA | C3B-C2B | 4.97 | 1.46 | 1.40 |
| 15 | B | 1235 | CLA | O2D-CGD | 4.97 | 1.46 | 1.33 |
| 15 | B | 1204 | CLA | C3B-C2B | 4.97 | 1.46 | 1.40 |
| 10 | B | 2002 | PQN | C10-C5 | 4.96 | 1.48 | 1.40 |
| 15 | A | 1121 | CLA | O2D-CGD | 4.96 | 1.46 | 1.33 |
| 15 | A | 1136 | CLA | O2D-CGD | 4.96 | 1.46 | 1.33 |
| 15 | A | 1106 | CLA | C3B-C2B | 4.96 | 1.46 | 1.40 |
| 15 | A | 1109 | CLA | O2D-CGD | 4.96 | 1.46 | 1.33 |
| 15 | B | 1203 | CLA | O2D-CGD | 4.96 | 1.46 | 1.33 |
| 10 | A | 2001 | PQN | C10-C5 | 4.96 | 1.48 | 1.40 |
| 15 | A | 1120 | CLA | O2D-CGD | 4.95 | 1.46 | 1.33 |
| 15 | A | 1112 | CLA | C3B-C2B | 4.95 | 1.46 | 1.40 |
| 15 | F | 1301 | CLA | O2D-CGD | 4.95 | 1.46 | 1.33 |
| 15 | A | 1127 | CLA | O2D-CGD | 4.94 | 1.46 | 1.33 |
| 15 | B | 1202 | CLA | O2D-CGD | 4.94 | 1.46 | 1.33 |
| 15 | A | 1138 | CLA | C3B-C2B | 4.94 | 1.46 | 1.40 |
| 15 | A | 1110 | CLA | C3B-C2B | 4.94 | 1.46 | 1.40 |
| 15 | B | 1214 | CLA | C3B-C2B | 4.94 | 1.46 | 1.40 |
| 15 | B | 1227 | CLA | O2D-CGD | 4.94 | 1.46 | 1.33 |
| 15 | B | 1232 | CLA | O2D-CGD | 4.94 | 1.46 | 1.33 |
| 15 | B | 1021 | CLA | O2D-CGD | 4.94 | 1.46 | 1.33 |
| 15 | A | 1130 | CLA | C3B-C2B | 4.94 | 1.46 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1219 | CLA | O2D-CGD | 4.93 | 1.46 | 1.33 |
| 15 | F | 1410 | CLA | C3B-C2B | 4.93 | 1.46 | 1.40 |
| 15 | B | 1208 | CLA | O2D-CGD | 4.93 | 1.46 | 1.33 |
| 15 | A | 1125 | CLA | C3B-C2B | 4.93 | 1.46 | 1.40 |
| 15 | A | 1117 | CLA | O2D-CGD | 4.93 | 1.46 | 1.33 |
| 15 | J | 1303 | CLA | O2D-CGD | 4.93 | 1.46 | 1.33 |
| 13 | A | 1108 | CL0 | O2D-CGD | 4.93 | 1.46 | 1.33 |
| 15 | A | 1801 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 15 | A | 1131 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 15 | K | 1402 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 15 | B | 1240 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 15 | B | 1237 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 15 | B | 1226 | CLA | C3B-C2B | 4.92 | 1.46 | 1.40 |
| 15 | A | 1022 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 15 | B | 1205 | CLA | C3B-C2B | 4.91 | 1.46 | 1.40 |
| 15 | A | 1116 | CLA | C3B-C2B | 4.91 | 1.46 | 1.40 |
| 15 | B | 1218 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 15 | B | 1216 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 15 | A | 1133 | CLA | C3B-C2B | 4.90 | 1.46 | 1.40 |
| 15 | B | 1215 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 15 | A | 1112 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 15 | B | 1203 | CLA | C3B-C2B | 4.90 | 1.46 | 1.40 |
| 15 | A | 1124 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 15 | B | 1205 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 15 | A | 1801 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 15 | A | 1133 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 15 | B | 1207 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 15 | B | 1220 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | A | 1124 | CLA | C3B-C2B | 4.88 | 1.46 | 1.40 |
| 13 | A | 1011 | CL0 | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | B | 1212 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | A | 1116 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | B | 1214 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | A | 1122 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | B | 1230 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | A | 1107 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | B | 1228 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | B | 1206 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 15 | A | 1118 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 15 | A | 1114 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 15 | A | 1126 | CLA | C3B-C2B | 4.87 | 1.46 | 1.40 |
| 15 | B | 1209 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 1105 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 15 | A | 1115 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 15 | A | 1106 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 15 | A | 1126 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 15 | A | 1129 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 15 | B | 1211 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 15 | A | 1113 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | B | 1224 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | B | 1201 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | B | 1204 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | B | 1239 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | A | 1117 | CLA | C3B-C2B | 4.85 | 1.46 | 1.40 |
| 15 | A | 1132 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | A | 1128 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | B | 1221 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 15 | B | 1229 | CLA | OBD-CAD | 4.84 | 1.29 | 1.22 |
| 15 | F | 1410 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 15 | A | 1140 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 15 | B | 1229 | CLA | C3B-C2B | 4.84 | 1.46 | 1.40 |
| 15 | B | 1213 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 15 | B | 1023 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 15 | J | 1302 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 15 | A | 1119 | CLA | C3B-C2B | 4.83 | 1.46 | 1.40 |
| 15 | B | 1238 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 15 | A | 1104 | CLA | C3B-C2B | 4.82 | 1.46 | 1.40 |
| 15 | A | 1130 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 15 | A | 1111 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 15 | B | 1223 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 15 | B | 1023 | CLA | C3B-C2B | 4.82 | 1.46 | 1.40 |
| 15 | A | 1124 | CLA | OBD-CAD | 4.81 | 1.29 | 1.22 |
| 15 | B | 1217 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 15 | A | 1137 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 15 | A | 1012 | CLA | C3B-C2B | 4.81 | 1.46 | 1.40 |
| 15 | B | 1222 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 15 | A | 1102 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 15 | B | 1222 | CLA | OBD-CAD | 4.80 | 1.29 | 1.22 |
| 15 | A | 1123 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 15 | B | 1236 | CLA | C3B-C2B | 4.80 | 1.46 | 1.40 |
| 15 | B | 1225 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 15 | A | 1122 | CLA | C3B-C2B | 4.79 | 1.46 | 1.40 |
| 15 | A | 1105 | CLA | C3B-C2B | 4.79 | 1.46 | 1.40 |
| 15 | B | 1236 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 1022 | CLA | C3B-C2B | 4.78 | 1.46 | 1.40 |
| 15 | A | 1101 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 15 | A | 1110 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 15 | A | 1138 | CLA | OBD-CAD | 4.77 | 1.29 | 1.22 |
| 15 | A | 1125 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 15 | B | 1202 | CLA | OBD-CAD | 4.77 | 1.29 | 1.22 |
| 15 | B | 1210 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 15 | A | 1102 | CLA | OBD-CAD | 4.76 | 1.29 | 1.22 |
| 15 | A | 1022 | CLA | OBD-CAD | 4.76 | 1.29 | 1.22 |
| 15 | A | 1135 | CLA | O2D-CGD | 4.76 | 1.45 | 1.33 |
| 15 | B | 1218 | CLA | OBD-CAD | 4.76 | 1.29 | 1.22 |
| 15 | B | 1229 | CLA | O2D-CGD | 4.76 | 1.45 | 1.33 |
| 15 | B | 1231 | CLA | O2D-CGD | 4.75 | 1.45 | 1.33 |
| 15 | B | 1228 | CLA | C3C-C2C | 4.75 | 1.46 | 1.36 |
| 15 | B | 1225 | CLA | OBD-CAD | 4.74 | 1.29 | 1.22 |
| 15 | A | 1130 | CLA | C3C-C2C | 4.74 | 1.46 | 1.36 |
| 15 | B | 1208 | CLA | C3C-C2C | 4.74 | 1.46 | 1.36 |
| 15 | A | 1101 | CLA | OBD-CAD | 4.74 | 1.29 | 1.22 |
| 15 | B | 1226 | CLA | O2D-CGD | 4.74 | 1.45 | 1.33 |
| 15 | A | 1120 | CLA | OBD-CAD | 4.72 | 1.29 | 1.22 |
| 15 | B | 1220 | CLA | C3C-C2C | 4.72 | 1.46 | 1.36 |
| 13 | A | 1011 | CL0 | C3B-C2B | 4.72 | 1.46 | 1.40 |
| 15 | A | 1134 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 15 | A | 1104 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 15 | B | 1222 | CLA | C3C-C2C | 4.71 | 1.46 | 1.36 |
| 15 | K | 1401 | CLA | OBD-CAD | 4.71 | 1.29 | 1.22 |
| 15 | B | 1207 | CLA | OBD-CAD | 4.71 | 1.29 | 1.22 |
| 15 | B | 1021 | CLA | OBD-CAD | 4.70 | 1.29 | 1.22 |
| 15 | B | 1227 | CLA | C3C-C2C | 4.70 | 1.46 | 1.36 |
| 15 | B | 1215 | CLA | OBD-CAD | 4.70 | 1.29 | 1.22 |
| 15 | B | 1213 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 15 | B | 1239 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 15 | B | 1240 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |
| 15 | B | 1223 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |
| 15 | B | 1224 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 15 | B | 1219 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 15 | B | 1216 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 15 | A | 1140 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 15 | A | 1106 | CLA | O2A-C1 | 4.69 | 1.61 | 1.46 |
| 15 | B | 1209 | CLA | OBD-CAD | 4.68 | 1.29 | 1.22 |
| 15 | B | 1214 | CLA | OBD-CAD | 4.68 | 1.29 | 1.22 |
| 15 | B | 1202 | CLA | C3C-C2C | 4.68 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 1109 | CLA | C3C-C2C | 4.68 | 1.46 | 1.36 |
| 15 | B | 1204 | CLA | OBD-CAD | 4.68 | 1.29 | 1.22 |
| 15 | A | 1116 | CLA | OBD-CAD | 4.68 | 1.29 | 1.22 |
| 15 | A | 1012 | CLA | O2A-C1 | 4.68 | 1.61 | 1.46 |
| 15 | B | 1021 | CLA | C3B-C2B | 4.68 | 1.46 | 1.40 |
| 15 | B | 1220 | CLA | OBD-CAD | 4.67 | 1.29 | 1.22 |
| 15 | A | 1117 | CLA | OBD-CAD | 4.67 | 1.29 | 1.22 |
| 15 | B | 1205 | CLA | OBD-CAD | 4.67 | 1.29 | 1.22 |
| 15 | B | 1212 | CLA | OBD-CAD | 4.67 | 1.29 | 1.22 |
| 15 | A | 1116 | CLA | C3C-C2C | 4.67 | 1.46 | 1.36 |
| 15 | A | 1022 | CLA | C3C-C2C | 4.67 | 1.46 | 1.36 |
| 15 | A | 1106 | CLA | OBD-CAD | 4.67 | 1.29 | 1.22 |
| 15 | B | 1013 | CLA | C3C-C2C | 4.66 | 1.46 | 1.36 |
| 15 | B | 1201 | CLA | OBD-CAD | 4.66 | 1.29 | 1.22 |
| 15 | A | 1122 | CLA | C3C-C2C | 4.66 | 1.46 | 1.36 |
| 15 | A | 1107 | CLA | C3C-C2C | 4.66 | 1.46 | 1.36 |
| 15 | B | 1217 | CLA | OBD-CAD | 4.66 | 1.29 | 1.22 |
| 15 | J | 1303 | CLA | C3C-C2C | 4.66 | 1.46 | 1.36 |
| 15 | B | 1226 | CLA | OBD-CAD | 4.66 | 1.29 | 1.22 |
| 15 | A | 1134 | CLA | OBD-CAD | 4.66 | 1.29 | 1.22 |
| 15 | B | 1240 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | A | 1138 | CLA | C3C-C2C | 4.65 | 1.46 | 1.36 |
| 15 | A | 1114 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | A | 1128 | CLA | C3B-C2B | 4.65 | 1.46 | 1.40 |
| 15 | A | 1131 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | A | 1111 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | A | 1112 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | J | 1302 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | F | 1410 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 15 | B | 1224 | CLA | O2A-C1 | 4.65 | 1.61 | 1.46 |
| 15 | A | 1137 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 15 | B | 1235 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 15 | A | 1118 | CLA | OBD-CAD | 4.64 | 1.29 | 1.22 |
| 15 | B | 1232 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 15 | B | 1212 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 15 | F | 1301 | CLA | OBD-CAD | 4.64 | 1.29 | 1.22 |
| 15 | A | 1127 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 15 | K | 1402 | CLA | OBD-CAD | 4.64 | 1.29 | 1.22 |
| 15 | B | 1232 | CLA | OBD-CAD | 4.63 | 1.29 | 1.22 |
| 15 | B | 1239 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | B | 1230 | CLA | OBD-CAD | 4.63 | 1.29 | 1.22 |
| 15 | B | 1226 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1021 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | A | 1124 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | A | 1140 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | B | 1216 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | A | 1132 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | A | 1012 | CLA | OBD-CAD | 4.63 | 1.29 | 1.22 |
| 15 | A | 1109 | CLA | O2A-C1 | 4.63 | 1.61 | 1.46 |
| 15 | B | 1229 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | B | 1234 | CLA | C3C-C2C | 4.63 | 1.46 | 1.36 |
| 15 | A | 1133 | CLA | OBD-CAD | 4.63 | 1.29 | 1.22 |
| 15 | A | 1801 | CLA | OBD-CAD | 4.62 | 1.29 | 1.22 |
| 15 | A | 1122 | CLA | OBD-CAD | 4.62 | 1.29 | 1.22 |
| 15 | J | 1303 | CLA | OBD-CAD | 4.62 | 1.29 | 1.22 |
| 15 | A | 1012 | CLA | C3C-C2C | 4.62 | 1.46 | 1.36 |
| 15 | A | 1115 | CLA | OBD-CAD | 4.62 | 1.28 | 1.22 |
| 15 | B | 1217 | CLA | C3C-C2C | 4.62 | 1.46 | 1.36 |
| 15 | B | 1231 | CLA | OBD-CAD | 4.62 | 1.28 | 1.22 |
| 15 | B | 1208 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 15 | B | 1206 | CLA | OBD-CAD | 4.62 | 1.28 | 1.22 |
| 15 | A | 1103 | CLA | OBD-CAD | 4.62 | 1.28 | 1.22 |
| 15 | A | 1126 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 15 | A | 1119 | CLA | C3C-C2C | 4.61 | 1.46 | 1.36 |
| 15 | A | 1105 | CLA | C3C-C2C | 4.61 | 1.46 | 1.36 |
| 15 | B | 1023 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 15 | A | 1135 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 15 | B | 1215 | CLA | O2A-C1 | 4.61 | 1.61 | 1.46 |
| 15 | A | 1128 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 15 | B | 1203 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 15 | B | 1214 | CLA | C3C-C2C | 4.61 | 1.46 | 1.36 |
| 15 | B | 1231 | CLA | C3C-C2C | 4.61 | 1.46 | 1.36 |
| 15 | A | 1114 | CLA | C3C-C2C | 4.61 | 1.46 | 1.36 |
| 15 | F | 1139 | CLA | C3C-C2C | 4.61 | 1.46 | 1.36 |
| 15 | A | 1134 | CLA | C3C-C2C | 4.60 | 1.46 | 1.36 |
| 15 | A | 1102 | CLA | C3C-C2C | 4.60 | 1.46 | 1.36 |
| 15 | A | 1112 | CLA | C3C-C2C | 4.60 | 1.46 | 1.36 |
| 15 | A | 1105 | CLA | OBD-CAD | 4.60 | 1.28 | 1.22 |
| 15 | A | 1117 | CLA | C3C-C2C | 4.60 | 1.46 | 1.36 |
| 15 | A | 1129 | CLA | C3C-C2C | 4.60 | 1.46 | 1.36 |
| 15 | F | 1301 | CLA | C3C-C2C | 4.60 | 1.46 | 1.36 |
| 15 | A | 1123 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |
| 15 | A | 1104 | CLA | C3C-C2C | 4.59 | 1.46 | 1.36 |
| 15 | A | 1104 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1238 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |
| 15 | K | 1402 | CLA | C3C-C2C | 4.59 | 1.46 | 1.36 |
| 15 | A | 1137 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |
| 15 | B | 1234 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |
| 15 | B | 1210 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |
| 15 | B | 1219 | CLA | C3C-C2C | 4.59 | 1.46 | 1.36 |
| 15 | B | 1013 | CLA | OBD-CAD | 4.59 | 1.28 | 1.22 |
| 15 | A | 1121 | CLA | C3C-C2C | 4.59 | 1.46 | 1.36 |
| 15 | B | 1218 | CLA | C3C-C2C | 4.58 | 1.46 | 1.36 |
| 15 | A | 1120 | CLA | C3C-C2C | 4.58 | 1.46 | 1.36 |
| 15 | A | 1107 | CLA | OBD-CAD | 4.58 | 1.28 | 1.22 |
| 15 | A | 1126 | CLA | C3C-C2C | 4.57 | 1.46 | 1.36 |
| 15 | A | 1132 | CLA | OBD-CAD | 4.58 | 1.28 | 1.22 |
| 15 | B | 1203 | CLA | C3C-C2C | 4.57 | 1.46 | 1.36 |
| 15 | A | 1119 | CLA | OBD-CAD | 4.57 | 1.28 | 1.22 |
| 15 | A | 1117 | CLA | O2A-C1 | 4.57 | 1.61 | 1.46 |
| 15 | A | 1135 | CLA | C3C-C2C | 4.57 | 1.46 | 1.36 |
| 15 | A | 1113 | CLA | OBD-CAD | 4.57 | 1.28 | 1.22 |
| 15 | F | 1410 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 15 | B | 1207 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 15 | B | 1234 | CLA | O2D-CGD | 4.56 | 1.45 | 1.33 |
| 15 | B | 1213 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 15 | B | 1209 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 15 | A | 1109 | CLA | OBD-CAD | 4.56 | 1.28 | 1.22 |
| 15 | B | 1238 | CLA | C3C-C2C | 4.55 | 1.46 | 1.36 |
| 15 | B | 1234 | CLA | O2A-C1 | 4.55 | 1.61 | 1.46 |
| 15 | B | 1215 | CLA | C3C-C2C | 4.55 | 1.46 | 1.36 |
| 13 | A | 1011 | CL0 | OBD-CAD | 4.55 | 1.28 | 1.22 |
| 15 | B | 1204 | CLA | C3C-C2C | 4.55 | 1.46 | 1.36 |
| 15 | B | 1232 | CLA | C3B-C2B | 4.55 | 1.46 | 1.40 |
| 15 | A | 1136 | CLA | OBD-CAD | 4.55 | 1.28 | 1.22 |
| 15 | K | 1401 | CLA | C3C-C2C | 4.54 | 1.46 | 1.36 |
| 15 | B | 1211 | CLA | OBD-CAD | 4.55 | 1.28 | 1.22 |
| 15 | B | 1220 | CLA | O2A-C1 | 4.54 | 1.61 | 1.46 |
| 15 | B | 1205 | CLA | C3C-C2C | 4.54 | 1.46 | 1.36 |
| 13 | A | 1011 | CL0 | C3C-C2C | 4.54 | 1.46 | 1.36 |
| 15 | A | 1130 | CLA | OBD-CAD | 4.54 | 1.28 | 1.22 |
| 15 | A | 1128 | CLA | C3C-C2C | 4.54 | 1.46 | 1.36 |
| 15 | F | 1139 | CLA | OBD-CAD | 4.53 | 1.28 | 1.22 |
| 15 | A | 1113 | CLA | C3C-C2C | 4.53 | 1.46 | 1.36 |
| 15 | A | 1121 | CLA | OBD-CAD | 4.53 | 1.28 | 1.22 |
| 15 | A | 1131 | CLA | C3C-C2C | 4.53 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1236 | CLA | OBD-CAD | 4.53 | 1.28 | 1.22 |
| 15 | B | 1206 | CLA | C3C-C2C | 4.53 | 1.46 | 1.36 |
| 15 | A | 1106 | CLA | C3C-C2C | 4.53 | 1.46 | 1.36 |
| 15 | B | 1201 | CLA | C3C-C2C | 4.53 | 1.46 | 1.36 |
| 15 | A | 1101 | CLA | C3C-C2C | 4.53 | 1.46 | 1.36 |
| 15 | J | 1302 | CLA | C3C-C2C | 4.52 | 1.46 | 1.36 |
| 15 | A | 1131 | CLA | O2A-C1 | 4.52 | 1.61 | 1.46 |
| 15 | B | 1224 | CLA | C3C-C2C | 4.52 | 1.46 | 1.36 |
| 15 | B | 1221 | CLA | C3C-C2C | 4.52 | 1.46 | 1.36 |
| 15 | B | 1237 | CLA | OBD-CAD | 4.52 | 1.28 | 1.22 |
| 15 | B | 1231 | CLA | O2A-C1 | 4.52 | 1.61 | 1.46 |
| 15 | B | 1211 | CLA | C3C-C2C | 4.52 | 1.46 | 1.36 |
| 15 | A | 1136 | CLA | C3C-C2C | 4.51 | 1.46 | 1.36 |
| 15 | B | 1023 | CLA | C3C-C2C | 4.51 | 1.46 | 1.36 |
| 15 | A | 1125 | CLA | C3C-C2C | 4.51 | 1.46 | 1.36 |
| 13 | A | 1108 | CL0 | OBD-CAD | 4.51 | 1.28 | 1.22 |
| 15 | A | 1135 | CLA | O2A-C1 | 4.51 | 1.61 | 1.46 |
| 15 | A | 1119 | CLA | O2A-C1 | 4.50 | 1.61 | 1.46 |
| 15 | A | 1125 | CLA | O2A-C1 | 4.50 | 1.61 | 1.46 |
| 15 | B | 1237 | CLA | C3C-C2C | 4.50 | 1.46 | 1.36 |
| 15 | B | 1227 | CLA | C3B-C2B | 4.50 | 1.46 | 1.40 |
| 15 | B | 1225 | CLA | C3C-C2C | 4.50 | 1.46 | 1.36 |
| 15 | A | 1116 | CLA | O2A-C1 | 4.50 | 1.61 | 1.46 |
| 15 | A | 1110 | CLA | OBD-CAD | 4.50 | 1.28 | 1.22 |
| 15 | A | 1138 | CLA | O2A-C1 | 4.50 | 1.61 | 1.46 |
| 15 | B | 1230 | CLA | C3C-C2C | 4.50 | 1.46 | 1.36 |
| 15 | A | 1133 | CLA | C3C-C2C | 4.50 | 1.46 | 1.36 |
| 15 | B | 1013 | CLA | O2A-C1 | 4.50 | 1.61 | 1.46 |
| 15 | B | 1205 | CLA | O2A-C1 | 4.49 | 1.61 | 1.46 |
| 15 | A | 1115 | CLA | C3C-C2C | 4.49 | 1.46 | 1.36 |
| 15 | B | 1213 | CLA | O2A-C1 | 4.49 | 1.60 | 1.46 |
| 15 | A | 1136 | CLA | O2A-C1 | 4.49 | 1.60 | 1.46 |
| 15 | B | 1221 | CLA | OBD-CAD | 4.48 | 1.28 | 1.22 |
| 15 | A | 1118 | CLA | C3C-C2C | 4.48 | 1.46 | 1.36 |
| 15 | A | 1102 | CLA | O2A-C1 | 4.48 | 1.60 | 1.46 |
| 15 | B | 1235 | CLA | O2A-C1 | 4.47 | 1.60 | 1.46 |
| 15 | B | 1235 | CLA | OBD-CAD | 4.47 | 1.28 | 1.22 |
| 15 | B | 1218 | CLA | O2A-C1 | 4.46 | 1.60 | 1.46 |
| 15 | A | 1119 | CLA | C5-C3 | 4.46 | 1.52 | 1.46 |
| 15 | B | 1210 | CLA | C3C-C2C | 4.46 | 1.46 | 1.36 |
| 15 | B | 1236 | CLA | C3C-C2C | 4.46 | 1.46 | 1.36 |
| 15 | A | 1110 | CLA | C3C-C2C | 4.45 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 1105 | CLA | O2A-C1 | 4.45 | 1.60 | 1.46 |
| 15 | A | 1123 | CLA | C3C-C2C | 4.45 | 1.46 | 1.36 |
| 13 | A | 1011 | CL0 | O2A-C1 | 4.45 | 1.60 | 1.46 |
| 15 | B | 1226 | CLA | O2A-C1 | 4.43 | 1.60 | 1.46 |
| 15 | A | 1111 | CLA | C3C-C2C | 4.43 | 1.46 | 1.36 |
| 15 | A | 1130 | CLA | O2A-C1 | 4.42 | 1.60 | 1.46 |
| 15 | B | 1236 | CLA | O2A-C1 | 4.42 | 1.60 | 1.46 |
| 15 | A | 1103 | CLA | C3C-C2C | 4.42 | 1.46 | 1.36 |
| 15 | A | 1128 | CLA | O2A-C1 | 4.42 | 1.60 | 1.46 |
| 15 | A | 1124 | CLA | O2A-C1 | 4.42 | 1.60 | 1.46 |
| 15 | B | 1219 | CLA | O2A-C1 | 4.42 | 1.60 | 1.46 |
| 15 | A | 1120 | CLA | O2A-C1 | 4.41 | 1.60 | 1.46 |
| 15 | B | 1221 | CLA | O2A-C1 | 4.41 | 1.60 | 1.46 |
| 15 | A | 1801 | CLA | O2A-C1 | 4.41 | 1.60 | 1.46 |
| 15 | A | 1114 | CLA | O2A-C1 | 4.40 | 1.60 | 1.46 |
| 15 | A | 1111 | CLA | O2A-C1 | 4.40 | 1.60 | 1.46 |
| 15 | F | 1410 | CLA | O2A-C1 | 4.39 | 1.60 | 1.46 |
| 15 | B | 1227 | CLA | OBD-CAD | 4.39 | 1.28 | 1.22 |
| 15 | A | 1137 | CLA | O2A-C1 | 4.39 | 1.60 | 1.46 |
| 15 | B | 1223 | CLA | O2A-C1 | 4.39 | 1.60 | 1.46 |
| 15 | A | 1127 | CLA | O2A-C1 | 4.39 | 1.60 | 1.46 |
| 15 | B | 1237 | CLA | O2A-C1 | 4.38 | 1.60 | 1.46 |
| 15 | A | 1125 | CLA | OBD-CAD | 4.37 | 1.28 | 1.22 |
| 15 | B | 1216 | CLA | O2A-C1 | 4.37 | 1.60 | 1.46 |
| 15 | B | 1228 | CLA | O2A-C1 | 4.37 | 1.60 | 1.46 |
| 15 | B | 1228 | CLA | OBD-CAD | 4.37 | 1.28 | 1.22 |
| 13 | A | 1108 | CL0 | C3C-C2C | 4.36 | 1.46 | 1.36 |
| 15 | B | 1239 | CLA | C1B-C2B | 4.36 | 1.50 | 1.43 |
| 15 | A | 1127 | CLA | OBD-CAD | 4.35 | 1.28 | 1.22 |
| 15 | B | 1021 | CLA | O2A-C1 | 4.34 | 1.60 | 1.46 |
| 15 | A | 1107 | CLA | O2A-C1 | 4.34 | 1.60 | 1.46 |
| 15 | B | 1202 | CLA | O2A-C1 | 4.34 | 1.60 | 1.46 |
| 15 | B | 1222 | CLA | O2A-C1 | 4.34 | 1.60 | 1.46 |
| 15 | B | 1229 | CLA | O2A-C1 | 4.34 | 1.60 | 1.46 |
| 15 | A | 1022 | CLA | O2A-C1 | 4.33 | 1.60 | 1.46 |
| 15 | A | 1126 | CLA | O2A-C1 | 4.33 | 1.60 | 1.46 |
| 15 | A | 1138 | CLA | CHC-C1C | 4.33 | 1.49 | 1.35 |
| 15 | A | 1140 | CLA | O2A-C1 | 4.33 | 1.60 | 1.46 |
| 15 | A | 1132 | CLA | O2A-C1 | 4.32 | 1.60 | 1.46 |
| 15 | B | 1214 | CLA | O2A-C1 | 4.32 | 1.60 | 1.46 |
| 15 | B | 1023 | CLA | O2A-C1 | 4.30 | 1.60 | 1.46 |
| 15 | A | 1123 | CLA | O2A-C1 | 4.29 | 1.60 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 1122 | CLA | O2A-C1 | 4.30 | 1.60 | 1.46 |
| 15 | A | 1110 | CLA | O2A-C1 | 4.29 | 1.60 | 1.46 |
| 15 | A | 1104 | CLA | O2A-C1 | 4.29 | 1.60 | 1.46 |
| 15 | B | 1210 | CLA | O2A-C1 | 4.29 | 1.60 | 1.46 |
| 15 | A | 1101 | CLA | O2A-C1 | 4.26 | 1.60 | 1.46 |
| 15 | B | 1225 | CLA | O2A-C1 | 4.26 | 1.60 | 1.46 |
| 15 | B | 1203 | CLA | O2A-C1 | 4.25 | 1.60 | 1.46 |
| 15 | A | 1129 | CLA | OBD-CAD | 4.24 | 1.28 | 1.22 |
| 15 | A | 1103 | CLA | O2A-C1 | 4.23 | 1.60 | 1.46 |
| 15 | B | 1203 | CLA | C1B-C2B | 4.23 | 1.50 | 1.43 |
| 15 | B | 1230 | CLA | O2A-C1 | 4.21 | 1.60 | 1.46 |
| 15 | B | 1228 | CLA | CHC-C1C | 4.21 | 1.49 | 1.35 |
| 15 | A | 1136 | CLA | C1B-C2B | 4.20 | 1.50 | 1.43 |
| 15 | A | 1126 | CLA | CHC-C1C | 4.18 | 1.49 | 1.35 |
| 15 | B | 1223 | CLA | OBD-CAD | 4.18 | 1.28 | 1.22 |
| 15 | B | 1236 | CLA | CHC-C1C | 4.17 | 1.49 | 1.35 |
| 15 | K | 1402 | CLA | C1B-C2B | 4.16 | 1.50 | 1.43 |
| 12 | A | 5003 | LHG | O8-C23 | 4.16 | 1.46 | 1.33 |
| 15 | B | 1235 | CLA | CHC-C1C | 4.15 | 1.49 | 1.35 |
| 15 | F | 1139 | CLA | O2A-C1 | 4.15 | 1.59 | 1.46 |
| 15 | A | 1125 | CLA | CHC-C1C | 4.14 | 1.49 | 1.35 |
| 17 | B | 5002 | LMG | O8-C28 | 4.14 | 1.45 | 1.33 |
| 15 | A | 1101 | CLA | CHC-C1C | 4.12 | 1.49 | 1.35 |
| 15 | A | 1112 | CLA | CHC-C1C | 4.12 | 1.49 | 1.35 |
| 15 | B | 1222 | CLA | C1B-C2B | 4.11 | 1.50 | 1.43 |
| 15 | A | 1122 | CLA | CHC-C1C | 4.11 | 1.49 | 1.35 |
| 15 | A | 1130 | CLA | CHC-C1C | 4.10 | 1.48 | 1.35 |
| 15 | B | 1234 | CLA | C1B-C2B | 4.10 | 1.50 | 1.43 |
| 15 | A | 1107 | CLA | CHC-C1C | 4.10 | 1.48 | 1.35 |
| 15 | J | 1303 | CLA | C1B-C2B | 4.08 | 1.50 | 1.43 |
| 15 | A | 1115 | CLA | CHC-C1C | 4.08 | 1.48 | 1.35 |
| 15 | A | 1111 | CLA | CHC-C1C | 4.08 | 1.48 | 1.35 |
| 15 | B | 1219 | CLA | C1B-C2B | 4.08 | 1.50 | 1.43 |
| 15 | A | 1140 | CLA | CHC-C1C | 4.08 | 1.48 | 1.35 |
| 15 | A | 1132 | CLA | C1B-C2B | 4.07 | 1.50 | 1.43 |
| 15 | B | 1220 | CLA | CHC-C1C | 4.06 | 1.48 | 1.35 |
| 15 | B | 1230 | CLA | CHC-C1C | 4.06 | 1.48 | 1.35 |
| 15 | B | 1223 | CLA | CHC-C1C | 4.06 | 1.48 | 1.35 |
| 15 | A | 1103 | CLA | CHC-C1C | 4.06 | 1.48 | 1.35 |
| 13 | A | 1108 | CL0 | C1B-C2B | 4.05 | 1.50 | 1.43 |
| 15 | A | 1137 | CLA | C1B-C2B | 4.05 | 1.50 | 1.43 |
| 15 | A | 1134 | CLA | CHC-C1C | 4.05 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 1117 | CLA | CHC-C1C | 4.04 | 1.48 | 1.35 |
| 12 | A | 5005 | LHG | O8-C23 | 4.04 | 1.45 | 1.33 |
| 15 | A | 1118 | CLA | C1B-C2B | 4.03 | 1.50 | 1.43 |
| 15 | B | 1240 | CLA | CHC-C1C | 4.03 | 1.48 | 1.35 |
| 15 | A | 1106 | CLA | CHC-C1C | 4.03 | 1.48 | 1.35 |
| 15 | B | 1205 | CLA | C1B-C2B | 4.03 | 1.50 | 1.43 |
| 15 | B | 1214 | CLA | CHC-C1C | 4.03 | 1.48 | 1.35 |
| 15 | A | 1109 | CLA | CHC-C1C | 4.03 | 1.48 | 1.35 |
| 12 | B | 5004 | LHG | O8-C23 | 4.03 | 1.45 | 1.33 |
| 15 | A | 1116 | CLA | C1B-C2B | 4.02 | 1.50 | 1.43 |
| 15 | A | 1022 | CLA | CHC-C1C | 4.02 | 1.48 | 1.35 |
| 15 | J | 1303 | CLA | CHC-C1C | 4.02 | 1.48 | 1.35 |
| 15 | A | 1120 | CLA | C1B-C2B | 4.01 | 1.50 | 1.43 |
| 15 | B | 1013 | CLA | CHC-C1C | 4.01 | 1.48 | 1.35 |
| 15 | F | 1301 | CLA | CHC-C1C | 4.01 | 1.48 | 1.35 |
| 15 | A | 1127 | CLA | CHC-C1C | 4.01 | 1.48 | 1.35 |
| 13 | A | 1108 | CL0 | CHC-C1C | 4.01 | 1.48 | 1.35 |
| 15 | B | 1227 | CLA | C1B-C2B | 4.00 | 1.50 | 1.43 |
| 15 | B | 1217 | CLA | CHC-C1C | 4.00 | 1.48 | 1.35 |
| 15 | A | 1132 | CLA | CHC-C1C | 4.00 | 1.48 | 1.35 |
| 15 | B | 1210 | CLA | CHC-C1C | 4.00 | 1.48 | 1.35 |
| 15 | B | 1202 | CLA | CHC-C1C | 4.00 | 1.48 | 1.35 |
| 15 | B | 1213 | CLA | CHC-C1C | 4.00 | 1.48 | 1.35 |
| 15 | B | 1215 | CLA | C1B-C2B | 4.00 | 1.50 | 1.43 |
| 15 | A | 1121 | CLA | C1B-C2B | 3.99 | 1.50 | 1.43 |
| 15 | B | 1211 | CLA | C1B-C2B | 3.99 | 1.50 | 1.43 |
| 15 | A | 1105 | CLA | C1B-C2B | 3.99 | 1.50 | 1.43 |
| 15 | B | 1211 | CLA | CHC-C1C | 3.99 | 1.48 | 1.35 |
| 15 | A | 1119 | CLA | CHC-C1C | 3.99 | 1.48 | 1.35 |
| 15 | B | 1226 | CLA | CHC-C1C | 3.99 | 1.48 | 1.35 |
| 15 | A | 1103 | CLA | C1B-C2B | 3.99 | 1.49 | 1.43 |
| 15 | B | 1207 | CLA | C1B-C2B | 3.99 | 1.49 | 1.43 |
| 12 | A | 5001 | LHG | O8-C23 | 3.98 | 1.45 | 1.33 |
| 15 | A | 1801 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | A | 1102 | CLA | CHC-C1C | 3.99 | 1.48 | 1.35 |
| 15 | B | 1225 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | K | 1401 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | K | 1402 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | F | 1410 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | B | 1217 | CLA | C1B-C2B | 3.98 | 1.49 | 1.43 |
| 15 | B | 1212 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | A | 1012 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1104 | CLA | CHC-C1C | 3.98 | 1.48 | 1.35 |
| 15 | K | 1401 | CLA | C1B-C2B | 3.98 | 1.49 | 1.43 |
| 15 | A | 1114 | CLA | CHC-C1C | 3.97 | 1.48 | 1.35 |
| 15 | A | 1116 | CLA | CHC-C1C | 3.97 | 1.48 | 1.35 |
| 15 | B | 1231 | CLA | C1B-C2B | 3.97 | 1.49 | 1.43 |
| 15 | B | 1207 | CLA | CHC-C1C | 3.97 | 1.48 | 1.35 |
| 15 | A | 1124 | CLA | CHC-C1C | 3.97 | 1.48 | 1.35 |
| 15 | B | 1023 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | A | 1129 | CLA | CHC-C1C | 3.97 | 1.48 | 1.35 |
| 15 | B | 1229 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | B | 1208 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | A | 1113 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | A | 1129 | CLA | C1B-C2B | 3.96 | 1.49 | 1.43 |
| 15 | B | 1021 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | B | 1219 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | B | 1208 | CLA | C1B-C2B | 3.96 | 1.49 | 1.43 |
| 15 | B | 1201 | CLA | CHC-C1C | 3.96 | 1.48 | 1.35 |
| 15 | A | 1137 | CLA | CHC-C1C | 3.95 | 1.48 | 1.35 |
| 15 | B | 1218 | CLA | CHC-C1C | 3.95 | 1.48 | 1.35 |
| 15 | B | 1209 | CLA | CHC-C1C | 3.95 | 1.48 | 1.35 |
| 15 | A | 1123 | CLA | C1B-C2B | 3.95 | 1.49 | 1.43 |
| 15 | B | 1206 | CLA | C1B-C2B | 3.95 | 1.49 | 1.43 |
| 15 | A | 1133 | CLA | CHC-C1C | 3.95 | 1.48 | 1.35 |
| 15 | B | 1237 | CLA | CHC-C1C | 3.95 | 1.48 | 1.35 |
| 15 | A | 1801 | CLA | C1B-C2B | 3.94 | 1.49 | 1.43 |
| 15 | B | 1202 | CLA | C1B-C2B | 3.94 | 1.49 | 1.43 |
| 15 | B | 1216 | CLA | CHC-C1C | 3.94 | 1.48 | 1.35 |
| 15 | B | 1213 | CLA | C1B-C2B | 3.93 | 1.49 | 1.43 |
| 15 | B | 1224 | CLA | CHC-C1C | 3.93 | 1.48 | 1.35 |
| 15 | B | 1234 | CLA | CHC-C1C | 3.93 | 1.48 | 1.35 |
| 15 | B | 1238 | CLA | C1B-C2B | 3.93 | 1.49 | 1.43 |
| 15 | A | 1120 | CLA | CHC-C1C | 3.93 | 1.48 | 1.35 |
| 15 | A | 1131 | CLA | C1B-C2B | 3.93 | 1.49 | 1.43 |
| 15 | B | 1204 | CLA | CHC-C1C | 3.93 | 1.48 | 1.35 |
| 15 | A | 1121 | CLA | CHC-C1C | 3.93 | 1.48 | 1.35 |
| 15 | F | 1139 | CLA | CHC-C1C | 3.92 | 1.48 | 1.35 |
| 15 | B | 1212 | CLA | C1B-C2B | 3.92 | 1.49 | 1.43 |
| 15 | B | 1229 | CLA | C1B-C2B | 3.92 | 1.49 | 1.43 |
| 15 | A | 1118 | CLA | CHC-C1C | 3.92 | 1.48 | 1.35 |
| 15 | J | 1302 | CLA | CHC-C1C | 3.92 | 1.48 | 1.35 |
| 15 | B | 1227 | CLA | CHC-C1C | 3.92 | 1.48 | 1.35 |
| 13 | A | 1011 | CL0 | C4A-NA | -3.91 | 1.31 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1204 | CLA | C1B-C2B | 3.91 | 1.49 | 1.43 |
| 15 | A | 1123 | CLA | CHC-C1C | 3.91 | 1.48 | 1.35 |
| 15 | A | 1135 | CLA | C1B-C2B | 3.91 | 1.49 | 1.43 |
| 15 | A | 1135 | CLA | CHC-C1C | 3.90 | 1.48 | 1.35 |
| 15 | A | 1105 | CLA | CHC-C1C | 3.89 | 1.48 | 1.35 |
| 15 | A | 1114 | CLA | C1B-C2B | 3.89 | 1.49 | 1.43 |
| 15 | A | 1136 | CLA | CHC-C1C | 3.89 | 1.48 | 1.35 |
| 15 | B | 1206 | CLA | CHC-C1C | 3.89 | 1.48 | 1.35 |
| 15 | A | 1106 | CLA | C1B-C2B | 3.89 | 1.49 | 1.43 |
| 15 | A | 1131 | CLA | CHC-C1C | 3.89 | 1.48 | 1.35 |
| 15 | B | 1221 | CLA | CHC-C1C | 3.89 | 1.48 | 1.35 |
| 15 | B | 1237 | CLA | C1B-C2B | 3.89 | 1.49 | 1.43 |
| 17 | B | 5002 | LMG | O7-C10 | 3.89 | 1.46 | 1.34 |
| 15 | A | 1109 | CLA | C1B-C2B | 3.88 | 1.49 | 1.43 |
| 15 | B | 1205 | CLA | CHC-C1C | 3.88 | 1.48 | 1.35 |
| 15 | B | 1221 | CLA | C1B-C2B | 3.88 | 1.49 | 1.43 |
| 15 | F | 1410 | CLA | C1B-C2B | 3.87 | 1.49 | 1.43 |
| 15 | A | 1110 | CLA | C1B-C2B | 3.88 | 1.49 | 1.43 |
| 15 | B | 1222 | CLA | CHC-C1C | 3.88 | 1.48 | 1.35 |
| 15 | B | 1238 | CLA | CHC-C1C | 3.88 | 1.48 | 1.35 |
| 15 | F | 1139 | CLA | C1B-C2B | 3.87 | 1.49 | 1.43 |
| 15 | J | 1302 | CLA | C1B-C2B | 3.86 | 1.49 | 1.43 |
| 15 | A | 1102 | CLA | C1B-C2B | 3.86 | 1.49 | 1.43 |
| 15 | A | 1110 | CLA | CHC-C1C | 3.85 | 1.48 | 1.35 |
| 12 | B | 5004 | LHG | O7-C7 | 3.85 | 1.45 | 1.34 |
| 15 | B | 1201 | CLA | C1B-C2B | 3.84 | 1.49 | 1.43 |
| 12 | A | 5001 | LHG | O7-C7 | 3.84 | 1.45 | 1.34 |
| 15 | B | 1240 | CLA | C1B-C2B | 3.84 | 1.49 | 1.43 |
| 15 | A | 1115 | CLA | C1B-C2B | 3.84 | 1.49 | 1.43 |
| 13 | A | 1011 | CL0 | CHC-C1C | 3.84 | 1.48 | 1.35 |
| 15 | A | 1140 | CLA | C1B-C2B | 3.83 | 1.49 | 1.43 |
| 15 | B | 1232 | CLA | CHC-C1C | 3.83 | 1.48 | 1.35 |
| 15 | B | 1215 | CLA | CHC-C1C | 3.83 | 1.48 | 1.35 |
| 15 | B | 1023 | CLA | C1B-C2B | 3.81 | 1.49 | 1.43 |
| 15 | B | 1013 | CLA | C4A-NA | -3.81 | 1.31 | 1.38 |
| 15 | B | 1239 | CLA | CHC-C1C | 3.81 | 1.47 | 1.35 |
| 15 | A | 1127 | CLA | C4D-C3D | -3.80 | 1.34 | 1.42 |
| 15 | B | 1231 | CLA | CHC-C1C | 3.80 | 1.47 | 1.35 |
| 15 | A | 1110 | CLA | C4D-C3D | -3.80 | 1.34 | 1.42 |
| 12 | A | 5003 | LHG | O7-C7 | 3.80 | 1.45 | 1.34 |
| 15 | A | 1111 | CLA | C1B-C2B | 3.79 | 1.49 | 1.43 |
| 15 | B | 1021 | CLA | C4A-NA | -3.79 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1129 | CLA | C4D-C3D | -3.78 | 1.34 | 1.42 |
| 15 | B | 1210 | CLA | C1B-C2B | 3.78 | 1.49 | 1.43 |
| 15 | B | 1203 | CLA | CHC-C1C | 3.77 | 1.47 | 1.35 |
| 15 | A | 1128 | CLA | CHC-C1C | 3.77 | 1.47 | 1.35 |
| 15 | B | 1232 | CLA | C1B-C2B | 3.76 | 1.49 | 1.43 |
| 15 | B | 1214 | CLA | C4A-NA | -3.75 | 1.32 | 1.38 |
| 15 | B | 1227 | CLA | C4D-C3D | -3.75 | 1.34 | 1.42 |
| 15 | A | 1124 | CLA | C1B-C2B | 3.75 | 1.49 | 1.43 |
| 12 | A | 5005 | LHG | O7-C7 | 3.74 | 1.45 | 1.34 |
| 15 | A | 1126 | CLA | C4D-C3D | -3.74 | 1.34 | 1.42 |
| 15 | A | 1130 | CLA | C4D-C3D | -3.74 | 1.34 | 1.42 |
| 15 | A | 1012 | CLA | C1B-C2B | 3.73 | 1.49 | 1.43 |
| 15 | A | 1113 | CLA | C1B-C2B | 3.73 | 1.49 | 1.43 |
| 15 | B | 1209 | CLA | C1B-C2B | 3.72 | 1.49 | 1.43 |
| 15 | A | 1107 | CLA | C4D-C3D | -3.72 | 1.34 | 1.42 |
| 15 | B | 1230 | CLA | C1B-C2B | 3.72 | 1.49 | 1.43 |
| 15 | A | 1125 | CLA | C4D-C3D | -3.72 | 1.34 | 1.42 |
| 15 | F | 1301 | CLA | C1B-C2B | 3.72 | 1.49 | 1.43 |
| 15 | B | 1218 | CLA | C1B-C2B | 3.71 | 1.49 | 1.43 |
| 15 | B | 1216 | CLA | C4D-C3D | -3.71 | 1.34 | 1.42 |
| 15 | A | 1122 | CLA | C4D-C3D | -3.70 | 1.34 | 1.42 |
| 15 | A | 1119 | CLA | C4D-C3D | -3.70 | 1.34 | 1.42 |
| 15 | A | 1134 | CLA | C1B-C2B | 3.70 | 1.49 | 1.43 |
| 13 | A | 1011 | CL0 | C4D-C3D | -3.69 | 1.34 | 1.42 |
| 15 | A | 1022 | CLA | C4D-C3D | -3.69 | 1.34 | 1.42 |
| 15 | B | 1013 | CLA | C1B-C2B | 3.68 | 1.49 | 1.43 |
| 15 | B | 1218 | CLA | C4D-C3D | -3.68 | 1.34 | 1.42 |
| 13 | A | 1108 | CL0 | C4D-C3D | -3.67 | 1.34 | 1.42 |
| 15 | B | 1211 | CLA | C4D-C3D | -3.67 | 1.34 | 1.42 |
| 15 | F | 1139 | CLA | C4D-C3D | -3.67 | 1.34 | 1.42 |
| 15 | B | 1230 | CLA | C4D-C3D | -3.67 | 1.34 | 1.42 |
| 15 | B | 1225 | CLA | C4D-C3D | -3.67 | 1.34 | 1.42 |
| 15 | B | 1228 | CLA | C4D-C3D | -3.67 | 1.34 | 1.42 |
| 15 | B | 1013 | CLA | C4D-C3D | -3.66 | 1.34 | 1.42 |
| 15 | B | 1223 | CLA | C4D-C3D | -3.66 | 1.34 | 1.42 |
| 15 | B | 1237 | CLA | C4D-C3D | -3.65 | 1.34 | 1.42 |
| 15 | B | 1224 | CLA | C4D-C3D | -3.65 | 1.34 | 1.42 |
| 15 | B | 1204 | CLA | C4D-C3D | -3.65 | 1.34 | 1.42 |
| 15 | B | 1226 | CLA | C4D-C3D | -3.65 | 1.34 | 1.42 |
| 15 | A | 1127 | CLA | C1B-C2B | 3.64 | 1.49 | 1.43 |
| 15 | A | 1131 | CLA | C4D-C3D | -3.64 | 1.34 | 1.42 |
| 15 | A | 1128 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1224 | CLA | C1B-C2B | 3.64 | 1.49 | 1.43 |
| 15 | B | 1208 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | A | 1112 | CLA | C1B-C2B | 3.64 | 1.49 | 1.43 |
| 15 | B | 1203 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 13 | A | 1011 | CL0 | C1B-C2B | 3.63 | 1.49 | 1.43 |
| 15 | A | 1103 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | B | 1213 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | A | 1022 | CLA | C1B-C2B | 3.63 | 1.49 | 1.43 |
| 15 | A | 1105 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | A | 1022 | CLA | C4A-NA | -3.63 | 1.32 | 1.38 |
| 15 | B | 1232 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | B | 1236 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | B | 1023 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | B | 1239 | CLA | C4D-C3D | -3.63 | 1.34 | 1.42 |
| 15 | A | 1133 | CLA | C1B-C2B | 3.62 | 1.49 | 1.43 |
| 15 | A | 1118 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | B | 1231 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | A | 1114 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | A | 1133 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | B | 1234 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | A | 1115 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | B | 1214 | CLA | C4D-C3D | -3.62 | 1.34 | 1.42 |
| 15 | A | 1121 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | B | 1235 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | A | 1109 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | A | 1104 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | A | 1136 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | K | 1402 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | B | 1226 | CLA | C1B-C2B | 3.61 | 1.49 | 1.43 |
| 15 | A | 1106 | CLA | C4D-C3D | -3.61 | 1.34 | 1.42 |
| 15 | A | 1104 | CLA | C1B-C2B | 3.60 | 1.49 | 1.43 |
| 15 | B | 1205 | CLA | C4D-C3D | -3.60 | 1.34 | 1.42 |
| 15 | B | 1238 | CLA | C4D-C3D | -3.60 | 1.34 | 1.42 |
| 15 | A | 1135 | CLA | C4D-C3D | -3.60 | 1.34 | 1.42 |
| 15 | A | 1113 | CLA | C4D-C3D | -3.60 | 1.34 | 1.42 |
| 15 | A | 1123 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |
| 15 | A | 1111 | CLA | C4D-C3D | -3.60 | 1.34 | 1.42 |
| 15 | F | 1301 | CLA | C4A-NA | -3.60 | 1.32 | 1.38 |
| 15 | B | 1021 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |
| 15 | B | 1021 | CLA | C1B-C2B | 3.59 | 1.49 | 1.43 |
| 15 | A | 1132 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |
| 15 | F | 1410 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1210 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |
| 15 | B | 1225 | CLA | C1B-C2B | 3.59 | 1.49 | 1.43 |
| 15 | B | 1222 | CLA | C4A-NA | -3.59 | 1.32 | 1.38 |
| 15 | A | 1120 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |
| 15 | A | 1140 | CLA | C4D-C3D | -3.59 | 1.34 | 1.42 |
| 15 | B | 1201 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | A | 1137 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | B | 1212 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | A | 1110 | CLA | C4A-NA | -3.58 | 1.32 | 1.38 |
| 15 | B | 1206 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | A | 1134 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | K | 1401 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | B | 1215 | CLA | C4D-C3D | -3.58 | 1.34 | 1.42 |
| 15 | B | 1219 | CLA | C4D-C3D | -3.57 | 1.34 | 1.42 |
| 15 | B | 1207 | CLA | C4D-C3D | -3.57 | 1.34 | 1.42 |
| 15 | J | 1303 | CLA | C4D-C3D | -3.57 | 1.34 | 1.42 |
| 15 | A | 1125 | CLA | C1B-C2B | 3.57 | 1.49 | 1.43 |
| 15 | B | 1220 | CLA | C4D-C3D | -3.57 | 1.34 | 1.42 |
| 15 | J | 1302 | CLA | C4D-C3D | -3.56 | 1.34 | 1.42 |
| 15 | A | 1116 | CLA | C4D-C3D | -3.56 | 1.34 | 1.42 |
| 15 | B | 1217 | CLA | C4D-C3D | -3.56 | 1.34 | 1.42 |
| 15 | A | 1102 | CLA | C4A-NA | -3.56 | 1.32 | 1.38 |
| 15 | A | 1112 | CLA | C4D-C3D | -3.56 | 1.34 | 1.42 |
| 15 | B | 1240 | CLA | C4D-C3D | -3.55 | 1.34 | 1.42 |
| 15 | B | 1209 | CLA | C4D-C3D | -3.55 | 1.34 | 1.42 |
| 15 | A | 1117 | CLA | C4D-C3D | -3.55 | 1.34 | 1.42 |
| 15 | B | 1235 | CLA | C1B-C2B | 3.55 | 1.49 | 1.43 |
| 15 | A | 1801 | CLA | C4D-C3D | -3.54 | 1.34 | 1.42 |
| 15 | A | 1106 | CLA | C4A-NA | -3.54 | 1.32 | 1.38 |
| 15 | A | 1104 | CLA | C4A-NA | -3.54 | 1.32 | 1.38 |
| 15 | B | 1220 | CLA | C1B-C2B | 3.54 | 1.49 | 1.43 |
| 15 | A | 1124 | CLA | C4D-C3D | -3.54 | 1.34 | 1.42 |
| 15 | B | 1236 | CLA | C1B-C2B | 3.53 | 1.49 | 1.43 |
| 15 | B | 1221 | CLA | C4D-C3D | -3.53 | 1.34 | 1.42 |
| 15 | B | 1202 | CLA | C4D-C3D | -3.53 | 1.34 | 1.42 |
| 15 | A | 1102 | CLA | C4D-C3D | -3.52 | 1.34 | 1.42 |
| 15 | F | 1301 | CLA | C4D-C3D | -3.52 | 1.34 | 1.42 |
| 15 | B | 1218 | CLA | C4A-NA | -3.51 | 1.32 | 1.38 |
| 15 | A | 1012 | CLA | C4A-NA | -3.51 | 1.32 | 1.38 |
| 15 | B | 1223 | CLA | C1B-C2B | 3.51 | 1.49 | 1.43 |
| 15 | A | 1112 | CLA | C4A-NA | -3.51 | 1.32 | 1.38 |
| 15 | B | 1203 | CLA | C4A-NA | -3.50 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1122 | CLA | C1B-C2B | 3.50 | 1.49 | 1.43 |
| 15 | A | 1138 | CLA | C4B-CHC | 3.49 | 1.49 | 1.39 |
| 15 | A | 1101 | CLA | C4D-C3D | -3.49 | 1.35 | 1.42 |
| 15 | B | 1222 | CLA | C4D-C3D | -3.48 | 1.35 | 1.42 |
| 15 | A | 1122 | CLA | C4A-NA | -3.48 | 1.32 | 1.38 |
| 15 | A | 1138 | CLA | C4D-C3D | -3.48 | 1.35 | 1.42 |
| 15 | A | 1124 | CLA | C4A-NA | -3.47 | 1.32 | 1.38 |
| 15 | B | 1206 | CLA | C4A-NA | -3.47 | 1.32 | 1.38 |
| 15 | B | 1230 | CLA | C4A-NA | -3.47 | 1.32 | 1.38 |
| 15 | B | 1228 | CLA | C1B-C2B | 3.47 | 1.49 | 1.43 |
| 15 | A | 1117 | CLA | C1B-C2B | 3.47 | 1.49 | 1.43 |
| 15 | B | 1217 | CLA | C4A-NA | -3.46 | 1.32 | 1.38 |
| 15 | F | 1410 | CLA | C4A-NA | -3.46 | 1.32 | 1.38 |
| 15 | A | 1128 | CLA | C1B-C2B | 3.45 | 1.49 | 1.43 |
| 15 | A | 1125 | CLA | C4A-NA | -3.45 | 1.32 | 1.38 |
| 15 | A | 1129 | CLA | C4A-NA | -3.44 | 1.32 | 1.38 |
| 15 | B | 1214 | CLA | C1B-C2B | 3.44 | 1.49 | 1.43 |
| 15 | A | 1128 | CLA | C4A-NA | -3.44 | 1.32 | 1.38 |
| 15 | B | 1202 | CLA | C4A-NA | -3.43 | 1.32 | 1.38 |
| 15 | B | 1229 | CLA | C4D-C3D | -3.43 | 1.35 | 1.42 |
| 15 | B | 1210 | CLA | C4A-NA | -3.43 | 1.32 | 1.38 |
| 15 | A | 1103 | CLA | C4A-NA | -3.43 | 1.32 | 1.38 |
| 15 | B | 1219 | CLA | C4A-NA | -3.42 | 1.32 | 1.38 |
| 15 | A | 1126 | CLA | C4A-NA | -3.42 | 1.32 | 1.38 |
| 15 | A | 1012 | CLA | C4D-C3D | -3.42 | 1.35 | 1.42 |
| 15 | B | 1224 | CLA | C4A-NA | -3.41 | 1.32 | 1.38 |
| 15 | A | 1130 | CLA | C4A-NA | -3.41 | 1.32 | 1.38 |
| 15 | B | 1236 | CLA | C4B-CHC | 3.40 | 1.49 | 1.39 |
| 15 | A | 1125 | CLA | C4B-CHC | 3.40 | 1.49 | 1.39 |
| 15 | B | 1216 | CLA | C4A-NA | -3.40 | 1.32 | 1.38 |
| 15 | B | 1236 | CLA | C4A-NA | -3.39 | 1.32 | 1.38 |
| 15 | A | 1127 | CLA | C4A-NA | -3.39 | 1.32 | 1.38 |
| 15 | B | 1204 | CLA | C4A-NA | -3.39 | 1.32 | 1.38 |
| 15 | A | 1111 | CLA | C4A-NA | -3.38 | 1.32 | 1.38 |
| 15 | A | 1101 | CLA | C4A-NA | -3.38 | 1.32 | 1.38 |
| 15 | B | 1211 | CLA | C4A-NA | -3.38 | 1.32 | 1.38 |
| 15 | B | 1213 | CLA | C4A-NA | -3.38 | 1.32 | 1.38 |
| 15 | B | 1215 | CLA | C4A-NA | -3.37 | 1.32 | 1.38 |
| 15 | B | 1234 | CLA | C4A-NA | -3.37 | 1.32 | 1.38 |
| 15 | B | 1228 | CLA | C4B-CHC | 3.37 | 1.49 | 1.39 |
| 15 | A | 1116 | CLA | C4A-NA | -3.37 | 1.32 | 1.38 |
| 15 | B | 1223 | CLA | C4A-NA | -3.36 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1101 | CLA | C4B-CHC | 3.36 | 1.49 | 1.39 |
| 15 | A | 1126 | CLA | C1D-C2D | 3.35 | 1.51 | 1.42 |
| 15 | A | 1117 | CLA | C4A-NA | -3.35 | 1.32 | 1.38 |
| 15 | A | 1135 | CLA | C4A-NA | -3.35 | 1.32 | 1.38 |
| 15 | B | 1216 | CLA | C1B-C2B | 3.35 | 1.49 | 1.43 |
| 15 | B | 1227 | CLA | C4A-NA | -3.35 | 1.32 | 1.38 |
| 15 | B | 1208 | CLA | C4A-NA | -3.35 | 1.32 | 1.38 |
| 15 | B | 1207 | CLA | C4A-NA | -3.34 | 1.32 | 1.38 |
| 15 | B | 1225 | CLA | C4A-NA | -3.34 | 1.32 | 1.38 |
| 15 | A | 1126 | CLA | C4B-CHC | 3.34 | 1.49 | 1.39 |
| 15 | K | 1401 | CLA | C4A-NA | -3.33 | 1.32 | 1.38 |
| 15 | A | 1122 | CLA | C4B-CHC | 3.33 | 1.49 | 1.39 |
| 15 | B | 1239 | CLA | C4A-NA | -3.33 | 1.32 | 1.38 |
| 15 | A | 1138 | CLA | C4A-NA | -3.32 | 1.32 | 1.38 |
| 15 | A | 1118 | CLA | C4A-NA | -3.32 | 1.32 | 1.38 |
| 15 | A | 1022 | CLA | C3D-C2D | 3.31 | 1.48 | 1.40 |
| 15 | B | 1231 | CLA | C4A-NA | -3.31 | 1.32 | 1.38 |
| 15 | F | 1139 | CLA | C4A-NA | -3.31 | 1.32 | 1.38 |
| 15 | A | 1126 | CLA | C1B-C2B | 3.31 | 1.48 | 1.43 |
| 15 | B | 1023 | CLA | C4A-NA | -3.31 | 1.32 | 1.38 |
| 15 | B | 1230 | CLA | C4B-CHC | 3.31 | 1.49 | 1.39 |
| 15 | B | 1228 | CLA | C4A-NA | -3.31 | 1.32 | 1.38 |
| 15 | B | 1235 | CLA | C4B-CHC | 3.30 | 1.48 | 1.39 |
| 15 | A | 1012 | CLA | C3D-C2D | 3.30 | 1.48 | 1.40 |
| 15 | B | 1212 | CLA | C4A-NA | -3.30 | 1.32 | 1.38 |
| 15 | A | 1107 | CLA | C4B-CHC | 3.30 | 1.48 | 1.39 |
| 14 | A | 4012 | BCR | C11-C12 | -3.30 | 1.25 | 1.34 |
| 15 | A | 1101 | CLA | C1B-C2B | 3.29 | 1.48 | 1.43 |
| 15 | A | 1112 | CLA | C4B-CHC | 3.29 | 1.48 | 1.39 |
| 15 | A | 1113 | CLA | C4A-NA | -3.29 | 1.32 | 1.38 |
| 13 | A | 1108 | CL0 | C1B-CHB | 3.28 | 1.48 | 1.39 |
| 15 | B | 1223 | CLA | C4B-CHC | 3.28 | 1.48 | 1.39 |
| 15 | B | 1220 | CLA | C4A-NA | -3.28 | 1.32 | 1.38 |
| 15 | B | 1220 | CLA | C4B-CHC | 3.28 | 1.48 | 1.39 |
| 15 | A | 1140 | CLA | C4B-CHC | 3.27 | 1.48 | 1.39 |
| 15 | A | 1107 | CLA | C4A-NA | -3.27 | 1.32 | 1.38 |
| 15 | B | 1226 | CLA | C4A-NA | -3.27 | 1.32 | 1.38 |
| 15 | A | 1109 | CLA | C4A-NA | -3.27 | 1.32 | 1.38 |
| 15 | A | 1119 | CLA | C4A-NA | -3.27 | 1.32 | 1.38 |
| 13 | A | 1108 | CL0 | C4A-NA | -3.27 | 1.32 | 1.38 |
| 15 | B | 1240 | CLA | C4A-NA | -3.26 | 1.32 | 1.38 |
| 15 | A | 1130 | CLA | C4B-CHC | 3.26 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1232 | CLA | C4A-NA | -3.25 | 1.32 | 1.38 |
| 15 | A | 1121 | CLA | C4A-NA | -3.24 | 1.32 | 1.38 |
| 15 | A | 1122 | CLA | C1D-C2D | 3.24 | 1.50 | 1.42 |
| 15 | B | 1209 | CLA | C4A-NA | -3.24 | 1.32 | 1.38 |
| 15 | B | 1239 | CLA | C1B-CHB | 3.24 | 1.48 | 1.39 |
| 15 | B | 1213 | CLA | C4B-CHC | 3.24 | 1.48 | 1.39 |
| 15 | B | 1229 | CLA | C1B-CHB | 3.23 | 1.48 | 1.39 |
| 15 | A | 1134 | CLA | C4B-CHC | 3.23 | 1.48 | 1.39 |
| 14 | B | 4006 | BCR | C11-C12 | -3.23 | 1.25 | 1.34 |
| 15 | A | 1132 | CLA | C4A-NA | -3.23 | 1.32 | 1.38 |
| 15 | A | 1133 | CLA | C4A-NA | -3.22 | 1.32 | 1.38 |
| 15 | B | 1221 | CLA | C1B-CHB | 3.23 | 1.48 | 1.39 |
| 15 | A | 1104 | CLA | C4B-CHC | 3.22 | 1.48 | 1.39 |
| 15 | A | 1131 | CLA | C4A-NA | -3.22 | 1.32 | 1.38 |
| 15 | B | 1240 | CLA | C4B-CHC | 3.21 | 1.48 | 1.39 |
| 15 | A | 1140 | CLA | C4A-NA | -3.21 | 1.32 | 1.38 |
| 15 | A | 1115 | CLA | C4A-NA | -3.21 | 1.32 | 1.38 |
| 15 | A | 1131 | CLA | C1B-CHB | 3.21 | 1.48 | 1.39 |
| 15 | F | 1410 | CLA | C4B-CHC | 3.21 | 1.48 | 1.39 |
| 15 | A | 1136 | CLA | C1B-CHB | 3.21 | 1.48 | 1.39 |
| 15 | A | 1115 | CLA | C4B-CHC | 3.21 | 1.48 | 1.39 |
| 15 | A | 1138 | CLA | C1B-C2B | 3.21 | 1.48 | 1.43 |
| 15 | F | 1301 | CLA | C4B-CHC | 3.21 | 1.48 | 1.39 |
| 15 | B | 1204 | CLA | C1D-C2D | 3.20 | 1.50 | 1.42 |
| 15 | A | 1129 | CLA | C1D-C2D | 3.20 | 1.50 | 1.42 |
| 15 | A | 1022 | CLA | C4B-CHC | 3.20 | 1.48 | 1.39 |
| 15 | B | 1211 | CLA | C4B-CHC | 3.20 | 1.48 | 1.39 |
| 15 | A | 1103 | CLA | C4B-CHC | 3.20 | 1.48 | 1.39 |
| 13 | A | 1108 | CL0 | C4B-CHC | 3.20 | 1.48 | 1.39 |
| 15 | A | 1132 | CLA | C4B-CHC | 3.20 | 1.48 | 1.39 |
| 15 | K | 1402 | CLA | C1B-CHB | 3.20 | 1.48 | 1.39 |
| 15 | A | 1120 | CLA | C4A-NA | -3.19 | 1.33 | 1.38 |
| 15 | A | 1127 | CLA | C4B-CHC | 3.19 | 1.48 | 1.39 |
| 15 | J | 1303 | CLA | C1B-CHB | 3.19 | 1.48 | 1.39 |
| 15 | A | 1109 | CLA | C1D-C2D | 3.19 | 1.50 | 1.42 |
| 15 | B | 1220 | CLA | C3D-C2D | 3.19 | 1.47 | 1.40 |
| 15 | B | 1225 | CLA | C4B-CHC | 3.19 | 1.48 | 1.39 |
| 15 | A | 1137 | CLA | C1B-CHB | 3.19 | 1.48 | 1.39 |
| 15 | A | 1132 | CLA | C1B-CHB | 3.19 | 1.48 | 1.39 |
| 15 | A | 1109 | CLA | C4B-CHC | 3.19 | 1.48 | 1.39 |
| 15 | B | 1013 | CLA | C4B-CHC | 3.19 | 1.48 | 1.39 |
| 15 | A | 1130 | CLA | C1B-C2B | 3.19 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1114 | CLA | C4A-NA | -3.19 | 1.33 | 1.38 |
| 15 | B | 1238 | CLA | C4A-NA | -3.19 | 1.33 | 1.38 |
| 15 | J | 1303 | CLA | C4B-CHC | 3.18 | 1.48 | 1.39 |
| 15 | B | 1208 | CLA | C1D-C2D | 3.18 | 1.50 | 1.42 |
| 15 | A | 1102 | CLA | C3D-C2D | 3.18 | 1.47 | 1.40 |
| 14 | F | 4016 | BCR | C11-C12 | -3.18 | 1.25 | 1.34 |
| 15 | J | 1302 | CLA | C4A-NA | -3.18 | 1.33 | 1.38 |
| 15 | B | 1202 | CLA | C4B-CHC | 3.18 | 1.48 | 1.39 |
| 15 | B | 1201 | CLA | C4A-NA | -3.18 | 1.33 | 1.38 |
| 15 | A | 1119 | CLA | C4B-CHC | 3.18 | 1.48 | 1.39 |
| 15 | B | 1213 | CLA | C1D-C2D | 3.17 | 1.50 | 1.42 |
| 15 | B | 1237 | CLA | C1B-CHB | 3.17 | 1.48 | 1.39 |
| 15 | F | 1139 | CLA | C4B-CHC | 3.17 | 1.48 | 1.39 |
| 15 | B | 1212 | CLA | C1B-CHB | 3.17 | 1.48 | 1.39 |
| 15 | A | 1111 | CLA | C4B-CHC | 3.17 | 1.48 | 1.39 |
| 15 | B | 1213 | CLA | C1B-CHB | 3.17 | 1.48 | 1.39 |
| 15 | A | 1117 | CLA | C4B-CHC | 3.17 | 1.48 | 1.39 |
| 15 | B | 1234 | CLA | C1B-CHB | 3.17 | 1.48 | 1.39 |
| 15 | B | 1214 | CLA | C4B-CHC | 3.17 | 1.48 | 1.39 |
| 15 | B | 1206 | CLA | C1D-C2D | 3.16 | 1.50 | 1.42 |
| 15 | A | 1121 | CLA | C1B-CHB | 3.16 | 1.48 | 1.39 |
| 15 | A | 1115 | CLA | C1B-CHB | 3.16 | 1.48 | 1.39 |
| 15 | A | 1135 | CLA | C1B-CHB | 3.16 | 1.48 | 1.39 |
| 15 | K | 1401 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 15 | J | 1302 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 15 | B | 1205 | CLA | C1B-CHB | 3.16 | 1.48 | 1.39 |
| 15 | A | 1801 | CLA | C4A-NA | -3.16 | 1.33 | 1.38 |
| 15 | A | 1801 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 14 | B | 4004 | BCR | C11-C12 | -3.16 | 1.26 | 1.34 |
| 15 | A | 1114 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 15 | B | 1238 | CLA | C1B-CHB | 3.16 | 1.48 | 1.39 |
| 15 | A | 1113 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 15 | A | 1012 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 15 | B | 1229 | CLA | C4B-CHC | 3.16 | 1.48 | 1.39 |
| 15 | F | 1139 | CLA | C1B-CHB | 3.15 | 1.48 | 1.39 |
| 15 | B | 1237 | CLA | C4B-CHC | 3.15 | 1.48 | 1.39 |
| 15 | B | 1218 | CLA | C4B-CHC | 3.15 | 1.48 | 1.39 |
| 15 | B | 1237 | CLA | C1D-C2D | 3.15 | 1.50 | 1.42 |
| 15 | K | 1402 | CLA | C4A-NA | -3.15 | 1.33 | 1.38 |
| 15 | A | 1134 | CLA | C4A-NA | -3.15 | 1.33 | 1.38 |
| 15 | A | 1801 | CLA | C1B-CHB | 3.15 | 1.48 | 1.39 |
| 15 | A | 1114 | CLA | C1B-CHB | 3.15 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1127 | CLA | C1B-CHB | 3.15 | 1.48 | 1.39 |
| 15 | B | 1212 | CLA | C4B-CHC | 3.15 | 1.48 | 1.39 |
| 15 | A | 1118 | CLA | C1B-CHB | 3.15 | 1.48 | 1.39 |
| 15 | A | 1107 | CLA | C1D-C2D | 3.15 | 1.50 | 1.42 |
| 15 | A | 1126 | CLA | CHD-C4C | 3.14 | 1.48 | 1.41 |
| 15 | B | 1208 | CLA | C1B-CHB | 3.14 | 1.48 | 1.39 |
| 15 | A | 1116 | CLA | C4B-CHC | 3.14 | 1.48 | 1.39 |
| 15 | A | 1117 | CLA | C3D-C2D | 3.14 | 1.47 | 1.40 |
| 15 | B | 1215 | CLA | C1B-CHB | 3.14 | 1.48 | 1.39 |
| 15 | A | 1140 | CLA | C1B-CHB | 3.14 | 1.48 | 1.39 |
| 15 | B | 1201 | CLA | C4B-CHC | 3.14 | 1.48 | 1.39 |
| 15 | A | 1123 | CLA | C1B-CHB | 3.14 | 1.48 | 1.39 |
| 15 | B | 1229 | CLA | C4A-NA | -3.14 | 1.33 | 1.38 |
| 15 | B | 1207 | CLA | C4B-CHC | 3.14 | 1.48 | 1.39 |
| 15 | A | 1119 | CLA | C1B-C2B | 3.14 | 1.48 | 1.43 |
| 15 | A | 1129 | CLA | C1B-CHB | 3.14 | 1.48 | 1.39 |
| 15 | B | 1226 | CLA | C1B-CHB | 3.14 | 1.48 | 1.39 |
| 15 | A | 1106 | CLA | C1D-C2D | 3.14 | 1.50 | 1.42 |
| 15 | A | 1105 | CLA | C1D-C2D | 3.13 | 1.50 | 1.42 |
| 15 | B | 1217 | CLA | C4B-CHC | 3.13 | 1.48 | 1.39 |
| 15 | B | 1231 | CLA | C1D-C2D | 3.14 | 1.50 | 1.42 |
| 15 | J | 1302 | CLA | C1B-CHB | 3.13 | 1.48 | 1.39 |
| 15 | A | 1120 | CLA | C1D-C2D | 3.13 | 1.50 | 1.42 |
| 15 | B | 1219 | CLA | C1B-CHB | 3.13 | 1.48 | 1.39 |
| 15 | B | 1221 | CLA | C4A-NA | -3.13 | 1.33 | 1.38 |
| 15 | A | 1130 | CLA | C1D-C2D | 3.13 | 1.50 | 1.42 |
| 15 | B | 1211 | CLA | C1B-CHB | 3.13 | 1.48 | 1.39 |
| 15 | B | 1203 | CLA | C1B-CHB | 3.13 | 1.48 | 1.39 |
| 15 | A | 1137 | CLA | C4B-CHC | 3.13 | 1.48 | 1.39 |
| 13 | A | 1108 | CL0 | CBA-CGA | 3.13 | 1.51 | 1.49 |
| 15 | A | 1124 | CLA | C4B-CHC | 3.12 | 1.48 | 1.39 |
| 15 | A | 1121 | CLA | C4B-CHC | 3.12 | 1.48 | 1.39 |
| 15 | B | 1219 | CLA | C1D-C2D | 3.12 | 1.50 | 1.42 |
| 15 | A | 1102 | CLA | C4B-CHC | 3.12 | 1.48 | 1.39 |
| 15 | B | 1221 | CLA | C4B-CHC | 3.12 | 1.48 | 1.39 |
| 15 | B | 1214 | CLA | C1D-C2D | 3.12 | 1.50 | 1.42 |
| 15 | A | 1133 | CLA | C4B-CHC | 3.12 | 1.48 | 1.39 |
| 15 | B | 1226 | CLA | C4B-CHC | 3.12 | 1.48 | 1.39 |
| 15 | A | 1124 | CLA | C1D-C2D | 3.12 | 1.50 | 1.42 |
| 15 | B | 1228 | CLA | C1D-C2D | 3.12 | 1.50 | 1.42 |
| 15 | J | 1303 | CLA | C4A-NA | -3.12 | 1.33 | 1.38 |
| 15 | B | 1209 | CLA | C1D-C2D | 3.11 | 1.50 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1216 | CLA | C4B-CHC | 3.11 | 1.48 | 1.39 |
| 15 | K | 1402 | CLA | C4B-CHC | 3.11 | 1.48 | 1.39 |
| 15 | B | 1224 | CLA | C4B-CHC | 3.11 | 1.48 | 1.39 |
| 15 | B | 1208 | CLA | C4B-CHC | 3.11 | 1.48 | 1.39 |
| 15 | A | 1136 | CLA | C1D-C2D | 3.11 | 1.50 | 1.42 |
| 15 | B | 1021 | CLA | C4B-CHC | 3.11 | 1.48 | 1.39 |
| 15 | B | 1235 | CLA | C4A-NA | -3.11 | 1.33 | 1.38 |
| 15 | A | 1123 | CLA | C1D-C2D | 3.11 | 1.50 | 1.42 |
| 15 | B | 1238 | CLA | C4B-CHC | 3.11 | 1.48 | 1.39 |
| 14 | B | 4010 | BCR | C11-C12 | -3.11 | 1.26 | 1.34 |
| 15 | A | 1103 | CLA | C1B-CHB | 3.11 | 1.48 | 1.39 |
| 15 | B | 1240 | CLA | C1B-CHB | 3.11 | 1.48 | 1.39 |
| 15 | A | 1114 | CLA | C1D-C2D | 3.10 | 1.50 | 1.42 |
| 15 | A | 1107 | CLA | C1B-C2B | 3.10 | 1.48 | 1.43 |
| 15 | B | 1202 | CLA | C1D-C2D | 3.10 | 1.50 | 1.42 |
| 15 | B | 1216 | CLA | C1D-C2D | 3.10 | 1.50 | 1.42 |
| 15 | B | 1239 | CLA | C1D-C2D | 3.10 | 1.50 | 1.42 |
| 15 | B | 1237 | CLA | C4A-NA | -3.10 | 1.33 | 1.38 |
| 15 | A | 1137 | CLA | C4A-NA | -3.10 | 1.33 | 1.38 |
| 15 | B | 1205 | CLA | C4B-CHC | 3.10 | 1.48 | 1.39 |
| 15 | B | 1220 | CLA | C1D-C2D | 3.10 | 1.50 | 1.42 |
| 15 | B | 1232 | CLA | C1B-CHB | 3.10 | 1.48 | 1.39 |
| 15 | B | 1013 | CLA | C3D-C2D | 3.10 | 1.47 | 1.40 |
| 15 | A | 1134 | CLA | C1D-C2D | 3.09 | 1.50 | 1.42 |
| 15 | B | 1222 | CLA | C3D-C2D | 3.09 | 1.47 | 1.40 |
| 15 | A | 1116 | CLA | C1D-C2D | 3.09 | 1.50 | 1.42 |
| 15 | A | 1129 | CLA | C4B-CHC | 3.09 | 1.48 | 1.39 |
| 15 | B | 1231 | CLA | C1B-CHB | 3.09 | 1.48 | 1.39 |
| 15 | A | 1105 | CLA | C4B-CHC | 3.09 | 1.48 | 1.39 |
| 15 | A | 1133 | CLA | C1B-CHB | 3.09 | 1.48 | 1.39 |
| 15 | A | 1105 | CLA | C4A-NA | -3.09 | 1.33 | 1.38 |
| 15 | B | 1214 | CLA | CHD-C4C | 3.09 | 1.48 | 1.41 |
| 15 | B | 1208 | CLA | CHD-C4C | 3.09 | 1.48 | 1.41 |
| 15 | A | 1106 | CLA | C4B-CHC | 3.08 | 1.48 | 1.39 |
| 15 | B | 1214 | CLA | C3D-C2D | 3.08 | 1.47 | 1.40 |
| 15 | B | 1201 | CLA | C1B-CHB | 3.08 | 1.48 | 1.39 |
| 15 | A | 1130 | CLA | CHD-C4C | 3.08 | 1.48 | 1.41 |
| 15 | B | 1204 | CLA | C1B-CHB | 3.08 | 1.48 | 1.39 |
| 15 | B | 1215 | CLA | C1D-C2D | 3.08 | 1.50 | 1.42 |
| 15 | B | 1203 | CLA | C1D-C2D | 3.07 | 1.50 | 1.42 |
| 15 | A | 1109 | CLA | C1B-CHB | 3.07 | 1.48 | 1.39 |
| 15 | A | 1131 | CLA | C1D-C2D | 3.07 | 1.50 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1103 | CLA | C1D-C2D | 3.07 | 1.50 | 1.42 |
| 15 | B | 1210 | CLA | C4B-CHC | 3.07 | 1.48 | 1.39 |
| 15 | B | 1207 | CLA | C1B-CHB | 3.07 | 1.48 | 1.39 |
| 15 | B | 1219 | CLA | C4B-CHC | 3.07 | 1.48 | 1.39 |
| 15 | B | 1217 | CLA | C1B-CHB | 3.07 | 1.48 | 1.39 |
| 15 | B | 1232 | CLA | C3D-C2D | 3.07 | 1.47 | 1.40 |
| 15 | B | 1239 | CLA | CHD-C4C | 3.07 | 1.48 | 1.41 |
| 15 | A | 1131 | CLA | C4B-CHC | 3.07 | 1.48 | 1.39 |
| 15 | B | 1236 | CLA | C1D-C2D | 3.07 | 1.50 | 1.42 |
| 15 | A | 1120 | CLA | C4B-CHC | 3.07 | 1.48 | 1.39 |
| 15 | A | 1106 | CLA | C3D-C2D | 3.07 | 1.47 | 1.40 |
| 15 | A | 1118 | CLA | C4B-CHC | 3.07 | 1.48 | 1.39 |
| 15 | B | 1207 | CLA | C1D-C2D | 3.07 | 1.50 | 1.42 |
| 15 | A | 1134 | CLA | C1B-CHB | 3.07 | 1.48 | 1.39 |
| 15 | B | 1205 | CLA | C4A-NA | -3.07 | 1.33 | 1.38 |
| 15 | A | 1116 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | B | 1023 | CLA | C4B-CHC | 3.07 | 1.48 | 1.39 |
| 15 | A | 1135 | CLA | C4B-CHC | 3.06 | 1.48 | 1.39 |
| 15 | B | 1230 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | A | 1111 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | A | 1113 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | A | 1138 | CLA | C3D-C2D | 3.06 | 1.47 | 1.40 |
| 15 | B | 1224 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | F | 1410 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | B | 1215 | CLA | C3D-C2D | 3.06 | 1.47 | 1.40 |
| 15 | A | 1104 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | B | 1238 | CLA | C3D-C2D | 3.06 | 1.47 | 1.40 |
| 15 | B | 1202 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | B | 1204 | CLA | C4B-CHC | 3.06 | 1.48 | 1.39 |
| 15 | B | 1240 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | A | 1121 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | K | 1402 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | A | 1138 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | B | 1230 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | A | 1120 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | K | 1401 | CLA | C1B-CHB | 3.06 | 1.48 | 1.39 |
| 15 | A | 1133 | CLA | C1D-C2D | 3.06 | 1.50 | 1.42 |
| 15 | B | 1023 | CLA | C1D-C2D | 3.05 | 1.50 | 1.42 |
| 15 | A | 1102 | CLA | C1D-C2D | 3.05 | 1.50 | 1.42 |
| 15 | A | 1117 | CLA | C1D-C2D | 3.05 | 1.50 | 1.42 |
| 15 | F | 1410 | CLA | C1D-C2D | 3.05 | 1.50 | 1.42 |
| 15 | B | 1220 | CLA | CHD-C4C | 3.05 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1206 | CLA | C4B-CHC | 3.05 | 1.48 | 1.39 |
| 15 | A | 1122 | CLA | CHD-C4C | 3.05 | 1.48 | 1.41 |
| 15 | B | 1219 | CLA | CHD-C4C | 3.05 | 1.48 | 1.41 |
| 15 | B | 1216 | CLA | C3D-C2D | 3.05 | 1.47 | 1.40 |
| 15 | A | 1119 | CLA | C1D-C2D | 3.04 | 1.50 | 1.42 |
| 15 | A | 1106 | CLA | CHD-C4C | 3.04 | 1.48 | 1.41 |
| 15 | A | 1105 | CLA | C1B-CHB | 3.04 | 1.48 | 1.39 |
| 15 | A | 1110 | CLA | C4B-CHC | 3.04 | 1.48 | 1.39 |
| 15 | B | 1238 | CLA | C1D-C2D | 3.04 | 1.50 | 1.42 |
| 15 | B | 1023 | CLA | C3D-C2D | 3.04 | 1.47 | 1.40 |
| 15 | A | 1136 | CLA | C4B-CHC | 3.04 | 1.48 | 1.39 |
| 15 | A | 1128 | CLA | C1B-CHB | 3.04 | 1.48 | 1.39 |
| 15 | B | 1209 | CLA | C4B-CHC | 3.04 | 1.48 | 1.39 |
| 15 | B | 1215 | CLA | C4B-CHC | 3.04 | 1.48 | 1.39 |
| 15 | B | 1227 | CLA | CBA-CGA | 3.04 | 1.51 | 1.49 |
| 15 | B | 1232 | CLA | C4B-CHC | 3.04 | 1.48 | 1.39 |
| 15 | B | 1235 | CLA | C1B-CHB | 3.04 | 1.48 | 1.39 |
| 15 | B | 1227 | CLA | C1D-C2D | 3.04 | 1.50 | 1.42 |
| 14 | B | 4014 | BCR | C11-C12 | -3.04 | 1.26 | 1.34 |
| 15 | B | 1206 | CLA | CHD-C4C | 3.04 | 1.48 | 1.41 |
| 14 | B | 4011 | BCR | C11-C12 | -3.03 | 1.26 | 1.34 |
| 15 | B | 1227 | CLA | C4B-CHC | 3.03 | 1.48 | 1.39 |
| 15 | B | 1218 | CLA | C1B-CHB | 3.03 | 1.48 | 1.39 |
| 15 | A | 1119 | CLA | C3D-C2D | 3.03 | 1.47 | 1.40 |
| 15 | F | 1301 | CLA | C3D-C2D | 3.03 | 1.47 | 1.40 |
| 15 | B | 1213 | CLA | CHD-C4C | 3.03 | 1.48 | 1.41 |
| 14 | B | 4005 | BCR | C11-C12 | -3.03 | 1.26 | 1.34 |
| 15 | A | 1124 | CLA | C3D-C2D | 3.03 | 1.47 | 1.40 |
| 15 | B | 1222 | CLA | C4B-CHC | 3.03 | 1.48 | 1.39 |
| 15 | A | 1112 | CLA | C1D-C2D | 3.03 | 1.50 | 1.42 |
| 15 | A | 1012 | CLA | C1B-CHB | 3.03 | 1.48 | 1.39 |
| 15 | B | 1234 | CLA | C4B-CHC | 3.03 | 1.48 | 1.39 |
| 15 | B | 1216 | CLA | C1B-CHB | 3.03 | 1.48 | 1.39 |
| 15 | J | 1303 | CLA | C1D-C2D | 3.02 | 1.50 | 1.42 |
| 15 | B | 1217 | CLA | C3D-C2D | 3.02 | 1.47 | 1.40 |
| 15 | B | 1228 | CLA | C1B-CHB | 3.02 | 1.48 | 1.39 |
| 15 | B | 1223 | CLA | C1B-CHB | 3.02 | 1.48 | 1.39 |
| 15 | B | 1213 | CLA | C3D-C2D | 3.02 | 1.47 | 1.40 |
| 15 | B | 1220 | CLA | C1B-CHB | 3.02 | 1.48 | 1.39 |
| 15 | K | 1401 | CLA | C1D-C2D | 3.02 | 1.50 | 1.42 |
| 15 | J | 1302 | CLA | C1D-C2D | 3.02 | 1.50 | 1.42 |
| 15 | A | 1113 | CLA | C1D-C2D | 3.02 | 1.50 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1125 | CLA | C1B-CHB | 3.02 | 1.48 | 1.39 |
| 15 | A | 1109 | CLA | C3D-C2D | 3.02 | 1.47 | 1.40 |
| 15 | B | 1209 | CLA | C1B-CHB | 3.01 | 1.48 | 1.39 |
| 15 | A | 1117 | CLA | CHD-C4C | 3.01 | 1.48 | 1.41 |
| 15 | A | 1128 | CLA | C3D-C2D | 3.00 | 1.47 | 1.40 |
| 15 | B | 1212 | CLA | C3D-C2D | 3.01 | 1.47 | 1.40 |
| 15 | A | 1135 | CLA | C1D-C2D | 3.01 | 1.50 | 1.42 |
| 15 | A | 1122 | CLA | C1B-CHB | 3.00 | 1.48 | 1.39 |
| 15 | B | 1215 | CLA | CHD-C4C | 3.00 | 1.48 | 1.41 |
| 15 | B | 1210 | CLA | C1D-C2D | 3.00 | 1.50 | 1.42 |
| 15 | B | 1208 | CLA | C3D-C2D | 3.00 | 1.47 | 1.40 |
| 15 | A | 1109 | CLA | CHD-C4C | 3.00 | 1.48 | 1.41 |
| 15 | B | 1204 | CLA | CHD-C4C | 3.00 | 1.48 | 1.41 |
| 15 | B | 1222 | CLA | C1B-CHB | 3.00 | 1.48 | 1.39 |
| 15 | A | 1112 | CLA | CBA-CGA | 3.00 | 1.51 | 1.49 |
| 15 | B | 1210 | CLA | C3D-C2D | 3.00 | 1.47 | 1.40 |
| 15 | A | 1110 | CLA | C1B-CHB | 3.00 | 1.48 | 1.39 |
| 15 | B | 1211 | CLA | C3D-C2D | 3.00 | 1.47 | 1.40 |
| 15 | A | 1112 | CLA | C3D-C2D | 3.00 | 1.47 | 1.40 |
| 15 | B | 1232 | CLA | C1D-C2D | 2.99 | 1.50 | 1.42 |
| 15 | B | 1216 | CLA | CHD-C4C | 3.00 | 1.48 | 1.41 |
| 15 | B | 1203 | CLA | C4B-CHC | 2.99 | 1.48 | 1.39 |
| 15 | B | 1021 | CLA | C1B-CHB | 2.99 | 1.48 | 1.39 |
| 15 | B | 1235 | CLA | C3D-C2D | 2.99 | 1.47 | 1.40 |
| 15 | B | 1218 | CLA | C3D-C2D | 2.99 | 1.47 | 1.40 |
| 15 | A | 1123 | CLA | C4B-CHC | 2.99 | 1.48 | 1.39 |
| 15 | A | 1133 | CLA | C3D-C2D | 2.99 | 1.47 | 1.40 |
| 15 | A | 1105 | CLA | C3D-C2D | 2.99 | 1.47 | 1.40 |
| 15 | B | 1234 | CLA | C1D-C2D | 2.99 | 1.50 | 1.42 |
| 15 | B | 1201 | CLA | C1D-C2D | 2.99 | 1.50 | 1.42 |
| 15 | A | 1123 | CLA | C4A-NA | -2.99 | 1.33 | 1.38 |
| 15 | A | 1120 | CLA | CHD-C4C | 2.99 | 1.48 | 1.41 |
| 14 | A | 4002 | BCR | C11-C12 | -2.99 | 1.26 | 1.34 |
| 15 | B | 1206 | CLA | C1B-CHB | 2.99 | 1.48 | 1.39 |
| 15 | A | 1118 | CLA | C1D-C2D | 2.98 | 1.50 | 1.42 |
| 15 | F | 1410 | CLA | C3D-C2D | 2.98 | 1.47 | 1.40 |
| 15 | A | 1135 | CLA | CHD-C4C | 2.98 | 1.48 | 1.41 |
| 15 | A | 1130 | CLA | C3D-C2D | 2.98 | 1.47 | 1.40 |
| 15 | B | 1227 | CLA | C1B-CHB | 2.98 | 1.48 | 1.39 |
| 15 | A | 1114 | CLA | CHD-C4C | 2.98 | 1.48 | 1.41 |
| 15 | B | 1201 | CLA | C3D-C2D | 2.98 | 1.47 | 1.40 |
| 15 | A | 1111 | CLA | C3D-C2D | 2.98 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1801 | CLA | C1D-C2D | 2.98 | 1.50 | 1.42 |
| 15 | A | 1112 | CLA | C1B-CHB | 2.98 | 1.48 | 1.39 |
| 15 | B | 1231 | CLA | C4B-CHC | 2.98 | 1.48 | 1.39 |
| 15 | B | 1231 | CLA | CHD-C4C | 2.98 | 1.48 | 1.41 |
| 15 | A | 1136 | CLA | C4A-NA | -2.98 | 1.33 | 1.38 |
| 15 | B | 1227 | CLA | CHD-C4C | 2.97 | 1.48 | 1.41 |
| 15 | A | 1124 | CLA | CHD-C4C | 2.98 | 1.48 | 1.41 |
| 15 | A | 1102 | CLA | C1B-CHB | 2.97 | 1.48 | 1.39 |
| 15 | A | 1132 | CLA | C1D-C2D | 2.97 | 1.50 | 1.42 |
| 15 | B | 1225 | CLA | C1B-CHB | 2.97 | 1.48 | 1.39 |
| 15 | B | 1240 | CLA | C3D-C2D | 2.97 | 1.47 | 1.40 |
| 15 | A | 1104 | CLA | C3D-C2D | 2.97 | 1.47 | 1.40 |
| 15 | B | 1217 | CLA | C1D-C2D | 2.97 | 1.50 | 1.42 |
| 15 | A | 1123 | CLA | CHD-C4C | 2.97 | 1.48 | 1.41 |
| 15 | B | 1221 | CLA | C3D-C2D | 2.97 | 1.47 | 1.40 |
| 15 | A | 1132 | CLA | C3D-C2D | 2.97 | 1.47 | 1.40 |
| 15 | B | 1237 | CLA | CHD-C4C | 2.97 | 1.48 | 1.41 |
| 15 | A | 1101 | CLA | C3D-C2D | 2.97 | 1.47 | 1.40 |
| 15 | B | 1224 | CLA | CHD-C4C | 2.97 | 1.48 | 1.41 |
| 15 | A | 1119 | CLA | CHD-C4C | 2.97 | 1.48 | 1.41 |
| 15 | B | 1218 | CLA | C1D-C2D | 2.97 | 1.50 | 1.42 |
| 15 | B | 1219 | CLA | C3D-C2D | 2.96 | 1.47 | 1.40 |
| 13 | A | 1011 | CL0 | C4B-CHC | 2.96 | 1.48 | 1.39 |
| 15 | A | 1105 | CLA | CHD-C4C | 2.96 | 1.48 | 1.41 |
| 15 | A | 1102 | CLA | CHD-C4C | 2.96 | 1.48 | 1.41 |
| 15 | A | 1121 | CLA | CHD-C4C | 2.96 | 1.48 | 1.41 |
| 15 | A | 1107 | CLA | CHD-C4C | 2.96 | 1.48 | 1.41 |
| 15 | A | 1022 | CLA | C1B-CHB | 2.96 | 1.48 | 1.39 |
| 15 | J | 1302 | CLA | CBA-CGA | 2.96 | 1.51 | 1.49 |
| 15 | B | 1021 | CLA | C3D-C2D | 2.96 | 1.47 | 1.40 |
| 15 | A | 1110 | CLA | C1D-C2D | 2.95 | 1.50 | 1.42 |
| 15 | B | 1203 | CLA | CHD-C4C | 2.95 | 1.48 | 1.41 |
| 15 | B | 1204 | CLA | C3D-C2D | 2.95 | 1.47 | 1.40 |
| 15 | A | 1114 | CLA | C3D-C2D | 2.95 | 1.47 | 1.40 |
| 15 | B | 1240 | CLA | CHD-C4C | 2.95 | 1.48 | 1.41 |
| 15 | A | 1128 | CLA | C4B-CHC | 2.95 | 1.48 | 1.39 |
| 15 | B | 1218 | CLA | CHD-C4C | 2.95 | 1.48 | 1.41 |
| 15 | A | 1113 | CLA | CBA-CGA | 2.95 | 1.51 | 1.49 |
| 15 | B | 1023 | CLA | C1B-CHB | 2.95 | 1.48 | 1.39 |
| 15 | B | 1206 | CLA | C3D-C2D | 2.95 | 1.47 | 1.40 |
| 15 | A | 1127 | CLA | C3D-C2D | 2.95 | 1.47 | 1.40 |
| 14 | A | 4003 | BCR | C11-C12 | -2.95 | 1.26 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1135 | CLA | C3D-C2D | 2.95 | 1.47 | 1.40 |
| 15 | B | 1212 | CLA | C1D-C2D | 2.95 | 1.50 | 1.42 |
| 15 | A | 1116 | CLA | CHD-C4C | 2.95 | 1.48 | 1.41 |
| 15 | A | 1115 | CLA | C3D-C2D | 2.95 | 1.47 | 1.40 |
| 15 | B | 1205 | CLA | C3D-C2D | 2.94 | 1.47 | 1.40 |
| 15 | A | 1116 | CLA | C3D-C2D | 2.94 | 1.47 | 1.40 |
| 15 | A | 1111 | CLA | C1B-CHB | 2.94 | 1.48 | 1.39 |
| 15 | A | 1121 | CLA | C3D-C2D | 2.94 | 1.47 | 1.40 |
| 15 | A | 1119 | CLA | C1B-CHB | 2.94 | 1.47 | 1.39 |
| 15 | B | 1210 | CLA | C1B-CHB | 2.94 | 1.47 | 1.39 |
| 15 | F | 1410 | CLA | CHD-C4C | 2.94 | 1.48 | 1.41 |
| 15 | A | 1137 | CLA | C1D-C2D | 2.94 | 1.50 | 1.42 |
| 15 | B | 1224 | CLA | C1B-CHB | 2.94 | 1.47 | 1.39 |
| 15 | B | 1224 | CLA | C3D-C2D | 2.94 | 1.47 | 1.40 |
| 15 | B | 1229 | CLA | C3D-C2D | 2.94 | 1.47 | 1.40 |
| 15 | B | 1225 | CLA | C1D-C2D | 2.94 | 1.50 | 1.42 |
| 15 | A | 1133 | CLA | CHD-C4C | 2.94 | 1.48 | 1.41 |
| 15 | B | 1209 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | A | 1801 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | B | 1235 | CLA | C1D-C2D | 2.93 | 1.50 | 1.42 |
| 15 | A | 1118 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | B | 1227 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 14 | B | 4017 | BCR | C11-C12 | -2.93 | 1.26 | 1.34 |
| 15 | A | 1138 | CLA | CHD-C4C | 2.93 | 1.48 | 1.41 |
| 15 | B | 1239 | CLA | C4B-CHC | 2.93 | 1.47 | 1.39 |
| 15 | B | 1202 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | A | 1103 | CLA | CHD-C4C | 2.93 | 1.48 | 1.41 |
| 15 | B | 1210 | CLA | CHD-C4C | 2.93 | 1.48 | 1.41 |
| 15 | A | 1022 | CLA | C1D-C2D | 2.93 | 1.50 | 1.42 |
| 15 | A | 1110 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | B | 1236 | CLA | C1B-CHB | 2.93 | 1.47 | 1.39 |
| 15 | A | 1131 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | A | 1113 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | A | 1140 | CLA | C1D-C2D | 2.93 | 1.50 | 1.42 |
| 15 | B | 1223 | CLA | C3D-C2D | 2.93 | 1.47 | 1.40 |
| 15 | B | 1217 | CLA | CHD-C4C | 2.93 | 1.48 | 1.41 |
| 15 | F | 1139 | CLA | C1D-C2D | 2.93 | 1.50 | 1.42 |
| 15 | F | 1301 | CLA | C1B-CHB | 2.93 | 1.47 | 1.39 |
| 15 | B | 1209 | CLA | CHD-C4C | 2.92 | 1.48 | 1.41 |
| 15 | B | 1222 | CLA | C1D-C2D | 2.92 | 1.49 | 1.42 |
| 15 | B | 1226 | CLA | C1D-C2D | 2.92 | 1.49 | 1.42 |
| 15 | F | 1301 | CLA | C1D-C2D | 2.92 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 4007 | BCR | C11-C12 | -2.92 | 1.26 | 1.34 |
| 13 | A | 1011 | CL0 | C3D-C2D | 2.92 | 1.47 | 1.40 |
| 15 | A | 1104 | CLA | C1B-CHB | 2.92 | 1.47 | 1.39 |
| 15 | A | 1113 | CLA | CHD-C4C | 2.92 | 1.48 | 1.41 |
| 15 | A | 1129 | CLA | CHD-C4C | 2.92 | 1.48 | 1.41 |
| 15 | B | 1236 | CLA | C3D-C2D | 2.91 | 1.47 | 1.40 |
| 15 | B | 1228 | CLA | C3D-C2D | 2.91 | 1.47 | 1.40 |
| 15 | A | 1012 | CLA | MG-NC | 2.91 | 2.15 | 2.07 |
| 15 | B | 1239 | CLA | C3D-C2D | 2.91 | 1.47 | 1.40 |
| 15 | A | 1117 | CLA | C1B-CHB | 2.91 | 1.47 | 1.39 |
| 15 | B | 1225 | CLA | C3D-C2D | 2.91 | 1.47 | 1.40 |
| 15 | A | 1123 | CLA | C3D-C2D | 2.91 | 1.47 | 1.40 |
| 14 | F | 4015 | BCR | C11-C12 | -2.91 | 1.26 | 1.34 |
| 15 | A | 1022 | CLA | CHD-C4C | 2.91 | 1.48 | 1.41 |
| 15 | B | 1238 | CLA | CHD-C4C | 2.91 | 1.48 | 1.41 |
| 15 | B | 1228 | CLA | CHD-C4C | 2.91 | 1.48 | 1.41 |
| 15 | B | 1234 | CLA | C3D-C2D | 2.90 | 1.47 | 1.40 |
| 15 | K | 1401 | CLA | CHD-C4C | 2.90 | 1.48 | 1.41 |
| 14 | B | 4009 | BCR | C11-C12 | -2.90 | 1.26 | 1.34 |
| 15 | A | 1138 | CLA | C1B-CHB | 2.90 | 1.47 | 1.39 |
| 15 | J | 1302 | CLA | C3D-C2D | 2.90 | 1.47 | 1.40 |
| 15 | B | 1207 | CLA | C3D-C2D | 2.90 | 1.47 | 1.40 |
| 15 | B | 1207 | CLA | CHD-C4C | 2.89 | 1.48 | 1.41 |
| 15 | B | 1203 | CLA | C3D-C2D | 2.90 | 1.47 | 1.40 |
| 15 | A | 1136 | CLA | CHD-C4C | 2.89 | 1.48 | 1.41 |
| 15 | B | 1211 | CLA | C1D-C2D | 2.89 | 1.49 | 1.42 |
| 15 | A | 1115 | CLA | C1D-C2D | 2.89 | 1.49 | 1.42 |
| 15 | B | 1236 | CLA | CHD-C4C | 2.89 | 1.48 | 1.41 |
| 15 | B | 1231 | CLA | C3D-C2D | 2.89 | 1.47 | 1.40 |
| 14 | A | 4008 | BCR | C11-C12 | -2.89 | 1.26 | 1.34 |
| 15 | A | 1101 | CLA | C1B-CHB | 2.89 | 1.47 | 1.39 |
| 15 | B | 1234 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | A | 1101 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 15 | A | 1131 | CLA | CHD-C4C | 2.89 | 1.48 | 1.41 |
| 14 | J | 4013 | BCR | C11-C12 | -2.88 | 1.26 | 1.34 |
| 15 | B | 1211 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | B | 1021 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 15 | A | 1106 | CLA | C1B-CHB | 2.88 | 1.47 | 1.39 |
| 15 | B | 1232 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | A | 1126 | CLA | C1B-CHB | 2.88 | 1.47 | 1.39 |
| 15 | J | 1303 | CLA | C3D-C2D | 2.88 | 1.47 | 1.40 |
| 15 | A | 1136 | CLA | C3D-C2D | 2.88 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1013 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 15 | B | 1202 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | A | 1801 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | B | 1229 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 15 | F | 1301 | CLA | CBA-CGA | 2.88 | 1.51 | 1.49 |
| 15 | A | 1104 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | B | 1023 | CLA | CHD-C4C | 2.87 | 1.48 | 1.41 |
| 15 | B | 1021 | CLA | CHD-C4C | 2.88 | 1.48 | 1.41 |
| 15 | J | 1302 | CLA | CHD-C4C | 2.87 | 1.48 | 1.41 |
| 15 | A | 1110 | CLA | CHD-C4C | 2.87 | 1.48 | 1.41 |
| 13 | A | 1011 | CL0 | C1B-CHB | 2.87 | 1.47 | 1.39 |
| 15 | B | 1212 | CLA | CHD-C4C | 2.87 | 1.48 | 1.41 |
| 15 | A | 1140 | CLA | C3D-C2D | 2.87 | 1.47 | 1.40 |
| 15 | K | 1402 | CLA | C3D-C2D | 2.87 | 1.47 | 1.40 |
| 15 | A | 1134 | CLA | CHD-C4C | 2.87 | 1.48 | 1.41 |
| 15 | A | 1134 | CLA | C3D-C2D | 2.87 | 1.47 | 1.40 |
| 15 | B | 1222 | CLA | CHD-C4C | 2.87 | 1.48 | 1.41 |
| 15 | K | 1402 | CLA | CHD-C4C | 2.86 | 1.48 | 1.41 |
| 15 | B | 1240 | CLA | CBA-CGA | 2.86 | 1.51 | 1.49 |
| 15 | A | 1137 | CLA | CHD-C4C | 2.86 | 1.48 | 1.41 |
| 15 | B | 1226 | CLA | C3D-C2D | 2.86 | 1.47 | 1.40 |
| 15 | F | 1139 | CLA | CHD-C4C | 2.86 | 1.48 | 1.41 |
| 15 | A | 1120 | CLA | C3D-C2D | 2.86 | 1.47 | 1.40 |
| 13 | A | 1108 | CL0 | C1D-C2D | 2.86 | 1.49 | 1.42 |
| 15 | A | 1111 | CLA | CHD-C4C | 2.85 | 1.48 | 1.41 |
| 15 | A | 1112 | CLA | CHD-C4C | 2.85 | 1.48 | 1.41 |
| 15 | B | 1201 | CLA | CHD-C4C | 2.85 | 1.48 | 1.41 |
| 15 | A | 1129 | CLA | C3D-C2D | 2.85 | 1.47 | 1.40 |
| 15 | A | 1137 | CLA | C3D-C2D | 2.85 | 1.47 | 1.40 |
| 15 | B | 1013 | CLA | C1B-CHB | 2.85 | 1.47 | 1.39 |
| 15 | A | 1107 | CLA | C1B-CHB | 2.84 | 1.47 | 1.39 |
| 15 | B | 1230 | CLA | C3D-C2D | 2.84 | 1.46 | 1.40 |
| 15 | B | 1226 | CLA | CHD-C4C | 2.84 | 1.48 | 1.41 |
| 15 | B | 1223 | CLA | C1D-C2D | 2.84 | 1.49 | 1.42 |
| 15 | F | 1301 | CLA | CHD-C4C | 2.84 | 1.48 | 1.41 |
| 15 | B | 1225 | CLA | CHD-C4C | 2.84 | 1.48 | 1.41 |
| 15 | J | 1303 | CLA | CHD-C4C | 2.84 | 1.48 | 1.41 |
| 15 | A | 1012 | CLA | CHD-C4C | 2.84 | 1.48 | 1.41 |
| 15 | B | 1212 | CLA | CBA-CGA | 2.84 | 1.51 | 1.49 |
| 15 | B | 1214 | CLA | C1B-CHB | 2.84 | 1.47 | 1.39 |
| 15 | A | 1103 | CLA | C3D-C2D | 2.84 | 1.46 | 1.40 |
| 15 | B | 1237 | CLA | C3D-C2D | 2.83 | 1.46 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | K | 1401 | CLA | C3D-C2D | 2.82 | 1.46 | 1.40 |
| 15 | A | 1140 | CLA | CHD-C4C | 2.82 | 1.47 | 1.41 |
| 15 | A | 1122 | CLA | C3D-C2D | 2.81 | 1.46 | 1.40 |
| 15 | A | 1123 | CLA | MG-NC | 2.81 | 2.15 | 2.07 |
| 15 | A | 1127 | CLA | C1D-C2D | 2.81 | 1.49 | 1.42 |
| 15 | A | 1118 | CLA | CHD-C4C | 2.80 | 1.47 | 1.41 |
| 15 | A | 1101 | CLA | CHD-C4C | 2.80 | 1.47 | 1.41 |
| 15 | A | 1130 | CLA | C1B-CHB | 2.80 | 1.47 | 1.39 |
| 15 | B | 1221 | CLA | C1D-C2D | 2.79 | 1.49 | 1.42 |
| 15 | A | 1801 | CLA | MG-NC | 2.79 | 2.15 | 2.07 |
| 15 | A | 1124 | CLA | C1B-CHB | 2.78 | 1.47 | 1.39 |
| 15 | B | 1205 | CLA | C1D-C2D | 2.78 | 1.49 | 1.42 |
| 15 | A | 1125 | CLA | C1D-C2D | 2.78 | 1.49 | 1.42 |
| 15 | B | 1223 | CLA | CHD-C4C | 2.78 | 1.47 | 1.41 |
| 15 | B | 1229 | CLA | CHD-C4C | 2.78 | 1.47 | 1.41 |
| 13 | A | 1108 | CL0 | MG-NC | 2.78 | 2.15 | 2.07 |
| 15 | A | 1137 | CLA | MG-NC | 2.77 | 2.15 | 2.07 |
| 15 | A | 1126 | CLA | C3D-C2D | 2.77 | 1.46 | 1.40 |
| 15 | B | 1209 | CLA | CBA-CGA | 2.77 | 1.51 | 1.49 |
| 15 | A | 1132 | CLA | CHD-C4C | 2.77 | 1.47 | 1.41 |
| 15 | B | 1221 | CLA | MG-NC | 2.77 | 2.15 | 2.07 |
| 15 | A | 1121 | CLA | MG-NC | 2.76 | 2.15 | 2.07 |
| 13 | A | 1011 | CL0 | CHD-C4C | 2.76 | 1.47 | 1.41 |
| 15 | A | 1128 | CLA | CHD-C4C | 2.76 | 1.47 | 1.41 |
| 13 | A | 1011 | CL0 | C1D-C2D | 2.75 | 1.49 | 1.42 |
| 15 | B | 1240 | CLA | MG-NC | 2.75 | 2.15 | 2.07 |
| 15 | J | 1303 | CLA | MG-NC | 2.75 | 2.15 | 2.07 |
| 15 | A | 1127 | CLA | CHD-C4C | 2.75 | 1.47 | 1.41 |
| 15 | B | 1215 | CLA | MG-NC | 2.75 | 2.15 | 2.07 |
| 15 | B | 1235 | CLA | CHD-C4C | 2.74 | 1.47 | 1.41 |
| 15 | A | 1128 | CLA | C1D-C2D | 2.74 | 1.49 | 1.42 |
| 15 | F | 1410 | CLA | MG-NC | 2.74 | 2.15 | 2.07 |
| 15 | A | 1107 | CLA | C3D-C2D | 2.73 | 1.46 | 1.40 |
| 15 | A | 1012 | CLA | C1D-C2D | 2.73 | 1.49 | 1.42 |
| 15 | B | 1013 | CLA | CHD-C4C | 2.72 | 1.47 | 1.41 |
| 15 | B | 1232 | CLA | CBA-CGA | 2.72 | 1.51 | 1.49 |
| 15 | B | 1232 | CLA | MG-NC | 2.72 | 2.15 | 2.07 |
| 15 | B | 1227 | CLA | MG-NC | 2.72 | 2.15 | 2.07 |
| 15 | A | 1116 | CLA | MG-NC | 2.72 | 2.15 | 2.07 |
| 15 | B | 1230 | CLA | CHD-C4C | 2.72 | 1.47 | 1.41 |
| 15 | B | 1223 | CLA | MG-NC | 2.72 | 2.15 | 2.07 |
| 15 | A | 1124 | CLA | MG-NC | 2.72 | 2.15 | 2.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1134 | CLA | MG-NC | 2.71 | 2.15 | 2.07 |
| 15 | A | 1135 | CLA | MG-NC | 2.71 | 2.15 | 2.07 |
| 14 | A | 4001 | BCR | C11-C12 | -2.71 | 1.27 | 1.34 |
| 13 | A | 1108 | CL0 | CHD-C4C | 2.71 | 1.47 | 1.41 |
| 15 | F | 1139 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | B | 1205 | CLA | CHD-C4C | 2.70 | 1.47 | 1.41 |
| 15 | B | 1021 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | A | 1022 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | A | 1114 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | A | 1125 | CLA | C3D-C2D | 2.70 | 1.46 | 1.40 |
| 15 | J | 1302 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | B | 1217 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | A | 1115 | CLA | CHD-C4C | 2.70 | 1.47 | 1.41 |
| 15 | A | 1131 | CLA | MG-NC | 2.70 | 2.15 | 2.07 |
| 15 | B | 1225 | CLA | MG-NC | 2.69 | 2.15 | 2.07 |
| 15 | B | 1206 | CLA | MG-NC | 2.69 | 2.15 | 2.07 |
| 15 | B | 1209 | CLA | MG-NC | 2.69 | 2.15 | 2.07 |
| 15 | B | 1238 | CLA | MG-NC | 2.69 | 2.15 | 2.07 |
| 15 | A | 1119 | CLA | MG-NC | 2.69 | 2.15 | 2.07 |
| 15 | F | 1139 | CLA | C3D-C2D | 2.69 | 1.46 | 1.40 |
| 15 | A | 1113 | CLA | MG-NC | 2.68 | 2.15 | 2.07 |
| 15 | A | 1127 | CLA | MG-NC | 2.68 | 2.15 | 2.07 |
| 15 | A | 1105 | CLA | MG-NC | 2.67 | 2.15 | 2.07 |
| 15 | B | 1216 | CLA | MG-NC | 2.67 | 2.15 | 2.07 |
| 15 | B | 1205 | CLA | MG-NC | 2.67 | 2.15 | 2.07 |
| 13 | A | 1108 | CL0 | C3D-C2D | 2.67 | 1.46 | 1.40 |
| 15 | A | 1120 | CLA | MG-NC | 2.67 | 2.15 | 2.07 |
| 15 | A | 1112 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | F | 1301 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | B | 1207 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | B | 1219 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | K | 1401 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | B | 1234 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | B | 1212 | CLA | MG-NC | 2.66 | 2.15 | 2.07 |
| 15 | B | 1213 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | A | 1133 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | B | 1220 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | K | 1402 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | B | 1239 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | B | 1237 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | A | 1130 | CLA | MG-NC | 2.65 | 2.15 | 2.07 |
| 15 | B | 1210 | CLA | MG-NC | 2.64 | 2.15 | 2.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1221 | CLA | CHD-C4C | 2.64 | 1.47 | 1.41 |
| 13 | A | 1011 | CL0 | MG-NC | 2.64 | 2.15 | 2.07 |
| 15 | A | 1125 | CLA | MG-NC | 2.64 | 2.15 | 2.07 |
| 15 | A | 1132 | CLA | MG-NC | 2.63 | 2.15 | 2.07 |
| 15 | B | 1208 | CLA | CBA-CGA | 2.63 | 1.51 | 1.49 |
| 15 | A | 1111 | CLA | MG-NC | 2.63 | 2.15 | 2.07 |
| 15 | B | 1201 | CLA | MG-NC | 2.62 | 2.15 | 2.07 |
| 15 | B | 1211 | CLA | MG-NC | 2.62 | 2.15 | 2.07 |
| 15 | A | 1117 | CLA | MG-NC | 2.61 | 2.15 | 2.07 |
| 15 | A | 1125 | CLA | CHD-C4C | 2.61 | 1.47 | 1.41 |
| 15 | B | 1202 | CLA | MG-NC | 2.61 | 2.14 | 2.07 |
| 15 | A | 1129 | CLA | MG-NC | 2.61 | 2.14 | 2.07 |
| 15 | B | 1230 | CLA | MG-NC | 2.61 | 2.14 | 2.07 |
| 15 | A | 1136 | CLA | MG-NC | 2.60 | 2.14 | 2.07 |
| 15 | B | 1229 | CLA | MG-NC | 2.60 | 2.14 | 2.07 |
| 15 | B | 1231 | CLA | MG-NC | 2.60 | 2.14 | 2.07 |
| 15 | B | 1203 | CLA | MG-NC | 2.60 | 2.14 | 2.07 |
| 15 | A | 1128 | CLA | MG-NC | 2.60 | 2.14 | 2.07 |
| 15 | B | 1214 | CLA | MG-NC | 2.60 | 2.14 | 2.07 |
| 15 | A | 1110 | CLA | MG-NC | 2.59 | 2.14 | 2.07 |
| 15 | B | 1218 | CLA | MG-NC | 2.59 | 2.14 | 2.07 |
| 15 | B | 1224 | CLA | MG-NC | 2.59 | 2.14 | 2.07 |
| 15 | A | 1101 | CLA | MG-NC | 2.59 | 2.14 | 2.07 |
| 15 | B | 1235 | CLA | MG-NC | 2.59 | 2.14 | 2.07 |
| 15 | A | 1102 | CLA | MG-NC | 2.58 | 2.14 | 2.07 |
| 15 | B | 1208 | CLA | MG-NC | 2.58 | 2.14 | 2.07 |
| 15 | B | 1226 | CLA | MG-NC | 2.58 | 2.14 | 2.07 |
| 15 | A | 1140 | CLA | MG-NC | 2.58 | 2.14 | 2.07 |
| 15 | B | 1204 | CLA | MG-NC | 2.57 | 2.14 | 2.07 |
| 15 | A | 1115 | CLA | MG-NC | 2.58 | 2.14 | 2.07 |
| 15 | A | 1109 | CLA | MG-NC | 2.57 | 2.14 | 2.07 |
| 15 | A | 1138 | CLA | MG-NC | 2.57 | 2.14 | 2.07 |
| 15 | B | 1222 | CLA | MG-NC | 2.57 | 2.14 | 2.07 |
| 15 | A | 1103 | CLA | MG-NC | 2.57 | 2.14 | 2.07 |
| 15 | B | 1236 | CLA | MG-NC | 2.55 | 2.14 | 2.07 |
| 15 | A | 1122 | CLA | MG-NC | 2.54 | 2.14 | 2.07 |
| 15 | B | 1228 | CLA | MG-NC | 2.54 | 2.14 | 2.07 |
| 15 | A | 1106 | CLA | MG-NC | 2.54 | 2.14 | 2.07 |
| 15 | A | 1104 | CLA | MG-NC | 2.50 | 2.14 | 2.07 |
| 15 | A | 1107 | CLA | MG-NC | 2.50 | 2.14 | 2.07 |
| 15 | B | 1023 | CLA | MG-NC | 2.50 | 2.14 | 2.07 |
| 15 | A | 1126 | CLA | MG-NC | 2.50 | 2.14 | 2.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1118 | CLA | MG-NC | 2.45 | 2.14 | 2.07 |
| 15 | B | 1013 | CLA | MG-NC | 2.45 | 2.14 | 2.07 |
| 15 | A | 1123 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 15 | B | 1236 | CLA | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 15 | B | 1236 | CLA | C5-C3 | 2.39 | 1.51 | 1.39 |
| 15 | A | 1124 | CLA | C4D-CHA | 2.37 | 1.48 | 1.38 |
| 15 | B | 1221 | CLA | C4D-CHA | 2.36 | 1.48 | 1.38 |
| 15 | A | 1107 | CLA | C5-C3 | 2.36 | 1.51 | 1.39 |
| 15 | B | 1222 | CLA | C4D-CHA | 2.35 | 1.48 | 1.38 |
| 15 | A | 1138 | CLA | C1C-C2C | 2.35 | 1.49 | 1.44 |
| 13 | A | 1011 | CL0 | C4D-CHA | 2.35 | 1.48 | 1.38 |
| 15 | B | 1213 | CLA | C5-C3 | 2.35 | 1.51 | 1.39 |
| 15 | A | 1801 | CLA | C4D-CHA | 2.34 | 1.48 | 1.38 |
| 15 | A | 1137 | CLA | C5-C3 | 2.33 | 1.51 | 1.39 |
| 15 | A | 1102 | CLA | C4D-CHA | 2.33 | 1.48 | 1.38 |
| 15 | B | 1209 | CLA | C4D-CHA | 2.33 | 1.48 | 1.38 |
| 15 | A | 1120 | CLA | C4D-CHA | 2.33 | 1.48 | 1.38 |
| 15 | B | 1209 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 15 | A | 1123 | CLA | C4D-CHA | 2.33 | 1.48 | 1.38 |
| 15 | A | 1101 | CLA | C4D-CHA | 2.32 | 1.48 | 1.38 |
| 15 | B | 1240 | CLA | C4D-CHA | 2.31 | 1.48 | 1.38 |
| 15 | J | 1303 | CLA | C4D-CHA | 2.31 | 1.48 | 1.38 |
| 15 | B | 1203 | CLA | C4D-CHA | 2.30 | 1.48 | 1.38 |
| 15 | A | 1114 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 15 | B | 1212 | CLA | C4D-CHA | 2.30 | 1.48 | 1.38 |
| 15 | B | 1201 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | B | 1239 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 15 | A | 1117 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | B | 1226 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | J | 1302 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | B | 1210 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | B | 1206 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 15 | B | 1207 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | A | 1012 | CLA | C4D-CHA | 2.29 | 1.48 | 1.38 |
| 15 | B | 1206 | CLA | C4D-CHA | 2.28 | 1.48 | 1.38 |
| 15 | A | 1128 | CLA | C1C-NC | -2.28 | 1.33 | 1.37 |
| 15 | B | 1217 | CLA | C4D-CHA | 2.28 | 1.48 | 1.38 |
| 15 | B | 1232 | CLA | C4D-CHA | 2.28 | 1.48 | 1.38 |
| 15 | A | 1112 | CLA | C4D-CHA | 2.28 | 1.48 | 1.38 |
| 15 | F | 1301 | CLA | C4D-CHA | 2.28 | 1.48 | 1.38 |
| 15 | A | 1106 | CLA | C4D-CHA | 2.28 | 1.48 | 1.38 |
| 15 | B | 1225 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1239 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |
| 15 | B | 1224 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |
| 15 | B | 1227 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |
| 15 | B | 1202 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |
| 15 | A | 1113 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |
| 15 | A | 1130 | CLA | C1D-CHD | 2.27 | 1.47 | 1.37 |
| 15 | A | 1103 | CLA | C4D-CHA | 2.27 | 1.48 | 1.38 |
| 15 | A | 1138 | CLA | C4D-CHA | 2.26 | 1.48 | 1.38 |
| 15 | B | 1216 | CLA | C4C-C3C | 2.26 | 1.49 | 1.45 |
| 15 | B | 1206 | CLA | C1D-CHD | 2.26 | 1.47 | 1.37 |
| 15 | A | 1123 | CLA | C1D-CHD | 2.26 | 1.47 | 1.37 |
| 15 | B | 1223 | CLA | C4D-CHA | 2.26 | 1.48 | 1.38 |
| 15 | A | 1119 | CLA | C4D-CHA | 2.26 | 1.48 | 1.38 |
| 15 | A | 1131 | CLA | C4D-CHA | 2.26 | 1.48 | 1.38 |
| 15 | A | 1120 | CLA | C1D-CHD | 2.26 | 1.47 | 1.37 |
| 15 | B | 1021 | CLA | C4D-CHA | 2.26 | 1.48 | 1.38 |
| 13 | A | 1108 | CL0 | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | A | 1125 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | B | 1219 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | B | 1235 | CLA | C1C-C2C | 2.25 | 1.49 | 1.44 |
| 15 | K | 1402 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | K | 1401 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | B | 1223 | CLA | C1C-C2C | 2.25 | 1.49 | 1.44 |
| 15 | A | 1128 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | F | 1410 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | A | 1126 | CLA | C1D-CHD | 2.25 | 1.47 | 1.37 |
| 15 | A | 1129 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | B | 1214 | CLA | C1D-CHD | 2.25 | 1.47 | 1.37 |
| 15 | B | 1220 | CLA | C4D-CHA | 2.25 | 1.48 | 1.38 |
| 15 | A | 1116 | CLA | C1D-CHD | 2.24 | 1.47 | 1.37 |
| 15 | A | 1134 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | A | 1133 | CLA | C4C-C3C | 2.24 | 1.49 | 1.45 |
| 15 | A | 1111 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | A | 1125 | CLA | C1C-C2C | 2.24 | 1.49 | 1.44 |
| 15 | A | 1121 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | A | 1133 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | B | 1229 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | A | 1118 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | B | 1227 | CLA | C1D-CHD | 2.24 | 1.47 | 1.37 |
| 15 | A | 1105 | CLA | C4C-C3C | 2.24 | 1.49 | 1.45 |
| 15 | B | 1235 | CLA | C4D-CHA | 2.24 | 1.48 | 1.38 |
| 15 | B | 1204 | CLA | C1D-CHD | 2.23 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | B | 1239 | CLA | C1D-CHD | 2.23 | 1.47 | 1.37 |
| 15 | B | 1237 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | B | 1214 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | A | 1132 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | A | 1116 | CLA | C4C-C3C | 2.23 | 1.49 | 1.45 |
| 15 | A | 1105 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | B | 1211 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | B | 1237 | CLA | C1D-CHD | 2.23 | 1.47 | 1.37 |
| 15 | B | 1215 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | B | 1209 | CLA | C1D-CHD | 2.23 | 1.47 | 1.37 |
| 15 | A | 1114 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | B | 1203 | CLA | C1D-CHD | 2.23 | 1.47 | 1.37 |
| 15 | B | 1238 | CLA | C4D-CHA | 2.23 | 1.48 | 1.38 |
| 15 | A | 1137 | CLA | C4D-CHA | 2.22 | 1.48 | 1.38 |
| 15 | B | 1216 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | A | 1135 | CLA | C4D-CHA | 2.22 | 1.48 | 1.38 |
| 15 | B | 1234 | CLA | C4D-CHA | 2.22 | 1.48 | 1.38 |
| 15 | B | 1208 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | A | 1102 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | B | 1231 | CLA | C4D-CHA | 2.22 | 1.48 | 1.38 |
| 15 | A | 1114 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | A | 1124 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | B | 1205 | CLA | C4D-CHA | 2.22 | 1.48 | 1.38 |
| 15 | B | 1231 | CLA | C1C-NC | -2.22 | 1.33 | 1.37 |
| 15 | A | 1130 | CLA | C4D-CHA | 2.22 | 1.48 | 1.38 |
| 15 | B | 1220 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | A | 1105 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | B | 1215 | CLA | C1D-CHD | 2.22 | 1.47 | 1.37 |
| 15 | B | 1213 | CLA | C1D-CHD | 2.21 | 1.47 | 1.37 |
| 15 | A | 1121 | CLA | C1D-CHD | 2.21 | 1.47 | 1.37 |
| 15 | A | 1117 | CLA | C1D-CHD | 2.21 | 1.47 | 1.37 |
| 15 | B | 1208 | CLA | C4D-CHA | 2.21 | 1.48 | 1.38 |
| 15 | A | 1116 | CLA | C4D-CHA | 2.21 | 1.47 | 1.38 |
| 15 | B | 1228 | CLA | C4D-CHA | 2.21 | 1.47 | 1.38 |
| 15 | A | 1133 | CLA | C1D-CHD | 2.21 | 1.47 | 1.37 |
| 15 | A | 1129 | CLA | C1D-CHD | 2.21 | 1.47 | 1.37 |
| 15 | A | 1106 | CLA | C1D-CHD | 2.21 | 1.47 | 1.37 |
| 15 | B | 1213 | CLA | C4D-CHA | 2.21 | 1.47 | 1.38 |
| 15 | A | 1126 | CLA | C4D-CHA | 2.21 | 1.47 | 1.38 |
| 15 | B | 1216 | CLA | C4D-CHA | 2.21 | 1.47 | 1.38 |
| 15 | B | 1204 | CLA | C4D-CHA | 2.21 | 1.47 | 1.38 |
| 15 | A | 1119 | CLA | C1D-CHD | 2.20 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1140 | CLA | C4D-CHA | 2.20 | 1.47 | 1.38 |
| 15 | A | 1113 | CLA | C4C-C3C | 2.20 | 1.49 | 1.45 |
| 15 | A | 1103 | CLA | C1D-CHD | 2.20 | 1.47 | 1.37 |
| 15 | B | 1204 | CLA | C4C-C3C | 2.20 | 1.49 | 1.45 |
| 15 | B | 1232 | CLA | C1D-CHD | 2.20 | 1.47 | 1.37 |
| 15 | A | 1107 | CLA | C1D-CHD | 2.20 | 1.47 | 1.37 |
| 15 | A | 1104 | CLA | C4D-CHA | 2.20 | 1.47 | 1.38 |
| 15 | A | 1022 | CLA | C4D-CHA | 2.19 | 1.47 | 1.38 |
| 15 | B | 1201 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | B | 1021 | CLA | C1D-CHD | 2.20 | 1.47 | 1.37 |
| 15 | B | 1240 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | A | 1138 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | B | 1219 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | A | 1107 | CLA | C1C-NC | -2.19 | 1.33 | 1.37 |
| 15 | A | 1137 | CLA | C4C-C3C | 2.19 | 1.49 | 1.45 |
| 15 | F | 1139 | CLA | C1C-C2C | 2.19 | 1.49 | 1.44 |
| 15 | A | 1120 | CLA | C4C-C3C | 2.19 | 1.49 | 1.45 |
| 15 | A | 1122 | CLA | C4D-CHA | 2.19 | 1.47 | 1.38 |
| 15 | A | 1122 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | K | 1401 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | A | 1136 | CLA | C4D-CHA | 2.19 | 1.47 | 1.38 |
| 15 | A | 1109 | CLA | C1D-CHD | 2.19 | 1.47 | 1.37 |
| 15 | B | 1218 | CLA | C4D-CHA | 2.19 | 1.47 | 1.38 |
| 15 | J | 1303 | CLA | C4C-C3C | 2.19 | 1.49 | 1.45 |
| 15 | B | 1215 | CLA | C4C-C3C | 2.19 | 1.49 | 1.45 |
| 15 | A | 1131 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | A | 1104 | CLA | C1C-C2C | 2.18 | 1.49 | 1.44 |
| 15 | B | 1224 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | A | 1121 | CLA | C4C-C3C | 2.18 | 1.49 | 1.45 |
| 15 | B | 1217 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | A | 1137 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | A | 1131 | CLA | C4C-C3C | 2.18 | 1.49 | 1.45 |
| 15 | B | 1210 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | B | 1023 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | B | 1228 | CLA | C1D-CHD | 2.18 | 1.47 | 1.37 |
| 15 | F | 1410 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | B | 1240 | CLA | C4C-C3C | 2.17 | 1.49 | 1.45 |
| 15 | B | 1207 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | B | 1225 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | F | 1139 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | J | 1303 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | A | 1113 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | B | 1218 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | B | 1236 | CLA | C4D-CHA | 2.17 | 1.47 | 1.38 |
| 15 | A | 1112 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | B | 1227 | CLA | C4C-C3C | 2.17 | 1.49 | 1.45 |
| 15 | B | 1023 | CLA | C4D-CHA | 2.17 | 1.47 | 1.38 |
| 15 | B | 1230 | CLA | C4D-CHA | 2.17 | 1.47 | 1.38 |
| 15 | K | 1401 | CLA | C4C-C3C | 2.17 | 1.49 | 1.45 |
| 15 | A | 1022 | CLA | C1D-CHD | 2.17 | 1.47 | 1.37 |
| 15 | A | 1135 | CLA | C1D-CHD | 2.16 | 1.47 | 1.37 |
| 15 | A | 1110 | CLA | C4D-CHA | 2.16 | 1.47 | 1.38 |
| 15 | A | 1135 | CLA | C4C-C3C | 2.16 | 1.49 | 1.45 |
| 15 | B | 1214 | CLA | C4C-C3C | 2.16 | 1.49 | 1.45 |
| 15 | B | 1226 | CLA | C1D-CHD | 2.16 | 1.47 | 1.37 |
| 15 | A | 1134 | CLA | C1D-CHD | 2.16 | 1.47 | 1.37 |
| 15 | B | 1211 | CLA | C1D-CHD | 2.16 | 1.47 | 1.37 |
| 15 | A | 1136 | CLA | C1D-CHD | 2.16 | 1.47 | 1.37 |
| 15 | A | 1109 | CLA | C4D-CHA | 2.16 | 1.47 | 1.38 |
| 15 | B | 1207 | CLA | C4C-C3C | 2.16 | 1.49 | 1.45 |
| 15 | B | 1013 | CLA | C4D-CHA | 2.16 | 1.47 | 1.38 |
| 15 | A | 1801 | CLA | C1D-CHD | 2.15 | 1.47 | 1.37 |
| 15 | B | 1231 | CLA | C1D-CHD | 2.15 | 1.47 | 1.37 |
| 15 | F | 1301 | CLA | C1D-CHD | 2.15 | 1.47 | 1.37 |
| 15 | A | 1115 | CLA | C4D-CHA | 2.15 | 1.47 | 1.38 |
| 15 | A | 1111 | CLA | C1D-CHD | 2.15 | 1.47 | 1.37 |
| 15 | A | 1109 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 15 | J | 1302 | CLA | C1D-CHD | 2.15 | 1.47 | 1.37 |
| 15 | K | 1402 | CLA | C1D-CHD | 2.15 | 1.47 | 1.37 |
| 15 | B | 1202 | CLA | C1D-CHD | 2.14 | 1.47 | 1.37 |
| 15 | B | 1237 | CLA | C4C-C3C | 2.14 | 1.49 | 1.45 |
| 15 | A | 1128 | CLA | C1D-CHD | 2.14 | 1.47 | 1.37 |
| 15 | A | 1130 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 15 | B | 1238 | CLA | C1D-CHD | 2.14 | 1.47 | 1.37 |
| 15 | F | 1139 | CLA | C4D-CHA | 2.14 | 1.47 | 1.38 |
| 15 | B | 1208 | CLA | C4C-C3C | 2.14 | 1.48 | 1.45 |
| 15 | A | 1127 | CLA | C4D-CHA | 2.14 | 1.47 | 1.38 |
| 15 | B | 1220 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 15 | A | 1101 | CLA | C1D-CHD | 2.14 | 1.47 | 1.37 |
| 15 | A | 1119 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 15 | B | 1203 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 15 | A | 1127 | CLA | C1D-CHD | 2.13 | 1.47 | 1.37 |
| 13 | A | 1011 | CL0 | C1D-CHD | 2.13 | 1.47 | 1.37 |
| 15 | A | 1134 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1107 | CLA | C4D-CHA | 2.13 | 1.47 | 1.38 |
| 15 | F | 1301 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 15 | A | 1111 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 15 | B | 1212 | CLA | C1D-CHD | 2.13 | 1.47 | 1.37 |
| 15 | A | 1110 | CLA | C1D-CHD | 2.12 | 1.47 | 1.37 |
| 15 | A | 1124 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 15 | B | 1222 | CLA | C1D-CHD | 2.12 | 1.47 | 1.37 |
| 15 | B | 1220 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 15 | B | 1234 | CLA | C1D-CHD | 2.12 | 1.47 | 1.37 |
| 15 | A | 1012 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 15 | B | 1230 | CLA | C1D-CHD | 2.12 | 1.47 | 1.37 |
| 15 | A | 1129 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 15 | A | 1122 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 15 | B | 1210 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 15 | B | 1232 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 15 | A | 1110 | CLA | C1A-NA | -2.11 | 1.27 | 1.32 |
| 15 | B | 1219 | CLA | C4C-C3C | 2.11 | 1.48 | 1.45 |
| 15 | A | 1104 | CLA | C1D-CHD | 2.11 | 1.47 | 1.37 |
| 15 | A | 1136 | CLA | C4C-C3C | 2.11 | 1.48 | 1.45 |
| 15 | A | 1140 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 15 | A | 1012 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 15 | B | 1205 | CLA | C1D-CHD | 2.11 | 1.47 | 1.37 |
| 15 | B | 1023 | CLA | C4C-C3C | 2.10 | 1.48 | 1.45 |
| 15 | A | 1140 | CLA | C1D-CHD | 2.10 | 1.47 | 1.37 |
| 15 | A | 1012 | CLA | C1D-CHD | 2.10 | 1.47 | 1.37 |
| 15 | A | 1118 | CLA | C1D-CHD | 2.10 | 1.47 | 1.37 |
| 15 | A | 1022 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 15 | B | 1236 | CLA | C1D-CHD | 2.10 | 1.47 | 1.37 |
| 15 | B | 1013 | CLA | C1D-CHD | 2.10 | 1.47 | 1.37 |
| 15 | B | 1221 | CLA | C1D-CHD | 2.10 | 1.47 | 1.37 |
| 14 | A | 4008 | BCR | C30-C25 | -2.10 | 1.50 | 1.53 |
| 13 | A | 1108 | CL0 | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 15 | K | 1402 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 15 | A | 1132 | CLA | C1D-CHD | 2.09 | 1.47 | 1.37 |
| 15 | B | 1230 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 15 | B | 1213 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 15 | J | 1302 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 15 | B | 1217 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 15 | B | 1240 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 15 | B | 1230 | CLA | C1A-NA | -2.07 | 1.27 | 1.32 |
| 15 | B | 1021 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 15 | B | 1223 | CLA | C1D-CHD | 2.07 | 1.46 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1110 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |
| 15 | B | 1235 | CLA | C1D-CHD | 2.07 | 1.46 | 1.37 |
| 15 | B | 1238 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 15 | A | 1107 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 15 | B | 1218 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 15 | A | 1107 | CLA | C1A-NA | -2.06 | 1.27 | 1.32 |
| 15 | B | 1228 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 15 | B | 1202 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 15 | B | 1213 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 13 | A | 1108 | CL0 | C1D-CHD | 2.06 | 1.46 | 1.37 |
| 15 | A | 1101 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 15 | F | 1410 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 15 | B | 1201 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 15 | A | 1112 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 15 | A | 1110 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 15 | B | 1217 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 14 | F | 4015 | BCR | C30-C25 | -2.05 | 1.50 | 1.53 |
| 15 | A | 1126 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 15 | A | 1130 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 15 | B | 1227 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 15 | A | 1102 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 15 | A | 1801 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 15 | B | 1221 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 15 | A | 1126 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 15 | B | 1229 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 15 | A | 1115 | CLA | C1D-CHD | 2.04 | 1.46 | 1.37 |
| 15 | F | 1139 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 15 | A | 1117 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 15 | B | 1021 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 15 | B | 1234 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 15 | B | 1229 | CLA | C1D-CHD | 2.03 | 1.46 | 1.37 |
| 15 | B | 1225 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 15 | A | 1112 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 15 | B | 1219 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 15 | A | 1119 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 15 | B | 1212 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 15 | A | 1115 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 15 | B | 1023 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 14 | B | 4009 | BCR | C30-C25 | -2.01 | 1.50 | 1.53 |
| 15 | B | 1221 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 15 | B | 1228 | CLA | C1A-NA | -2.01 | 1.27 | 1.32 |
| 15 | B | 1211 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 1801 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 15 | A | 1131 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 15 | A | 1120 | CLA | C4-C3 | 2.01 | 1.50 | 1.47 |
| 15 | B | 1228 | CLA | C4C-C3C | 2.01 | 1.48 | 1.45 |
| 15 | B | 1023 | CLA | C1A-NA | -2.01 | 1.27 | 1.32 |
| 15 | B | 1013 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 15 | A | 1801 | CLA | C1C-NC | -2.00 | 1.34 | 1.37 |
| 15 | B | 1239 | CLA | C1C-NC | -2.00 | 1.34 | 1.37 |
| 15 | A | 1106 | CLA | C4C-C3C | 2.00 | 1.48 | 1.45 |
| 15 | J | 1303 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |

All (2699) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 4009 | BCR | C16-C17-C18 | 26.43 | 165.49 | 127.29 |
| 14 | F | 4016 | BCR | C20-C21-C22 | 25.03 | 163.47 | 127.29 |
| 14 | B | 4006 | BCR | C20-C21-C22 | 23.66 | 161.49 | 127.29 |
| 14 | A | 4008 | BCR | C20-C21-C22 | 22.96 | 160.48 | 127.29 |
| 14 | A | 4007 | BCR | C20-C21-C22 | 22.96 | 160.48 | 127.29 |
| 14 | B | 4014 | BCR | C16-C17-C18 | 22.80 | 160.24 | 127.29 |
| 14 | B | 4010 | BCR | C20-C21-C22 | 22.77 | 160.21 | 127.29 |
| 14 | F | 4015 | BCR | C20-C21-C22 | 21.92 | 158.97 | 127.29 |
| 14 | A | 4008 | BCR | C16-C17-C18 | 21.92 | 158.97 | 127.29 |
| 14 | A | 4007 | BCR | C16-C17-C18 | 21.63 | 158.55 | 127.29 |
| 14 | J | 4013 | BCR | C20-C21-C22 | 21.60 | 158.50 | 127.29 |
| 14 | F | 4015 | BCR | C16-C17-C18 | 21.55 | 158.44 | 127.29 |
| 14 | B | 4011 | BCR | C16-C17-C18 | 21.55 | 158.44 | 127.29 |
| 14 | A | 4003 | BCR | C16-C17-C18 | 21.02 | 157.67 | 127.29 |
| 14 | B | 4010 | BCR | C16-C17-C18 | 20.93 | 157.54 | 127.29 |
| 14 | A | 4002 | BCR | C20-C21-C22 | 20.81 | 157.36 | 127.29 |
| 14 | B | 4017 | BCR | C20-C21-C22 | 20.71 | 157.23 | 127.29 |
| 14 | F | 4016 | BCR | C16-C17-C18 | 20.42 | 156.80 | 127.29 |
| 14 | J | 4013 | BCR | C16-C17-C18 | 20.27 | 156.59 | 127.29 |
| 14 | B | 4006 | BCR | C16-C17-C18 | 20.20 | 156.48 | 127.29 |
| 14 | B | 4005 | BCR | C20-C21-C22 | 20.06 | 156.28 | 127.29 |
| 14 | A | 4001 | BCR | C20-C21-C22 | 19.96 | 156.15 | 127.29 |
| 14 | B | 4009 | BCR | C20-C21-C22 | 19.91 | 156.06 | 127.29 |
| 14 | B | 4017 | BCR | C16-C17-C18 | 19.71 | 155.78 | 127.29 |
| 14 | A | 4003 | BCR | C20-C21-C22 | 19.54 | 155.53 | 127.29 |
| 14 | B | 4014 | BCR | C20-C21-C22 | 19.50 | 155.48 | 127.29 |
| 14 | B | 4004 | BCR | C20-C21-C22 | 19.45 | 155.40 | 127.29 |
| 14 | A | 4002 | BCR | C15-C16-C17 | 19.33 | 166.01 | 123.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | F | 4016 | BCR | C15-C16-C17 | 19.23 | 165.79 | 123.45 |
| 14 | A | 4012 | BCR | C16-C17-C18 | 19.19 | 155.03 | 127.29 |
| 14 | A | 4001 | BCR | C16-C17-C18 | 19.14 | 154.96 | 127.29 |
| 14 | B | 4005 | BCR | C15-C16-C17 | 19.11 | 165.52 | 123.45 |
| 14 | B | 4011 | BCR | C20-C21-C22 | 19.10 | 154.90 | 127.29 |
| 14 | B | 4005 | BCR | C16-C17-C18 | 18.87 | 154.56 | 127.29 |
| 14 | B | 4017 | BCR | C15-C16-C17 | 18.85 | 164.95 | 123.45 |
| 14 | A | 4012 | BCR | C15-C16-C17 | 18.79 | 164.81 | 123.45 |
| 14 | A | 4002 | BCR | C16-C17-C18 | 18.75 | 154.39 | 127.29 |
| 14 | A | 4003 | BCR | C15-C16-C17 | 18.67 | 164.55 | 123.45 |
| 14 | A | 4012 | BCR | C20-C21-C22 | 18.66 | 154.26 | 127.29 |
| 14 | B | 4004 | BCR | C15-C16-C17 | 18.65 | 164.51 | 123.45 |
| 14 | A | 4001 | BCR | C15-C16-C17 | 18.41 | 163.98 | 123.45 |
| 14 | B | 4006 | BCR | C15-C16-C17 | 18.36 | 163.88 | 123.45 |
| 14 | B | 4004 | BCR | C16-C17-C18 | 18.18 | 153.56 | 127.29 |
| 14 | J | 4013 | BCR | C15-C16-C17 | 18.08 | 163.25 | 123.45 |
| 14 | B | 4011 | BCR | C15-C16-C17 | 18.00 | 163.09 | 123.45 |
| 14 | A | 4007 | BCR | C15-C16-C17 | 17.95 | 162.96 | 123.45 |
| 14 | B | 4010 | BCR | C15-C16-C17 | 17.74 | 162.50 | 123.45 |
| 14 | A | 4008 | BCR | C15-C16-C17 | 17.51 | 162.01 | 123.45 |
| 14 | B | 4014 | BCR | C15-C16-C17 | 17.31 | 161.57 | 123.45 |
| 14 | B | 4011 | BCR | C11-C10-C9 | 16.91 | 151.74 | 127.29 |
| 14 | F | 4015 | BCR | C15-C16-C17 | 16.53 | 159.85 | 123.45 |
| 14 | F | 4015 | BCR | C10-C11-C12 | 16.23 | 177.72 | 123.23 |
| 14 | B | 4005 | BCR | C10-C11-C12 | 16.07 | 177.17 | 123.23 |
| 14 | B | 4014 | BCR | C10-C11-C12 | 16.05 | 177.11 | 123.23 |
| 14 | J | 4013 | BCR | C10-C11-C12 | 16.05 | 177.10 | 123.23 |
| 14 | A | 4008 | BCR | C10-C11-C12 | 15.99 | 176.90 | 123.23 |
| 14 | B | 4017 | BCR | C10-C11-C12 | 15.99 | 176.89 | 123.23 |
| 14 | B | 4006 | BCR | C10-C11-C12 | 15.97 | 176.83 | 123.23 |
| 14 | A | 4002 | BCR | C10-C11-C12 | 15.91 | 176.64 | 123.23 |
| 14 | A | 4007 | BCR | C10-C11-C12 | 15.75 | 176.12 | 123.23 |
| 14 | B | 4010 | BCR | C10-C11-C12 | 15.72 | 176.01 | 123.23 |
| 14 | B | 4004 | BCR | C10-C11-C12 | 15.59 | 175.56 | 123.23 |
| 14 | F | 4016 | BCR | C10-C11-C12 | 15.51 | 175.29 | 123.23 |
| 14 | A | 4003 | BCR | C10-C11-C12 | 15.41 | 174.95 | 123.23 |
| 14 | B | 4009 | BCR | C16-C15-C14 | 15.37 | 157.29 | 123.45 |
| 14 | B | 4009 | BCR | C15-C16-C17 | 14.83 | 156.10 | 123.45 |
| 14 | B | 4011 | BCR | C10-C11-C12 | 14.49 | 171.87 | 123.23 |
| 14 | A | 4012 | BCR | C10-C11-C12 | 14.24 | 171.03 | 123.23 |
| 14 | B | 4009 | BCR | C10-C11-C12 | 14.12 | 170.63 | 123.23 |
| 14 | F | 4015 | BCR | C16-C15-C14 | 13.99 | 154.25 | 123.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 4014 | BCR | C16-C15-C14 | 13.99 | 154.24 | 123.45 |
| 14 | A | 4001 | BCR | C10-C11-C12 | 13.88 | 169.83 | 123.23 |
| 14 | B | 4017 | BCR | C11-C10-C9 | 13.76 | 147.18 | 127.29 |
| 14 | B | 4014 | BCR | C11-C10-C9 | 13.47 | 146.75 | 127.29 |
| 14 | B | 4006 | BCR | C11-C10-C9 | 13.17 | 146.32 | 127.29 |
| 14 | B | 4010 | BCR | C11-C10-C9 | 13.17 | 146.32 | 127.29 |
| 14 | A | 4008 | BCR | C11-C10-C9 | 13.08 | 146.20 | 127.29 |
| 14 | A | 4008 | BCR | C16-C15-C14 | 12.95 | 151.97 | 123.45 |
| 14 | J | 4013 | BCR | C11-C10-C9 | 12.92 | 145.96 | 127.29 |
| 14 | A | 4007 | BCR | C11-C10-C9 | 12.90 | 145.94 | 127.29 |
| 14 | B | 4004 | BCR | C21-C20-C19 | 12.79 | 166.17 | 123.23 |
| 14 | J | 4013 | BCR | C16-C15-C14 | 12.68 | 151.38 | 123.45 |
| 14 | B | 4010 | BCR | C16-C15-C14 | 12.67 | 151.35 | 123.45 |
| 14 | B | 4005 | BCR | C11-C10-C9 | 12.65 | 145.57 | 127.29 |
| 14 | A | 4001 | BCR | C21-C20-C19 | 12.63 | 165.64 | 123.23 |
| 14 | A | 4003 | BCR | C16-C15-C14 | 12.61 | 151.22 | 123.45 |
| 14 | B | 4004 | BCR | C16-C15-C14 | 12.56 | 151.10 | 123.45 |
| 14 | A | 4012 | BCR | C21-C20-C19 | 12.50 | 165.18 | 123.23 |
| 14 | B | 4014 | BCR | C21-C20-C19 | 12.42 | 164.92 | 123.23 |
| 14 | A | 4002 | BCR | C11-C10-C9 | 12.41 | 145.23 | 127.29 |
| 14 | A | 4007 | BCR | C16-C15-C14 | 12.41 | 150.78 | 123.45 |
| 14 | A | 4003 | BCR | C21-C20-C19 | 12.38 | 164.79 | 123.23 |
| 14 | B | 4004 | BCR | C11-C10-C9 | 12.37 | 145.18 | 127.29 |
| 14 | B | 4005 | BCR | C21-C20-C19 | 12.35 | 164.70 | 123.23 |
| 14 | B | 4009 | BCR | C21-C20-C19 | 12.24 | 164.32 | 123.23 |
| 14 | A | 4001 | BCR | C16-C15-C14 | 12.22 | 150.36 | 123.45 |
| 14 | B | 4017 | BCR | C21-C20-C19 | 12.20 | 164.19 | 123.23 |
| 14 | B | 4011 | BCR | C16-C15-C14 | 12.19 | 150.29 | 123.45 |
| 14 | B | 4011 | BCR | C11-C12-C13 | 12.10 | 161.04 | 126.37 |
| 14 | A | 4002 | BCR | C21-C20-C19 | 12.07 | 163.73 | 123.23 |
| 14 | B | 4017 | BCR | C16-C15-C14 | 12.03 | 149.93 | 123.45 |
| 14 | F | 4015 | BCR | C11-C10-C9 | 11.89 | 144.48 | 127.29 |
| 14 | B | 4011 | BCR | C21-C20-C19 | 11.76 | 162.71 | 123.23 |
| 14 | B | 4006 | BCR | C16-C15-C14 | 11.66 | 149.13 | 123.45 |
| 14 | F | 4016 | BCR | C21-C20-C19 | 11.63 | 162.28 | 123.23 |
| 14 | B | 4005 | BCR | C16-C15-C14 | 11.56 | 148.90 | 123.45 |
| 14 | F | 4015 | BCR | C21-C20-C19 | 11.52 | 161.92 | 123.23 |
| 14 | F | 4016 | BCR | C11-C10-C9 | 11.45 | 143.84 | 127.29 |
| 14 | B | 4009 | BCR | C11-C10-C9 | 11.44 | 143.82 | 127.29 |
| 14 | A | 4008 | BCR | C21-C20-C19 | 11.40 | 161.50 | 123.23 |
| 14 | A | 4003 | BCR | C11-C10-C9 | 11.37 | 143.73 | 127.29 |
| 14 | F | 4016 | BCR | C16-C15-C14 | 11.35 | 148.45 | 123.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 4007 | BCR | C21-C20-C19 | 11.28 | 161.09 | 123.23 |
| 14 | A | 4002 | BCR | C11-C12-C13 | 11.27 | 158.66 | 126.37 |
| 14 | B | 4010 | BCR | C21-C20-C19 | 11.24 | 160.97 | 123.23 |
| 14 | A | 4012 | BCR | C16-C15-C14 | 11.18 | 148.06 | 123.45 |
| 14 | A | 4007 | BCR | C11-C12-C13 | 11.12 | 158.23 | 126.37 |
| 14 | B | 4006 | BCR | C21-C20-C19 | 11.09 | 160.47 | 123.23 |
| 14 | A | 4002 | BCR | C16-C15-C14 | 11.08 | 147.85 | 123.45 |
| 14 | B | 4005 | BCR | C11-C12-C13 | 10.90 | 157.59 | 126.37 |
| 14 | J | 4013 | BCR | C21-C20-C19 | 10.89 | 159.80 | 123.23 |
| 14 | J | 4013 | BCR | C11-C12-C13 | 10.78 | 157.25 | 126.37 |
| 14 | A | 4008 | BCR | C11-C12-C13 | 10.77 | 157.22 | 126.37 |
| 14 | F | 4015 | BCR | C11-C12-C13 | 10.71 | 157.06 | 126.37 |
| 14 | A | 4012 | BCR | C11-C12-C13 | 10.70 | 157.01 | 126.37 |
| 14 | B | 4010 | BCR | C11-C12-C13 | 10.64 | 156.85 | 126.37 |
| 14 | B | 4006 | BCR | C11-C12-C13 | 10.64 | 156.85 | 126.37 |
| 14 | B | 4004 | BCR | C11-C12-C13 | 10.54 | 156.54 | 126.37 |
| 14 | A | 4012 | BCR | C11-C10-C9 | 10.48 | 142.44 | 127.29 |
| 14 | B | 4017 | BCR | C11-C12-C13 | 10.34 | 155.99 | 126.37 |
| 14 | A | 4003 | BCR | C11-C12-C13 | 10.32 | 155.91 | 126.37 |
| 14 | A | 4001 | BCR | C11-C10-C9 | 10.30 | 142.18 | 127.29 |
| 14 | B | 4014 | BCR | C11-C12-C13 | 10.20 | 155.58 | 126.37 |
| 14 | A | 4001 | BCR | C11-C12-C13 | 9.47 | 153.49 | 126.37 |
| 14 | B | 4009 | BCR | C11-C12-C13 | 9.34 | 153.13 | 126.37 |
| 15 | A | 1125 | CLA | C1D-C2D-C3D | -9.06 | 98.10 | 106.97 |
| 15 | B | 1235 | CLA | C1D-C2D-C3D | -8.70 | 98.44 | 106.97 |
| 15 | B | 1229 | CLA | C1D-C2D-C3D | -8.69 | 98.45 | 106.97 |
| 14 | F | 4016 | BCR | C11-C12-C13 | 8.69 | 151.27 | 126.37 |
| 15 | B | 1223 | CLA | C1D-C2D-C3D | -8.58 | 98.56 | 106.97 |
| 15 | B | 1222 | CLA | C1D-C2D-C3D | -8.55 | 98.59 | 106.97 |
| 15 | B | 1231 | CLA | C1D-C2D-C3D | -8.54 | 98.60 | 106.97 |
| 15 | A | 1132 | CLA | C1D-C2D-C3D | -8.48 | 98.66 | 106.97 |
| 15 | A | 1134 | CLA | C1D-C2D-C3D | -8.48 | 98.66 | 106.97 |
| 15 | A | 1118 | CLA | C1D-C2D-C3D | -8.47 | 98.67 | 106.97 |
| 15 | A | 1129 | CLA | C1D-C2D-C3D | -8.47 | 98.67 | 106.97 |
| 14 | F | 4016 | BCR | C20-C19-C18 | 8.45 | 150.57 | 126.37 |
| 14 | A | 4007 | BCR | C20-C19-C18 | 8.45 | 150.57 | 126.37 |
| 15 | B | 1236 | CLA | C1D-C2D-C3D | -8.44 | 98.70 | 106.97 |
| 15 | A | 1109 | CLA | C1D-C2D-C3D | -8.44 | 98.70 | 106.97 |
| 15 | A | 1102 | CLA | C1D-C2D-C3D | -8.43 | 98.71 | 106.97 |
| 15 | B | 1228 | CLA | C1D-C2D-C3D | -8.42 | 98.72 | 106.97 |
| 15 | A | 1012 | CLA | C1D-C2D-C3D | -8.40 | 98.74 | 106.97 |
| 15 | B | 1212 | CLA | C1D-C2D-C3D | -8.40 | 98.74 | 106.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1801 | CLA | C1D-C2D-C3D | -8.39 | 98.75 | 106.97 |
| 15 | A | 1131 | CLA | C1D-C2D-C3D | -8.39 | 98.75 | 106.97 |
| 15 | B | 1227 | CLA | C1D-C2D-C3D | -8.38 | 98.76 | 106.97 |
| 15 | F | 1410 | CLA | C1D-C2D-C3D | -8.38 | 98.76 | 106.97 |
| 15 | B | 1224 | CLA | C1D-C2D-C3D | -8.38 | 98.76 | 106.97 |
| 15 | A | 1104 | CLA | C1D-C2D-C3D | -8.37 | 98.77 | 106.97 |
| 15 | K | 1402 | CLA | C1D-C2D-C3D | -8.37 | 98.77 | 106.97 |
| 14 | A | 4008 | BCR | C20-C19-C18 | 8.35 | 150.30 | 126.37 |
| 15 | A | 1110 | CLA | C1D-C2D-C3D | -8.35 | 98.79 | 106.97 |
| 15 | J | 1303 | CLA | C1D-C2D-C3D | -8.35 | 98.79 | 106.97 |
| 14 | B | 4010 | BCR | C20-C19-C18 | 8.35 | 150.28 | 126.37 |
| 15 | B | 1238 | CLA | C1D-C2D-C3D | -8.33 | 98.81 | 106.97 |
| 15 | J | 1302 | CLA | C1D-C2D-C3D | -8.33 | 98.81 | 106.97 |
| 15 | B | 1234 | CLA | C1D-C2D-C3D | -8.33 | 98.81 | 106.97 |
| 15 | A | 1138 | CLA | C1D-C2D-C3D | -8.31 | 98.82 | 106.97 |
| 15 | B | 1202 | CLA | C1D-C2D-C3D | -8.31 | 98.82 | 106.97 |
| 15 | A | 1111 | CLA | C1D-C2D-C3D | -8.31 | 98.83 | 106.97 |
| 15 | A | 1106 | CLA | C1D-C2D-C3D | -8.31 | 98.83 | 106.97 |
| 15 | B | 1240 | CLA | C1D-C2D-C3D | -8.31 | 98.83 | 106.97 |
| 15 | B | 1232 | CLA | C1D-C2D-C3D | -8.30 | 98.84 | 106.97 |
| 13 | A | 1108 | CL0 | C1D-C2D-C3D | -8.30 | 98.84 | 106.97 |
| 15 | F | 1301 | CLA | C1D-C2D-C3D | -8.29 | 98.85 | 106.97 |
| 15 | B | 1221 | CLA | C1D-C2D-C3D | -8.28 | 98.85 | 106.97 |
| 15 | A | 1136 | CLA | C1D-C2D-C3D | -8.28 | 98.85 | 106.97 |
| 15 | B | 1203 | CLA | C1D-C2D-C3D | -8.28 | 98.86 | 106.97 |
| 15 | B | 1210 | CLA | C1D-C2D-C3D | -8.27 | 98.86 | 106.97 |
| 15 | B | 1207 | CLA | C1D-C2D-C3D | -8.27 | 98.87 | 106.97 |
| 15 | A | 1140 | CLA | C1D-C2D-C3D | -8.27 | 98.87 | 106.97 |
| 15 | A | 1115 | CLA | C1D-C2D-C3D | -8.26 | 98.87 | 106.97 |
| 15 | A | 1113 | CLA | C1D-C2D-C3D | -8.26 | 98.88 | 106.97 |
| 15 | A | 1126 | CLA | C1D-C2D-C3D | -8.25 | 98.89 | 106.97 |
| 15 | A | 1105 | CLA | C1D-C2D-C3D | -8.24 | 98.90 | 106.97 |
| 15 | B | 1226 | CLA | C1D-C2D-C3D | -8.23 | 98.90 | 106.97 |
| 15 | B | 1219 | CLA | C1D-C2D-C3D | -8.23 | 98.90 | 106.97 |
| 15 | A | 1114 | CLA | C1D-C2D-C3D | -8.23 | 98.91 | 106.97 |
| 15 | A | 1124 | CLA | C1D-C2D-C3D | -8.23 | 98.91 | 106.97 |
| 15 | B | 1215 | CLA | C1D-C2D-C3D | -8.21 | 98.93 | 106.97 |
| 15 | B | 1208 | CLA | C1D-C2D-C3D | -8.21 | 98.93 | 106.97 |
| 15 | K | 1401 | CLA | C1D-C2D-C3D | -8.20 | 98.93 | 106.97 |
| 15 | B | 1217 | CLA | C1D-C2D-C3D | -8.19 | 98.94 | 106.97 |
| 15 | F | 1139 | CLA | C1D-C2D-C3D | -8.17 | 98.97 | 106.97 |
| 15 | A | 1123 | CLA | C1D-C2D-C3D | -8.16 | 98.97 | 106.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1135 | CLA | C1D-C2D-C3D | -8.16 | 98.97 | 106.97 |
| 15 | A | 1117 | CLA | C1D-C2D-C3D | -8.16 | 98.98 | 106.97 |
| 15 | B | 1013 | CLA | C1D-C2D-C3D | -8.15 | 98.98 | 106.97 |
| 15 | B | 1023 | CLA | C1D-C2D-C3D | -8.15 | 98.99 | 106.97 |
| 15 | A | 1120 | CLA | C1D-C2D-C3D | -8.15 | 98.99 | 106.97 |
| 15 | B | 1206 | CLA | C1D-C2D-C3D | -8.13 | 99.00 | 106.97 |
| 15 | B | 1237 | CLA | C1D-C2D-C3D | -8.13 | 99.00 | 106.97 |
| 15 | A | 1121 | CLA | C1D-C2D-C3D | -8.12 | 99.01 | 106.97 |
| 15 | B | 1239 | CLA | C1D-C2D-C3D | -8.12 | 99.01 | 106.97 |
| 15 | A | 1022 | CLA | C1D-C2D-C3D | -8.12 | 99.01 | 106.97 |
| 15 | B | 1230 | CLA | C1D-C2D-C3D | -8.12 | 99.02 | 106.97 |
| 15 | B | 1213 | CLA | C1D-C2D-C3D | -8.12 | 99.02 | 106.97 |
| 15 | B | 1209 | CLA | C1D-C2D-C3D | -8.11 | 99.02 | 106.97 |
| 15 | A | 1122 | CLA | C1D-C2D-C3D | -8.11 | 99.02 | 106.97 |
| 15 | B | 1204 | CLA | C1D-C2D-C3D | -8.11 | 99.02 | 106.97 |
| 15 | A | 1130 | CLA | C1D-C2D-C3D | -8.10 | 99.03 | 106.97 |
| 15 | B | 1216 | CLA | C1D-C2D-C3D | -8.09 | 99.04 | 106.97 |
| 15 | A | 1112 | CLA | C1D-C2D-C3D | -8.08 | 99.05 | 106.97 |
| 15 | A | 1137 | CLA | C1D-C2D-C3D | -8.08 | 99.06 | 106.97 |
| 15 | A | 1119 | CLA | C1D-C2D-C3D | -8.08 | 99.06 | 106.97 |
| 15 | B | 1220 | CLA | C1D-C2D-C3D | -8.07 | 99.06 | 106.97 |
| 15 | A | 1133 | CLA | C1D-C2D-C3D | -8.07 | 99.07 | 106.97 |
| 15 | A | 1116 | CLA | C1D-C2D-C3D | -8.06 | 99.07 | 106.97 |
| 15 | A | 1103 | CLA | C1D-C2D-C3D | -8.04 | 99.09 | 106.97 |
| 15 | B | 1201 | CLA | C1D-C2D-C3D | -8.03 | 99.10 | 106.97 |
| 15 | B | 1214 | CLA | C1D-C2D-C3D | -8.02 | 99.11 | 106.97 |
| 15 | A | 1107 | CLA | C1D-C2D-C3D | -8.02 | 99.11 | 106.97 |
| 13 | A | 1011 | CL0 | C1D-C2D-C3D | -7.99 | 99.15 | 106.97 |
| 15 | B | 1218 | CLA | C1D-C2D-C3D | -7.98 | 99.15 | 106.97 |
| 15 | B | 1225 | CLA | C1D-C2D-C3D | -7.96 | 99.17 | 106.97 |
| 15 | A | 1101 | CLA | C1D-C2D-C3D | -7.91 | 99.22 | 106.97 |
| 15 | B | 1211 | CLA | C1D-C2D-C3D | -7.90 | 99.23 | 106.97 |
| 15 | A | 1128 | CLA | C1D-C2D-C3D | -7.90 | 99.23 | 106.97 |
| 14 | B | 4006 | BCR | C20-C19-C18 | 7.89 | 148.96 | 126.37 |
| 15 | B | 1021 | CLA | C1D-C2D-C3D | -7.87 | 99.26 | 106.97 |
| 14 | J | 4013 | BCR | C20-C19-C18 | 7.85 | 148.86 | 126.37 |
| 15 | A | 1126 | CLA | CMD-C2D-C1D | 7.81 | 141.59 | 126.16 |
| 15 | A | 1127 | CLA | C1D-C2D-C3D | -7.79 | 99.33 | 106.97 |
| 14 | B | 4011 | BCR | C20-C19-C18 | 7.79 | 148.69 | 126.37 |
| 15 | B | 1205 | CLA | C1D-C2D-C3D | -7.78 | 99.35 | 106.97 |
| 15 | B | 1215 | CLA | C2C-C1C-NC | 7.72 | 116.45 | 110.22 |
| 15 | B | 1239 | CLA | C2C-C1C-NC | 7.71 | 116.45 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 13 | A | 1011 | CL0 | C2C-C1C-NC | 7.63 | 116.38 | 110.22 |
| 15 | A | 1135 | CLA | C2C-C1C-NC | 7.58 | 116.35 | 110.22 |
| 15 | B | 1207 | CLA | C2C-C1C-NC | 7.57 | 116.33 | 110.22 |
| 15 | B | 1203 | CLA | C2C-C1C-NC | 7.56 | 116.33 | 110.22 |
| 15 | A | 1131 | CLA | C2C-C1C-NC | 7.56 | 116.32 | 110.22 |
| 15 | A | 1128 | CLA | C2C-C1C-NC | 7.52 | 116.30 | 110.22 |
| 15 | A | 1123 | CLA | C2C-C1C-NC | 7.49 | 116.27 | 110.22 |
| 15 | A | 1136 | CLA | C2C-C1C-NC | 7.48 | 116.26 | 110.22 |
| 15 | A | 1137 | CLA | C2C-C1C-NC | 7.45 | 116.24 | 110.22 |
| 14 | F | 4015 | BCR | C20-C19-C18 | 7.44 | 147.67 | 126.37 |
| 15 | B | 1231 | CLA | C2C-C1C-NC | 7.44 | 116.23 | 110.22 |
| 15 | A | 1801 | CLA | C2C-C1C-NC | 7.42 | 116.21 | 110.22 |
| 15 | A | 1133 | CLA | C2C-C1C-NC | 7.42 | 116.21 | 110.22 |
| 15 | B | 1232 | CLA | C2C-C1C-NC | 7.42 | 116.21 | 110.22 |
| 15 | J | 1302 | CLA | C2C-C1C-NC | 7.40 | 116.20 | 110.22 |
| 15 | B | 1209 | CLA | C2C-C1C-NC | 7.37 | 116.17 | 110.22 |
| 15 | A | 1120 | CLA | C2C-C1C-NC | 7.34 | 116.15 | 110.22 |
| 15 | B | 1221 | CLA | C2C-C1C-NC | 7.33 | 116.14 | 110.22 |
| 15 | A | 1113 | CLA | C2C-C1C-NC | 7.33 | 116.14 | 110.22 |
| 15 | A | 1105 | CLA | C2C-C1C-NC | 7.32 | 116.13 | 110.22 |
| 15 | B | 1227 | CLA | C2C-C1C-NC | 7.31 | 116.13 | 110.22 |
| 15 | B | 1205 | CLA | C2C-C1C-NC | 7.31 | 116.12 | 110.22 |
| 15 | A | 1012 | CLA | C2C-C1C-NC | 7.28 | 116.10 | 110.22 |
| 15 | B | 1204 | CLA | C2C-C1C-NC | 7.27 | 116.09 | 110.22 |
| 15 | J | 1303 | CLA | C2C-C1C-NC | 7.26 | 116.08 | 110.22 |
| 15 | B | 1222 | CLA | C2C-C1C-NC | 7.22 | 116.05 | 110.22 |
| 15 | A | 1110 | CLA | C2C-C1C-NC | 7.21 | 116.05 | 110.22 |
| 15 | B | 1225 | CLA | C2C-C1C-NC | 7.21 | 116.04 | 110.22 |
| 15 | A | 1114 | CLA | C2C-C1C-NC | 7.20 | 116.04 | 110.22 |
| 15 | B | 1226 | CLA | C2C-C1C-NC | 7.20 | 116.04 | 110.22 |
| 14 | B | 4014 | BCR | C20-C19-C18 | 7.19 | 146.97 | 126.37 |
| 15 | A | 1116 | CLA | C2C-C1C-NC | 7.19 | 116.03 | 110.22 |
| 15 | A | 1127 | CLA | C2C-C1C-NC | 7.19 | 116.03 | 110.22 |
| 15 | K | 1402 | CLA | C2C-C1C-NC | 7.18 | 116.02 | 110.22 |
| 15 | B | 1238 | CLA | C2C-C1C-NC | 7.18 | 116.02 | 110.22 |
| 15 | A | 1129 | CLA | CMD-C2D-C1D | 7.18 | 140.35 | 126.16 |
| 15 | A | 1121 | CLA | C2C-C1C-NC | 7.16 | 116.00 | 110.22 |
| 15 | A | 1122 | CLA | CMD-C2D-C1D | 7.14 | 140.27 | 126.16 |
| 15 | A | 1129 | CLA | C2C-C1C-NC | 7.14 | 115.99 | 110.22 |
| 15 | B | 1234 | CLA | C2C-C1C-NC | 7.13 | 115.98 | 110.22 |
| 15 | K | 1401 | CLA | C2C-C1C-NC | 7.10 | 115.96 | 110.22 |
| 15 | A | 1118 | CLA | C2C-C1C-NC | 7.09 | 115.95 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15 | A | 1124 | CLA | C2C-C1C-NC | 7.09 | 115.94 | 110.22 |
| 15 | B | 1206 | CLA | C2C-C1C-NC | 7.09 | 115.94 | 110.22 |
| 15 | A | 1022 | CLA | C2C-C1C-NC | 7.06 | 115.92 | 110.22 |
| 15 | B | 1229 | CLA | C2C-C1C-NC | 7.03 | 115.90 | 110.22 |
| 15 | B | 1217 | CLA | C2C-C1C-NC | 7.02 | 115.89 | 110.22 |
| 15 | B | 1212 | CLA | C2C-C1C-NC | 7.02 | 115.89 | 110.22 |
| 15 | A | 1126 | CLA | C2B-C1B-NB | 7.02 | 114.19 | 109.50 |
| 15 | B | 1201 | CLA | C2C-C1C-NC | 7.00 | 115.88 | 110.22 |
| 15 | B | 1216 | CLA | C2C-C1C-NC | 7.00 | 115.88 | 110.22 |
| 15 | B | 1224 | CLA | C2C-C1C-NC | 7.00 | 115.88 | 110.22 |
| 15 | B | 1219 | CLA | C2C-C1C-NC | 7.00 | 115.87 | 110.22 |
| 15 | B | 1218 | CLA | C2C-C1C-NC | 6.99 | 115.87 | 110.22 |
| 13 | A | 1108 | CL0 | C2C-C1C-NC | 6.99 | 115.87 | 110.22 |
| 15 | F | 1139 | CLA | C2C-C1C-NC | 6.99 | 115.86 | 110.22 |
| 15 | B | 1237 | CLA | C2C-C1C-NC | 6.99 | 115.86 | 110.22 |
| 15 | B | 1023 | CLA | C2C-C1C-NC | 6.97 | 115.85 | 110.22 |
| 15 | A | 1134 | CLA | C2C-C1C-NC | 6.96 | 115.84 | 110.22 |
| 15 | F | 1410 | CLA | C2C-C1C-NC | 6.96 | 115.84 | 110.22 |
| 15 | B | 1208 | CLA | C2C-C1C-NC | 6.94 | 115.83 | 110.22 |
| 15 | A | 1124 | CLA | C2B-C1B-NB | 6.93 | 114.13 | 109.50 |
| 15 | B | 1240 | CLA | C2C-C1C-NC | 6.93 | 115.81 | 110.22 |
| 15 | A | 1107 | CLA | CMD-C2D-C1D | 6.92 | 139.84 | 126.16 |
| 15 | B | 1021 | CLA | C2C-C1C-NC | 6.92 | 115.81 | 110.22 |
| 15 | B | 1237 | CLA | CMD-C2D-C1D | 6.91 | 139.81 | 126.16 |
| 15 | B | 1202 | CLA | C2C-C1C-NC | 6.90 | 115.79 | 110.22 |
| 15 | A | 1138 | CLA | C2B-C1B-NB | 6.90 | 114.11 | 109.50 |
| 15 | B | 1231 | CLA | CMD-C2D-C1D | 6.88 | 139.76 | 126.16 |
| 15 | A | 1119 | CLA | C2C-C1C-NC | 6.87 | 115.77 | 110.22 |
| 15 | A | 1112 | CLA | C2C-C1C-NC | 6.86 | 115.76 | 110.22 |
| 15 | B | 1230 | CLA | C2C-C1C-NC | 6.86 | 115.76 | 110.22 |
| 15 | A | 1132 | CLA | C2C-C1C-NC | 6.85 | 115.76 | 110.22 |
| 15 | B | 1013 | CLA | O2A-C1-C2 | 6.83 | 123.76 | 108.12 |
| 15 | A | 1102 | CLA | C2C-C1C-NC | 6.81 | 115.72 | 110.22 |
| 15 | B | 1213 | CLA | C2C-C1C-NC | 6.79 | 115.70 | 110.22 |
| 15 | A | 1106 | CLA | C2C-C1C-NC | 6.79 | 115.70 | 110.22 |
| 14 | A | 4003 | BCR | C20-C19-C18 | 6.77 | 145.77 | 126.37 |
| 15 | B | 1230 | CLA | CMD-C2D-C1D | 6.77 | 139.54 | 126.16 |
| 15 | A | 1120 | CLA | CMD-C2D-C1D | 6.77 | 139.54 | 126.16 |
| 15 | A | 1102 | CLA | C2B-C1B-NB | 6.77 | 114.02 | 109.50 |
| 15 | B | 1224 | CLA | CMD-C2D-C1D | 6.76 | 139.52 | 126.16 |
| 15 | F | 1301 | CLA | C2C-C1C-NC | 6.74 | 115.66 | 110.22 |
| 15 | B | 1204 | CLA | CMD-C2D-C1D | 6.73 | 139.47 | 126.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15 | B | 1239 | CLA | CMD-C2D-C1D | 6.73 | 139.46 | 126.16 |
| 15 | B | 1206 | CLA | CMD-C2D-C1D | 6.72 | 139.45 | 126.16 |
| 15 | B | 1214 | CLA | C2B-C1B-NB | 6.72 | 113.99 | 109.50 |
| 15 | A | 1115 | CLA | C2C-C1C-NC | 6.71 | 115.64 | 110.22 |
| 15 | A | 1130 | CLA | C2B-C1B-NB | 6.71 | 113.98 | 109.50 |
| 15 | B | 1223 | CLA | C2C-C1C-NC | 6.71 | 115.64 | 110.22 |
| 15 | A | 1134 | CLA | CMD-C2D-C1D | 6.70 | 139.40 | 126.16 |
| 15 | A | 1125 | CLA | CMD-C2D-C1D | 6.69 | 139.39 | 126.16 |
| 15 | B | 1203 | CLA | CMD-C2D-C1D | 6.67 | 139.34 | 126.16 |
| 15 | A | 1106 | CLA | C2B-C1B-NB | 6.67 | 113.95 | 109.50 |
| 15 | B | 1214 | CLA | C2C-C1C-NC | 6.66 | 115.60 | 110.22 |
| 15 | K | 1401 | CLA | CMD-C2D-C1D | 6.66 | 139.32 | 126.16 |
| 15 | B | 1210 | CLA | C2B-C1B-NB | 6.65 | 113.94 | 109.50 |
| 13 | A | 1108 | CL0 | CMD-C2D-C1D | 6.64 | 139.29 | 126.16 |
| 15 | A | 1117 | CLA | C2C-C1C-NC | 6.64 | 115.58 | 110.22 |
| 15 | B | 1228 | CLA | CMD-C2D-C1D | 6.64 | 139.28 | 126.16 |
| 15 | B | 1211 | CLA | C2C-C1C-NC | 6.64 | 115.58 | 110.22 |
| 15 | A | 1104 | CLA | C2C-C1C-NC | 6.63 | 115.58 | 110.22 |
| 15 | B | 1209 | CLA | CMD-C2D-C1D | 6.63 | 139.26 | 126.16 |
| 15 | A | 1103 | CLA | CMD-C2D-C1D | 6.61 | 139.22 | 126.16 |
| 15 | A | 1123 | CLA | CMD-C2D-C1D | 6.60 | 139.21 | 126.16 |
| 15 | A | 1109 | CLA | CMD-C2D-C1D | 6.60 | 139.21 | 126.16 |
| 15 | F | 1139 | CLA | CMD-C2D-C1D | 6.60 | 139.20 | 126.16 |
| 15 | A | 1130 | CLA | CMD-C2D-C1D | 6.59 | 139.19 | 126.16 |
| 14 | B | 4009 | BCR | C20-C19-C18 | 6.57 | 145.19 | 126.37 |
| 14 | B | 4017 | BCR | C20-C19-C18 | 6.57 | 145.18 | 126.37 |
| 15 | B | 1227 | CLA | CMD-C2D-C1D | 6.57 | 139.14 | 126.16 |
| 15 | B | 1013 | CLA | C2B-C1B-NB | 6.57 | 113.89 | 109.50 |
| 15 | A | 1012 | CLA | O2A-C1-C2 | 6.56 | 123.15 | 108.12 |
| 15 | A | 1114 | CLA | CMD-C2D-C1D | 6.56 | 139.13 | 126.16 |
| 15 | B | 1215 | CLA | O2A-C1-C2 | 6.56 | 123.14 | 108.12 |
| 14 | A | 4002 | BCR | C20-C19-C18 | 6.56 | 145.15 | 126.37 |
| 15 | J | 1303 | CLA | CMD-C2D-C1D | 6.55 | 139.11 | 126.16 |
| 14 | A | 4012 | BCR | C20-C19-C18 | 6.54 | 145.10 | 126.37 |
| 14 | B | 4005 | BCR | C20-C19-C18 | 6.54 | 145.09 | 126.37 |
| 15 | B | 1236 | CLA | CMD-C2D-C1D | 6.54 | 139.08 | 126.16 |
| 15 | B | 1013 | CLA | C2C-C1C-NC | 6.54 | 115.50 | 110.22 |
| 15 | A | 1113 | CLA | CMD-C2D-C1D | 6.53 | 139.07 | 126.16 |
| 15 | B | 1222 | CLA | C2B-C1B-NB | 6.53 | 113.86 | 109.50 |
| 15 | A | 1111 | CLA | C2C-C1C-NC | 6.52 | 115.49 | 110.22 |
| 15 | B | 1210 | CLA | C2C-C1C-NC | 6.52 | 115.49 | 110.22 |
| 15 | B | 1219 | CLA | CMD-C2D-C1D | 6.52 | 139.05 | 126.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15 | K | 1402 | CLA | CMD-C2D-C1D | 6.52 | 139.05 | 126.16 |
| 15 | B | 1220 | CLA | C2C-C1C-NC | 6.51 | 115.48 | 110.22 |
| 15 | B | 1213 | CLA | CMD-C2D-C1D | 6.51 | 139.02 | 126.16 |
| 15 | A | 1136 | CLA | CMD-C2D-C1D | 6.50 | 139.01 | 126.16 |
| 15 | B | 1207 | CLA | CMD-C2D-C1D | 6.50 | 139.00 | 126.16 |
| 15 | A | 1106 | CLA | CMD-C2D-C1D | 6.50 | 139.00 | 126.16 |
| 15 | B | 1208 | CLA | CMD-C2D-C1D | 6.48 | 138.97 | 126.16 |
| 15 | A | 1104 | CLA | CMD-C2D-C1D | 6.48 | 138.96 | 126.16 |
| 15 | J | 1302 | CLA | CMD-C2D-C1D | 6.47 | 138.96 | 126.16 |
| 15 | A | 1801 | CLA | CMD-C2D-C1D | 6.47 | 138.94 | 126.16 |
| 15 | B | 1219 | CLA | C2B-C1B-NB | 6.46 | 113.82 | 109.50 |
| 15 | A | 1105 | CLA | CMD-C2D-C1D | 6.46 | 138.93 | 126.16 |
| 15 | A | 1116 | CLA | CMD-C2D-C1D | 6.46 | 138.93 | 126.16 |
| 15 | A | 1130 | CLA | C2C-C1C-NC | 6.45 | 115.43 | 110.22 |
| 15 | A | 1140 | CLA | C2C-C1C-NC | 6.45 | 115.43 | 110.22 |
| 15 | A | 1110 | CLA | CMD-C2D-C1D | 6.45 | 138.91 | 126.16 |
| 15 | A | 1101 | CLA | C2C-C1C-NC | 6.45 | 115.43 | 110.22 |
| 15 | B | 1202 | CLA | CMD-C2D-C1D | 6.45 | 138.90 | 126.16 |
| 15 | B | 1234 | CLA | CMD-C2D-C1D | 6.45 | 138.90 | 126.16 |
| 15 | F | 1410 | CLA | CMD-C2D-C1D | 6.44 | 138.88 | 126.16 |
| 15 | B | 1216 | CLA | CMD-C2D-C1D | 6.44 | 138.88 | 126.16 |
| 15 | A | 1104 | CLA | C2B-C1B-NB | 6.42 | 113.79 | 109.50 |
| 15 | A | 1131 | CLA | CMD-C2D-C1D | 6.42 | 138.85 | 126.16 |
| 15 | B | 1214 | CLA | CMD-C2D-C1D | 6.42 | 138.84 | 126.16 |
| 15 | B | 1226 | CLA | CMD-C2D-C1D | 6.42 | 138.84 | 126.16 |
| 15 | A | 1124 | CLA | CMD-C2D-C1D | 6.41 | 138.83 | 126.16 |
| 15 | B | 1236 | CLA | C2B-C1B-NB | 6.41 | 113.78 | 109.50 |
| 15 | A | 1121 | CLA | CMD-C2D-C1D | 6.41 | 138.82 | 126.16 |
| 15 | A | 1103 | CLA | C2C-C1C-NC | 6.40 | 115.39 | 110.22 |
| 15 | B | 1240 | CLA | CMD-C2D-C1D | 6.39 | 138.79 | 126.16 |
| 14 | A | 4001 | BCR | C20-C19-C18 | 6.39 | 144.66 | 126.37 |
| 15 | B | 1206 | CLA | C2B-C1B-NB | 6.38 | 113.76 | 109.50 |
| 15 | B | 1235 | CLA | C2C-C1C-NC | 6.38 | 115.37 | 110.22 |
| 15 | A | 1140 | CLA | CMD-C2D-C1D | 6.37 | 138.75 | 126.16 |
| 15 | A | 1111 | CLA | CMD-C2D-C1D | 6.37 | 138.74 | 126.16 |
| 15 | A | 1118 | CLA | CMD-C2D-C1D | 6.36 | 138.74 | 126.16 |
| 15 | A | 1112 | CLA | CMD-C2D-C1D | 6.35 | 138.71 | 126.16 |
| 15 | A | 1133 | CLA | CMD-C2D-C1D | 6.35 | 138.71 | 126.16 |
| 15 | B | 1223 | CLA | CMD-C2D-C1D | 6.35 | 138.70 | 126.16 |
| 15 | B | 1203 | CLA | O2A-C1-C2 | 6.35 | 122.65 | 108.12 |
| 15 | A | 1135 | CLA | CMD-C2D-C1D | 6.33 | 138.68 | 126.16 |
| 15 | A | 1109 | CLA | C2C-C1C-NC | 6.33 | 115.33 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1210 | CLA | CMD-C2D-C1D | 6.33 | 138.66 | 126.16 |
| 15 | A | 1137 | CLA | CMD-C2D-C1D | 6.32 | 138.65 | 126.16 |
| 13 | A | 1011 | CL0 | CMD-C2D-C1D | 6.31 | 138.64 | 126.16 |
| 15 | B | 1228 | CLA | C2C-C1C-NC | 6.30 | 115.31 | 110.22 |
| 15 | F | 1301 | CLA | C2B-C1B-NB | 6.30 | 113.70 | 109.50 |
| 15 | A | 1122 | CLA | C2C-C1C-NC | 6.29 | 115.30 | 110.22 |
| 15 | A | 1101 | CLA | CAA-C2A-C3A | -6.29 | 97.58 | 113.32 |
| 15 | A | 1117 | CLA | C2B-C1B-NB | 6.28 | 113.69 | 109.50 |
| 15 | B | 1021 | CLA | CMD-C2D-C1D | 6.28 | 138.57 | 126.16 |
| 15 | B | 1229 | CLA | CMD-C2D-C1D | 6.28 | 138.57 | 126.16 |
| 15 | B | 1225 | CLA | CMD-C2D-C1D | 6.27 | 138.55 | 126.16 |
| 15 | B | 1218 | CLA | CMD-C2D-C1D | 6.27 | 138.55 | 126.16 |
| 15 | A | 1107 | CLA | C2B-C1B-NB | 6.26 | 113.68 | 109.50 |
| 15 | A | 1132 | CLA | CMD-C2D-C1D | 6.25 | 138.51 | 126.16 |
| 15 | B | 1201 | CLA | CMD-C2D-C1D | 6.25 | 138.50 | 126.16 |
| 15 | B | 1238 | CLA | CMD-C2D-C1D | 6.24 | 138.50 | 126.16 |
| 15 | A | 1119 | CLA | CMD-C2D-C1D | 6.22 | 138.45 | 126.16 |
| 15 | B | 1220 | CLA | C2B-C1B-NB | 6.21 | 113.65 | 109.50 |
| 15 | B | 1215 | CLA | CMD-C2D-C1D | 6.21 | 138.43 | 126.16 |
| 15 | A | 1107 | CLA | C2C-C1C-NC | 6.20 | 115.23 | 110.22 |
| 14 | B | 4004 | BCR | C20-C19-C18 | 6.20 | 144.12 | 126.37 |
| 15 | A | 1105 | CLA | C3B-CAB-CBB | -6.19 | 113.12 | 125.95 |
| 15 | B | 1023 | CLA | CMD-C2D-C1D | 6.19 | 138.40 | 126.16 |
| 15 | B | 1211 | CLA | CMD-C2D-C1D | 6.18 | 138.38 | 126.16 |
| 15 | A | 1127 | CLA | CMD-C2D-C1D | 6.18 | 138.37 | 126.16 |
| 15 | A | 1110 | CLA | C2B-C1B-NB | 6.18 | 113.62 | 109.50 |
| 15 | B | 1212 | CLA | CMD-C2D-C1D | 6.17 | 138.36 | 126.16 |
| 15 | A | 1119 | CLA | C2B-C1B-NB | 6.17 | 113.62 | 109.50 |
| 15 | A | 1122 | CLA | C2B-C1B-NB | 6.16 | 113.62 | 109.50 |
| 15 | B | 1217 | CLA | CMD-C2D-C1D | 6.16 | 138.33 | 126.16 |
| 15 | B | 1232 | CLA | CMD-C2D-C1D | 6.15 | 138.32 | 126.16 |
| 15 | A | 1112 | CLA | C2B-C1B-NB | 6.15 | 113.61 | 109.50 |
| 15 | A | 1101 | CLA | C2B-C1B-NB | 6.14 | 113.60 | 109.50 |
| 15 | A | 1115 | CLA | CMD-C2D-C1D | 6.14 | 138.30 | 126.16 |
| 15 | A | 1117 | CLA | CMD-C2D-C1D | 6.14 | 138.29 | 126.16 |
| 15 | B | 1235 | CLA | CMD-C2D-C1D | 6.14 | 138.29 | 126.16 |
| 15 | A | 1111 | CLA | C2B-C1B-NB | 6.11 | 113.58 | 109.50 |
| 15 | A | 1109 | CLA | C2B-C1B-NB | 6.10 | 113.57 | 109.50 |
| 15 | A | 1101 | CLA | CMD-C2D-C1D | 6.09 | 138.19 | 126.16 |
| 15 | B | 1240 | CLA | C2B-C1B-NB | 6.09 | 113.56 | 109.50 |
| 15 | B | 1236 | CLA | C2C-C1C-NC | 6.08 | 115.14 | 110.22 |
| 15 | B | 1201 | CLA | C2B-C1B-NB | 6.07 | 113.55 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 4009 | BCR | C15-C14-C13 | -6.06 | 118.53 | 127.29 |
| 15 | B | 1220 | CLA | O2A-C1-C2 | 6.06 | 121.99 | 108.12 |
| 15 | A | 1138 | CLA | CMD-C2D-C1D | 6.06 | 138.13 | 126.16 |
| 15 | B | 1220 | CLA | CMD-C2D-C1D | 6.04 | 138.10 | 126.16 |
| 15 | B | 1208 | CLA | C2B-C1B-NB | 6.04 | 113.53 | 109.50 |
| 15 | A | 1102 | CLA | CMD-C2D-C1D | 6.04 | 138.09 | 126.16 |
| 15 | A | 1125 | CLA | C2B-C1B-NB | 6.03 | 113.53 | 109.50 |
| 15 | A | 1135 | CLA | O2A-C1-C2 | 6.03 | 121.93 | 108.12 |
| 15 | A | 1124 | CLA | O2A-C1-C2 | 6.02 | 121.92 | 108.12 |
| 15 | F | 1410 | CLA | C2B-C1B-NB | 6.01 | 113.51 | 109.50 |
| 15 | B | 1218 | CLA | O2A-C1-C2 | 6.00 | 121.86 | 108.12 |
| 15 | B | 1228 | CLA | C2B-C1B-NB | 6.00 | 113.51 | 109.50 |
| 15 | A | 1127 | CLA | O2A-C1-C2 | 5.98 | 121.82 | 108.12 |
| 15 | A | 1125 | CLA | C2C-C1C-NC | 5.98 | 115.05 | 110.22 |
| 15 | F | 1301 | CLA | CMD-C2D-C1D | 5.98 | 137.98 | 126.16 |
| 15 | A | 1126 | CLA | C2C-C1C-NC | 5.98 | 115.05 | 110.22 |
| 15 | A | 1022 | CLA | C2B-C1B-NB | 5.97 | 113.49 | 109.50 |
| 13 | A | 1011 | CL0 | C2B-C1B-NB | 5.96 | 113.48 | 109.50 |
| 15 | A | 1105 | CLA | O2A-C1-C2 | 5.95 | 121.75 | 108.12 |
| 15 | B | 1224 | CLA | C2B-C1B-NB | 5.95 | 113.47 | 109.50 |
| 15 | B | 1222 | CLA | O2D-CGD-CBD | 5.95 | 123.35 | 111.34 |
| 15 | A | 1105 | CLA | C2B-C1B-NB | 5.94 | 113.47 | 109.50 |
| 15 | B | 1227 | CLA | C2B-C1B-NB | 5.94 | 113.47 | 109.50 |
| 15 | B | 1222 | CLA | CMD-C2D-C1D | 5.93 | 137.87 | 126.16 |
| 15 | B | 1230 | CLA | C4-C3-C5 | 5.91 | 124.37 | 115.39 |
| 15 | A | 1801 | CLA | C2B-C1B-NB | 5.90 | 113.44 | 109.50 |
| 15 | K | 1401 | CLA | C2B-C1B-NB | 5.89 | 113.44 | 109.50 |
| 15 | B | 1217 | CLA | C2B-C1B-NB | 5.89 | 113.43 | 109.50 |
| 15 | B | 1231 | CLA | C2B-C1B-NB | 5.89 | 113.43 | 109.50 |
| 15 | A | 1128 | CLA | CMD-C2D-C1D | 5.89 | 137.80 | 126.16 |
| 15 | B | 1221 | CLA | CMD-C2D-C1D | 5.87 | 137.77 | 126.16 |
| 15 | B | 1216 | CLA | C2B-C1B-NB | 5.87 | 113.42 | 109.50 |
| 15 | B | 1013 | CLA | CMD-C2D-C1D | 5.87 | 137.76 | 126.16 |
| 15 | B | 1205 | CLA | O2D-CGD-CBD | 5.86 | 123.18 | 111.34 |
| 15 | A | 1110 | CLA | O2A-C1-C2 | 5.84 | 121.49 | 108.12 |
| 15 | B | 1223 | CLA | C2B-C1B-NB | 5.84 | 113.40 | 109.50 |
| 15 | B | 1239 | CLA | O2A-CGA-O1A | -5.83 | 110.21 | 122.93 |
| 15 | B | 1213 | CLA | C2B-C1B-NB | 5.82 | 113.39 | 109.50 |
| 15 | A | 1012 | CLA | C2B-C1B-NB | 5.82 | 113.39 | 109.50 |
| 15 | B | 1226 | CLA | O2D-CGD-CBD | 5.81 | 123.08 | 111.34 |
| 15 | B | 1202 | CLA | C2B-C1B-NB | 5.81 | 113.38 | 109.50 |
| 15 | B | 1231 | CLA | O2A-C1-C2 | 5.80 | 121.41 | 108.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1234 | CLA | O2A-C1-C2 | 5.80 | 121.40 | 108.12 |
| 15 | A | 1109 | CLA | O2A-C1-C2 | 5.79 | 121.37 | 108.12 |
| 15 | B | 1237 | CLA | C2B-C1B-NB | 5.78 | 113.36 | 109.50 |
| 15 | A | 1120 | CLA | C2B-C1B-NB | 5.77 | 113.36 | 109.50 |
| 15 | A | 1121 | CLA | O2A-CGA-O1A | -5.77 | 110.35 | 122.93 |
| 15 | B | 1225 | CLA | C2B-C1B-NB | 5.76 | 113.35 | 109.50 |
| 15 | B | 1238 | CLA | C2B-C1B-NB | 5.75 | 113.34 | 109.50 |
| 15 | B | 1212 | CLA | C2B-C1B-NB | 5.73 | 113.33 | 109.50 |
| 15 | A | 1117 | CLA | O2A-C1-C2 | 5.73 | 121.24 | 108.12 |
| 15 | B | 1023 | CLA | C2B-C1B-NB | 5.73 | 113.32 | 109.50 |
| 15 | B | 1209 | CLA | C2B-C1B-NB | 5.71 | 113.32 | 109.50 |
| 15 | B | 1213 | CLA | O2A-C1-C2 | 5.70 | 121.16 | 108.12 |
| 15 | B | 1215 | CLA | C2B-C1B-NB | 5.69 | 113.30 | 109.50 |
| 15 | B | 1226 | CLA | O2A-C1-C2 | 5.68 | 121.13 | 108.12 |
| 15 | A | 1134 | CLA | C2B-C1B-NB | 5.67 | 113.29 | 109.50 |
| 15 | B | 1219 | CLA | O2A-C1-C2 | 5.67 | 121.10 | 108.12 |
| 15 | B | 1203 | CLA | C2B-C1B-NB | 5.67 | 113.28 | 109.50 |
| 15 | B | 1205 | CLA | CMD-C2D-C1D | 5.64 | 137.31 | 126.16 |
| 15 | A | 1140 | CLA | C2B-C1B-NB | 5.63 | 113.26 | 109.50 |
| 15 | A | 1106 | CLA | O2D-CGD-CBD | 5.63 | 122.71 | 111.34 |
| 15 | B | 1218 | CLA | C2B-C1B-NB | 5.62 | 113.25 | 109.50 |
| 15 | A | 1113 | CLA | C2B-C1B-NB | 5.62 | 113.25 | 109.50 |
| 15 | A | 1022 | CLA | CMD-C2D-C1D | 5.61 | 137.25 | 126.16 |
| 15 | A | 1106 | CLA | O2A-C1-C2 | 5.61 | 120.97 | 108.12 |
| 15 | F | 1410 | CLA | C4-C3-C5 | 5.60 | 123.90 | 115.39 |
| 14 | J | 4013 | BCR | C7-C8-C9 | -5.60 | 117.84 | 126.22 |
| 15 | B | 1204 | CLA | C2B-C1B-NB | 5.59 | 113.23 | 109.50 |
| 15 | A | 1116 | CLA | C2B-C1B-NB | 5.58 | 113.23 | 109.50 |
| 14 | B | 4011 | BCR | C34-C9-C10 | -5.58 | 114.98 | 122.92 |
| 15 | B | 1204 | CLA | O2A-CGA-O1A | -5.57 | 110.77 | 122.93 |
| 15 | B | 1229 | CLA | C2D-C1D-ND | 5.56 | 115.91 | 109.56 |
| 15 | B | 1234 | CLA | C2B-C1B-NB | 5.56 | 113.21 | 109.50 |
| 15 | A | 1128 | CLA | C2B-C1B-NB | 5.55 | 113.20 | 109.50 |
| 13 | A | 1011 | CL0 | O2A-C1-C2 | 5.54 | 120.82 | 108.12 |
| 15 | B | 1211 | CLA | C2B-C1B-NB | 5.53 | 113.19 | 109.50 |
| 15 | B | 1235 | CLA | C2D-C1D-ND | 5.53 | 115.87 | 109.56 |
| 15 | A | 1121 | CLA | C2B-C1B-NB | 5.52 | 113.19 | 109.50 |
| 15 | B | 1235 | CLA | C2B-C1B-NB | 5.51 | 113.18 | 109.50 |
| 15 | J | 1303 | CLA | O2A-CGA-O1A | -5.51 | 110.91 | 122.93 |
| 15 | B | 1021 | CLA | C2B-C1B-NB | 5.51 | 113.18 | 109.50 |
| 15 | A | 1131 | CLA | O2A-C1-C2 | 5.51 | 120.74 | 108.12 |
| 15 | B | 1232 | CLA | C2B-C1B-NB | 5.51 | 113.18 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1128 | CLA | O2D-CGD-CBD | 5.50 | 122.46 | 111.34 |
| 15 | A | 1115 | CLA | O2A-CGA-O1A | -5.50 | 110.93 | 122.93 |
| 15 | A | 1125 | CLA | C2D-C1D-ND | 5.48 | 115.81 | 109.56 |
| 15 | B | 1223 | CLA | O2A-C1-C2 | 5.48 | 120.67 | 108.12 |
| 15 | B | 1201 | CLA | O2A-CGA-O1A | -5.48 | 110.99 | 122.93 |
| 15 | A | 1133 | CLA | O2A-CGA-O1A | -5.47 | 110.99 | 122.93 |
| 15 | A | 1103 | CLA | C2B-C1B-NB | 5.47 | 113.15 | 109.50 |
| 15 | K | 1401 | CLA | O2A-CGA-O1A | -5.45 | 111.03 | 122.93 |
| 15 | B | 1211 | CLA | O2A-CGA-O1A | -5.45 | 111.04 | 122.93 |
| 15 | B | 1013 | CLA | C3B-CAB-CBB | -5.45 | 114.67 | 125.95 |
| 15 | B | 1207 | CLA | O2A-CGA-O1A | -5.44 | 111.06 | 122.93 |
| 15 | A | 1118 | CLA | O2A-CGA-O1A | -5.44 | 111.07 | 122.93 |
| 15 | A | 1135 | CLA | C2B-C1B-NB | 5.44 | 113.13 | 109.50 |
| 15 | F | 1139 | CLA | C2B-C1B-NB | 5.43 | 113.13 | 109.50 |
| 15 | A | 1109 | CLA | C4-C3-C5 | 5.43 | 123.63 | 115.39 |
| 15 | B | 1229 | CLA | C2B-C1B-NB | 5.43 | 113.12 | 109.50 |
| 15 | A | 1111 | CLA | O2A-C1-C2 | 5.42 | 120.54 | 108.12 |
| 15 | A | 1123 | CLA | O2D-CGD-CBD | 5.40 | 122.25 | 111.34 |
| 15 | A | 1129 | CLA | O2A-CGA-O1A | -5.40 | 111.15 | 122.93 |
| 15 | K | 1402 | CLA | O2A-CGA-O1A | -5.38 | 111.19 | 122.93 |
| 15 | A | 1105 | CLA | C3B-C2B-C1B | -5.38 | 100.73 | 106.69 |
| 15 | B | 1201 | CLA | O2D-CGD-CBD | 5.36 | 122.17 | 111.34 |
| 15 | A | 1118 | CLA | C2D-C1D-ND | 5.34 | 115.65 | 109.56 |
| 15 | A | 1138 | CLA | C2C-C1C-NC | 5.34 | 114.53 | 110.22 |
| 15 | B | 1207 | CLA | C2B-C1B-NB | 5.34 | 113.06 | 109.50 |
| 15 | B | 1225 | CLA | C4-C3-C5 | 5.33 | 123.49 | 115.39 |
| 15 | A | 1101 | CLA | O2D-CGD-CBD | 5.33 | 122.10 | 111.34 |
| 15 | A | 1114 | CLA | C2B-C1B-NB | 5.32 | 113.05 | 109.50 |
| 15 | A | 1120 | CLA | O2A-C1-C2 | 5.32 | 120.29 | 108.12 |
| 15 | A | 1118 | CLA | C2B-C1B-NB | 5.31 | 113.05 | 109.50 |
| 15 | J | 1303 | CLA | C2B-C1B-NB | 5.31 | 113.05 | 109.50 |
| 15 | A | 1132 | CLA | C2D-C1D-ND | 5.31 | 115.62 | 109.56 |
| 15 | A | 1124 | CLA | C3B-C2B-C1B | -5.30 | 100.81 | 106.69 |
| 15 | A | 1103 | CLA | O2A-C1-C2 | 5.30 | 120.26 | 108.12 |
| 15 | B | 1013 | CLA | C3B-C2B-C1B | -5.29 | 100.82 | 106.69 |
| 15 | A | 1137 | CLA | C2B-C1B-NB | 5.29 | 113.03 | 109.50 |
| 15 | A | 1125 | CLA | O2A-C1-C2 | 5.28 | 120.22 | 108.12 |
| 15 | A | 1123 | CLA | C2B-C1B-NB | 5.28 | 113.03 | 109.50 |
| 15 | B | 1222 | CLA | C2D-C1D-ND | 5.28 | 115.58 | 109.56 |
| 15 | A | 1119 | CLA | O2A-C1-C2 | 5.28 | 120.21 | 108.12 |
| 15 | B | 1215 | CLA | C4-C3-C5 | 5.28 | 123.40 | 115.39 |
| 15 | B | 1221 | CLA | C2B-C1B-NB | 5.27 | 113.02 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1205 | CLA | C2B-C1B-NB | 5.27 | 113.02 | 109.50 |
| 15 | A | 1012 | CLA | C2D-C1D-ND | 5.27 | 115.57 | 109.56 |
| 15 | A | 1125 | CLA | O2D-CGD-CBD | 5.25 | 121.94 | 111.34 |
| 15 | B | 1230 | CLA | O2A-C1-C2 | 5.25 | 120.14 | 108.12 |
| 15 | A | 1128 | CLA | O2A-C1-C2 | 5.24 | 120.12 | 108.12 |
| 15 | A | 1138 | CLA | C2D-C1D-ND | 5.24 | 115.54 | 109.56 |
| 15 | A | 1133 | CLA | C2B-C1B-NB | 5.24 | 113.00 | 109.50 |
| 15 | A | 1109 | CLA | C2D-C1D-ND | 5.24 | 115.54 | 109.56 |
| 14 | B | 4017 | BCR | C24-C23-C22 | -5.23 | 118.39 | 126.22 |
| 15 | A | 1126 | CLA | C3B-C2B-C1B | -5.22 | 100.90 | 106.69 |
| 15 | B | 1013 | CLA | O2A-CGA-O1A | -5.22 | 109.84 | 123.48 |
| 15 | B | 1222 | CLA | C3B-C2B-C1B | -5.22 | 100.91 | 106.69 |
| 15 | B | 1236 | CLA | O2A-C1-C2 | 5.21 | 120.06 | 108.12 |
| 15 | B | 1221 | CLA | C2D-C1D-ND | 5.21 | 115.50 | 109.56 |
| 15 | B | 1023 | CLA | O2A-C1-C2 | 5.21 | 120.04 | 108.12 |
| 15 | A | 1115 | CLA | C2D-C1D-ND | 5.20 | 115.49 | 109.56 |
| 15 | B | 1230 | CLA | C2B-C1B-NB | 5.18 | 112.96 | 109.50 |
| 15 | A | 1130 | CLA | O2A-C1-C2 | 5.17 | 119.97 | 108.12 |
| 15 | J | 1302 | CLA | C2B-C1B-NB | 5.17 | 112.95 | 109.50 |
| 15 | B | 1206 | CLA | O2A-CGA-O1A | -5.17 | 111.66 | 122.93 |
| 15 | A | 1115 | CLA | C2B-C1B-NB | 5.17 | 112.95 | 109.50 |
| 15 | B | 1228 | CLA | C2D-C1D-ND | 5.17 | 115.45 | 109.56 |
| 15 | A | 1119 | CLA | O2A-CGA-O1A | -5.17 | 109.98 | 123.48 |
| 15 | K | 1402 | CLA | C2D-C1D-ND | 5.16 | 115.45 | 109.56 |
| 15 | B | 1212 | CLA | C2D-C1D-ND | 5.16 | 115.44 | 109.56 |
| 15 | B | 1221 | CLA | O2A-CGA-O1A | -5.16 | 110.00 | 123.48 |
| 15 | A | 1134 | CLA | O2A-CGA-O1A | -5.16 | 111.68 | 122.93 |
| 15 | B | 1205 | CLA | O2A-CGA-O1A | -5.15 | 110.02 | 123.48 |
| 15 | A | 1140 | CLA | C2D-C1D-ND | 5.15 | 115.44 | 109.56 |
| 15 | B | 1223 | CLA | C2D-C1D-ND | 5.15 | 115.43 | 109.56 |
| 15 | A | 1106 | CLA | C3B-C2B-C1B | -5.15 | 100.98 | 106.69 |
| 15 | B | 1013 | CLA | C2D-C1D-ND | 5.15 | 115.43 | 109.56 |
| 15 | A | 1022 | CLA | O2A-C1-C2 | 5.14 | 119.90 | 108.12 |
| 15 | A | 1138 | CLA | C3B-C2B-C1B | -5.14 | 100.99 | 106.69 |
| 15 | A | 1131 | CLA | C2D-C1D-ND | 5.14 | 115.43 | 109.56 |
| 15 | A | 1114 | CLA | O2A-C1-C2 | 5.14 | 119.89 | 108.12 |
| 15 | B | 1239 | CLA | C2B-C1B-NB | 5.14 | 112.93 | 109.50 |
| 14 | F | 4016 | BCR | C38-C26-C25 | -5.13 | 118.70 | 124.50 |
| 15 | A | 1131 | CLA | O2D-CGD-CBD | 5.13 | 121.70 | 111.34 |
| 15 | B | 1236 | CLA | C2D-C1D-ND | 5.12 | 115.40 | 109.56 |
| 15 | A | 1136 | CLA | C2D-C1D-ND | 5.12 | 115.40 | 109.56 |
| 15 | J | 1303 | CLA | C2D-C1D-ND | 5.12 | 115.40 | 109.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1235 | CLA | O2A-CGA-O1A | -5.12 | 110.11 | 123.48 |
| 15 | J | 1302 | CLA | C2D-C1D-ND | 5.11 | 115.39 | 109.56 |
| 15 | A | 1116 | CLA | C3B-C2B-C1B | -5.11 | 101.02 | 106.69 |
| 15 | B | 1227 | CLA | O2D-CGD-CBD | 5.11 | 121.66 | 111.34 |
| 15 | A | 1126 | CLA | O2A-C1-C2 | 5.11 | 119.82 | 108.12 |
| 15 | B | 1202 | CLA | C2D-C1D-ND | 5.11 | 115.39 | 109.56 |
| 15 | B | 1021 | CLA | O2A-C1-C2 | 5.11 | 119.82 | 108.12 |
| 15 | A | 1134 | CLA | C2D-C1D-ND | 5.10 | 115.38 | 109.56 |
| 15 | B | 1023 | CLA | C3B-C2B-C1B | -5.10 | 101.03 | 106.69 |
| 15 | A | 1104 | CLA | O2A-C1-C2 | 5.09 | 119.79 | 108.12 |
| 15 | A | 1111 | CLA | C3B-C2B-C1B | -5.10 | 101.04 | 106.69 |
| 15 | B | 1210 | CLA | O2A-C1-C2 | 5.09 | 119.78 | 108.12 |
| 15 | A | 1137 | CLA | O2A-C1-C2 | 5.08 | 119.76 | 108.12 |
| 15 | A | 1129 | CLA | C2B-C1B-NB | 5.08 | 112.89 | 109.50 |
| 15 | A | 1132 | CLA | C2B-C1B-NB | 5.08 | 112.89 | 109.50 |
| 15 | A | 1102 | CLA | O2A-C1-C2 | 5.08 | 119.75 | 108.12 |
| 15 | F | 1410 | CLA | O2A-C1-C2 | 5.07 | 119.73 | 108.12 |
| 15 | B | 1236 | CLA | C3B-C2B-C1B | -5.07 | 101.07 | 106.69 |
| 15 | A | 1132 | CLA | O2A-C1-C2 | 5.07 | 119.74 | 108.12 |
| 15 | A | 1130 | CLA | C3B-C2B-C1B | -5.07 | 101.07 | 106.69 |
| 14 | A | 4001 | BCR | C7-C8-C9 | -5.07 | 118.63 | 126.22 |
| 15 | F | 1301 | CLA | C2D-C1D-ND | 5.06 | 115.34 | 109.56 |
| 15 | A | 1102 | CLA | C3B-C2B-C1B | -5.06 | 101.08 | 106.69 |
| 15 | A | 1104 | CLA | C2D-C1D-ND | 5.06 | 115.33 | 109.56 |
| 15 | B | 1211 | CLA | O2D-CGD-CBD | 5.06 | 121.55 | 111.34 |
| 15 | A | 1136 | CLA | O2A-CGA-O1A | -5.05 | 110.28 | 123.48 |
| 15 | B | 1221 | CLA | O2D-CGD-CBD | 5.05 | 121.54 | 111.34 |
| 13 | A | 1108 | CL0 | C2D-C1D-ND | 5.05 | 115.32 | 109.56 |
| 15 | A | 1132 | CLA | O2A-CGA-O1A | -5.04 | 110.31 | 123.48 |
| 15 | A | 1131 | CLA | C2B-C1B-NB | 5.04 | 112.86 | 109.50 |
| 15 | K | 1402 | CLA | C2B-C1B-NB | 5.04 | 112.86 | 109.50 |
| 15 | A | 1110 | CLA | C3B-C2B-C1B | -5.04 | 101.11 | 106.69 |
| 15 | K | 1401 | CLA | C3B-C2B-C1B | -5.03 | 101.11 | 106.69 |
| 15 | B | 1210 | CLA | C3B-C2B-C1B | -5.03 | 101.11 | 106.69 |
| 15 | B | 1217 | CLA | C1-O2A-CGA | 5.02 | 121.18 | 115.30 |
| 15 | B | 1207 | CLA | C2D-C1D-ND | 5.02 | 115.28 | 109.56 |
| 15 | B | 1234 | CLA | C2D-C1D-ND | 5.02 | 115.28 | 109.56 |
| 15 | A | 1132 | CLA | O2D-CGD-CBD | 5.01 | 121.46 | 111.34 |
| 15 | A | 1111 | CLA | C2D-C1D-ND | 5.01 | 115.27 | 109.56 |
| 15 | B | 1227 | CLA | C3B-C2B-C1B | -5.01 | 101.14 | 106.69 |
| 15 | A | 1110 | CLA | C2D-C1D-ND | 5.01 | 115.27 | 109.56 |
| 15 | B | 1212 | CLA | O2D-CGD-CBD | 5.00 | 121.45 | 111.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1801 | CLA | O2A-CGA-O1A | -5.00 | 110.41 | 123.48 |
| 15 | A | 1102 | CLA | C2D-C1D-ND | 5.00 | 115.26 | 109.56 |
| 15 | B | 1238 | CLA | C2D-C1D-ND | 4.99 | 115.25 | 109.56 |
| 15 | B | 1219 | CLA | C3B-C2B-C1B | -4.99 | 101.16 | 106.69 |
| 15 | F | 1139 | CLA | C2D-C1D-ND | 4.99 | 115.25 | 109.56 |
| 14 | A | 4012 | BCR | C38-C26-C25 | -4.99 | 118.86 | 124.50 |
| 15 | F | 1410 | CLA | C2D-C1D-ND | 4.99 | 115.25 | 109.56 |
| 15 | A | 1801 | CLA | C2D-C1D-ND | 4.99 | 115.25 | 109.56 |
| 15 | A | 1113 | CLA | C2D-C1D-ND | 4.99 | 115.25 | 109.56 |
| 15 | B | 1226 | CLA | C2D-C1D-ND | 4.98 | 115.24 | 109.56 |
| 15 | B | 1202 | CLA | O2A-CGA-O1A | -4.98 | 110.48 | 123.48 |
| 15 | B | 1224 | CLA | C3B-C2B-C1B | -4.97 | 101.17 | 106.69 |
| 15 | A | 1125 | CLA | C3B-C2B-C1B | -4.97 | 101.18 | 106.69 |
| 15 | B | 1210 | CLA | O2A-CGA-O1A | -4.97 | 110.49 | 123.48 |
| 13 | A | 1011 | CL0 | O2D-CGD-CBD | 4.97 | 121.38 | 111.34 |
| 15 | B | 1231 | CLA | C2D-C1D-ND | 4.97 | 115.22 | 109.56 |
| 15 | A | 1114 | CLA | C2D-C1D-ND | 4.96 | 115.22 | 109.56 |
| 15 | A | 1126 | CLA | O2D-CGD-CBD | 4.96 | 121.36 | 111.34 |
| 14 | J | 4013 | BCR | C3-C4-C5 | -4.96 | 105.66 | 113.81 |
| 15 | B | 1214 | CLA | C3B-C2B-C1B | -4.96 | 101.19 | 106.69 |
| 15 | A | 1106 | CLA | C2D-C1D-ND | 4.96 | 115.22 | 109.56 |
| 15 | B | 1220 | CLA | C3B-C2B-C1B | -4.95 | 101.20 | 106.69 |
| 15 | B | 1202 | CLA | C3B-C2B-C1B | -4.95 | 101.20 | 106.69 |
| 15 | B | 1240 | CLA | C2D-C1D-ND | 4.95 | 115.21 | 109.56 |
| 15 | A | 1137 | CLA | C2D-C1D-ND | 4.95 | 115.21 | 109.56 |
| 15 | K | 1401 | CLA | C2D-C1D-ND | 4.95 | 115.21 | 109.56 |
| 15 | B | 1219 | CLA | C2D-C1D-ND | 4.95 | 115.20 | 109.56 |
| 15 | B | 1231 | CLA | O2A-CGA-O1A | -4.95 | 110.55 | 123.48 |
| 15 | B | 1023 | CLA | C2D-C1D-ND | 4.95 | 115.20 | 109.56 |
| 15 | B | 1232 | CLA | C2D-C1D-ND | 4.94 | 115.20 | 109.56 |
| 15 | A | 1022 | CLA | C3B-C2B-C1B | -4.94 | 101.21 | 106.69 |
| 15 | A | 1102 | CLA | O2D-CGD-CBD | 4.94 | 121.32 | 111.34 |
| 15 | F | 1410 | CLA | C3B-C2B-C1B | -4.94 | 101.22 | 106.69 |
| 15 | B | 1217 | CLA | C2D-C1D-ND | 4.94 | 115.19 | 109.56 |
| 14 | A | 4003 | BCR | C7-C8-C9 | -4.94 | 118.83 | 126.22 |
| 15 | A | 1112 | CLA | C2D-C1D-ND | 4.94 | 115.19 | 109.56 |
| 14 | B | 4006 | BCR | C38-C26-C25 | -4.93 | 118.92 | 124.50 |
| 15 | B | 1226 | CLA | C2B-C1B-NB | 4.93 | 112.79 | 109.50 |
| 15 | B | 1217 | CLA | C3B-C2B-C1B | -4.93 | 101.22 | 106.69 |
| 15 | A | 1137 | CLA | O2D-CGD-CBD | 4.93 | 121.29 | 111.34 |
| 15 | B | 1224 | CLA | C2D-C1D-ND | 4.93 | 115.18 | 109.56 |
| 15 | A | 1103 | CLA | C2D-C1D-ND | 4.92 | 115.18 | 109.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1104 | CLA | C3B-C2B-C1B | -4.92 | 101.23 | 106.69 |
| 15 | F | 1301 | CLA | C3B-C2B-C1B | -4.92 | 101.23 | 106.69 |
| 15 | B | 1210 | CLA | C2D-C1D-ND | 4.92 | 115.17 | 109.56 |
| 15 | B | 1225 | CLA | C3B-C2B-C1B | -4.91 | 101.25 | 106.69 |
| 15 | B | 1224 | CLA | O2D-CGD-CBD | 4.90 | 121.24 | 111.34 |
| 15 | A | 1102 | CLA | O2A-CGA-O1A | -4.90 | 110.67 | 123.48 |
| 15 | A | 1122 | CLA | C4-C3-C5 | 4.90 | 122.83 | 115.39 |
| 15 | A | 1112 | CLA | C3B-C2B-C1B | -4.90 | 101.26 | 106.69 |
| 15 | B | 1229 | CLA | O2A-C1-C2 | 4.89 | 119.32 | 108.12 |
| 15 | B | 1224 | CLA | O2A-C1-C2 | 4.89 | 119.31 | 108.12 |
| 15 | B | 1234 | CLA | C3B-C2B-C1B | -4.89 | 101.27 | 106.69 |
| 15 | A | 1121 | CLA | O2A-CGA-CBA | 4.89 | 125.56 | 110.50 |
| 15 | B | 1206 | CLA | C3B-C2B-C1B | -4.89 | 101.27 | 106.69 |
| 15 | B | 1228 | CLA | C3B-C2B-C1B | -4.88 | 101.28 | 106.69 |
| 15 | B | 1208 | CLA | C2D-C1D-ND | 4.88 | 115.12 | 109.56 |
| 15 | A | 1131 | CLA | O2A-CGA-O1A | -4.87 | 110.75 | 123.48 |
| 15 | A | 1111 | CLA | O2A-CGA-O1A | -4.87 | 110.76 | 123.48 |
| 15 | B | 1201 | CLA | C3B-C2B-C1B | -4.87 | 101.30 | 106.69 |
| 15 | B | 1230 | CLA | O2A-CGA-O1A | -4.86 | 110.77 | 123.48 |
| 15 | A | 1136 | CLA | C2B-C1B-NB | 4.86 | 112.75 | 109.50 |
| 15 | B | 1240 | CLA | C3B-C2B-C1B | -4.86 | 101.30 | 106.69 |
| 15 | B | 1217 | CLA | O2D-CGD-CBD | 4.86 | 121.16 | 111.34 |
| 15 | A | 1137 | CLA | C3B-C2B-C1B | -4.86 | 101.30 | 106.69 |
| 15 | A | 1116 | CLA | O2A-C1-C2 | 4.86 | 119.25 | 108.12 |
| 15 | A | 1109 | CLA | C3B-C2B-C1B | -4.86 | 101.30 | 106.69 |
| 15 | B | 1204 | CLA | C3B-C2B-C1B | -4.85 | 101.31 | 106.69 |
| 15 | A | 1801 | CLA | C3B-C2B-C1B | -4.86 | 101.31 | 106.69 |
| 15 | B | 1229 | CLA | C3B-C2B-C1B | -4.86 | 101.31 | 106.69 |
| 15 | A | 1132 | CLA | C3B-C2B-C1B | -4.85 | 101.31 | 106.69 |
| 15 | A | 1101 | CLA | C2D-C1D-ND | 4.85 | 115.09 | 109.56 |
| 15 | A | 1121 | CLA | C2D-C1D-ND | 4.85 | 115.09 | 109.56 |
| 15 | A | 1135 | CLA | O2A-CGA-O1A | -4.85 | 110.81 | 123.48 |
| 15 | A | 1117 | CLA | C2D-C1D-ND | 4.85 | 115.09 | 109.56 |
| 15 | A | 1135 | CLA | C2D-C1D-ND | 4.85 | 115.09 | 109.56 |
| 15 | K | 1401 | CLA | O2A-CGA-CBA | 4.85 | 125.44 | 110.50 |
| 15 | B | 1213 | CLA | C2D-C1D-ND | 4.84 | 115.08 | 109.56 |
| 15 | B | 1021 | CLA | O2A-CGA-O1A | -4.84 | 110.83 | 123.48 |
| 15 | B | 1227 | CLA | C2D-C1D-ND | 4.84 | 115.08 | 109.56 |
| 15 | A | 1101 | CLA | O2A-C1-C2 | 4.84 | 119.20 | 108.12 |
| 13 | A | 1108 | CL0 | C2B-C1B-NB | 4.84 | 112.73 | 109.50 |
| 15 | A | 1130 | CLA | O2D-CGD-CBD | 4.84 | 121.11 | 111.34 |
| 15 | B | 1220 | CLA | C2D-C1D-ND | 4.83 | 115.07 | 109.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1230 | CLA | C2D-C1D-ND | 4.82 | 115.06 | 109.56 |
| 15 | A | 1128 | CLA | C2D-C1D-ND | 4.82 | 115.05 | 109.56 |
| 15 | A | 1105 | CLA | O2A-CGA-O1A | -4.82 | 110.89 | 123.48 |
| 15 | A | 1107 | CLA | C3B-C2B-C1B | -4.82 | 101.35 | 106.69 |
| 15 | B | 1203 | CLA | C2D-C1D-ND | 4.81 | 115.05 | 109.56 |
| 15 | A | 1116 | CLA | C2D-C1D-ND | 4.81 | 115.05 | 109.56 |
| 15 | A | 1127 | CLA | C2B-C1B-NB | 4.81 | 112.71 | 109.50 |
| 15 | A | 1104 | CLA | O2A-CGA-O1A | -4.81 | 110.91 | 123.48 |
| 15 | B | 1211 | CLA | C3B-C2B-C1B | -4.81 | 101.36 | 106.69 |
| 15 | A | 1134 | CLA | C3B-C2B-C1B | -4.81 | 101.36 | 106.69 |
| 15 | A | 1105 | CLA | C2D-C1D-ND | 4.81 | 115.05 | 109.56 |
| 15 | A | 1107 | CLA | O2A-CGA-O1A | -4.81 | 110.92 | 123.48 |
| 15 | B | 1215 | CLA | C3B-C2B-C1B | -4.81 | 101.36 | 106.69 |
| 15 | A | 1117 | CLA | C3B-C2B-C1B | -4.80 | 101.36 | 106.69 |
| 15 | A | 1107 | CLA | C2D-C1D-ND | 4.80 | 115.03 | 109.56 |
| 15 | B | 1208 | CLA | C3B-C2B-C1B | -4.80 | 101.37 | 106.69 |
| 15 | A | 1801 | CLA | O2A-C1-C2 | 4.80 | 119.10 | 108.12 |
| 15 | A | 1122 | CLA | C2D-C1D-ND | 4.80 | 115.03 | 109.56 |
| 15 | A | 1116 | CLA | O2D-CGD-CBD | 4.80 | 121.03 | 111.34 |
| 15 | A | 1109 | CLA | O2A-CGA-O1A | -4.79 | 110.95 | 123.48 |
| 15 | B | 1218 | CLA | O2A-CGA-O1A | -4.79 | 110.96 | 123.48 |
| 15 | B | 1235 | CLA | C3B-C2B-C1B | -4.79 | 101.38 | 106.69 |
| 13 | A | 1011 | CL0 | C1C-C2C-C3C | -4.79 | 100.94 | 106.96 |
| 15 | B | 1204 | CLA | C2D-C1D-ND | 4.79 | 115.02 | 109.56 |
| 15 | A | 1022 | CLA | C2D-C1D-ND | 4.78 | 115.02 | 109.56 |
| 15 | B | 1201 | CLA | C2D-C1D-ND | 4.78 | 115.01 | 109.56 |
| 15 | B | 1205 | CLA | C2D-C1D-ND | 4.78 | 115.01 | 109.56 |
| 15 | B | 1221 | CLA | O2A-CGA-CBA | 4.78 | 126.52 | 111.90 |
| 15 | A | 1127 | CLA | C2D-C1D-ND | 4.78 | 115.01 | 109.56 |
| 15 | A | 1119 | CLA | C2D-C1D-ND | 4.77 | 115.01 | 109.56 |
| 15 | B | 1226 | CLA | O2A-CGA-O1A | -4.77 | 111.00 | 123.48 |
| 15 | A | 1129 | CLA | C2D-C1D-ND | 4.77 | 115.00 | 109.56 |
| 15 | B | 1214 | CLA | O2A-CGA-O1A | -4.77 | 111.01 | 123.48 |
| 15 | B | 1209 | CLA | O2D-CGD-CBD | 4.77 | 120.98 | 111.34 |
| 15 | B | 1213 | CLA | C3B-C2B-C1B | -4.77 | 101.40 | 106.69 |
| 15 | B | 1225 | CLA | O2A-C1-C2 | 4.77 | 119.04 | 108.12 |
| 15 | A | 1105 | CLA | O2D-CGD-CBD | 4.77 | 120.97 | 111.34 |
| 15 | A | 1138 | CLA | O2A-C1-C2 | 4.77 | 119.04 | 108.12 |
| 15 | B | 1235 | CLA | O2D-CGD-CBD | 4.77 | 120.97 | 111.34 |
| 15 | A | 1124 | CLA | C2D-C1D-ND | 4.77 | 115.00 | 109.56 |
| 14 | A | 4002 | BCR | C24-C23-C22 | -4.77 | 119.08 | 126.22 |
| 15 | A | 1120 | CLA | C2D-C1D-ND | 4.76 | 115.00 | 109.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1211 | CLA | C2D-C1D-ND | 4.76 | 114.99 | 109.56 |
| 15 | B | 1216 | CLA | C2D-C1D-ND | 4.76 | 114.99 | 109.56 |
| 15 | K | 1402 | CLA | C3B-C2B-C1B | -4.76 | 101.41 | 106.69 |
| 15 | B | 1209 | CLA | C2D-C1D-ND | 4.76 | 114.99 | 109.56 |
| 15 | A | 1120 | CLA | C3B-C2B-C1B | -4.76 | 101.42 | 106.69 |
| 13 | A | 1011 | CL0 | C2D-C1D-ND | 4.76 | 114.98 | 109.56 |
| 15 | B | 1239 | CLA | O2A-CGA-CBA | 4.76 | 125.16 | 110.50 |
| 15 | B | 1234 | CLA | O2D-CGD-CBD | 4.75 | 120.94 | 111.34 |
| 15 | B | 1212 | CLA | C3B-C2B-C1B | -4.75 | 101.42 | 106.69 |
| 15 | B | 1021 | CLA | C2D-C1D-ND | 4.75 | 114.98 | 109.56 |
| 15 | F | 1410 | CLA | O2D-CGD-CBD | 4.75 | 120.93 | 111.34 |
| 15 | A | 1012 | CLA | CMD-C2D-C1D | 4.75 | 135.54 | 126.16 |
| 15 | B | 1202 | CLA | O2D-CGD-CBD | 4.75 | 120.93 | 111.34 |
| 15 | A | 1104 | CLA | C1C-C2C-C3C | -4.74 | 100.99 | 106.96 |
| 15 | B | 1203 | CLA | C3B-C2B-C1B | -4.74 | 101.43 | 106.69 |
| 15 | A | 1123 | CLA | C2D-C1D-ND | 4.74 | 114.97 | 109.56 |
| 15 | A | 1123 | CLA | O2A-CGA-O1A | -4.74 | 111.09 | 123.48 |
| 15 | J | 1303 | CLA | C3B-C2B-C1B | -4.73 | 101.44 | 106.69 |
| 15 | B | 1237 | CLA | C3B-C2B-C1B | -4.73 | 101.45 | 106.69 |
| 14 | A | 4008 | BCR | C33-C5-C6 | -4.73 | 119.16 | 124.50 |
| 14 | A | 4003 | BCR | C38-C26-C25 | -4.73 | 119.16 | 124.50 |
| 15 | B | 1205 | CLA | O2A-C1-C2 | 4.73 | 118.94 | 108.12 |
| 15 | B | 1223 | CLA | C3B-C2B-C1B | -4.73 | 101.45 | 106.69 |
| 15 | B | 1209 | CLA | C3B-C2B-C1B | -4.72 | 101.45 | 106.69 |
| 15 | A | 1136 | CLA | C3B-C2B-C1B | -4.72 | 101.45 | 106.69 |
| 15 | A | 1022 | CLA | O2A-CGA-O1A | -4.71 | 111.17 | 123.48 |
| 15 | B | 1230 | CLA | C3B-C2B-C1B | -4.71 | 101.47 | 106.69 |
| 15 | B | 1236 | CLA | O2D-CGD-CBD | 4.70 | 120.84 | 111.34 |
| 15 | B | 1238 | CLA | C3B-C2B-C1B | -4.70 | 101.47 | 106.69 |
| 15 | B | 1214 | CLA | O2D-CGD-CBD | 4.70 | 120.84 | 111.34 |
| 15 | B | 1221 | CLA | C3B-C2B-C1B | -4.70 | 101.48 | 106.69 |
| 15 | A | 1133 | CLA | C2D-C1D-ND | 4.70 | 114.92 | 109.56 |
| 15 | B | 1206 | CLA | C2D-C1D-ND | 4.70 | 114.92 | 109.56 |
| 15 | A | 1130 | CLA | O2A-CGA-O1A | -4.70 | 111.20 | 123.48 |
| 15 | B | 1218 | CLA | C2D-C1D-ND | 4.70 | 114.92 | 109.56 |
| 15 | B | 1215 | CLA | C2D-C1D-ND | 4.69 | 114.92 | 109.56 |
| 14 | B | 4014 | BCR | C7-C8-C9 | -4.69 | 119.19 | 126.22 |
| 15 | B | 1237 | CLA | C2D-C1D-ND | 4.69 | 114.91 | 109.56 |
| 15 | B | 1215 | CLA | O2D-CGD-CBD | 4.69 | 120.82 | 111.34 |
| 15 | A | 1118 | CLA | C1C-C2C-C3C | -4.69 | 101.06 | 106.96 |
| 15 | A | 1118 | CLA | O2D-CGD-CBD | 4.69 | 120.81 | 111.34 |
| 15 | B | 1207 | CLA | C3B-C2B-C1B | -4.69 | 101.49 | 106.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1121 | CLA | C3B-C2B-C1B | -4.69 | 101.49 | 106.69 |
| 15 | A | 1112 | CLA | O2D-CGD-CBD | 4.68 | 120.80 | 111.34 |
| 15 | A | 1114 | CLA | C3B-C2B-C1B | -4.68 | 101.50 | 106.69 |
| 15 | A | 1114 | CLA | O2D-CGD-CBD | 4.68 | 120.79 | 111.34 |
| 15 | A | 1103 | CLA | C3B-C2B-C1B | -4.68 | 101.50 | 106.69 |
| 15 | B | 1219 | CLA | O2A-CGA-O1A | -4.68 | 111.26 | 123.48 |
| 15 | B | 1230 | CLA | O2D-CGD-CBD | 4.67 | 120.78 | 111.34 |
| 13 | A | 1011 | CL0 | O2A-CGA-O1A | -4.67 | 111.27 | 123.48 |
| 15 | B | 1217 | CLA | O2A-CGA-O1A | -4.67 | 111.28 | 123.48 |
| 15 | B | 1236 | CLA | CMC-C2C-C1C | 4.67 | 131.60 | 124.95 |
| 15 | A | 1135 | CLA | C3B-C2B-C1B | -4.66 | 101.52 | 106.69 |
| 15 | A | 1136 | CLA | O2A-CGA-CBA | 4.66 | 126.17 | 111.90 |
| 15 | B | 1202 | CLA | O2A-C1-C2 | 4.66 | 118.79 | 108.12 |
| 15 | B | 1231 | CLA | C1C-C2C-C3C | -4.66 | 101.10 | 106.96 |
| 15 | A | 1110 | CLA | O2A-CGA-O1A | -4.65 | 111.32 | 123.48 |
| 15 | A | 1140 | CLA | O2A-CGA-O1A | -4.65 | 111.33 | 123.48 |
| 15 | A | 1118 | CLA | C3B-C2B-C1B | -4.65 | 101.53 | 106.69 |
| 15 | A | 1101 | CLA | C3B-C2B-C1B | -4.65 | 101.54 | 106.69 |
| 15 | B | 1214 | CLA | C2D-C1D-ND | 4.65 | 114.86 | 109.56 |
| 15 | A | 1126 | CLA | C2D-C1D-ND | 4.65 | 114.86 | 109.56 |
| 15 | A | 1136 | CLA | O2D-CGD-CBD | 4.65 | 120.72 | 111.34 |
| 15 | B | 1236 | CLA | O2A-CGA-O1A | -4.64 | 111.34 | 123.48 |
| 15 | B | 1223 | CLA | O2D-CGD-CBD | 4.64 | 120.72 | 111.34 |
| 15 | A | 1137 | CLA | O2A-CGA-O1A | -4.64 | 111.35 | 123.48 |
| 15 | A | 1140 | CLA | C3B-C2B-C1B | -4.64 | 101.54 | 106.69 |
| 15 | B | 1239 | CLA | C2D-C1D-ND | 4.63 | 114.84 | 109.56 |
| 15 | B | 1225 | CLA | C2D-C1D-ND | 4.62 | 114.83 | 109.56 |
| 14 | B | 4009 | BCR | C24-C23-C22 | -4.62 | 119.30 | 126.22 |
| 15 | B | 1239 | CLA | O2D-CGD-CBD | 4.62 | 120.68 | 111.34 |
| 15 | B | 1203 | CLA | C1C-C2C-C3C | -4.62 | 101.15 | 106.96 |
| 14 | B | 4009 | BCR | C7-C8-C9 | -4.62 | 119.30 | 126.22 |
| 12 | B | 5004 | LHG | O7-C7-C8 | 4.62 | 121.38 | 111.54 |
| 15 | A | 1140 | CLA | O2A-C1-C2 | 4.62 | 118.69 | 108.12 |
| 15 | B | 1220 | CLA | O2A-CGA-O1A | -4.61 | 111.42 | 123.48 |
| 15 | B | 1228 | CLA | O2A-CGA-O1A | -4.61 | 111.42 | 123.48 |
| 15 | B | 1214 | CLA | C4-C3-C5 | 4.61 | 122.39 | 115.39 |
| 15 | B | 1215 | CLA | C1C-C2C-C3C | -4.61 | 101.16 | 106.96 |
| 15 | B | 1231 | CLA | C3B-C2B-C1B | -4.61 | 101.58 | 106.69 |
| 15 | B | 1205 | CLA | C3B-C2B-C1B | -4.60 | 101.59 | 106.69 |
| 15 | B | 1216 | CLA | C3B-C2B-C1B | -4.60 | 101.59 | 106.69 |
| 15 | B | 1232 | CLA | C1C-C2C-C3C | -4.60 | 101.17 | 106.96 |
| 15 | A | 1012 | CLA | C3B-C2B-C1B | -4.60 | 101.59 | 106.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | F | 1139 | CLA | O2A-C1-C2 | 4.59 | 118.64 | 108.12 |
| 15 | B | 1228 | CLA | O2A-C1-C2 | 4.59 | 118.63 | 108.12 |
| 15 | B | 1218 | CLA | O2D-CGD-CBD | 4.59 | 120.60 | 111.34 |
| 15 | A | 1122 | CLA | C3B-C2B-C1B | -4.59 | 101.61 | 106.69 |
| 15 | A | 1135 | CLA | C1C-C2C-C3C | -4.59 | 101.19 | 106.96 |
| 15 | B | 1229 | CLA | C1C-C2C-C3C | -4.58 | 101.19 | 106.96 |
| 15 | B | 1239 | CLA | C3B-C2B-C1B | -4.58 | 101.61 | 106.69 |
| 15 | A | 1128 | CLA | O2A-CGA-O1A | -4.58 | 111.51 | 123.48 |
| 15 | A | 1130 | CLA | C2D-C1D-ND | 4.58 | 114.78 | 109.56 |
| 15 | A | 1131 | CLA | O2A-CGA-CBA | 4.57 | 125.89 | 111.90 |
| 15 | B | 1239 | CLA | C1C-C2C-C3C | -4.57 | 101.21 | 106.96 |
| 15 | J | 1303 | CLA | O2A-CGA-CBA | 4.57 | 124.58 | 110.50 |
| 15 | A | 1115 | CLA | C3B-C2B-C1B | -4.56 | 101.63 | 106.69 |
| 15 | A | 1120 | CLA | O2A-CGA-O1A | -4.56 | 111.55 | 123.48 |
| 15 | A | 1119 | CLA | C3B-C2B-C1B | -4.56 | 101.63 | 106.69 |
| 15 | B | 1219 | CLA | O2D-CGD-CBD | 4.56 | 120.56 | 111.34 |
| 15 | A | 1115 | CLA | O2A-CGA-CBA | 4.56 | 124.56 | 110.50 |
| 15 | A | 1132 | CLA | O2A-CGA-CBA | 4.56 | 125.86 | 111.90 |
| 15 | B | 1207 | CLA | O2D-CGD-CBD | 4.56 | 120.55 | 111.34 |
| 15 | B | 1218 | CLA | C3B-C2B-C1B | -4.56 | 101.64 | 106.69 |
| 15 | A | 1133 | CLA | C3B-C2B-C1B | -4.56 | 101.64 | 106.69 |
| 15 | A | 1140 | CLA | O2D-CGD-CBD | 4.56 | 120.55 | 111.34 |
| 15 | A | 1012 | CLA | O2A-CGA-O1A | -4.56 | 111.57 | 123.48 |
| 15 | A | 1123 | CLA | C3B-C2B-C1B | -4.55 | 101.64 | 106.69 |
| 15 | A | 1129 | CLA | O2D-CGD-CBD | 4.55 | 120.54 | 111.34 |
| 15 | A | 1131 | CLA | C1C-C2C-C3C | -4.55 | 101.23 | 106.96 |
| 15 | B | 1219 | CLA | C1C-C2C-C3C | -4.55 | 101.24 | 106.96 |
| 15 | B | 1226 | CLA | C1C-C2C-C3C | -4.55 | 101.23 | 106.96 |
| 15 | A | 1801 | CLA | C1C-C2C-C3C | -4.55 | 101.24 | 106.96 |
| 15 | B | 1213 | CLA | O2D-CGD-CBD | 4.54 | 120.51 | 111.34 |
| 15 | B | 1214 | CLA | C4-C3-C2 | -4.54 | 114.48 | 123.52 |
| 14 | F | 4015 | BCR | C24-C23-C22 | -4.54 | 119.42 | 126.22 |
| 14 | A | 4008 | BCR | C24-C23-C22 | -4.54 | 119.43 | 126.22 |
| 15 | B | 1207 | CLA | C1C-C2C-C3C | -4.54 | 101.25 | 106.96 |
| 12 | A | 5003 | LHG | O7-C7-C8 | 4.54 | 121.21 | 111.54 |
| 15 | B | 1227 | CLA | C1C-C2C-C3C | -4.53 | 101.25 | 106.96 |
| 15 | A | 1122 | CLA | O2A-CGA-O1A | -4.54 | 111.63 | 123.48 |
| 13 | A | 1108 | CL0 | C1C-C2C-C3C | -4.54 | 101.25 | 106.96 |
| 15 | B | 1224 | CLA | C1C-C2C-C3C | -4.53 | 101.26 | 106.96 |
| 15 | A | 1107 | CLA | O2D-CGD-CBD | 4.53 | 120.50 | 111.34 |
| 15 | J | 1302 | CLA | C1C-C2C-C3C | -4.53 | 101.26 | 106.96 |
| 15 | A | 1114 | CLA | O2A-CGA-O1A | -4.53 | 111.64 | 123.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | F | 1410 | CLA | O2A-CGA-O1A | -4.53 | 111.65 | 123.48 |
| 15 | B | 1234 | CLA | O2A-CGA-O1A | -4.53 | 111.64 | 123.48 |
| 15 | A | 1012 | CLA | O2D-CGD-CBD | 4.53 | 120.48 | 111.34 |
| 15 | A | 1133 | CLA | C1C-C2C-C3C | -4.52 | 101.27 | 106.96 |
| 15 | A | 1128 | CLA | C1C-C2C-C3C | -4.52 | 101.27 | 106.96 |
| 15 | A | 1129 | CLA | C3B-C2B-C1B | -4.52 | 101.68 | 106.69 |
| 15 | B | 1204 | CLA | O2A-CGA-CBA | 4.52 | 124.42 | 110.50 |
| 15 | B | 1204 | CLA | C1C-C2C-C3C | -4.52 | 101.28 | 106.96 |
| 14 | B | 4014 | BCR | C24-C23-C22 | -4.52 | 119.46 | 126.22 |
| 15 | B | 1224 | CLA | O2A-CGA-CBA | 4.52 | 125.72 | 111.90 |
| 15 | B | 1023 | CLA | O2A-CGA-O1A | -4.52 | 111.68 | 123.48 |
| 14 | B | 4009 | BCR | C33-C5-C6 | -4.51 | 119.40 | 124.50 |
| 15 | A | 1123 | CLA | O2A-C1-C2 | 4.51 | 118.45 | 108.12 |
| 15 | B | 1222 | CLA | C1C-C2C-C3C | -4.51 | 101.29 | 106.96 |
| 15 | A | 1113 | CLA | C3B-C2B-C1B | -4.51 | 101.69 | 106.69 |
| 15 | A | 1116 | CLA | O2A-CGA-O1A | -4.50 | 111.71 | 123.48 |
| 15 | A | 1022 | CLA | C1C-C2C-C3C | -4.50 | 101.30 | 106.96 |
| 15 | A | 1105 | CLA | C1C-C2C-C3C | -4.50 | 101.30 | 106.96 |
| 15 | B | 1238 | CLA | C1C-C2C-C3C | -4.50 | 101.30 | 106.96 |
| 15 | A | 1120 | CLA | C1C-C2C-C3C | -4.50 | 101.30 | 106.96 |
| 15 | B | 1213 | CLA | C1C-C2C-C3C | -4.50 | 101.30 | 106.96 |
| 15 | B | 1205 | CLA | C1C-C2C-C3C | -4.50 | 101.30 | 106.96 |
| 14 | B | 4011 | BCR | C24-C23-C22 | -4.49 | 119.49 | 126.22 |
| 15 | B | 1235 | CLA | O2A-C1-C2 | 4.49 | 118.41 | 108.12 |
| 14 | B | 4004 | BCR | C33-C5-C6 | -4.49 | 119.43 | 124.50 |
| 15 | A | 1106 | CLA | C1C-C2C-C3C | -4.49 | 101.31 | 106.96 |
| 15 | A | 1136 | CLA | C1C-C2C-C3C | -4.48 | 101.32 | 106.96 |
| 15 | B | 1215 | CLA | O2A-CGA-O1A | -4.48 | 111.77 | 123.48 |
| 15 | A | 1137 | CLA | C1C-C2C-C3C | -4.48 | 101.32 | 106.96 |
| 14 | B | 4014 | BCR | C33-C5-C6 | -4.48 | 119.44 | 124.50 |
| 15 | A | 1134 | CLA | O2A-CGA-CBA | 4.47 | 124.30 | 110.50 |
| 15 | B | 1221 | CLA | C1C-C2C-C3C | -4.47 | 101.33 | 106.96 |
| 15 | B | 1237 | CLA | O2A-C1-C2 | 4.47 | 118.37 | 108.12 |
| 15 | A | 1129 | CLA | C1C-C2C-C3C | -4.47 | 101.33 | 106.96 |
| 14 | A | 4012 | BCR | C24-C23-C22 | -4.47 | 119.53 | 126.22 |
| 15 | F | 1139 | CLA | C1C-C2C-C3C | -4.46 | 101.34 | 106.96 |
| 15 | K | 1402 | CLA | O2A-CGA-CBA | 4.46 | 124.26 | 110.50 |
| 15 | A | 1127 | CLA | C1C-C2C-C3C | -4.45 | 101.36 | 106.96 |
| 15 | B | 1208 | CLA | C1C-C2C-C3C | -4.45 | 101.36 | 106.96 |
| 15 | A | 1124 | CLA | C1C-C2C-C3C | -4.45 | 101.36 | 106.96 |
| 15 | B | 1218 | CLA | C1C-C2C-C3C | -4.45 | 101.36 | 106.96 |
| 15 | B | 1225 | CLA | C1C-C2C-C3C | -4.45 | 101.36 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1212 | CLA | C1C-C2C-C3C | -4.45 | 101.36 | 106.96 |
| 15 | A | 1127 | CLA | C3B-C2B-C1B | -4.44 | 101.76 | 106.69 |
| 15 | B | 1202 | CLA | C1C-C2C-C3C | -4.44 | 101.37 | 106.96 |
| 15 | A | 1103 | CLA | O2D-CGD-CBD | 4.44 | 120.31 | 111.34 |
| 15 | A | 1127 | CLA | O2A-CGA-O1A | -4.44 | 111.88 | 123.48 |
| 13 | A | 1011 | CL0 | C3B-C2B-C1B | -4.44 | 101.77 | 106.69 |
| 15 | K | 1402 | CLA | C1C-C2C-C3C | -4.44 | 101.38 | 106.96 |
| 15 | B | 1224 | CLA | O2A-CGA-O1A | -4.43 | 111.89 | 123.48 |
| 15 | B | 1237 | CLA | O2A-CGA-O1A | -4.43 | 111.89 | 123.48 |
| 14 | B | 4014 | BCR | C38-C26-C25 | -4.43 | 119.49 | 124.50 |
| 15 | B | 1023 | CLA | C3B-CAB-CBB | -4.43 | 116.79 | 125.95 |
| 15 | B | 1232 | CLA | C3B-C2B-C1B | -4.42 | 101.79 | 106.69 |
| 15 | A | 1115 | CLA | O2D-CGD-CBD | 4.42 | 120.27 | 111.34 |
| 15 | A | 1117 | CLA | O2A-CGA-O1A | -4.42 | 111.92 | 123.48 |
| 15 | A | 1110 | CLA | C1C-C2C-C3C | -4.42 | 101.40 | 106.96 |
| 15 | B | 1236 | CLA | C1C-C2C-C3C | -4.41 | 101.41 | 106.96 |
| 15 | A | 1133 | CLA | O2D-CGD-CBD | 4.41 | 120.26 | 111.34 |
| 15 | B | 1201 | CLA | C1C-C2C-C3C | -4.41 | 101.41 | 106.96 |
| 15 | B | 1204 | CLA | O2D-CGD-CBD | 4.41 | 120.25 | 111.34 |
| 15 | B | 1218 | CLA | O2A-CGA-CBA | 4.41 | 125.39 | 111.90 |
| 14 | F | 4015 | BCR | C33-C5-C6 | -4.41 | 119.52 | 124.50 |
| 15 | F | 1410 | CLA | C1C-C2C-C3C | -4.41 | 101.42 | 106.96 |
| 15 | A | 1801 | CLA | O2A-CGA-CBA | 4.40 | 125.38 | 111.90 |
| 15 | A | 1122 | CLA | O2A-C1-C2 | 4.40 | 118.21 | 108.12 |
| 15 | A | 1104 | CLA | O2A-CGA-CBA | 4.40 | 125.38 | 111.90 |
| 15 | A | 1113 | CLA | C1C-C2C-C3C | -4.40 | 101.42 | 106.96 |
| 15 | B | 1206 | CLA | C1C-C2C-C3C | -4.40 | 101.42 | 106.96 |
| 15 | A | 1109 | CLA | C1C-C2C-C3C | -4.40 | 101.42 | 106.96 |
| 15 | B | 1223 | CLA | O2A-CGA-O1A | -4.40 | 111.98 | 123.48 |
| 15 | F | 1301 | CLA | O2D-CGD-CBD | 4.40 | 120.23 | 111.34 |
| 15 | B | 1217 | CLA | C1C-C2C-C3C | -4.40 | 101.43 | 106.96 |
| 10 | B | 2002 | PQN | C14-C13-C15 | 4.40 | 122.06 | 115.39 |
| 15 | B | 1209 | CLA | C1C-C2C-C3C | -4.40 | 101.43 | 106.96 |
| 15 | A | 1121 | CLA | C1C-C2C-C3C | -4.40 | 101.43 | 106.96 |
| 15 | A | 1125 | CLA | O2A-CGA-O1A | -4.40 | 111.99 | 123.48 |
| 15 | B | 1021 | CLA | C1C-C2C-C3C | -4.40 | 101.43 | 106.96 |
| 15 | A | 1022 | CLA | O2D-CGD-CBD | 4.39 | 120.22 | 111.34 |
| 15 | A | 1114 | CLA | C1C-C2C-C3C | -4.39 | 101.44 | 106.96 |
| 13 | A | 1108 | CL0 | CMC-C2C-C1C | 4.39 | 131.21 | 124.95 |
| 15 | B | 1216 | CLA | C1C-C2C-C3C | -4.39 | 101.44 | 106.96 |
| 15 | B | 1229 | CLA | O2D-CGD-CBD | 4.39 | 120.20 | 111.34 |
| 15 | A | 1104 | CLA | O2D-CGD-CBD | 4.38 | 120.20 | 111.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1013 | CLA | C1C-C2C-C3C | -4.38 | 101.45 | 106.96 |
| 15 | B | 1226 | CLA | C3B-C2B-C1B | -4.38 | 101.84 | 106.69 |
| 15 | B | 1211 | CLA | O2A-CGA-CBA | 4.38 | 123.99 | 110.50 |
| 15 | B | 1235 | CLA | C1C-C2C-C3C | -4.37 | 101.46 | 106.96 |
| 15 | B | 1237 | CLA | C1C-C2C-C3C | -4.37 | 101.46 | 106.96 |
| 15 | A | 1116 | CLA | C1C-C2C-C3C | -4.37 | 101.46 | 106.96 |
| 15 | A | 1129 | CLA | O2A-CGA-CBA | 4.37 | 123.96 | 110.50 |
| 15 | J | 1302 | CLA | C3B-C2B-C1B | -4.36 | 101.85 | 106.69 |
| 15 | A | 1118 | CLA | O2A-CGA-CBA | 4.36 | 123.94 | 110.50 |
| 15 | F | 1301 | CLA | C1C-C2C-C3C | -4.36 | 101.48 | 106.96 |
| 15 | B | 1234 | CLA | C1C-C2C-C3C | -4.36 | 101.48 | 106.96 |
| 15 | A | 1111 | CLA | O2A-CGA-CBA | 4.36 | 125.23 | 111.90 |
| 15 | B | 1230 | CLA | C1C-C2C-C3C | -4.35 | 101.48 | 106.96 |
| 15 | B | 1013 | CLA | O2A-CGA-CBA | 4.35 | 125.22 | 111.90 |
| 15 | B | 1021 | CLA | C3B-C2B-C1B | -4.35 | 101.87 | 106.69 |
| 15 | A | 1119 | CLA | C1C-C2C-C3C | -4.35 | 101.49 | 106.96 |
| 15 | B | 1214 | CLA | C1C-C2C-C3C | -4.34 | 101.49 | 106.96 |
| 14 | B | 4017 | BCR | C33-C5-C6 | -4.34 | 119.59 | 124.50 |
| 15 | A | 1121 | CLA | O2D-CGD-CBD | 4.34 | 120.11 | 111.34 |
| 15 | B | 1201 | CLA | O2A-CGA-CBA | 4.34 | 123.89 | 110.50 |
| 15 | B | 1230 | CLA | O2A-CGA-CBA | 4.34 | 125.19 | 111.90 |
| 15 | A | 1102 | CLA | C1C-C2C-C3C | -4.34 | 101.50 | 106.96 |
| 15 | B | 1223 | CLA | C1C-C2C-C3C | -4.34 | 101.50 | 106.96 |
| 15 | B | 1225 | CLA | O2A-CGA-O1A | -4.33 | 112.16 | 123.48 |
| 15 | A | 1111 | CLA | O2D-CGD-CBD | 4.33 | 120.09 | 111.34 |
| 15 | A | 1112 | CLA | C1C-C2C-C3C | -4.33 | 101.51 | 106.96 |
| 15 | K | 1401 | CLA | C1C-C2C-C3C | -4.32 | 101.52 | 106.96 |
| 15 | A | 1107 | CLA | O2A-C1-C2 | 4.32 | 118.01 | 108.12 |
| 15 | A | 1134 | CLA | C1C-C2C-C3C | -4.31 | 101.53 | 106.96 |
| 15 | A | 1119 | CLA | O2A-CGA-CBA | 4.32 | 125.11 | 111.90 |
| 15 | J | 1303 | CLA | O2D-CGD-CBD | 4.32 | 120.06 | 111.34 |
| 15 | J | 1303 | CLA | C1C-C2C-C3C | -4.31 | 101.53 | 106.96 |
| 15 | A | 1123 | CLA | C1C-C2C-C3C | -4.31 | 101.53 | 106.96 |
| 15 | B | 1237 | CLA | O2D-CGD-CBD | 4.31 | 120.05 | 111.34 |
| 15 | A | 1126 | CLA | O2A-CGA-O1A | -4.31 | 112.22 | 123.48 |
| 15 | B | 1229 | CLA | O2A-CGA-O1A | -4.30 | 112.25 | 123.48 |
| 15 | B | 1214 | CLA | O2A-C1-C2 | 4.29 | 117.95 | 108.12 |
| 13 | A | 1108 | CL0 | C3B-C2B-C1B | -4.29 | 101.93 | 106.69 |
| 15 | B | 1225 | CLA | O2D-CGD-CBD | 4.29 | 120.01 | 111.34 |
| 15 | A | 1012 | CLA | C1C-C2C-C3C | -4.29 | 101.56 | 106.96 |
| 15 | A | 1106 | CLA | O2A-CGA-O1A | -4.29 | 112.27 | 123.48 |
| 15 | K | 1401 | CLA | O2D-CGD-CBD | 4.28 | 119.99 | 111.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1240 | CLA | C1C-C2C-C3C | -4.28 | 101.58 | 106.96 |
| 15 | A | 1133 | CLA | O2A-CGA-CBA | 4.28 | 123.69 | 110.50 |
| 15 | B | 1021 | CLA | O2A-CGA-CBA | 4.28 | 125.00 | 111.90 |
| 15 | A | 1022 | CLA | OBD-CAD-CBD | -4.28 | 119.48 | 125.94 |
| 15 | A | 1130 | CLA | C1C-C2C-C3C | -4.28 | 101.58 | 106.96 |
| 15 | A | 1122 | CLA | O2D-CGD-CBD | 4.28 | 119.98 | 111.34 |
| 15 | A | 1119 | CLA | O2D-CGD-CBD | 4.27 | 119.97 | 111.34 |
| 15 | B | 1231 | CLA | O2A-CGA-CBA | 4.27 | 124.98 | 111.90 |
| 15 | B | 1210 | CLA | O2A-CGA-CBA | 4.27 | 124.96 | 111.90 |
| 15 | B | 1203 | CLA | O2A-CGA-O1A | -4.27 | 112.33 | 123.48 |
| 15 | B | 1235 | CLA | O2A-CGA-CBA | 4.27 | 124.95 | 111.90 |
| 15 | B | 1023 | CLA | C1C-C2C-C3C | -4.26 | 101.60 | 106.96 |
| 15 | B | 1211 | CLA | C1C-C2C-C3C | -4.26 | 101.60 | 106.96 |
| 15 | B | 1210 | CLA | O2D-CGD-CBD | 4.26 | 119.94 | 111.34 |
| 15 | B | 1207 | CLA | O2A-CGA-CBA | 4.25 | 123.62 | 110.50 |
| 15 | B | 1214 | CLA | O2A-CGA-CBA | 4.25 | 124.92 | 111.90 |
| 15 | A | 1122 | CLA | C1C-C2C-C3C | -4.25 | 101.61 | 106.96 |
| 15 | B | 1213 | CLA | O2A-CGA-O1A | -4.24 | 112.39 | 123.48 |
| 15 | B | 1220 | CLA | C1C-C2C-C3C | -4.24 | 101.62 | 106.96 |
| 15 | A | 1131 | CLA | C3B-C2B-C1B | -4.24 | 101.99 | 106.69 |
| 15 | J | 1302 | CLA | O2D-CGD-CBD | 4.23 | 119.89 | 111.34 |
| 15 | B | 1238 | CLA | O2D-CGD-CBD | 4.23 | 119.90 | 111.34 |
| 15 | B | 1216 | CLA | O2D-CGD-CBD | 4.23 | 119.89 | 111.34 |
| 15 | A | 1132 | CLA | C1C-C2C-C3C | -4.23 | 101.64 | 106.96 |
| 15 | A | 1140 | CLA | C1C-C2C-C3C | -4.23 | 101.64 | 106.96 |
| 15 | B | 1222 | CLA | O2A-CGA-O1A | -4.22 | 112.44 | 123.48 |
| 15 | F | 1139 | CLA | C3B-C2B-C1B | -4.22 | 102.01 | 106.69 |
| 15 | A | 1117 | CLA | O2D-CGD-CBD | 4.22 | 119.87 | 111.34 |
| 15 | A | 1103 | CLA | C1C-C2C-C3C | -4.22 | 101.65 | 106.96 |
| 15 | A | 1117 | CLA | C1C-C2C-C3C | -4.22 | 101.65 | 106.96 |
| 15 | A | 1102 | CLA | O2A-CGA-CBA | 4.22 | 124.81 | 111.90 |
| 15 | B | 1220 | CLA | O2D-CGD-CBD | 4.22 | 119.86 | 111.34 |
| 15 | A | 1116 | CLA | O2A-CGA-CBA | 4.21 | 124.79 | 111.90 |
| 15 | A | 1127 | CLA | O2D-CGD-CBD | 4.21 | 119.85 | 111.34 |
| 15 | B | 1208 | CLA | O2D-CGD-CBD | 4.21 | 119.84 | 111.34 |
| 14 | A | 4003 | BCR | C24-C23-C22 | -4.21 | 119.92 | 126.22 |
| 15 | B | 1216 | CLA | O2A-CGA-O1A | -4.21 | 112.48 | 123.48 |
| 15 | A | 1122 | CLA | C4-C3-C2 | -4.21 | 115.15 | 123.52 |
| 15 | A | 1138 | CLA | O2A-CGA-O1A | -4.20 | 112.52 | 123.48 |
| 15 | B | 1221 | CLA | O2A-C1-C2 | 4.19 | 117.72 | 108.12 |
| 15 | B | 1206 | CLA | O2A-CGA-CBA | 4.19 | 123.42 | 110.50 |
| 15 | A | 1120 | CLA | O2A-CGA-CBA | 4.18 | 124.71 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1203 | CLA | O2D-CGD-CBD | 4.17 | 119.77 | 111.34 |
| 14 | F | 4015 | BCR | C7-C8-C9 | -4.17 | 119.97 | 126.22 |
| 15 | A | 1109 | CLA | O2A-CGA-CBA | 4.17 | 124.67 | 111.90 |
| 15 | B | 1217 | CLA | O2A-CGA-CBA | 4.17 | 124.65 | 111.90 |
| 14 | B | 4017 | BCR | C7-C8-C9 | -4.16 | 119.99 | 126.22 |
| 15 | A | 1130 | CLA | O2A-CGA-CBA | 4.16 | 124.63 | 111.90 |
| 14 | B | 4010 | BCR | C33-C5-C6 | -4.15 | 119.81 | 124.50 |
| 14 | A | 4001 | BCR | C33-C5-C6 | -4.15 | 119.81 | 124.50 |
| 15 | F | 1139 | CLA | O2A-CGA-O1A | -4.15 | 112.64 | 123.48 |
| 15 | A | 1101 | CLA | C1C-C2C-C3C | -4.13 | 101.76 | 106.96 |
| 15 | F | 1139 | CLA | O2D-CGD-CBD | 4.13 | 119.69 | 111.34 |
| 15 | A | 1138 | CLA | O2D-CGD-CBD | 4.13 | 119.68 | 111.34 |
| 14 | B | 4004 | BCR | C38-C26-C25 | -4.12 | 119.84 | 124.50 |
| 14 | B | 4011 | BCR | C33-C5-C6 | -4.12 | 119.84 | 124.50 |
| 15 | B | 1228 | CLA | C1C-C2C-C3C | -4.12 | 101.77 | 106.96 |
| 15 | A | 1101 | CLA | O2A-CGA-O1A | -4.12 | 112.72 | 123.48 |
| 15 | A | 1120 | CLA | O2D-CGD-CBD | 4.11 | 119.64 | 111.34 |
| 15 | B | 1228 | CLA | O2D-CGD-CBD | 4.11 | 119.64 | 111.34 |
| 15 | B | 1240 | CLA | O2D-CGD-CBD | 4.11 | 119.64 | 111.34 |
| 15 | A | 1113 | CLA | O2D-CGD-CBD | 4.10 | 119.63 | 111.34 |
| 15 | A | 1127 | CLA | C4-C3-C5 | 4.10 | 121.62 | 115.39 |
| 15 | A | 1124 | CLA | O2D-CGD-CBD | 4.10 | 119.62 | 111.34 |
| 15 | A | 1107 | CLA | O2A-CGA-CBA | 4.09 | 124.42 | 111.90 |
| 15 | A | 1135 | CLA | O2A-CGA-CBA | 4.09 | 124.41 | 111.90 |
| 15 | B | 1231 | CLA | O2D-CGD-CBD | 4.09 | 119.60 | 111.34 |
| 15 | B | 1205 | CLA | O2A-CGA-CBA | 4.08 | 124.39 | 111.90 |
| 12 | A | 5001 | LHG | O7-C7-C8 | 4.08 | 120.23 | 111.54 |
| 15 | A | 1126 | CLA | C1C-C2C-C3C | -4.07 | 101.83 | 106.96 |
| 15 | A | 1135 | CLA | O2D-CGD-CBD | 4.07 | 119.57 | 111.34 |
| 15 | B | 1206 | CLA | O2D-CGD-CBD | 4.07 | 119.57 | 111.34 |
| 14 | A | 4012 | BCR | C33-C5-C6 | -4.07 | 119.90 | 124.50 |
| 15 | B | 1202 | CLA | O2A-CGA-CBA | 4.07 | 124.35 | 111.90 |
| 15 | A | 1110 | CLA | O2D-CGD-CBD | 4.06 | 119.55 | 111.34 |
| 15 | A | 1111 | CLA | C1C-C2C-C3C | -4.06 | 101.85 | 106.96 |
| 15 | B | 1216 | CLA | O2A-C1-C2 | 4.06 | 117.42 | 108.12 |
| 15 | A | 1022 | CLA | C3B-CAB-CBB | -4.06 | 117.54 | 125.95 |
| 15 | A | 1137 | CLA | O2A-CGA-CBA | 4.06 | 124.32 | 111.90 |
| 15 | A | 1801 | CLA | O2D-CGD-CBD | 4.06 | 119.53 | 111.34 |
| 14 | B | 4011 | BCR | C7-C8-C9 | -4.05 | 120.15 | 126.22 |
| 15 | B | 1023 | CLA | O2D-CGD-CBD | 4.05 | 119.53 | 111.34 |
| 15 | A | 1107 | CLA | CAA-C2A-C1A | -4.05 | 101.78 | 112.51 |
| 15 | A | 1115 | CLA | C1C-C2C-C3C | -4.04 | 101.88 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | F | 4015 | BCR | C15-C14-C13 | -4.04 | 121.45 | 127.29 |
| 14 | B | 4011 | BCR | C38-C26-C25 | -4.03 | 119.94 | 124.50 |
| 15 | B | 1223 | CLA | O2A-CGA-CBA | 4.03 | 124.22 | 111.90 |
| 17 | B | 5002 | LMG | O7-C10-C11 | 4.02 | 120.11 | 111.54 |
| 15 | B | 1021 | CLA | O2D-CGD-CBD | 4.02 | 119.46 | 111.34 |
| 15 | B | 1219 | CLA | O2A-CGA-CBA | 4.02 | 124.20 | 111.90 |
| 15 | A | 1103 | CLA | O2A-CGA-O1A | -4.02 | 112.98 | 123.48 |
| 15 | A | 1107 | CLA | C1C-C2C-C3C | -4.02 | 101.91 | 106.96 |
| 14 | A | 4003 | BCR | C33-C5-C6 | -4.01 | 119.97 | 124.50 |
| 15 | A | 1110 | CLA | O2A-CGA-CBA | 4.01 | 124.17 | 111.90 |
| 15 | B | 1226 | CLA | O2A-CGA-CBA | 4.00 | 124.15 | 111.90 |
| 15 | B | 1215 | CLA | O2A-CGA-CBA | 4.00 | 124.14 | 111.90 |
| 14 | A | 4002 | BCR | C33-C5-C6 | -3.99 | 119.99 | 124.50 |
| 15 | A | 1117 | CLA | O2A-CGA-CBA | 3.99 | 124.10 | 111.90 |
| 15 | B | 1236 | CLA | O2A-CGA-CBA | 3.98 | 124.09 | 111.90 |
| 15 | B | 1234 | CLA | O2A-CGA-CBA | 3.98 | 124.08 | 111.90 |
| 15 | A | 1127 | CLA | O2A-CGA-CBA | 3.98 | 124.08 | 111.90 |
| 15 | A | 1012 | CLA | OBD-CAD-CBD | -3.98 | 119.93 | 125.94 |
| 15 | B | 1204 | CLA | C3B-CAB-CBB | -3.97 | 117.72 | 125.95 |
| 15 | A | 1140 | CLA | O2A-CGA-CBA | 3.97 | 124.07 | 111.90 |
| 14 | F | 4016 | BCR | C33-C5-C6 | -3.96 | 120.02 | 124.50 |
| 15 | A | 1132 | CLA | C3B-CAB-CBB | -3.96 | 117.76 | 125.95 |
| 15 | A | 1125 | CLA | OBD-CAD-C3D | -3.96 | 120.16 | 128.15 |
| 15 | B | 1210 | CLA | C1C-C2C-C3C | -3.96 | 101.98 | 106.96 |
| 13 | A | 1011 | CL0 | O2A-CGA-CBA | 3.95 | 124.00 | 111.90 |
| 14 | B | 4006 | BCR | C34-C9-C10 | -3.95 | 117.30 | 122.92 |
| 15 | K | 1402 | CLA | O2D-CGD-CBD | 3.94 | 119.31 | 111.34 |
| 15 | A | 1109 | CLA | O2D-CGD-CBD | 3.94 | 119.30 | 111.34 |
| 14 | A | 4012 | BCR | C37-C22-C21 | -3.94 | 117.31 | 122.92 |
| 14 | A | 4003 | BCR | C34-C9-C10 | -3.93 | 117.32 | 122.92 |
| 14 | B | 4010 | BCR | C38-C26-C25 | -3.93 | 120.06 | 124.50 |
| 12 | A | 5005 | LHG | O7-C7-C8 | 3.93 | 119.91 | 111.54 |
| 15 | F | 1410 | CLA | C4-C3-C2 | -3.92 | 115.71 | 123.52 |
| 15 | A | 1136 | CLA | O2A-C1-C2 | 3.92 | 117.09 | 108.12 |
| 14 | B | 4005 | BCR | C33-C5-C6 | -3.91 | 120.08 | 124.50 |
| 15 | A | 1124 | CLA | O2A-CGA-O1A | -3.91 | 113.26 | 123.48 |
| 15 | A | 1138 | CLA | CMC-C2C-C1C | 3.91 | 130.52 | 124.95 |
| 15 | A | 1114 | CLA | O2A-CGA-CBA | 3.89 | 123.80 | 111.90 |
| 15 | A | 1125 | CLA | O2A-CGA-CBA | 3.89 | 123.80 | 111.90 |
| 15 | A | 1125 | CLA | C1C-C2C-C3C | -3.89 | 102.07 | 106.96 |
| 15 | B | 1232 | CLA | O2D-CGD-CBD | 3.88 | 119.18 | 111.34 |
| 15 | A | 1128 | CLA | C3B-C2B-C1B | -3.88 | 102.39 | 106.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 4001 | BCR | C24-C23-C22 | -3.87 | 120.42 | 126.22 |
| 14 | A | 4008 | BCR | C38-C26-C27 | 3.87 | 120.73 | 113.39 |
| 15 | B | 1219 | CLA | CMB-C2B-C3B | 3.87 | 132.45 | 125.16 |
| 14 | B | 4004 | BCR | C19-C18-C17 | 3.87 | 124.92 | 118.98 |
| 15 | B | 1220 | CLA | O2A-CGA-CBA | 3.86 | 123.72 | 111.90 |
| 15 | B | 1237 | CLA | C4-C3-C5 | 3.86 | 121.25 | 115.39 |
| 15 | B | 1228 | CLA | O2A-CGA-CBA | 3.85 | 123.70 | 111.90 |
| 15 | B | 1023 | CLA | O2A-CGA-CBA | 3.85 | 123.69 | 111.90 |
| 15 | B | 1013 | CLA | O2D-CGD-CBD | 3.83 | 119.08 | 111.34 |
| 15 | A | 1022 | CLA | O2A-CGA-CBA | 3.83 | 123.61 | 111.90 |
| 15 | B | 1229 | CLA | O2A-CGA-CBA | 3.82 | 123.59 | 111.90 |
| 15 | A | 1138 | CLA | C1C-C2C-C3C | -3.82 | 102.16 | 106.96 |
| 15 | A | 1104 | CLA | CMC-C2C-C1C | 3.80 | 130.38 | 124.95 |
| 14 | B | 4014 | BCR | C37-C22-C21 | -3.80 | 117.51 | 122.92 |
| 15 | B | 1237 | CLA | C4-C3-C2 | -3.79 | 115.98 | 123.52 |
| 14 | B | 4011 | BCR | C37-C22-C21 | -3.78 | 117.53 | 122.92 |
| 15 | B | 1213 | CLA | O2A-CGA-CBA | 3.78 | 123.47 | 111.90 |
| 14 | A | 4001 | BCR | C38-C26-C25 | -3.77 | 120.24 | 124.50 |
| 14 | A | 4008 | BCR | C7-C8-C9 | -3.77 | 120.58 | 126.22 |
| 15 | B | 1230 | CLA | C4-C3-C2 | -3.77 | 116.03 | 123.52 |
| 14 | A | 4008 | BCR | C27-C26-C25 | -3.76 | 117.89 | 122.86 |
| 14 | A | 4001 | BCR | C36-C18-C17 | -3.76 | 117.56 | 122.92 |
| 15 | A | 1012 | CLA | O2A-CGA-CBA | 3.75 | 123.39 | 111.90 |
| 15 | A | 1123 | CLA | O2A-CGA-CBA | 3.74 | 123.34 | 111.90 |
| 14 | A | 4007 | BCR | C38-C26-C25 | -3.74 | 120.28 | 124.50 |
| 15 | A | 1128 | CLA | O2A-CGA-CBA | 3.73 | 123.33 | 111.90 |
| 14 | B | 4005 | BCR | C7-C8-C9 | -3.73 | 120.64 | 126.22 |
| 14 | B | 4004 | BCR | C36-C18-C17 | -3.72 | 117.62 | 122.92 |
| 15 | A | 1106 | CLA | O2A-CGA-CBA | 3.72 | 123.30 | 111.90 |
| 15 | A | 1105 | CLA | O2A-CGA-CBA | 3.72 | 123.28 | 111.90 |
| 15 | B | 1235 | CLA | C4D-ND-C1D | -3.71 | 102.09 | 106.57 |
| 14 | B | 4006 | BCR | C33-C5-C6 | -3.70 | 120.32 | 124.50 |
| 15 | F | 1410 | CLA | O2A-CGA-CBA | 3.70 | 123.22 | 111.90 |
| 15 | A | 1109 | CLA | C4D-ND-C1D | -3.69 | 102.10 | 106.57 |
| 15 | B | 1228 | CLA | C4D-ND-C1D | -3.69 | 102.11 | 106.57 |
| 15 | B | 1211 | CLA | CMC-C2C-C1C | 3.69 | 130.21 | 124.95 |
| 14 | A | 4002 | BCR | C38-C26-C27 | 3.69 | 120.38 | 113.39 |
| 15 | A | 1125 | CLA | CMC-C2C-C1C | 3.69 | 130.21 | 124.95 |
| 14 | B | 4005 | BCR | C24-C23-C22 | -3.69 | 120.70 | 126.22 |
| 15 | A | 1138 | CLA | O2A-CGA-CBA | 3.69 | 123.18 | 111.90 |
| 15 | A | 1118 | CLA | C4D-ND-C1D | -3.68 | 102.12 | 106.57 |
| 15 | A | 1135 | CLA | C4-C3-C5 | 3.68 | 120.97 | 115.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1237 | CLA | O2A-CGA-CBA | 3.68 | 123.15 | 111.90 |
| 14 | B | 4017 | BCR | C3-C4-C5 | -3.67 | 107.77 | 113.81 |
| 15 | A | 1136 | CLA | C4D-ND-C1D | -3.67 | 102.13 | 106.57 |
| 14 | B | 4009 | BCR | C34-C9-C10 | -3.67 | 117.69 | 122.92 |
| 15 | A | 1116 | CLA | C3B-CAB-CBB | -3.65 | 118.39 | 125.95 |
| 15 | A | 1022 | CLA | OBD-CAD-C3D | -3.63 | 120.81 | 128.15 |
| 15 | B | 1235 | CLA | CMC-C2C-C1C | 3.63 | 130.13 | 124.95 |
| 15 | A | 1126 | CLA | O2A-CGA-CBA | 3.63 | 123.01 | 111.90 |
| 14 | A | 4007 | BCR | C38-C26-C27 | 3.63 | 120.26 | 113.39 |
| 15 | A | 1132 | CLA | C4D-ND-C1D | -3.62 | 102.19 | 106.57 |
| 15 | K | 1402 | CLA | C4D-ND-C1D | -3.62 | 102.19 | 106.57 |
| 14 | A | 4001 | BCR | C37-C22-C21 | -3.62 | 117.77 | 122.92 |
| 15 | B | 1224 | CLA | C3B-CAB-CBB | -3.58 | 118.55 | 125.95 |
| 15 | B | 1229 | CLA | C4D-ND-C1D | -3.58 | 102.25 | 106.57 |
| 14 | B | 4011 | BCR | C33-C5-C4 | 3.57 | 120.16 | 113.39 |
| 15 | A | 1131 | CLA | C4D-ND-C1D | -3.57 | 102.25 | 106.57 |
| 14 | A | 4003 | BCR | C37-C22-C21 | -3.56 | 117.85 | 122.92 |
| 15 | B | 1228 | CLA | CMB-C2B-C3B | 3.56 | 131.87 | 125.16 |
| 15 | F | 1139 | CLA | O2A-CGA-CBA | 3.56 | 122.79 | 111.90 |
| 15 | A | 1134 | CLA | O2D-CGD-CBD | 3.55 | 118.52 | 111.34 |
| 15 | A | 1107 | CLA | C4D-ND-C1D | -3.55 | 102.28 | 106.57 |
| 15 | A | 1115 | CLA | C4D-ND-C1D | -3.55 | 102.28 | 106.57 |
| 15 | A | 1103 | CLA | C4D-ND-C1D | -3.55 | 102.28 | 106.57 |
| 15 | A | 1122 | CLA | C4D-ND-C1D | -3.53 | 102.30 | 106.57 |
| 14 | A | 4001 | BCR | C19-C18-C17 | 3.52 | 124.39 | 118.98 |
| 14 | A | 4012 | BCR | C36-C18-C17 | -3.51 | 117.92 | 122.92 |
| 14 | B | 4005 | BCR | C36-C18-C17 | -3.51 | 117.92 | 122.92 |
| 15 | B | 1202 | CLA | C4D-ND-C1D | -3.50 | 102.34 | 106.57 |
| 15 | F | 1410 | CLA | CMC-C2C-C1C | 3.50 | 129.94 | 124.95 |
| 15 | A | 1140 | CLA | C4D-ND-C1D | -3.50 | 102.34 | 106.57 |
| 15 | J | 1303 | CLA | C4D-ND-C1D | -3.49 | 102.35 | 106.57 |
| 12 | B | 5004 | LHG | C5-O7-C7 | -3.49 | 109.66 | 117.86 |
| 15 | A | 1138 | CLA | C4D-ND-C1D | -3.48 | 102.36 | 106.57 |
| 15 | B | 1013 | CLA | C1-O2A-CGA | 3.47 | 127.10 | 117.00 |
| 15 | B | 1225 | CLA | CMC-C2C-C1C | 3.47 | 129.89 | 124.95 |
| 14 | F | 4016 | BCR | C35-C13-C14 | -3.47 | 117.98 | 122.92 |
| 15 | A | 1104 | CLA | C1-C2-C3 | -3.47 | 120.22 | 126.23 |
| 14 | B | 4009 | BCR | C19-C18-C17 | 3.46 | 124.31 | 118.98 |
| 15 | A | 1012 | CLA | C3B-CAB-CBB | -3.46 | 118.78 | 125.95 |
| 15 | A | 1125 | CLA | C3C-C4C-NC | 3.46 | 114.32 | 110.15 |
| 15 | B | 1230 | CLA | CMC-C2C-C1C | 3.46 | 129.88 | 124.95 |
| 15 | F | 1139 | CLA | C4D-ND-C1D | -3.46 | 102.39 | 106.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1114 | CLA | C4D-ND-C1D | -3.45 | 102.39 | 106.57 |
| 15 | B | 1013 | CLA | C4D-ND-C1D | -3.45 | 102.40 | 106.57 |
| 15 | B | 1225 | CLA | O2A-CGA-CBA | 3.45 | 122.46 | 111.90 |
| 14 | F | 4016 | BCR | C3-C4-C5 | -3.45 | 108.14 | 113.81 |
| 15 | B | 1237 | CLA | CMC-C2C-C1C | 3.45 | 129.87 | 124.95 |
| 14 | B | 4005 | BCR | C19-C18-C17 | 3.45 | 124.28 | 118.98 |
| 15 | J | 1302 | CLA | C4D-ND-C1D | -3.44 | 102.41 | 106.57 |
| 15 | A | 1134 | CLA | C4D-ND-C1D | -3.44 | 102.41 | 106.57 |
| 14 | B | 4009 | BCR | C36-C18-C17 | -3.44 | 118.02 | 122.92 |
| 15 | A | 1135 | CLA | C4-C3-C2 | -3.44 | 116.68 | 123.52 |
| 15 | B | 1207 | CLA | C4D-ND-C1D | -3.43 | 102.42 | 106.57 |
| 14 | F | 4016 | BCR | C12-C13-C14 | 3.43 | 124.26 | 118.98 |
| 15 | B | 1216 | CLA | O2A-CGA-CBA | 3.43 | 122.40 | 111.90 |
| 15 | A | 1125 | CLA | C4D-ND-C1D | -3.42 | 102.43 | 106.57 |
| 15 | B | 1215 | CLA | C4-C3-C2 | -3.42 | 116.70 | 123.52 |
| 14 | B | 4009 | BCR | C38-C26-C27 | 3.42 | 119.88 | 113.39 |
| 15 | A | 1101 | CLA | O2A-CGA-CBA | 3.42 | 122.37 | 111.90 |
| 15 | B | 1223 | CLA | C1-C2-C3 | -3.42 | 120.30 | 126.23 |
| 13 | A | 1108 | CL0 | C4D-ND-C1D | -3.42 | 102.44 | 106.57 |
| 15 | B | 1203 | CLA | O2A-CGA-CBA | 3.41 | 122.35 | 111.90 |
| 15 | B | 1220 | CLA | CMB-C2B-C3B | 3.41 | 131.59 | 125.16 |
| 15 | K | 1401 | CLA | C4D-ND-C1D | -3.41 | 102.45 | 106.57 |
| 15 | A | 1111 | CLA | C4D-ND-C1D | -3.41 | 102.45 | 106.57 |
| 15 | B | 1213 | CLA | CMC-C2C-C1C | 3.40 | 129.80 | 124.95 |
| 15 | A | 1137 | CLA | C4D-ND-C1D | -3.40 | 102.46 | 106.57 |
| 14 | B | 4004 | BCR | C37-C22-C21 | -3.40 | 118.08 | 122.92 |
| 14 | B | 4017 | BCR | C19-C18-C17 | 3.40 | 124.20 | 118.98 |
| 15 | A | 1124 | CLA | C3B-CAB-CBB | -3.40 | 118.92 | 125.95 |
| 15 | A | 1122 | CLA | CMC-C2C-C1C | 3.40 | 129.79 | 124.95 |
| 15 | B | 1236 | CLA | C4D-ND-C1D | -3.39 | 102.47 | 106.57 |
| 15 | B | 1204 | CLA | C4D-ND-C1D | -3.39 | 102.48 | 106.57 |
| 15 | F | 1139 | CLA | CMC-C2C-C1C | 3.38 | 129.77 | 124.95 |
| 15 | A | 1126 | CLA | C3B-CAB-CBB | -3.38 | 118.95 | 125.95 |
| 15 | B | 1229 | CLA | C1-C2-C3 | -3.38 | 120.36 | 126.23 |
| 15 | B | 1219 | CLA | C4D-ND-C1D | -3.38 | 102.48 | 106.57 |
| 15 | A | 1109 | CLA | CMC-C2C-C1C | 3.37 | 129.76 | 124.95 |
| 15 | B | 1023 | CLA | C4D-ND-C1D | -3.37 | 102.49 | 106.57 |
| 15 | B | 1221 | CLA | C4D-ND-C1D | -3.37 | 102.49 | 106.57 |
| 15 | A | 1113 | CLA | C4D-ND-C1D | -3.37 | 102.49 | 106.57 |
| 14 | A | 4001 | BCR | C34-C9-C10 | -3.37 | 118.12 | 122.92 |
| 15 | A | 1104 | CLA | C4D-ND-C1D | -3.37 | 102.50 | 106.57 |
| 15 | B | 1213 | CLA | C4D-ND-C1D | -3.36 | 102.51 | 106.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 4017 | BCR | C34-C9-C10 | -3.36 | 118.14 | 122.92 |
| 15 | A | 1112 | CLA | C4D-ND-C1D | -3.36 | 102.51 | 106.57 |
| 15 | F | 1301 | CLA | CMC-C2C-C1C | 3.35 | 129.73 | 124.95 |
| 15 | B | 1230 | CLA | C4D-ND-C1D | -3.35 | 102.52 | 106.57 |
| 15 | B | 1212 | CLA | C4D-ND-C1D | -3.35 | 102.52 | 106.57 |
| 15 | B | 1208 | CLA | C4D-ND-C1D | -3.35 | 102.52 | 106.57 |
| 15 | A | 1127 | CLA | C4D-ND-C1D | -3.34 | 102.53 | 106.57 |
| 14 | A | 4002 | BCR | C19-C18-C17 | 3.34 | 124.12 | 118.98 |
| 15 | A | 1116 | CLA | C4D-ND-C1D | -3.34 | 102.53 | 106.57 |
| 15 | A | 1106 | CLA | CMC-C2C-C1C | 3.33 | 129.71 | 124.95 |
| 14 | B | 4005 | BCR | C37-C22-C21 | -3.33 | 118.18 | 122.92 |
| 15 | B | 1223 | CLA | CMC-C2C-C1C | 3.33 | 129.70 | 124.95 |
| 13 | A | 1108 | CL0 | O2D-CGD-CBD | 3.32 | 118.06 | 111.34 |
| 15 | A | 1110 | CLA | C4D-ND-C1D | -3.32 | 102.55 | 106.57 |
| 15 | B | 1234 | CLA | C4D-ND-C1D | -3.32 | 102.55 | 106.57 |
| 15 | A | 1012 | CLA | C3C-C4C-NC | 3.32 | 114.15 | 110.15 |
| 15 | B | 1201 | CLA | CMC-C2C-C1C | 3.31 | 129.68 | 124.95 |
| 15 | A | 1126 | CLA | C4D-ND-C1D | -3.31 | 102.56 | 106.57 |
| 14 | J | 4013 | BCR | C33-C5-C4 | 3.31 | 119.67 | 113.39 |
| 14 | J | 4013 | BCR | C38-C26-C27 | 3.31 | 119.66 | 113.39 |
| 12 | A | 5003 | LHG | C5-O7-C7 | -3.31 | 110.09 | 117.86 |
| 14 | B | 4017 | BCR | C36-C18-C17 | -3.30 | 118.21 | 122.92 |
| 15 | B | 1226 | CLA | C4D-ND-C1D | -3.31 | 102.57 | 106.57 |
| 15 | B | 1208 | CLA | CMB-C2B-C3B | 3.30 | 131.39 | 125.16 |
| 15 | B | 1224 | CLA | C4D-ND-C1D | -3.29 | 102.59 | 106.57 |
| 15 | A | 1105 | CLA | CMC-C2C-C1C | 3.29 | 129.64 | 124.95 |
| 15 | A | 1122 | CLA | O2A-CGA-CBA | 3.29 | 121.97 | 111.90 |
| 15 | A | 1110 | CLA | C1-C2-C3 | -3.29 | 120.53 | 126.23 |
| 15 | B | 1217 | CLA | CMC-C2C-C1C | 3.29 | 129.64 | 124.95 |
| 15 | A | 1022 | CLA | CMC-C2C-C1C | 3.29 | 129.63 | 124.95 |
| 14 | A | 4003 | BCR | C33-C5-C4 | 3.28 | 119.61 | 113.39 |
| 15 | B | 1237 | CLA | C4D-ND-C1D | -3.28 | 102.60 | 106.57 |
| 15 | A | 1112 | CLA | CMC-C2C-C1C | 3.28 | 129.63 | 124.95 |
| 14 | B | 4005 | BCR | C38-C26-C25 | -3.28 | 120.80 | 124.50 |
| 14 | F | 4015 | BCR | C38-C26-C25 | -3.28 | 120.80 | 124.50 |
| 15 | B | 1202 | CLA | C3B-CAB-CBB | -3.28 | 119.17 | 125.95 |
| 15 | A | 1106 | CLA | C4D-ND-C1D | -3.27 | 102.61 | 106.57 |
| 15 | B | 1217 | CLA | C3B-CAB-CBB | -3.27 | 119.17 | 125.95 |
| 15 | A | 1126 | CLA | CMC-C2C-C1C | 3.27 | 129.61 | 124.95 |
| 15 | B | 1216 | CLA | C3B-CAB-CBB | -3.27 | 119.19 | 125.95 |
| 14 | A | 4002 | BCR | C38-C26-C25 | -3.27 | 120.81 | 124.50 |
| 14 | B | 4011 | BCR | C8-C9-C10 | 3.26 | 124.00 | 118.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | F | 4015 | BCR | C38-C26-C27 | 3.26 | 119.56 | 113.39 |
| 15 | B | 1216 | CLA | C4D-ND-C1D | -3.26 | 102.63 | 106.57 |
| 14 | A | 4002 | BCR | C36-C18-C17 | -3.26 | 118.28 | 122.92 |
| 14 | B | 4010 | BCR | C24-C23-C22 | -3.26 | 121.34 | 126.22 |
| 15 | B | 1222 | CLA | C4D-ND-C1D | -3.25 | 102.64 | 106.57 |
| 14 | B | 4006 | BCR | C33-C5-C4 | 3.25 | 119.56 | 113.39 |
| 14 | A | 4002 | BCR | C34-C9-C10 | -3.25 | 118.28 | 122.92 |
| 15 | A | 1119 | CLA | CMB-C2B-C3B | 3.25 | 131.29 | 125.16 |
| 14 | B | 4006 | BCR | C36-C18-C17 | -3.25 | 118.29 | 122.92 |
| 15 | B | 1231 | CLA | C4D-ND-C1D | -3.25 | 102.64 | 106.57 |
| 15 | A | 1121 | CLA | C4D-ND-C1D | -3.25 | 102.65 | 106.57 |
| 14 | A | 4012 | BCR | C7-C8-C9 | -3.24 | 121.36 | 126.22 |
| 15 | K | 1401 | CLA | C3B-CAB-CBB | -3.24 | 119.24 | 125.95 |
| 10 | A | 2001 | PQN | C14-C13-C15 | 3.24 | 120.31 | 115.39 |
| 15 | B | 1238 | CLA | C4D-ND-C1D | -3.24 | 102.65 | 106.57 |
| 14 | B | 4011 | BCR | C23-C22-C21 | 3.24 | 123.96 | 118.98 |
| 15 | B | 1210 | CLA | CMB-C2B-C3B | 3.24 | 131.26 | 125.16 |
| 15 | B | 1218 | CLA | C4-C3-C5 | 3.23 | 122.60 | 114.55 |
| 14 | B | 4009 | BCR | C3-C4-C5 | -3.23 | 108.50 | 113.81 |
| 14 | B | 4009 | BCR | C38-C26-C25 | -3.23 | 120.85 | 124.50 |
| 15 | B | 1214 | CLA | CMC-C2C-C1C | 3.23 | 129.55 | 124.95 |
| 15 | B | 1234 | CLA | CGD-CBD-CHA | -3.22 | 106.17 | 113.65 |
| 13 | A | 1011 | CL0 | CMC-C2C-C1C | 3.22 | 129.54 | 124.95 |
| 15 | A | 1130 | CLA | CMC-C2C-C1C | 3.22 | 129.54 | 124.95 |
| 15 | A | 1129 | CLA | C4D-ND-C1D | -3.22 | 102.68 | 106.57 |
| 15 | F | 1410 | CLA | C4D-ND-C1D | -3.22 | 102.68 | 106.57 |
| 15 | A | 1105 | CLA | C4D-ND-C1D | -3.21 | 102.68 | 106.57 |
| 15 | B | 1219 | CLA | CMC-C2C-C1C | 3.22 | 129.53 | 124.95 |
| 15 | A | 1117 | CLA | C3B-CAB-CBB | -3.22 | 119.29 | 125.95 |
| 15 | B | 1240 | CLA | C4D-ND-C1D | -3.21 | 102.69 | 106.57 |
| 15 | A | 1135 | CLA | C4D-ND-C1D | -3.21 | 102.69 | 106.57 |
| 15 | B | 1223 | CLA | C3C-C4C-NC | 3.21 | 114.02 | 110.15 |
| 15 | B | 1220 | CLA | CMC-C2C-C1C | 3.21 | 129.53 | 124.95 |
| 14 | B | 4011 | BCR | C38-C26-C27 | 3.21 | 119.47 | 113.39 |
| 15 | B | 1229 | CLA | CMC-C2C-C1C | 3.21 | 129.52 | 124.95 |
| 15 | B | 1211 | CLA | C4D-ND-C1D | -3.20 | 102.70 | 106.57 |
| 15 | A | 1012 | CLA | C4-C3-C5 | 3.20 | 120.25 | 115.39 |
| 15 | B | 1231 | CLA | C4-C3-C5 | 3.20 | 120.25 | 115.39 |
| 15 | A | 1110 | CLA | C3B-CAB-CBB | -3.20 | 119.33 | 125.95 |
| 15 | A | 1123 | CLA | C4D-ND-C1D | -3.20 | 102.71 | 106.57 |
| 14 | A | 4007 | BCR | C33-C5-C6 | -3.20 | 120.89 | 124.50 |
| 14 | B | 4006 | BCR | C7-C8-C9 | -3.19 | 121.44 | 126.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1210 | CLA | CMC-C2C-C1C | 3.19 | 129.50 | 124.95 |
| 15 | B | 1220 | CLA | C4D-ND-C1D | -3.19 | 102.71 | 106.57 |
| 15 | B | 1230 | CLA | C3C-C4C-NC | 3.19 | 114.00 | 110.15 |
| 15 | B | 1210 | CLA | C4D-ND-C1D | -3.19 | 102.72 | 106.57 |
| 15 | F | 1410 | CLA | C3B-CAB-CBB | -3.19 | 119.36 | 125.95 |
| 15 | B | 1209 | CLA | C4D-ND-C1D | -3.18 | 102.72 | 106.57 |
| 14 | A | 4001 | BCR | C38-C26-C27 | 3.18 | 119.42 | 113.39 |
| 15 | B | 1203 | CLA | C4D-ND-C1D | -3.18 | 102.72 | 106.57 |
| 15 | A | 1120 | CLA | C4D-ND-C1D | -3.18 | 102.72 | 106.57 |
| 15 | F | 1301 | CLA | C4D-ND-C1D | -3.18 | 102.72 | 106.57 |
| 14 | A | 4001 | BCR | C3-C4-C5 | -3.18 | 108.58 | 113.81 |
| 15 | A | 1101 | CLA | CGD-CBD-CHA | -3.18 | 106.28 | 113.65 |
| 15 | B | 1205 | CLA | C3B-CAB-CBB | -3.18 | 119.37 | 125.95 |
| 15 | B | 1219 | CLA | C4-C3-C5 | 3.18 | 120.22 | 115.39 |
| 15 | A | 1101 | CLA | CMC-C2C-C1C | 3.18 | 129.48 | 124.95 |
| 15 | B | 1238 | CLA | CMC-C2C-C1C | 3.18 | 129.48 | 124.95 |
| 15 | B | 1223 | CLA | C4D-ND-C1D | -3.17 | 102.73 | 106.57 |
| 15 | B | 1227 | CLA | C4D-ND-C1D | -3.17 | 102.74 | 106.57 |
| 14 | A | 4007 | BCR | C24-C23-C22 | -3.17 | 121.47 | 126.22 |
| 15 | A | 1121 | CLA | CMC-C2C-C1C | 3.16 | 129.46 | 124.95 |
| 14 | B | 4014 | BCR | C23-C22-C21 | 3.16 | 123.84 | 118.98 |
| 15 | A | 1131 | CLA | CMC-C2C-C1C | 3.16 | 129.46 | 124.95 |
| 15 | A | 1102 | CLA | CMB-C2B-C3B | 3.16 | 131.12 | 125.16 |
| 15 | A | 1138 | CLA | CED-O2D-CGD | 3.16 | 123.53 | 116.00 |
| 15 | A | 1119 | CLA | C4D-ND-C1D | -3.16 | 102.75 | 106.57 |
| 15 | B | 1206 | CLA | CMC-C2C-C1C | 3.16 | 129.45 | 124.95 |
| 15 | B | 1217 | CLA | C4D-ND-C1D | -3.16 | 102.75 | 106.57 |
| 15 | J | 1302 | CLA | CMC-C2C-C1C | 3.16 | 129.45 | 124.95 |
| 14 | A | 4007 | BCR | C3-C4-C5 | -3.16 | 108.62 | 113.81 |
| 15 | B | 1232 | CLA | C4D-ND-C1D | -3.15 | 102.76 | 106.57 |
| 15 | A | 1801 | CLA | C3C-C4C-NC | 3.15 | 113.95 | 110.15 |
| 15 | A | 1101 | CLA | C4D-ND-C1D | -3.15 | 102.76 | 106.57 |
| 15 | A | 1124 | CLA | C1-O2A-CGA | 3.15 | 126.16 | 117.00 |
| 14 | J | 4013 | BCR | C30-C25-C26 | -3.15 | 118.03 | 122.59 |
| 15 | A | 1107 | CLA | C1-C2-C3 | -3.14 | 122.13 | 126.05 |
| 15 | A | 1132 | CLA | C1-C2-C3 | -3.14 | 120.78 | 126.23 |
| 15 | A | 1133 | CLA | C4D-ND-C1D | -3.14 | 102.78 | 106.57 |
| 15 | B | 1221 | CLA | C3C-C4C-NC | 3.13 | 113.93 | 110.15 |
| 15 | B | 1021 | CLA | CMC-C2C-C1C | 3.14 | 129.42 | 124.95 |
| 15 | A | 1132 | CLA | C4-C3-C5 | 3.13 | 120.14 | 115.39 |
| 15 | A | 1123 | CLA | O2D-CGD-O1D | -3.12 | 117.52 | 123.79 |
| 15 | B | 1218 | CLA | C4-C3-C2 | -3.12 | 117.31 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1221 | CLA | C4-C3-C2 | -3.12 | 117.31 | 123.52 |
| 15 | B | 1218 | CLA | C4D-ND-C1D | -3.12 | 102.80 | 106.57 |
| 15 | B | 1205 | CLA | C4D-ND-C1D | -3.12 | 102.80 | 106.57 |
| 15 | B | 1206 | CLA | C4D-ND-C1D | -3.12 | 102.80 | 106.57 |
| 15 | A | 1123 | CLA | CAC-C3C-C4C | 3.11 | 129.52 | 124.85 |
| 15 | A | 1117 | CLA | C4D-ND-C1D | -3.11 | 102.81 | 106.57 |
| 15 | B | 1212 | CLA | CMC-C2C-C1C | 3.11 | 129.38 | 124.95 |
| 15 | A | 1140 | CLA | CMC-C2C-C1C | 3.11 | 129.38 | 124.95 |
| 15 | K | 1402 | CLA | C3B-CAB-CBB | -3.10 | 119.53 | 125.95 |
| 15 | A | 1134 | CLA | CMC-C2C-C1C | 3.10 | 129.37 | 124.95 |
| 15 | A | 1127 | CLA | CMC-C2C-C1C | 3.10 | 129.37 | 124.95 |
| 15 | A | 1012 | CLA | CMC-C2C-C1C | 3.10 | 129.37 | 124.95 |
| 14 | A | 4002 | BCR | C7-C8-C9 | -3.10 | 121.58 | 126.22 |
| 15 | B | 1201 | CLA | C4D-ND-C1D | -3.10 | 102.83 | 106.57 |
| 15 | A | 1103 | CLA | O2A-CGA-CBA | 3.09 | 121.36 | 111.90 |
| 14 | B | 4010 | BCR | C3-C4-C5 | -3.09 | 108.73 | 113.81 |
| 15 | A | 1123 | CLA | CMC-C2C-C1C | 3.09 | 129.35 | 124.95 |
| 15 | B | 1021 | CLA | C4D-ND-C1D | -3.09 | 102.83 | 106.57 |
| 15 | A | 1107 | CLA | C4B-CHC-C1C | 3.09 | 131.53 | 127.47 |
| 15 | A | 1801 | CLA | C4D-ND-C1D | -3.09 | 102.84 | 106.57 |
| 15 | B | 1226 | CLA | O2D-CGD-O1D | -3.09 | 117.59 | 123.79 |
| 15 | B | 1222 | CLA | O2D-CGD-O1D | -3.08 | 117.60 | 123.79 |
| 15 | B | 1219 | CLA | C4-C3-C2 | -3.08 | 117.38 | 123.52 |
| 15 | A | 1118 | CLA | CMC-C2C-C1C | 3.08 | 129.34 | 124.95 |
| 15 | B | 1214 | CLA | C4D-ND-C1D | -3.08 | 102.85 | 106.57 |
| 14 | B | 4017 | BCR | C38-C26-C27 | 3.07 | 119.21 | 113.39 |
| 15 | B | 1239 | CLA | C4D-ND-C1D | -3.07 | 102.86 | 106.57 |
| 15 | A | 1127 | CLA | C3C-C4C-NC | 3.07 | 113.85 | 110.15 |
| 14 | A | 4002 | BCR | C27-C26-C25 | -3.07 | 118.81 | 122.86 |
| 14 | B | 4004 | BCR | C33-C5-C4 | 3.07 | 119.20 | 113.39 |
| 14 | B | 4010 | BCR | C36-C18-C17 | -3.06 | 118.56 | 122.92 |
| 15 | B | 1216 | CLA | CMB-C2B-C3B | 3.06 | 130.93 | 125.16 |
| 15 | B | 1234 | CLA | C3B-CAB-CBB | -3.06 | 119.62 | 125.95 |
| 15 | A | 1124 | CLA | C4D-ND-C1D | -3.06 | 102.87 | 106.57 |
| 15 | A | 1102 | CLA | C4D-ND-C1D | -3.06 | 102.87 | 106.57 |
| 15 | A | 1102 | CLA | CMC-C2C-C1C | 3.06 | 129.31 | 124.95 |
| 15 | A | 1115 | CLA | C3C-C4C-NC | 3.05 | 113.83 | 110.15 |
| 15 | K | 1402 | CLA | CMC-C2C-C1C | 3.05 | 129.30 | 124.95 |
| 14 | J | 4013 | BCR | C4-C5-C6 | -3.05 | 118.83 | 122.86 |
| 15 | A | 1128 | CLA | C4D-ND-C1D | -3.05 | 102.89 | 106.57 |
| 15 | A | 1124 | CLA | CMC-C2C-C1C | 3.04 | 129.28 | 124.95 |
| 15 | A | 1111 | CLA | CMC-C2C-C1C | 3.03 | 129.28 | 124.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1221 | CLA | CMC-C2C-C1C | 3.03 | 129.27 | 124.95 |
| 15 | A | 1113 | CLA | CMC-C2C-C1C | 3.03 | 129.27 | 124.95 |
| 15 | A | 1117 | CLA | CMC-C2C-C1C | 3.03 | 129.27 | 124.95 |
| 13 | A | 1011 | CL0 | CHB-C4A-NA | 3.03 | 128.61 | 124.38 |
| 15 | B | 1205 | CLA | CMC-C2C-C1C | 3.03 | 129.26 | 124.95 |
| 14 | J | 4013 | BCR | C36-C18-C17 | -3.03 | 118.61 | 122.92 |
| 15 | A | 1110 | CLA | CMC-C2C-C1C | 3.02 | 129.26 | 124.95 |
| 15 | A | 1130 | CLA | CMB-C2B-C3B | 3.02 | 130.86 | 125.16 |
| 15 | B | 1204 | CLA | CMC-C2C-C1C | 3.02 | 129.26 | 124.95 |
| 15 | B | 1234 | CLA | C4-C3-C2 | -3.02 | 117.50 | 123.52 |
| 15 | B | 1218 | CLA | CMC-C2C-C1C | 3.02 | 129.26 | 124.95 |
| 15 | A | 1133 | CLA | CMC-C2C-C1C | 3.02 | 129.25 | 124.95 |
| 14 | A | 4012 | BCR | C19-C18-C17 | 3.02 | 123.62 | 118.98 |
| 15 | B | 1205 | CLA | O2D-CGD-O1D | -3.01 | 117.74 | 123.79 |
| 15 | A | 1801 | CLA | C3B-CAB-CBB | -3.01 | 119.71 | 125.95 |
| 15 | A | 1130 | CLA | C2B-C1B-CHB | -3.01 | 120.29 | 126.00 |
| 14 | B | 4017 | BCR | C33-C5-C4 | 3.01 | 119.10 | 113.39 |
| 15 | B | 1231 | CLA | C4-C3-C2 | -3.01 | 117.53 | 123.52 |
| 15 | J | 1303 | CLA | C3C-C4C-NC | 3.01 | 113.78 | 110.15 |
| 15 | B | 1225 | CLA | C4D-ND-C1D | -3.00 | 102.94 | 106.57 |
| 14 | A | 4003 | BCR | C36-C18-C17 | -3.01 | 118.64 | 122.92 |
| 14 | B | 4009 | BCR | C37-C22-C21 | -3.00 | 118.64 | 122.92 |
| 15 | A | 1138 | CLA | C2B-C1B-CHB | -3.00 | 120.31 | 126.00 |
| 15 | A | 1138 | CLA | C4-C3-C5 | 3.00 | 119.95 | 115.39 |
| 15 | A | 1124 | CLA | C3A-C4A-CHB | -3.00 | 118.09 | 124.33 |
| 15 | B | 1240 | CLA | CMC-C2C-C1C | 3.00 | 129.22 | 124.95 |
| 15 | A | 1130 | CLA | C4D-ND-C1D | -3.00 | 102.95 | 106.57 |
| 15 | A | 1126 | CLA | CMD-C2D-C3D | -2.99 | 119.51 | 125.16 |
| 15 | A | 1125 | CLA | C3B-CAB-CBB | -2.99 | 119.75 | 125.95 |
| 15 | A | 1101 | CLA | C3C-C4C-NC | 2.99 | 113.75 | 110.15 |
| 15 | B | 1229 | CLA | C3B-CAB-CBB | -2.99 | 119.77 | 125.95 |
| 15 | B | 1215 | CLA | CMC-C2C-C1C | 2.99 | 129.21 | 124.95 |
| 15 | A | 1135 | CLA | CGD-CBD-CHA | -2.98 | 106.73 | 113.65 |
| 14 | J | 4013 | BCR | C38-C26-C25 | -2.98 | 121.13 | 124.50 |
| 15 | A | 1012 | CLA | C4D-ND-C1D | -2.98 | 102.96 | 106.57 |
| 15 | B | 1213 | CLA | C2A-C1A-NA | 2.98 | 115.15 | 111.33 |
| 15 | A | 1122 | CLA | C4B-CHC-C1C | 2.98 | 131.39 | 127.47 |
| 15 | B | 1235 | CLA | C3C-C4C-NC | 2.98 | 113.74 | 110.15 |
| 15 | A | 1115 | CLA | CMC-C2C-C1C | 2.98 | 129.19 | 124.95 |
| 14 | B | 4004 | BCR | C7-C8-C9 | -2.97 | 121.77 | 126.22 |
| 15 | B | 1222 | CLA | O2A-C1-C2 | 2.97 | 114.93 | 108.12 |
| 15 | B | 1205 | CLA | C3C-C4C-NC | 2.97 | 113.73 | 110.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 4004 | BCR | C38-C26-C27 | 2.97 | 119.02 | 113.39 |
| 15 | B | 1224 | CLA | CMC-C2C-C1C | 2.97 | 129.19 | 124.95 |
| 15 | B | 1202 | CLA | O2D-CGD-O1D | -2.97 | 117.82 | 123.79 |
| 15 | B | 1225 | CLA | C3C-C4C-NC | 2.97 | 113.73 | 110.15 |
| 15 | A | 1104 | CLA | C4-C3-C5 | 2.97 | 119.90 | 115.39 |
| 15 | B | 1215 | CLA | C4D-ND-C1D | -2.97 | 102.98 | 106.57 |
| 15 | A | 1119 | CLA | CMC-C2C-C1C | 2.97 | 129.18 | 124.95 |
| 15 | A | 1123 | CLA | C3B-CAB-CBB | -2.96 | 119.81 | 125.95 |
| 15 | A | 1135 | CLA | CMC-C2C-C1C | 2.96 | 129.18 | 124.95 |
| 14 | B | 4017 | BCR | C27-C26-C25 | -2.96 | 118.95 | 122.86 |
| 15 | A | 1132 | CLA | C3C-C4C-NC | 2.96 | 113.72 | 110.15 |
| 14 | B | 4011 | BCR | C28-C27-C26 | -2.96 | 108.94 | 113.81 |
| 15 | B | 1229 | CLA | C3C-C4C-NC | 2.96 | 113.72 | 110.15 |
| 15 | A | 1022 | CLA | C4D-ND-C1D | -2.95 | 103.00 | 106.57 |
| 15 | B | 1240 | CLA | C3B-CAB-CBB | -2.96 | 119.83 | 125.95 |
| 15 | A | 1106 | CLA | C1-O2A-CGA | 2.96 | 125.60 | 117.00 |
| 15 | B | 1221 | CLA | O2D-CGD-O1D | -2.95 | 117.86 | 123.79 |
| 15 | A | 1128 | CLA | O2D-CGD-O1D | -2.95 | 117.87 | 123.79 |
| 15 | A | 1138 | CLA | CMB-C2B-C3B | 2.95 | 130.72 | 125.16 |
| 14 | B | 4006 | BCR | C3-C4-C5 | -2.95 | 108.96 | 113.81 |
| 15 | A | 1131 | CLA | C4B-CHC-C1C | 2.94 | 131.34 | 127.47 |
| 15 | A | 1101 | CLA | CBA-CAA-C2A | 2.94 | 121.13 | 113.95 |
| 15 | A | 1107 | CLA | CMC-C2C-C1C | 2.94 | 129.14 | 124.95 |
| 15 | A | 1130 | CLA | C3A-C4A-NA | 2.94 | 114.36 | 110.81 |
| 15 | A | 1113 | CLA | C4B-CHC-C1C | 2.93 | 131.33 | 127.47 |
| 14 | A | 4008 | BCR | C33-C5-C4 | 2.93 | 118.95 | 113.39 |
| 15 | A | 1106 | CLA | C3B-CAB-CBB | -2.93 | 119.88 | 125.95 |
| 15 | A | 1129 | CLA | CMC-C2C-C1C | 2.93 | 129.13 | 124.95 |
| 14 | A | 4008 | BCR | C30-C25-C26 | -2.93 | 118.34 | 122.59 |
| 13 | A | 1011 | CL0 | C4D-ND-C1D | -2.93 | 103.03 | 106.57 |
| 15 | F | 1410 | CLA | C2A-C1A-NA | 2.93 | 115.08 | 111.33 |
| 15 | A | 1138 | CLA | C1-C2-C3 | -2.93 | 121.15 | 126.23 |
| 15 | A | 1116 | CLA | CMC-C2C-C1C | 2.93 | 129.12 | 124.95 |
| 15 | J | 1303 | CLA | CMC-C2C-C1C | 2.92 | 129.12 | 124.95 |
| 15 | A | 1101 | CLA | O2D-CGD-O1D | -2.92 | 117.93 | 123.79 |
| 15 | B | 1222 | CLA | O2A-CGA-CBA | 2.92 | 120.83 | 111.90 |
| 15 | A | 1107 | CLA | C3A-C4A-NA | 2.92 | 114.34 | 110.81 |
| 13 | A | 1108 | CL0 | C4D-C3D-CAD | 2.92 | 111.64 | 108.05 |
| 15 | A | 1106 | CLA | O2D-CGD-O1D | -2.91 | 117.94 | 123.79 |
| 15 | B | 1222 | CLA | C3C-C4C-NC | 2.91 | 113.66 | 110.15 |
| 14 | J | 4013 | BCR | C15-C14-C13 | -2.91 | 123.08 | 127.29 |
| 15 | B | 1228 | CLA | CMC-C2C-C1C | 2.91 | 129.09 | 124.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1220 | CLA | C1-O2A-CGA | 2.90 | 125.44 | 117.00 |
| 15 | A | 1124 | CLA | O2A-CGA-CBA | 2.90 | 120.79 | 111.90 |
| 15 | A | 1120 | CLA | CMC-C2C-C1C | 2.90 | 129.09 | 124.95 |
| 15 | B | 1223 | CLA | C4-C3-C5 | 2.90 | 119.80 | 115.39 |
| 15 | A | 1125 | CLA | O2D-CGD-O1D | -2.90 | 117.97 | 123.79 |
| 15 | A | 1101 | CLA | C3A-C4A-CHB | -2.90 | 118.30 | 124.33 |
| 15 | B | 1021 | CLA | CMA-C3A-C4A | -2.90 | 103.13 | 112.40 |
| 15 | K | 1401 | CLA | CMC-C2C-C1C | 2.90 | 129.08 | 124.95 |
| 15 | A | 1012 | CLA | OBD-CAD-C3D | -2.90 | 122.29 | 128.15 |
| 13 | A | 1011 | CL0 | C3C-C4C-NC | 2.89 | 113.64 | 110.15 |
| 15 | A | 1022 | CLA | C3C-C4C-NC | 2.89 | 113.63 | 110.15 |
| 15 | A | 1119 | CLA | C2B-C1B-CHB | -2.89 | 120.53 | 126.00 |
| 14 | J | 4013 | BCR | C37-C22-C21 | -2.88 | 118.81 | 122.92 |
| 15 | F | 1301 | CLA | C3C-C4C-NC | 2.88 | 113.62 | 110.15 |
| 15 | A | 1114 | CLA | CMC-C2C-C1C | 2.88 | 129.05 | 124.95 |
| 15 | A | 1137 | CLA | C3C-C4C-NC | 2.88 | 113.62 | 110.15 |
| 15 | B | 1209 | CLA | C3B-CAB-CBB | -2.87 | 120.00 | 125.95 |
| 15 | B | 1222 | CLA | C4-C3-C5 | 2.88 | 119.76 | 115.39 |
| 15 | B | 1219 | CLA | C4B-C3B-CAB | -2.87 | 121.36 | 127.18 |
| 15 | A | 1136 | CLA | CMC-C2C-C1C | 2.87 | 129.05 | 124.95 |
| 15 | B | 1216 | CLA | CMC-C2C-C1C | 2.87 | 129.05 | 124.95 |
| 15 | A | 1022 | CLA | C4-C3-C5 | 2.87 | 119.75 | 115.39 |
| 15 | A | 1126 | CLA | C2B-C1B-CHB | -2.87 | 120.56 | 126.00 |
| 14 | A | 4012 | BCR | C23-C22-C21 | 2.87 | 123.39 | 118.98 |
| 15 | A | 1112 | CLA | C3C-C4C-NC | 2.87 | 113.61 | 110.15 |
| 15 | A | 1103 | CLA | CMC-C2C-C1C | 2.87 | 129.04 | 124.95 |
| 15 | B | 1240 | CLA | C3C-C4C-NC | 2.86 | 113.60 | 110.15 |
| 15 | A | 1126 | CLA | C4D-C3D-CAD | 2.86 | 111.57 | 108.05 |
| 14 | F | 4016 | BCR | C36-C18-C17 | -2.86 | 118.84 | 122.92 |
| 15 | A | 1140 | CLA | C3C-C4C-NC | 2.86 | 113.59 | 110.15 |
| 15 | B | 1225 | CLA | CBA-CAA-C2A | 2.85 | 120.93 | 113.95 |
| 15 | A | 1103 | CLA | C4D-C3D-CAD | 2.85 | 111.56 | 108.05 |
| 15 | A | 1101 | CLA | C4-C3-C2 | -2.85 | 117.84 | 123.52 |
| 15 | B | 1227 | CLA | CMC-C2C-C1C | 2.85 | 129.01 | 124.95 |
| 14 | A | 4002 | BCR | C3-C4-C5 | -2.85 | 109.13 | 113.81 |
| 15 | A | 1110 | CLA | C2A-C1A-NA | 2.85 | 114.98 | 111.33 |
| 15 | B | 1225 | CLA | C3B-CAB-CBB | -2.85 | 120.06 | 125.95 |
| 15 | F | 1139 | CLA | C4D-C3D-CAD | 2.85 | 111.55 | 108.05 |
| 15 | B | 1225 | CLA | C5-C3-C2 | -2.84 | 115.59 | 121.06 |
| 15 | B | 1207 | CLA | CMC-C2C-C1C | 2.84 | 129.00 | 124.95 |
| 15 | A | 1128 | CLA | C3C-C4C-NC | 2.84 | 113.58 | 110.15 |
| 15 | A | 1125 | CLA | C4D-C3D-CAD | 2.84 | 111.55 | 108.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1227 | CLA | C3C-C4C-NC | 2.84 | 113.57 | 110.15 |
| 15 | F | 1139 | CLA | C3C-C4C-NC | 2.84 | 113.57 | 110.15 |
| 15 | B | 1226 | CLA | CMC-C2C-C1C | 2.84 | 129.00 | 124.95 |
| 15 | B | 1220 | CLA | C2A-C1A-NA | 2.84 | 114.96 | 111.33 |
| 15 | A | 1129 | CLA | C2A-C1A-NA | 2.83 | 114.96 | 111.33 |
| 14 | A | 4012 | BCR | C34-C9-C10 | -2.83 | 118.89 | 122.92 |
| 14 | A | 4003 | BCR | C23-C22-C21 | 2.83 | 123.33 | 118.98 |
| 13 | A | 1011 | CL0 | O2D-CGD-O1D | -2.83 | 118.10 | 123.79 |
| 15 | B | 1232 | CLA | CMC-C2C-C1C | 2.83 | 128.98 | 124.95 |
| 15 | A | 1116 | CLA | C2A-C1A-NA | 2.83 | 114.95 | 111.33 |
| 15 | A | 1107 | CLA | C2B-C1B-CHB | -2.83 | 120.64 | 126.00 |
| 14 | A | 4001 | BCR | C30-C25-C26 | -2.82 | 118.50 | 122.59 |
| 12 | A | 5001 | LHG | C5-O7-C7 | -2.82 | 111.23 | 117.86 |
| 15 | A | 1103 | CLA | C3B-CAB-CBB | -2.82 | 120.11 | 125.95 |
| 15 | B | 1230 | CLA | CAA-C2A-C1A | -2.82 | 105.04 | 112.51 |
| 14 | F | 4016 | BCR | C38-C26-C27 | 2.81 | 118.72 | 113.39 |
| 15 | J | 1302 | CLA | C3C-C4C-NC | 2.81 | 113.54 | 110.15 |
| 15 | A | 1124 | CLA | C3A-C4A-NA | 2.81 | 114.21 | 110.81 |
| 15 | B | 1207 | CLA | C3C-C4C-NC | 2.81 | 113.54 | 110.15 |
| 15 | B | 1218 | CLA | C2A-C1A-NA | 2.81 | 114.93 | 111.33 |
| 14 | J | 4013 | BCR | C34-C9-C10 | -2.81 | 118.92 | 122.92 |
| 15 | B | 1223 | CLA | C3B-CAB-CBB | -2.81 | 120.13 | 125.95 |
| 15 | B | 1021 | CLA | C3C-C4C-NC | 2.81 | 113.53 | 110.15 |
| 15 | B | 1203 | CLA | CMC-C2C-C1C | 2.81 | 128.95 | 124.95 |
| 14 | B | 4005 | BCR | C3-C4-C5 | -2.80 | 109.20 | 113.81 |
| 15 | A | 1126 | CLA | CMB-C2B-C3B | 2.80 | 130.44 | 125.16 |
| 15 | B | 1021 | CLA | CBA-CAA-C2A | 2.80 | 120.80 | 113.95 |
| 14 | A | 4002 | BCR | C34-C9-C8 | 2.80 | 122.61 | 118.09 |
| 15 | B | 1227 | CLA | O2D-CGD-O1D | -2.80 | 118.17 | 123.79 |
| 15 | B | 1224 | CLA | O2D-CGD-O1D | -2.80 | 118.17 | 123.79 |
| 15 | B | 1209 | CLA | CMC-C2C-C1C | 2.79 | 128.93 | 124.95 |
| 15 | B | 1236 | CLA | C1-C2-C3 | -2.79 | 122.56 | 126.05 |
| 13 | A | 1108 | CL0 | C3C-C4C-NC | 2.79 | 113.51 | 110.15 |
| 15 | B | 1013 | CLA | C3C-C4C-NC | 2.79 | 113.52 | 110.15 |
| 15 | A | 1801 | CLA | C4D-C3D-CAD | 2.79 | 111.48 | 108.05 |
| 15 | J | 1302 | CLA | C4B-CHC-C1C | 2.79 | 131.14 | 127.47 |
| 15 | A | 1134 | CLA | C3C-C4C-NC | 2.79 | 113.51 | 110.15 |
| 15 | B | 1226 | CLA | C3C-C4C-NC | 2.79 | 113.51 | 110.15 |
| 15 | K | 1402 | CLA | C3C-C4C-NC | 2.78 | 113.50 | 110.15 |
| 15 | B | 1236 | CLA | C3C-C4C-NC | 2.78 | 113.50 | 110.15 |
| 15 | B | 1212 | CLA | C3C-C4C-NC | 2.78 | 113.50 | 110.15 |
| 15 | A | 1122 | CLA | C2A-C1A-NA | 2.78 | 114.89 | 111.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1202 | CLA | C1-C2-C3 | -2.77 | 121.42 | 126.23 |
| 15 | A | 1138 | CLA | C3A-C4A-CHB | -2.77 | 118.56 | 124.33 |
| 15 | A | 1102 | CLA | C4-C3-C5 | 2.77 | 119.59 | 115.39 |
| 15 | A | 1120 | CLA | C4D-C3D-CAD | 2.77 | 111.45 | 108.05 |
| 15 | B | 1232 | CLA | C3C-C4C-NC | 2.77 | 113.48 | 110.15 |
| 14 | J | 4013 | BCR | C27-C26-C25 | -2.77 | 119.21 | 122.86 |
| 15 | A | 1113 | CLA | C3C-C4C-NC | 2.76 | 113.48 | 110.15 |
| 14 | A | 4008 | BCR | C38-C26-C25 | -2.76 | 121.38 | 124.50 |
| 14 | A | 4008 | BCR | C3-C4-C5 | -2.76 | 109.28 | 113.81 |
| 15 | A | 1138 | CLA | C3B-CAB-CBB | -2.76 | 120.24 | 125.95 |
| 15 | B | 1211 | CLA | C2A-C1A-NA | 2.75 | 114.86 | 111.33 |
| 15 | B | 1211 | CLA | O2D-CGD-O1D | -2.75 | 118.26 | 123.79 |
| 15 | B | 1021 | CLA | C4D-C3D-CAD | 2.75 | 111.44 | 108.05 |
| 15 | B | 1206 | CLA | C3B-CAB-CBB | -2.75 | 120.25 | 125.95 |
| 15 | B | 1206 | CLA | C4D-C3D-CAD | 2.75 | 111.44 | 108.05 |
| 15 | B | 1215 | CLA | C1-C2-C3 | -2.75 | 121.45 | 126.23 |
| 15 | B | 1214 | CLA | C2A-C1A-NA | 2.75 | 114.85 | 111.33 |
| 15 | B | 1207 | CLA | C3B-CAB-CBB | -2.75 | 120.26 | 125.95 |
| 14 | A | 4003 | BCR | C3-C4-C5 | -2.75 | 109.29 | 113.81 |
| 14 | B | 4006 | BCR | C34-C9-C8 | 2.75 | 122.53 | 118.09 |
| 14 | B | 4010 | BCR | C34-C9-C10 | -2.75 | 119.01 | 122.92 |
| 13 | A | 1011 | CL0 | C3A-C4A-CHB | -2.75 | 118.62 | 124.33 |
| 15 | B | 1217 | CLA | C3C-C4C-NC | 2.74 | 113.46 | 110.15 |
| 15 | A | 1135 | CLA | C3C-C4C-NC | 2.74 | 113.46 | 110.15 |
| 15 | A | 1102 | CLA | O2D-CGD-O1D | -2.74 | 118.28 | 123.79 |
| 14 | A | 4012 | BCR | C3-C4-C5 | -2.74 | 109.31 | 113.81 |
| 15 | F | 1410 | CLA | C3C-C4C-NC | 2.73 | 113.45 | 110.15 |
| 15 | A | 1109 | CLA | C4-C3-C2 | -2.74 | 118.07 | 123.52 |
| 15 | A | 1137 | CLA | CMC-C2C-C1C | 2.73 | 128.85 | 124.95 |
| 15 | B | 1205 | CLA | C1-C2-C3 | -2.73 | 121.49 | 126.23 |
| 15 | B | 1208 | CLA | C2A-C1A-NA | 2.73 | 114.83 | 111.33 |
| 15 | A | 1127 | CLA | C4D-C3D-CAD | 2.73 | 111.41 | 108.05 |
| 12 | A | 5005 | LHG | O8-C23-C24 | 2.73 | 120.25 | 111.90 |
| 14 | B | 4017 | BCR | C37-C22-C21 | -2.73 | 119.03 | 122.92 |
| 15 | B | 1234 | CLA | C3C-C4C-NC | 2.73 | 113.44 | 110.15 |
| 15 | F | 1139 | CLA | C4B-CHC-C1C | 2.73 | 131.06 | 127.47 |
| 15 | A | 1123 | CLA | C4D-C3D-CAD | 2.73 | 111.40 | 108.05 |
| 15 | B | 1214 | CLA | CMB-C2B-C3B | 2.72 | 130.29 | 125.16 |
| 15 | A | 1101 | CLA | C4D-C3D-CAD | 2.72 | 111.39 | 108.05 |
| 15 | A | 1012 | CLA | C1-O2A-CGA | 2.72 | 124.91 | 117.00 |
| 15 | A | 1116 | CLA | C3C-C4C-NC | 2.71 | 113.42 | 110.15 |
| 15 | A | 1121 | CLA | C3C-C4C-NC | 2.71 | 113.42 | 110.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1201 | CLA | O2D-CGD-O1D | -2.71 | 118.35 | 123.79 |
| 14 | B | 4009 | BCR | C27-C26-C25 | -2.71 | 119.28 | 122.86 |
| 15 | A | 1136 | CLA | C3C-C4C-NC | 2.71 | 113.42 | 110.15 |
| 15 | A | 1127 | CLA | CMB-C2B-C3B | 2.71 | 130.26 | 125.16 |
| 15 | A | 1107 | CLA | CMB-C2B-C3B | 2.71 | 130.26 | 125.16 |
| 15 | B | 1228 | CLA | C3C-C4C-NC | 2.71 | 113.42 | 110.15 |
| 15 | B | 1216 | CLA | C2A-C1A-NA | 2.71 | 114.80 | 111.33 |
| 15 | B | 1218 | CLA | C4D-C3D-CAD | 2.71 | 111.38 | 108.05 |
| 14 | F | 4016 | BCR | C34-C9-C10 | -2.71 | 119.06 | 122.92 |
| 14 | A | 4007 | BCR | C33-C5-C4 | 2.71 | 118.52 | 113.39 |
| 14 | B | 4009 | BCR | C33-C5-C4 | 2.70 | 118.51 | 113.39 |
| 15 | A | 1022 | CLA | C2A-C1A-NA | 2.70 | 114.79 | 111.33 |
| 15 | J | 1303 | CLA | C4D-C3D-CAD | 2.70 | 111.37 | 108.05 |
| 12 | B | 5004 | LHG | O8-C23-C24 | 2.70 | 120.16 | 111.90 |
| 15 | B | 1215 | CLA | C3C-C4C-NC | 2.70 | 113.40 | 110.15 |
| 14 | B | 4004 | BCR | C34-C9-C10 | -2.70 | 119.08 | 122.92 |
| 15 | A | 1114 | CLA | C2A-C1A-NA | 2.69 | 114.78 | 111.33 |
| 15 | B | 1239 | CLA | C4D-C3D-CAD | 2.69 | 111.36 | 108.05 |
| 15 | F | 1139 | CLA | C4-C3-C2 | -2.69 | 118.16 | 123.52 |
| 14 | A | 4003 | BCR | C38-C26-C27 | 2.69 | 118.49 | 113.39 |
| 14 | F | 4016 | BCR | C8-C7-C6 | -2.69 | 119.29 | 127.23 |
| 15 | B | 1234 | CLA | CMC-C2C-C1C | 2.69 | 128.78 | 124.95 |
| 14 | B | 4014 | BCR | C15-C14-C13 | -2.69 | 123.40 | 127.29 |
| 15 | A | 1129 | CLA | C4D-C3D-CAD | 2.69 | 111.36 | 108.05 |
| 15 | A | 1119 | CLA | C3C-C4C-NC | 2.69 | 113.39 | 110.15 |
| 15 | B | 1219 | CLA | C2A-C1A-NA | 2.68 | 114.77 | 111.33 |
| 15 | B | 1237 | CLA | C4D-C3D-CAD | 2.68 | 111.35 | 108.05 |
| 15 | A | 1110 | CLA | C3C-C4C-NC | 2.68 | 113.38 | 110.15 |
| 14 | B | 4004 | BCR | C23-C22-C21 | 2.68 | 123.10 | 118.98 |
| 15 | A | 1110 | CLA | C4-C3-C5 | 2.68 | 119.45 | 115.39 |
| 15 | A | 1135 | CLA | C2A-C1A-NA | 2.67 | 114.76 | 111.33 |
| 15 | A | 1112 | CLA | C3A-C4A-CHB | -2.67 | 118.78 | 124.33 |
| 15 | B | 1215 | CLA | C2A-C1A-NA | 2.67 | 114.75 | 111.33 |
| 15 | A | 1131 | CLA | C3C-C4C-NC | 2.67 | 113.37 | 110.15 |
| 15 | B | 1211 | CLA | C3C-C4C-NC | 2.67 | 113.37 | 110.15 |
| 15 | A | 1121 | CLA | C4D-C3D-CAD | 2.67 | 111.33 | 108.05 |
| 15 | B | 1222 | CLA | C1-O2A-CGA | 2.67 | 124.76 | 117.00 |
| 15 | B | 1201 | CLA | C3C-C4C-NC | 2.66 | 113.36 | 110.15 |
| 15 | A | 1132 | CLA | CMC-C2C-C1C | 2.66 | 128.75 | 124.95 |
| 15 | B | 1234 | CLA | C2A-C1A-NA | 2.66 | 114.74 | 111.33 |
| 15 | A | 1133 | CLA | C3C-C4C-NC | 2.66 | 113.36 | 110.15 |
| 15 | A | 1101 | CLA | C4B-CHC-C1C | 2.66 | 130.97 | 127.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1101 | CLA | CHB-C4A-NA | 2.66 | 128.09 | 124.38 |
| 15 | A | 1105 | CLA | C3C-C4C-NC | 2.66 | 113.35 | 110.15 |
| 15 | B | 1219 | CLA | C2B-C3B-CAB | 2.66 | 132.76 | 127.33 |
| 14 | B | 4010 | BCR | C34-C9-C8 | 2.66 | 122.39 | 118.09 |
| 15 | B | 1236 | CLA | C2B-C1B-CHB | -2.66 | 120.96 | 126.00 |
| 15 | A | 1116 | CLA | C4D-C3D-CAD | 2.66 | 111.32 | 108.05 |
| 14 | J | 4013 | BCR | C33-C5-C6 | -2.66 | 121.50 | 124.50 |
| 15 | A | 1129 | CLA | C3C-C4C-NC | 2.66 | 113.35 | 110.15 |
| 15 | A | 1107 | CLA | C4D-C3D-CAD | 2.65 | 111.31 | 108.05 |
| 15 | B | 1223 | CLA | OBD-CAD-C3D | -2.66 | 122.78 | 128.15 |
| 15 | K | 1401 | CLA | C3C-C4C-NC | 2.65 | 113.35 | 110.15 |
| 15 | B | 1224 | CLA | CMB-C2B-C3B | 2.65 | 130.16 | 125.16 |
| 15 | B | 1236 | CLA | C2A-C1A-NA | 2.65 | 114.73 | 111.33 |
| 17 | B | 5002 | LMG | O8-C28-C29 | 2.65 | 120.02 | 111.90 |
| 14 | B | 4010 | BCR | C33-C5-C4 | 2.65 | 118.42 | 113.39 |
| 14 | A | 4007 | BCR | C7-C8-C9 | -2.65 | 122.25 | 126.22 |
| 15 | B | 1209 | CLA | O2D-CGD-O1D | -2.65 | 118.47 | 123.79 |
| 15 | B | 1222 | CLA | O1D-CGD-CBD | -2.65 | 119.04 | 124.45 |
| 15 | B | 1214 | CLA | C2B-C1B-CHB | -2.65 | 120.98 | 126.00 |
| 15 | B | 1202 | CLA | CMC-C2C-C1C | 2.65 | 128.73 | 124.95 |
| 15 | A | 1122 | CLA | C4D-C3D-CAD | 2.65 | 111.31 | 108.05 |
| 15 | B | 1214 | CLA | C3A-C4A-CHB | -2.65 | 118.83 | 124.33 |
| 15 | B | 1223 | CLA | CMB-C2B-C3B | 2.65 | 130.15 | 125.16 |
| 14 | F | 4016 | BCR | C23-C24-C25 | -2.65 | 119.43 | 127.23 |
| 15 | A | 1101 | CLA | C2B-C1B-CHB | -2.64 | 121.00 | 126.00 |
| 15 | B | 1238 | CLA | C3C-C4C-NC | 2.64 | 113.33 | 110.15 |
| 15 | B | 1223 | CLA | O2D-CGD-O1D | -2.64 | 118.49 | 123.79 |
| 15 | J | 1302 | CLA | C4D-C3D-CAD | 2.64 | 111.29 | 108.05 |
| 15 | B | 1217 | CLA | C2A-C1A-NA | 2.64 | 114.71 | 111.33 |
| 15 | A | 1117 | CLA | C2B-C1B-CHB | -2.64 | 121.00 | 126.00 |
| 15 | B | 1222 | CLA | CMC-C2C-C1C | 2.64 | 128.71 | 124.95 |
| 14 | B | 4006 | BCR | C24-C23-C22 | -2.64 | 122.27 | 126.22 |
| 15 | B | 1209 | CLA | C4D-C3D-CAD | 2.64 | 111.29 | 108.05 |
| 15 | A | 1119 | CLA | C3A-C4A-NA | 2.64 | 114.00 | 110.81 |
| 15 | B | 1221 | CLA | CMB-C2B-C3B | 2.64 | 130.13 | 125.16 |
| 15 | B | 1216 | CLA | C4-C3-C5 | 2.63 | 119.39 | 115.39 |
| 15 | A | 1103 | CLA | O2D-CGD-O1D | -2.64 | 118.50 | 123.79 |
| 15 | A | 1136 | CLA | C3B-CAB-CBB | -2.63 | 120.50 | 125.95 |
| 15 | B | 1234 | CLA | C5-C3-C2 | 2.63 | 126.12 | 121.06 |
| 14 | B | 4011 | BCR | C3-C4-C5 | -2.63 | 109.49 | 113.81 |
| 15 | B | 1205 | CLA | O1D-CGD-CBD | -2.63 | 119.08 | 124.45 |
| 15 | B | 1209 | CLA | C3A-C4A-CHB | -2.63 | 118.87 | 124.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1235 | CLA | O2D-CGD-O1D | -2.63 | 118.52 | 123.79 |
| 15 | A | 1129 | CLA | O2D-CGD-O1D | -2.63 | 118.52 | 123.79 |
| 15 | B | 1013 | CLA | CMC-C2C-C1C | 2.63 | 128.69 | 124.95 |
| 15 | B | 1013 | CLA | C1-C2-C3 | -2.63 | 121.67 | 126.23 |
| 14 | B | 4005 | BCR | C23-C22-C21 | 2.63 | 123.02 | 118.98 |
| 15 | F | 1301 | CLA | C2A-C1A-NA | 2.62 | 114.69 | 111.33 |
| 15 | A | 1130 | CLA | C3A-C4A-CHB | -2.62 | 118.87 | 124.33 |
| 15 | B | 1220 | CLA | C2B-C1B-CHB | -2.62 | 121.03 | 126.00 |
| 15 | A | 1137 | CLA | O2D-CGD-O1D | -2.62 | 118.53 | 123.79 |
| 15 | B | 1202 | CLA | C3C-C4C-NC | 2.62 | 113.31 | 110.15 |
| 15 | B | 1215 | CLA | O2D-CGD-O1D | -2.62 | 118.52 | 123.79 |
| 14 | A | 4008 | BCR | C15-C14-C13 | -2.62 | 123.50 | 127.29 |
| 15 | B | 1205 | CLA | C4D-C3D-CAD | 2.62 | 111.27 | 108.05 |
| 15 | A | 1134 | CLA | C3B-CAB-CBB | -2.62 | 120.53 | 125.95 |
| 15 | A | 1128 | CLA | C4D-C3D-CAD | 2.62 | 111.27 | 108.05 |
| 15 | B | 1228 | CLA | C2A-C1A-NA | 2.62 | 114.68 | 111.33 |
| 15 | A | 1131 | CLA | O2D-CGD-O1D | -2.62 | 118.53 | 123.79 |
| 15 | B | 1222 | CLA | C3A-C4A-CHB | -2.62 | 118.89 | 124.33 |
| 15 | B | 1238 | CLA | C2A-C1A-NA | 2.62 | 114.68 | 111.33 |
| 15 | B | 1212 | CLA | O2D-CGD-O1D | -2.62 | 118.54 | 123.79 |
| 15 | A | 1130 | CLA | C3C-C4C-NC | 2.61 | 113.30 | 110.15 |
| 15 | K | 1401 | CLA | C4D-C3D-CAD | 2.61 | 111.26 | 108.05 |
| 14 | A | 4012 | BCR | C38-C26-C27 | 2.61 | 118.34 | 113.39 |
| 15 | A | 1138 | CLA | C3A-C4A-NA | 2.61 | 113.97 | 110.81 |
| 15 | A | 1124 | CLA | C3C-C4C-NC | 2.61 | 113.30 | 110.15 |
| 15 | B | 1236 | CLA | O2D-CGD-O1D | -2.61 | 118.55 | 123.79 |
| 14 | B | 4010 | BCR | C38-C26-C27 | 2.61 | 118.34 | 113.39 |
| 15 | A | 1109 | CLA | C4D-C3D-CAD | 2.61 | 111.26 | 108.05 |
| 15 | A | 1012 | CLA | C3A-C4A-CHB | -2.61 | 118.91 | 124.33 |
| 15 | B | 1231 | CLA | C3C-C4C-NC | 2.61 | 113.29 | 110.15 |
| 15 | B | 1217 | CLA | O2D-CGD-O1D | -2.60 | 118.56 | 123.79 |
| 13 | A | 1108 | CL0 | C4B-CHC-C1C | 2.60 | 130.89 | 127.47 |
| 15 | B | 1201 | CLA | CMB-C2B-C3B | 2.60 | 130.06 | 125.16 |
| 15 | B | 1230 | CLA | C2A-C1A-NA | 2.60 | 114.66 | 111.33 |
| 15 | B | 1222 | CLA | CHB-C4A-NA | 2.60 | 128.00 | 124.38 |
| 15 | A | 1117 | CLA | C3C-C4C-NC | 2.60 | 113.28 | 110.15 |
| 15 | A | 1111 | CLA | C3B-CAB-CBB | -2.59 | 120.58 | 125.95 |
| 15 | B | 1220 | CLA | C3C-C4C-NC | 2.58 | 113.27 | 110.15 |
| 15 | B | 1209 | CLA | C3C-C4C-NC | 2.59 | 113.27 | 110.15 |
| 15 | B | 1234 | CLA | O2D-CGD-O1D | -2.59 | 118.60 | 123.79 |
| 15 | B | 1216 | CLA | C2B-C1B-CHB | -2.59 | 121.10 | 126.00 |
| 15 | A | 1118 | CLA | O2D-CGD-O1D | -2.58 | 118.61 | 123.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1134 | CLA | C4D-C3D-CAD | 2.58 | 111.23 | 108.05 |
| 15 | A | 1123 | CLA | CHD-C4C-NC | -2.58 | 122.48 | 124.28 |
| 15 | A | 1102 | CLA | C3C-C4C-NC | 2.58 | 113.26 | 110.15 |
| 12 | A | 5005 | LHG | C5-O7-C7 | -2.58 | 111.80 | 117.86 |
| 15 | A | 1111 | CLA | C3A-C4A-CHB | -2.58 | 118.97 | 124.33 |
| 15 | K | 1401 | CLA | C3A-C4A-CHB | -2.58 | 118.97 | 124.33 |
| 14 | F | 4016 | BCR | C34-C9-C8 | 2.57 | 122.25 | 118.09 |
| 15 | A | 1123 | CLA | C3C-C4C-NC | 2.57 | 113.25 | 110.15 |
| 14 | A | 4007 | BCR | C27-C26-C25 | -2.57 | 119.46 | 122.86 |
| 15 | B | 1224 | CLA | C2A-C1A-NA | 2.57 | 114.62 | 111.33 |
| 15 | B | 1204 | CLA | C4D-C3D-CAD | 2.57 | 111.21 | 108.05 |
| 15 | A | 1122 | CLA | C2B-C1B-CHB | -2.57 | 121.13 | 126.00 |
| 15 | A | 1131 | CLA | C2A-C1A-NA | 2.57 | 114.62 | 111.33 |
| 14 | A | 4003 | BCR | C15-C14-C13 | -2.57 | 123.58 | 127.29 |
| 15 | B | 1207 | CLA | O2D-CGD-O1D | -2.56 | 118.64 | 123.79 |
| 15 | A | 1119 | CLA | C3B-CAB-CBB | -2.56 | 120.64 | 125.95 |
| 14 | A | 4007 | BCR | C34-C9-C10 | -2.56 | 119.27 | 122.92 |
| 15 | A | 1114 | CLA | C3C-C4C-NC | 2.56 | 113.24 | 110.15 |
| 15 | A | 1801 | CLA | O2D-CGD-O1D | -2.56 | 118.65 | 123.79 |
| 15 | A | 1801 | CLA | C4-C3-C2 | -2.56 | 118.42 | 123.52 |
| 15 | A | 1120 | CLA | C3C-C4C-NC | 2.56 | 113.24 | 110.15 |
| 15 | A | 1134 | CLA | CMB-C2B-C3B | 2.56 | 129.98 | 125.16 |
| 15 | B | 1204 | CLA | C2A-C1A-NA | 2.56 | 114.61 | 111.33 |
| 15 | A | 1137 | CLA | C4D-C3D-CAD | 2.56 | 111.20 | 108.05 |
| 15 | K | 1401 | CLA | C2A-C1A-NA | 2.56 | 114.61 | 111.33 |
| 15 | A | 1117 | CLA | C3A-C4A-NA | 2.56 | 113.90 | 110.81 |
| 15 | B | 1237 | CLA | C3B-CAB-CBB | -2.56 | 120.65 | 125.95 |
| 15 | A | 1106 | CLA | CAA-C2A-C1A | -2.56 | 105.74 | 112.51 |
| 15 | A | 1114 | CLA | O2D-CGD-O1D | -2.55 | 118.66 | 123.79 |
| 15 | B | 1239 | CLA | CMC-C2C-C1C | 2.55 | 128.59 | 124.95 |
| 15 | B | 1237 | CLA | C3C-C4C-NC | 2.55 | 113.23 | 110.15 |
| 15 | B | 1210 | CLA | C3C-C4C-NC | 2.55 | 113.23 | 110.15 |
| 15 | A | 1103 | CLA | C2A-C1A-NA | 2.55 | 114.60 | 111.33 |
| 15 | A | 1110 | CLA | O2D-CGD-O1D | -2.55 | 118.67 | 123.79 |
| 15 | A | 1104 | CLA | C2A-C1A-NA | 2.55 | 114.60 | 111.33 |
| 15 | B | 1203 | CLA | C2A-C1A-NA | 2.55 | 114.60 | 111.33 |
| 15 | A | 1120 | CLA | C3A-C4A-CHB | -2.55 | 119.03 | 124.33 |
| 15 | B | 1206 | CLA | C2A-C1A-NA | 2.55 | 114.60 | 111.33 |
| 15 | A | 1118 | CLA | C3C-C4C-NC | 2.55 | 113.22 | 110.15 |
| 15 | A | 1105 | CLA | O2D-CGD-O1D | -2.55 | 118.67 | 123.79 |
| 14 | B | 4014 | BCR | C34-C9-C10 | -2.55 | 119.29 | 122.92 |
| 15 | B | 1023 | CLA | CMC-C2C-C1C | 2.55 | 128.58 | 124.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1206 | CLA | C3A-C4A-CHB | -2.55 | 119.03 | 124.33 |
| 15 | A | 1126 | CLA | O2D-CGD-O1D | -2.55 | 118.68 | 123.79 |
| 15 | A | 1127 | CLA | C2A-C1A-NA | 2.55 | 114.59 | 111.33 |
| 15 | A | 1113 | CLA | C2A-C1A-NA | 2.54 | 114.59 | 111.33 |
| 15 | B | 1207 | CLA | C2A-C1A-NA | 2.54 | 114.59 | 111.33 |
| 15 | A | 1130 | CLA | O2D-CGD-O1D | -2.54 | 118.69 | 123.79 |
| 15 | B | 1215 | CLA | C1-O2A-CGA | 2.54 | 124.38 | 117.00 |
| 15 | A | 1132 | CLA | C2A-C1A-NA | 2.54 | 114.58 | 111.33 |
| 15 | A | 1124 | CLA | C4D-C3D-CAD | 2.54 | 111.17 | 108.05 |
| 15 | A | 1104 | CLA | C3C-C4C-NC | 2.54 | 113.21 | 110.15 |
| 15 | B | 1220 | CLA | CED-O2D-CGD | 2.53 | 122.03 | 116.00 |
| 15 | A | 1138 | CLA | C3C-C4C-NC | 2.53 | 113.20 | 110.15 |
| 15 | B | 1224 | CLA | C4D-C3D-CAD | 2.53 | 111.17 | 108.05 |
| 14 | A | 4007 | BCR | C23-C24-C25 | -2.53 | 119.75 | 127.23 |
| 15 | A | 1116 | CLA | C4B-CHC-C1C | 2.53 | 130.80 | 127.47 |
| 15 | A | 1107 | CLA | C3A-C4A-CHB | -2.53 | 119.06 | 124.33 |
| 15 | B | 1203 | CLA | C4D-C3D-CAD | 2.53 | 111.16 | 108.05 |
| 12 | A | 5003 | LHG | O8-C23-C24 | 2.53 | 119.65 | 111.90 |
| 15 | K | 1402 | CLA | C4D-C3D-CAD | 2.53 | 111.16 | 108.05 |
| 15 | A | 1107 | CLA | C3C-C4C-NC | 2.53 | 113.19 | 110.15 |
| 15 | A | 1136 | CLA | C4D-C3D-CAD | 2.53 | 111.16 | 108.05 |
| 15 | B | 1202 | CLA | C4D-C3D-CAD | 2.53 | 111.16 | 108.05 |
| 15 | B | 1218 | CLA | C3C-C4C-NC | 2.52 | 113.19 | 110.15 |
| 15 | B | 1230 | CLA | C4D-C3D-CAD | 2.52 | 111.16 | 108.05 |
| 15 | A | 1112 | CLA | C4D-C3D-CAD | 2.52 | 111.15 | 108.05 |
| 15 | A | 1140 | CLA | C4D-C3D-CAD | 2.52 | 111.15 | 108.05 |
| 15 | A | 1102 | CLA | C3A-C4A-CHB | -2.52 | 119.09 | 124.33 |
| 15 | B | 1228 | CLA | C2B-C1B-CHB | -2.52 | 121.23 | 126.00 |
| 15 | B | 1202 | CLA | C3A-C4A-CHB | -2.52 | 119.09 | 124.33 |
| 15 | A | 1138 | CLA | C4B-CHC-C1C | 2.52 | 130.78 | 127.47 |
| 13 | A | 1108 | CL0 | C2A-C1A-NA | 2.52 | 114.56 | 111.33 |
| 15 | F | 1301 | CLA | C3A-C4A-CHB | -2.52 | 119.10 | 124.33 |
| 15 | B | 1203 | CLA | C3C-C4C-NC | 2.51 | 113.18 | 110.15 |
| 14 | J | 4013 | BCR | C23-C24-C25 | -2.51 | 119.81 | 127.23 |
| 15 | A | 1111 | CLA | C2A-C1A-NA | 2.52 | 114.55 | 111.33 |
| 15 | A | 1112 | CLA | C3B-CAB-CBB | -2.52 | 120.74 | 125.95 |
| 15 | A | 1114 | CLA | C4B-CHC-C1C | 2.51 | 130.78 | 127.47 |
| 15 | A | 1137 | CLA | CMB-C2B-C3B | 2.51 | 129.90 | 125.16 |
| 15 | A | 1801 | CLA | C3A-C4A-CHB | -2.51 | 119.11 | 124.33 |
| 15 | B | 1219 | CLA | C4D-C3D-CAD | 2.51 | 111.14 | 108.05 |
| 15 | A | 1130 | CLA | C2A-C1A-NA | 2.51 | 114.55 | 111.33 |
| 15 | B | 1227 | CLA | C4D-C3D-CAD | 2.51 | 111.14 | 108.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1226 | CLA | O1D-CGD-CBD | -2.51 | 119.32 | 124.45 |
| 15 | A | 1132 | CLA | O2D-CGD-O1D | -2.51 | 118.75 | 123.79 |
| 15 | B | 1209 | CLA | CMB-C2B-C3B | 2.51 | 129.88 | 125.16 |
| 15 | B | 1232 | CLA | C3B-CAB-CBB | -2.51 | 120.76 | 125.95 |
| 15 | B | 1207 | CLA | C4D-C3D-CAD | 2.51 | 111.13 | 108.05 |
| 15 | B | 1236 | CLA | C3A-C4A-NA | 2.51 | 113.84 | 110.81 |
| 15 | A | 1022 | CLA | O2D-CGD-O1D | -2.50 | 118.76 | 123.79 |
| 15 | B | 1225 | CLA | CMB-C2B-C3B | 2.50 | 129.88 | 125.16 |
| 15 | A | 1115 | CLA | C4B-CHC-C1C | 2.50 | 130.77 | 127.47 |
| 15 | B | 1208 | CLA | CMC-C2C-C1C | 2.51 | 128.52 | 124.95 |
| 15 | B | 1023 | CLA | O2D-CGD-O1D | -2.50 | 118.76 | 123.79 |
| 14 | A | 4001 | BCR | C33-C5-C4 | 2.51 | 118.14 | 113.39 |
| 14 | J | 4013 | BCR | C2-C1-C6 | 2.50 | 114.36 | 110.37 |
| 15 | K | 1401 | CLA | C4B-CHC-C1C | 2.50 | 130.76 | 127.47 |
| 15 | A | 1104 | CLA | C2B-C1B-CHB | -2.50 | 121.26 | 126.00 |
| 14 | F | 4015 | BCR | C36-C18-C17 | -2.50 | 119.36 | 122.92 |
| 15 | A | 1129 | CLA | OBD-CAD-C3D | -2.50 | 123.10 | 128.15 |
| 15 | A | 1106 | CLA | O1D-CGD-CBD | -2.50 | 119.35 | 124.45 |
| 14 | A | 4007 | BCR | C28-C27-C26 | -2.50 | 109.71 | 113.81 |
| 15 | A | 1124 | CLA | C2B-C1B-CHB | -2.50 | 121.27 | 126.00 |
| 15 | A | 1119 | CLA | C3A-C4A-CHB | -2.50 | 119.14 | 124.33 |
| 15 | B | 1235 | CLA | C4-C3-C5 | 2.50 | 119.18 | 115.39 |
| 13 | A | 1011 | CL0 | C4D-C3D-CAD | 2.50 | 111.12 | 108.05 |
| 15 | B | 1213 | CLA | O2D-CGD-O1D | -2.49 | 118.79 | 123.79 |
| 15 | B | 1228 | CLA | C4B-CHC-C1C | 2.49 | 130.75 | 127.47 |
| 15 | A | 1121 | CLA | C2A-C1A-NA | 2.49 | 114.52 | 111.33 |
| 15 | B | 1210 | CLA | CAC-C3C-C4C | 2.49 | 128.59 | 124.85 |
| 15 | A | 1113 | CLA | C3A-C4A-CHB | -2.49 | 119.16 | 124.33 |
| 15 | B | 1223 | CLA | C2B-C1B-CHB | -2.49 | 121.28 | 126.00 |
| 15 | A | 1115 | CLA | C4D-C3D-CAD | 2.49 | 111.11 | 108.05 |
| 15 | B | 1202 | CLA | C2A-C1A-NA | 2.49 | 114.52 | 111.33 |
| 15 | A | 1125 | CLA | C2A-C1A-NA | 2.49 | 114.52 | 111.33 |
| 15 | B | 1217 | CLA | C4D-C3D-CAD | 2.48 | 111.11 | 108.05 |
| 15 | B | 1013 | CLA | C3A-C4A-CHB | -2.49 | 119.16 | 124.33 |
| 15 | A | 1109 | CLA | C1-O2A-CGA | 2.48 | 124.22 | 117.00 |
| 15 | B | 1023 | CLA | C3A-C4A-CHB | -2.48 | 119.17 | 124.33 |
| 15 | B | 1229 | CLA | C4D-C3D-CAD | 2.48 | 111.11 | 108.05 |
| 15 | A | 1012 | CLA | O2D-CGD-O1D | -2.48 | 118.81 | 123.79 |
| 15 | B | 1236 | CLA | C4D-C3D-CAD | 2.48 | 111.10 | 108.05 |
| 15 | B | 1239 | CLA | O2D-CGD-O1D | -2.48 | 118.81 | 123.79 |
| 15 | A | 1109 | CLA | C3B-CAB-CBB | -2.48 | 120.82 | 125.95 |
| 14 | A | 4002 | BCR | C30-C25-C26 | -2.48 | 119.00 | 122.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1125 | CLA | CGD-CBD-CHA | -2.48 | 107.91 | 113.65 |
| 15 | B | 1239 | CLA | C2A-C1A-NA | 2.48 | 114.50 | 111.33 |
| 15 | A | 1102 | CLA | C2A-C1A-NA | 2.48 | 114.50 | 111.33 |
| 15 | B | 1013 | CLA | C2B-C1B-CHB | -2.48 | 121.31 | 126.00 |
| 15 | B | 1223 | CLA | C4D-C3D-CAD | 2.47 | 111.09 | 108.05 |
| 15 | B | 1216 | CLA | C3C-C4C-NC | 2.47 | 113.13 | 110.15 |
| 15 | A | 1109 | CLA | C3C-C4C-NC | 2.47 | 113.13 | 110.15 |
| 14 | B | 4011 | BCR | C1-C6-C5 | -2.47 | 119.02 | 122.59 |
| 15 | B | 1219 | CLA | O2D-CGD-O1D | -2.46 | 118.84 | 123.79 |
| 15 | A | 1116 | CLA | O2D-CGD-O1D | -2.47 | 118.84 | 123.79 |
| 15 | B | 1239 | CLA | C3C-C4C-NC | 2.47 | 113.12 | 110.15 |
| 15 | A | 1140 | CLA | O2D-CGD-O1D | -2.47 | 118.84 | 123.79 |
| 15 | B | 1214 | CLA | C4D-C3D-CAD | 2.46 | 111.08 | 108.05 |
| 15 | A | 1136 | CLA | O2D-CGD-O1D | -2.46 | 118.84 | 123.79 |
| 13 | A | 1011 | CL0 | C3B-CAB-CBB | -2.46 | 120.85 | 125.95 |
| 15 | K | 1402 | CLA | C2A-C1A-NA | 2.46 | 114.49 | 111.33 |
| 15 | J | 1302 | CLA | O2D-CGD-O1D | -2.46 | 118.85 | 123.79 |
| 15 | B | 1225 | CLA | C4D-C3D-CAD | 2.46 | 111.07 | 108.05 |
| 15 | B | 1216 | CLA | C1-O2A-CGA | 2.46 | 124.15 | 117.00 |
| 15 | B | 1210 | CLA | C3A-C4A-CHB | -2.46 | 119.22 | 124.33 |
| 15 | A | 1101 | CLA | CMB-C2B-C3B | 2.46 | 129.79 | 125.16 |
| 14 | A | 4007 | BCR | C36-C18-C17 | -2.45 | 119.43 | 122.92 |
| 14 | B | 4006 | BCR | C37-C22-C21 | -2.45 | 119.43 | 122.92 |
| 15 | A | 1117 | CLA | C4-C3-C5 | 2.45 | 119.11 | 115.39 |
| 15 | A | 1114 | CLA | C4D-C3D-CAD | 2.45 | 111.06 | 108.05 |
| 15 | A | 1137 | CLA | C2A-C1A-NA | 2.45 | 114.47 | 111.33 |
| 15 | B | 1023 | CLA | C3C-C4C-NC | 2.45 | 113.10 | 110.15 |
| 15 | B | 1210 | CLA | C2A-C1A-NA | 2.45 | 114.47 | 111.33 |
| 14 | B | 4010 | BCR | C30-C25-C26 | -2.45 | 119.05 | 122.59 |
| 15 | A | 1125 | CLA | C2B-C1B-CHB | -2.45 | 121.36 | 126.00 |
| 14 | A | 4008 | BCR | C23-C24-C25 | -2.45 | 120.02 | 127.23 |
| 14 | F | 4016 | BCR | C33-C5-C4 | 2.45 | 118.03 | 113.39 |
| 15 | A | 1112 | CLA | C2A-C1A-NA | 2.45 | 114.46 | 111.33 |
| 15 | A | 1133 | CLA | C4D-C3D-CAD | 2.44 | 111.06 | 108.05 |
| 15 | A | 1111 | CLA | C3C-C4C-NC | 2.44 | 113.09 | 110.15 |
| 15 | B | 1013 | CLA | CMB-C2B-C3B | 2.44 | 129.76 | 125.16 |
| 15 | B | 1240 | CLA | CMB-C2B-C3B | 2.44 | 129.76 | 125.16 |
| 15 | A | 1115 | CLA | C2A-C1A-NA | 2.44 | 114.46 | 111.33 |
| 15 | B | 1226 | CLA | C4D-C3D-CAD | 2.44 | 111.05 | 108.05 |
| 14 | F | 4015 | BCR | C27-C26-C25 | -2.44 | 119.64 | 122.86 |
| 15 | A | 1127 | CLA | OBD-CAD-C3D | -2.44 | 123.22 | 128.15 |
| 15 | A | 1133 | CLA | C3A-C4A-CHB | -2.44 | 119.26 | 124.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1130 | CLA | CGD-CBD-CHA | -2.44 | 108.00 | 113.65 |
| 15 | A | 1121 | CLA | C3B-CAB-CBB | -2.44 | 120.91 | 125.95 |
| 15 | A | 1106 | CLA | C3A-C4A-CHB | -2.44 | 119.26 | 124.33 |
| 15 | B | 1227 | CLA | C3A-C4A-CHB | -2.43 | 119.27 | 124.33 |
| 15 | B | 1240 | CLA | C3A-C4A-CHB | -2.43 | 119.27 | 124.33 |
| 15 | B | 1217 | CLA | C3A-C4A-CHB | -2.43 | 119.27 | 124.33 |
| 15 | B | 1212 | CLA | C4D-C3D-CAD | 2.43 | 111.05 | 108.05 |
| 15 | B | 1201 | CLA | O1D-CGD-CBD | -2.43 | 119.48 | 124.45 |
| 15 | B | 1023 | CLA | C4-C3-C5 | 2.43 | 119.08 | 115.39 |
| 14 | A | 4002 | BCR | C35-C13-C12 | 2.43 | 122.02 | 118.09 |
| 15 | B | 1218 | CLA | O2D-CGD-O1D | -2.43 | 118.91 | 123.79 |
| 14 | A | 4002 | BCR | C37-C22-C21 | -2.43 | 119.46 | 122.92 |
| 15 | B | 1225 | CLA | C2A-C1A-NA | 2.43 | 114.44 | 111.33 |
| 15 | B | 1203 | CLA | C3B-CAB-CBB | -2.43 | 120.93 | 125.95 |
| 15 | A | 1122 | CLA | C3C-C4C-NC | 2.43 | 113.08 | 110.15 |
| 15 | F | 1301 | CLA | C4D-C3D-CAD | 2.43 | 111.03 | 108.05 |
| 15 | B | 1213 | CLA | C3C-C4C-NC | 2.42 | 113.07 | 110.15 |
| 14 | B | 4005 | BCR | C38-C26-C27 | 2.42 | 117.98 | 113.39 |
| 15 | F | 1410 | CLA | O2D-CGD-O1D | -2.42 | 118.93 | 123.79 |
| 15 | B | 1221 | CLA | C4A-NA-C1A | 2.42 | 109.79 | 106.38 |
| 15 | A | 1125 | CLA | CMB-C2B-C3B | 2.42 | 129.72 | 125.16 |
| 15 | A | 1134 | CLA | C3A-C4A-CHB | -2.42 | 119.30 | 124.33 |
| 15 | A | 1116 | CLA | C3A-C4A-CHB | -2.42 | 119.30 | 124.33 |
| 14 | A | 4001 | BCR | C15-C14-C13 | -2.42 | 123.79 | 127.29 |
| 15 | B | 1224 | CLA | C3A-C4A-CHB | -2.42 | 119.30 | 124.33 |
| 15 | J | 1303 | CLA | C3A-C4A-CHB | -2.42 | 119.30 | 124.33 |
| 15 | A | 1140 | CLA | C4-C3-C5 | 2.42 | 119.06 | 115.39 |
| 15 | B | 1215 | CLA | C3B-CAB-CBB | -2.42 | 120.94 | 125.95 |
| 15 | B | 1207 | CLA | C3A-C4A-CHB | -2.42 | 119.31 | 124.33 |
| 15 | A | 1107 | CLA | C4-C3-C2 | -2.41 | 118.75 | 123.66 |
| 15 | K | 1402 | CLA | C4B-CHC-C1C | 2.41 | 130.65 | 127.47 |
| 15 | A | 1103 | CLA | C3A-C4A-CHB | -2.41 | 119.31 | 124.33 |
| 14 | F | 4015 | BCR | C35-C13-C14 | -2.41 | 119.48 | 122.92 |
| 15 | A | 1106 | CLA | C3C-C4C-NC | 2.41 | 113.06 | 110.15 |
| 16 | B | 1301 | LMU | O1'-C1'-C2' | -2.41 | 105.06 | 108.15 |
| 15 | B | 1232 | CLA | C4D-C3D-CAD | 2.41 | 111.02 | 108.05 |
| 14 | B | 4014 | BCR | C38-C26-C27 | 2.41 | 117.96 | 113.39 |
| 15 | A | 1111 | CLA | CAC-C3C-C4C | 2.41 | 128.47 | 124.85 |
| 15 | A | 1125 | CLA | CHD-C4C-C3C | -2.41 | 121.27 | 124.97 |
| 15 | A | 1128 | CLA | C3A-C4A-CHB | -2.41 | 119.32 | 124.33 |
| 15 | B | 1236 | CLA | CMB-C2B-C3B | 2.41 | 129.70 | 125.16 |
| 14 | B | 4005 | BCR | C33-C5-C4 | 2.41 | 117.95 | 113.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1107 | CLA | CAA-C2A-C3A | -2.41 | 107.29 | 113.32 |
| 15 | B | 1230 | CLA | O2D-CGD-O1D | -2.41 | 118.96 | 123.79 |
| 15 | A | 1126 | CLA | C3A-C4A-CHB | -2.41 | 119.33 | 124.33 |
| 15 | A | 1125 | CLA | C3A-C4A-CHB | -2.41 | 119.33 | 124.33 |
| 15 | A | 1117 | CLA | C1-O2A-CGA | 2.41 | 123.99 | 117.00 |
| 15 | A | 1103 | CLA | CHB-C4A-NA | 2.41 | 127.74 | 124.38 |
| 15 | A | 1110 | CLA | C3A-C4A-NA | 2.40 | 113.72 | 110.81 |
| 14 | B | 4005 | BCR | C34-C9-C10 | -2.40 | 119.49 | 122.92 |
| 15 | A | 1136 | CLA | C4A-NA-C1A | 2.40 | 109.77 | 106.38 |
| 15 | A | 1106 | CLA | C2A-C1A-NA | 2.40 | 114.41 | 111.33 |
| 15 | J | 1303 | CLA | C4B-CHC-C1C | 2.40 | 130.63 | 127.47 |
| 14 | A | 4003 | BCR | C19-C18-C17 | 2.40 | 122.67 | 118.98 |
| 15 | A | 1138 | CLA | C4D-C3D-CAD | 2.40 | 111.00 | 108.05 |
| 15 | B | 1237 | CLA | O2D-CGD-O1D | -2.40 | 118.97 | 123.79 |
| 15 | B | 1021 | CLA | O2D-CGD-O1D | -2.40 | 118.97 | 123.79 |
| 15 | B | 1220 | CLA | C3A-C4A-NA | 2.40 | 113.71 | 110.81 |
| 15 | B | 1218 | CLA | C1-C2-C3 | -2.40 | 122.07 | 126.23 |
| 15 | B | 1206 | CLA | C3C-C4C-NC | 2.40 | 113.04 | 110.15 |
| 15 | A | 1125 | CLA | C1-O2A-CGA | 2.40 | 123.97 | 117.00 |
| 15 | B | 1231 | CLA | CMC-C2C-C1C | 2.40 | 128.37 | 124.95 |
| 15 | B | 1209 | CLA | C3A-C4A-NA | 2.40 | 113.71 | 110.81 |
| 15 | B | 1214 | CLA | O2D-CGD-O1D | -2.40 | 118.98 | 123.79 |
| 15 | A | 1113 | CLA | C4D-C3D-CAD | 2.40 | 111.00 | 108.05 |
| 15 | A | 1115 | CLA | O2D-CGD-O1D | -2.39 | 118.98 | 123.79 |
| 15 | A | 1135 | CLA | CMB-C2B-C3B | 2.39 | 129.67 | 125.16 |
| 15 | B | 1235 | CLA | C3A-C4A-CHB | -2.39 | 119.36 | 124.33 |
| 15 | A | 1118 | CLA | C4D-C3D-CAD | 2.39 | 110.99 | 108.05 |
| 15 | B | 1219 | CLA | C3C-C4C-NC | 2.39 | 113.03 | 110.15 |
| 15 | A | 1107 | CLA | O2D-CGD-O1D | -2.39 | 119.00 | 123.79 |
| 15 | A | 1109 | CLA | O2D-CGD-O1D | -2.39 | 118.99 | 123.79 |
| 15 | B | 1214 | CLA | C3A-C4A-NA | 2.39 | 113.70 | 110.81 |
| 14 | A | 4003 | BCR | C28-C27-C26 | -2.39 | 109.89 | 113.81 |
| 15 | A | 1133 | CLA | O2D-CGD-O1D | -2.38 | 119.00 | 123.79 |
| 14 | A | 4002 | BCR | C33-C5-C4 | 2.38 | 117.91 | 113.39 |
| 15 | A | 1132 | CLA | C4D-C3D-CAD | 2.38 | 110.98 | 108.05 |
| 15 | B | 1229 | CLA | C4-C3-C2 | -2.38 | 118.77 | 123.52 |
| 15 | J | 1302 | CLA | C3A-C4A-CHB | -2.38 | 119.38 | 124.33 |
| 15 | B | 1224 | CLA | C3C-C4C-NC | 2.38 | 113.02 | 110.15 |
| 15 | A | 1122 | CLA | C3A-C4A-NA | 2.38 | 113.69 | 110.81 |
| 15 | A | 1012 | CLA | CHB-C4A-NA | 2.38 | 127.70 | 124.38 |
| 15 | A | 1134 | CLA | C4B-CHC-C1C | 2.38 | 130.60 | 127.47 |
| 14 | A | 4008 | BCR | C34-C9-C10 | -2.38 | 119.53 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1128 | CLA | C4B-CHC-C1C | 2.38 | 130.60 | 127.47 |
| 15 | A | 1117 | CLA | C2A-C1A-NA | 2.38 | 114.38 | 111.33 |
| 15 | B | 1211 | CLA | C4D-C3D-CAD | 2.38 | 110.98 | 108.05 |
| 15 | A | 1106 | CLA | C4B-CHC-C1C | 2.38 | 130.60 | 127.47 |
| 15 | B | 1229 | CLA | O2D-CGD-O1D | -2.38 | 119.02 | 123.79 |
| 15 | B | 1201 | CLA | C3A-C4A-CHB | -2.38 | 119.39 | 124.33 |
| 15 | B | 1214 | CLA | C3B-CAB-CBB | -2.38 | 121.03 | 125.95 |
| 14 | B | 4009 | BCR | C30-C25-C26 | -2.37 | 119.16 | 122.59 |
| 15 | B | 1222 | CLA | CAA-C2A-C1A | -2.37 | 106.22 | 112.51 |
| 15 | B | 1213 | CLA | C4D-C3D-CAD | 2.37 | 110.97 | 108.05 |
| 15 | A | 1123 | CLA | C3A-C4A-CHB | -2.37 | 119.40 | 124.33 |
| 15 | B | 1221 | CLA | C2A-C1A-NA | 2.37 | 114.37 | 111.33 |
| 15 | A | 1112 | CLA | CHB-C4A-NA | 2.37 | 127.69 | 124.38 |
| 15 | A | 1122 | CLA | O2D-CGD-O1D | -2.37 | 119.03 | 123.79 |
| 10 | A | 2001 | PQN | C11-C12-C13 | -2.37 | 122.75 | 126.76 |
| 15 | B | 1021 | CLA | C2A-C1A-NA | 2.37 | 114.37 | 111.33 |
| 14 | B | 4004 | BCR | C1-C6-C5 | -2.37 | 119.16 | 122.59 |
| 15 | B | 1240 | CLA | C4D-C3D-CAD | 2.37 | 110.96 | 108.05 |
| 15 | A | 1116 | CLA | C4-C3-C5 | 2.37 | 118.99 | 115.39 |
| 15 | A | 1111 | CLA | CMB-C2B-C3B | 2.37 | 129.62 | 125.16 |
| 15 | A | 1102 | CLA | C2B-C1B-CHB | -2.37 | 121.51 | 126.00 |
| 15 | B | 1235 | CLA | C4B-CHC-C1C | 2.37 | 130.59 | 127.47 |
| 15 | B | 1208 | CLA | O2D-CGD-O1D | -2.36 | 119.04 | 123.79 |
| 15 | B | 1201 | CLA | C4D-C3D-CAD | 2.36 | 110.96 | 108.05 |
| 14 | B | 4009 | BCR | C8-C9-C10 | 2.36 | 122.61 | 118.98 |
| 15 | B | 1013 | CLA | CED-O2D-CGD | 2.36 | 121.63 | 116.00 |
| 14 | B | 4017 | BCR | C38-C26-C25 | -2.36 | 121.83 | 124.50 |
| 14 | F | 4016 | BCR | C7-C6-C5 | -2.36 | 115.91 | 121.59 |
| 15 | A | 1122 | CLA | CMD-C2D-C3D | -2.36 | 120.70 | 125.16 |
| 15 | A | 1104 | CLA | C3A-C4A-CHB | -2.36 | 119.42 | 124.33 |
| 15 | F | 1301 | CLA | CMB-C2B-C3B | 2.36 | 129.61 | 125.16 |
| 15 | B | 1225 | CLA | O2D-CGD-O1D | -2.36 | 119.06 | 123.79 |
| 15 | A | 1112 | CLA | O2D-CGD-O1D | -2.36 | 119.06 | 123.79 |
| 15 | B | 1013 | CLA | O2D-CGD-O1D | -2.36 | 119.06 | 123.79 |
| 15 | B | 1222 | CLA | C4A-NA-C1A | 2.36 | 109.70 | 106.38 |
| 14 | B | 4010 | BCR | C37-C22-C21 | -2.36 | 119.56 | 122.92 |
| 14 | F | 4015 | BCR | C3-C4-C5 | -2.35 | 109.94 | 113.81 |
| 15 | B | 1214 | CLA | C3C-C4C-NC | 2.35 | 112.99 | 110.15 |
| 15 | B | 1208 | CLA | C3C-C4C-NC | 2.35 | 112.99 | 110.15 |
| 15 | B | 1021 | CLA | C4A-NA-C1A | 2.35 | 109.70 | 106.38 |
| 15 | B | 1213 | CLA | C4-C3-C2 | -2.35 | 118.87 | 123.66 |
| 13 | A | 1108 | CL0 | C3A-C4A-CHB | -2.35 | 119.44 | 124.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1109 | CLA | C2A-C1A-NA | 2.35 | 114.34 | 111.33 |
| 15 | A | 1124 | CLA | CHB-C4A-NA | 2.35 | 127.66 | 124.38 |
| 15 | A | 1118 | CLA | C3B-CAB-CBB | -2.35 | 121.09 | 125.95 |
| 14 | B | 4017 | BCR | C30-C25-C26 | -2.35 | 119.19 | 122.59 |
| 15 | A | 1131 | CLA | C4D-C3D-CAD | 2.35 | 110.94 | 108.05 |
| 15 | A | 1111 | CLA | C4D-C3D-CAD | 2.35 | 110.94 | 108.05 |
| 15 | B | 1212 | CLA | C2A-C1A-NA | 2.35 | 114.34 | 111.33 |
| 15 | B | 1228 | CLA | C3A-C4A-CHB | -2.35 | 119.45 | 124.33 |
| 15 | B | 1228 | CLA | C4D-C3D-CAD | 2.35 | 110.94 | 108.05 |
| 15 | B | 1210 | CLA | C2B-C1B-CHB | -2.35 | 121.55 | 126.00 |
| 15 | B | 1220 | CLA | O2D-CGD-O1D | -2.35 | 119.08 | 123.79 |
| 14 | B | 4011 | BCR | C35-C13-C12 | 2.35 | 121.88 | 118.09 |
| 15 | B | 1231 | CLA | C4D-C3D-CAD | 2.35 | 110.94 | 108.05 |
| 15 | B | 1210 | CLA | O2D-CGD-O1D | -2.35 | 119.08 | 123.79 |
| 15 | A | 1126 | CLA | C4-C3-C5 | 2.35 | 118.95 | 115.39 |
| 15 | B | 1205 | CLA | C4A-NA-C1A | 2.34 | 109.68 | 106.38 |
| 15 | F | 1301 | CLA | O2D-CGD-O1D | -2.34 | 119.09 | 123.79 |
| 15 | B | 1229 | CLA | C4A-NA-C1A | 2.34 | 109.68 | 106.38 |
| 15 | A | 1128 | CLA | O1D-CGD-CBD | -2.34 | 119.67 | 124.45 |
| 15 | A | 1105 | CLA | C3A-C4A-CHB | -2.34 | 119.47 | 124.33 |
| 15 | B | 1204 | CLA | O2D-CGD-O1D | -2.34 | 119.10 | 123.79 |
| 15 | A | 1121 | CLA | O2D-CGD-O1D | -2.34 | 119.09 | 123.79 |
| 15 | B | 1221 | CLA | CHD-C4C-NC | -2.34 | 122.65 | 124.28 |
| 15 | J | 1303 | CLA | C2A-C1A-NA | 2.34 | 114.32 | 111.33 |
| 15 | B | 1206 | CLA | CAC-C3C-C4C | 2.34 | 128.36 | 124.85 |
| 15 | A | 1118 | CLA | C4A-NA-C1A | 2.33 | 109.67 | 106.38 |
| 15 | F | 1410 | CLA | C3A-C4A-CHB | -2.33 | 119.47 | 124.33 |
| 15 | B | 1222 | CLA | C3B-CAB-CBB | -2.33 | 121.12 | 125.95 |
| 15 | A | 1126 | CLA | C1-C2-C3 | -2.34 | 122.18 | 126.23 |
| 15 | A | 1111 | CLA | CHB-C4A-NA | 2.34 | 127.64 | 124.38 |
| 15 | A | 1140 | CLA | CMB-C2B-C3B | 2.34 | 129.56 | 125.16 |
| 15 | A | 1136 | CLA | C1-O2A-CGA | 2.33 | 123.79 | 117.00 |
| 13 | A | 1011 | CL0 | C4A-NA-C1A | 2.33 | 109.67 | 106.38 |
| 15 | A | 1120 | CLA | C3A-C4A-NA | 2.33 | 113.63 | 110.81 |
| 15 | F | 1301 | CLA | CHB-C4A-NA | 2.33 | 127.63 | 124.38 |
| 15 | J | 1302 | CLA | C2A-C1A-NA | 2.33 | 114.32 | 111.33 |
| 15 | B | 1240 | CLA | C2A-C1A-NA | 2.33 | 114.32 | 111.33 |
| 15 | A | 1128 | CLA | CMC-C2C-C1C | 2.33 | 128.27 | 124.95 |
| 15 | B | 1210 | CLA | C4D-C3D-CAD | 2.33 | 110.92 | 108.05 |
| 15 | B | 1204 | CLA | C3C-C4C-NC | 2.33 | 112.96 | 110.15 |
| 15 | A | 1119 | CLA | C4D-C3D-CAD | 2.33 | 110.92 | 108.05 |
| 15 | B | 1221 | CLA | C3A-C4A-CHB | -2.33 | 119.49 | 124.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1216 | CLA | O2D-CGD-O1D | -2.33 | 119.11 | 123.79 |
| 15 | B | 1239 | CLA | C3B-CAB-CBB | -2.33 | 121.13 | 125.95 |
| 15 | B | 1231 | CLA | CED-O2D-CGD | 2.33 | 121.54 | 116.00 |
| 15 | B | 1203 | CLA | O2D-CGD-O1D | -2.33 | 119.12 | 123.79 |
| 15 | A | 1117 | CLA | CMB-C2B-C3B | 2.33 | 129.54 | 125.16 |
| 15 | A | 1106 | CLA | C4D-C3D-CAD | 2.33 | 110.91 | 108.05 |
| 15 | B | 1219 | CLA | C3A-C4A-CHB | -2.33 | 119.49 | 124.33 |
| 15 | B | 1204 | CLA | CGD-CBD-CHA | -2.32 | 108.26 | 113.65 |
| 15 | F | 1410 | CLA | C4D-C3D-CAD | 2.32 | 110.91 | 108.05 |
| 15 | A | 1105 | CLA | C4D-C3D-CAD | 2.32 | 110.91 | 108.05 |
| 15 | A | 1117 | CLA | C3A-C4A-CHB | -2.32 | 119.50 | 124.33 |
| 15 | A | 1120 | CLA | O2D-CGD-O1D | -2.32 | 119.13 | 123.79 |
| 15 | A | 1127 | CLA | O2D-CGD-O1D | -2.32 | 119.13 | 123.79 |
| 15 | A | 1119 | CLA | O2D-CGD-O1D | -2.32 | 119.13 | 123.79 |
| 15 | A | 1105 | CLA | C2A-C1A-NA | 2.32 | 114.30 | 111.33 |
| 15 | A | 1124 | CLA | CMB-C2B-C3B | 2.32 | 129.53 | 125.16 |
| 15 | A | 1109 | CLA | C1-C2-C3 | -2.32 | 122.20 | 126.23 |
| 15 | A | 1104 | CLA | O2D-CGD-O1D | -2.32 | 119.13 | 123.79 |
| 15 | A | 1115 | CLA | CMB-C2B-C3B | 2.32 | 129.53 | 125.16 |
| 15 | A | 1120 | CLA | C3B-CAB-CBB | -2.32 | 121.15 | 125.95 |
| 15 | B | 1202 | CLA | CHB-C4A-NA | 2.32 | 127.61 | 124.38 |
| 15 | B | 1240 | CLA | C2B-C1B-CHB | -2.32 | 121.61 | 126.00 |
| 15 | B | 1240 | CLA | C3A-C4A-NA | 2.31 | 113.61 | 110.81 |
| 15 | B | 1201 | CLA | C3B-CAB-CBB | -2.31 | 121.16 | 125.95 |
| 15 | B | 1021 | CLA | C4-C3-C5 | 2.31 | 118.90 | 115.39 |
| 15 | B | 1013 | CLA | CHB-C4A-NA | 2.31 | 127.61 | 124.38 |
| 15 | B | 1013 | CLA | C4-C3-C5 | 2.31 | 118.90 | 115.39 |
| 15 | B | 1223 | CLA | C3A-C4A-CHB | -2.31 | 119.52 | 124.33 |
| 15 | F | 1301 | CLA | C3B-CAB-CBB | -2.31 | 121.16 | 125.95 |
| 15 | B | 1215 | CLA | CAA-C2A-C1A | -2.31 | 106.38 | 112.51 |
| 14 | B | 4014 | BCR | C36-C18-C17 | -2.31 | 119.62 | 122.92 |
| 15 | A | 1122 | CLA | C3A-C4A-CHB | -2.31 | 119.52 | 124.33 |
| 10 | A | 2001 | PQN | C2M-C2-C1 | 2.31 | 120.10 | 116.31 |
| 15 | A | 1022 | CLA | C2B-C1B-CHB | -2.31 | 121.62 | 126.00 |
| 15 | B | 1209 | CLA | CAC-C3C-C4C | 2.31 | 128.32 | 124.85 |
| 15 | B | 1218 | CLA | C3A-C4A-CHB | -2.31 | 119.53 | 124.33 |
| 15 | A | 1136 | CLA | C4B-CHC-C1C | 2.31 | 130.51 | 127.47 |
| 15 | A | 1118 | CLA | C3A-C4A-CHB | -2.31 | 119.53 | 124.33 |
| 15 | A | 1129 | CLA | C3A-C4A-CHB | -2.31 | 119.53 | 124.33 |
| 15 | A | 1134 | CLA | C2A-C1A-NA | 2.31 | 114.28 | 111.33 |
| 15 | A | 1101 | CLA | C3A-C4A-NA | 2.30 | 113.60 | 110.81 |
| 15 | B | 1236 | CLA | C3A-C4A-CHB | -2.30 | 119.54 | 124.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1021 | CLA | CHB-C4A-NA | 2.30 | 127.59 | 124.38 |
| 15 | A | 1135 | CLA | C4D-C3D-CAD | 2.30 | 110.88 | 108.05 |
| 15 | B | 1228 | CLA | C3A-C4A-NA | 2.30 | 113.60 | 110.81 |
| 16 | J | 1304 | LMU | C1B-O1B-C4' | -2.30 | 112.15 | 118.00 |
| 15 | A | 1801 | CLA | C1-C2-C3 | -2.30 | 122.23 | 126.23 |
| 14 | A | 4008 | BCR | C36-C18-C17 | -2.30 | 119.64 | 122.92 |
| 15 | B | 1236 | CLA | C4B-CHC-C1C | 2.30 | 130.50 | 127.47 |
| 15 | B | 1223 | CLA | C2A-C1A-NA | 2.30 | 114.28 | 111.33 |
| 15 | B | 1231 | CLA | CAA-C2A-C3A | -2.30 | 107.56 | 113.32 |
| 14 | A | 4008 | BCR | C28-C27-C26 | -2.30 | 110.04 | 113.81 |
| 15 | A | 1128 | CLA | C2B-C1B-CHB | -2.30 | 121.65 | 126.00 |
| 14 | B | 4017 | BCR | C34-C9-C8 | 2.29 | 121.80 | 118.09 |
| 15 | B | 1203 | CLA | C4A-NA-C1A | 2.30 | 109.61 | 106.38 |
| 15 | B | 1222 | CLA | C4D-C3D-CAD | 2.30 | 110.87 | 108.05 |
| 15 | A | 1131 | CLA | O1D-CGD-CBD | -2.29 | 119.76 | 124.45 |
| 14 | A | 4001 | BCR | C30-C25-C24 | 2.29 | 122.05 | 115.69 |
| 15 | A | 1135 | CLA | C3B-CAB-CBB | -2.29 | 121.21 | 125.95 |
| 15 | A | 1131 | CLA | C1-C2-C3 | -2.29 | 122.25 | 126.23 |
| 15 | A | 1137 | CLA | C3A-C4A-CHB | -2.29 | 119.57 | 124.33 |
| 15 | A | 1137 | CLA | C3B-CAB-CBB | -2.29 | 121.21 | 125.95 |
| 15 | A | 1123 | CLA | C4-C3-C5 | 2.29 | 118.87 | 115.39 |
| 14 | B | 4014 | BCR | C33-C5-C4 | 2.29 | 117.73 | 113.39 |
| 15 | A | 1117 | CLA | O2D-CGD-O1D | -2.29 | 119.19 | 123.79 |
| 15 | B | 1236 | CLA | C3B-CAB-CBB | -2.29 | 121.21 | 125.95 |
| 15 | B | 1023 | CLA | C4D-C3D-CAD | 2.29 | 110.86 | 108.05 |
| 15 | A | 1140 | CLA | C2B-C1B-CHB | -2.29 | 121.66 | 126.00 |
| 10 | B | 2002 | PQN | C2M-C2-C1 | 2.29 | 120.06 | 116.31 |
| 15 | A | 1107 | CLA | CAA-CBA-CGA | -2.29 | 106.50 | 113.24 |
| 15 | B | 1230 | CLA | CMB-C2B-C3B | 2.29 | 129.47 | 125.16 |
| 15 | B | 1229 | CLA | C3A-C4A-CHB | -2.29 | 119.57 | 124.33 |
| 15 | J | 1303 | CLA | O2D-CGD-O1D | -2.29 | 119.20 | 123.79 |
| 15 | B | 1211 | CLA | C4B-CHC-C1C | 2.29 | 130.48 | 127.47 |
| 15 | B | 1205 | CLA | C4-C3-C5 | 2.28 | 118.86 | 115.39 |
| 15 | A | 1132 | CLA | O1D-CGD-CBD | -2.28 | 119.78 | 124.45 |
| 15 | A | 1012 | CLA | CMB-C2B-C3B | 2.28 | 129.46 | 125.16 |
| 15 | A | 1127 | CLA | C4B-CHC-C1C | 2.28 | 130.47 | 127.47 |
| 15 | B | 1215 | CLA | C4D-C3D-CAD | 2.28 | 110.86 | 108.05 |
| 15 | B | 1217 | CLA | C3A-C4A-NA | 2.28 | 113.57 | 110.81 |
| 15 | B | 1216 | CLA | C3A-C4A-NA | 2.28 | 113.57 | 110.81 |
| 15 | F | 1301 | CLA | C2B-C1B-CHB | -2.28 | 121.67 | 126.00 |
| 15 | B | 1227 | CLA | CHB-C4A-NA | 2.28 | 127.56 | 124.38 |
| 15 | A | 1134 | CLA | C2B-C1B-CHB | -2.28 | 121.68 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1114 | CLA | C3A-C4A-CHB | -2.28 | 119.59 | 124.33 |
| 15 | B | 1220 | CLA | C3A-C4A-CHB | -2.28 | 119.59 | 124.33 |
| 15 | B | 1218 | CLA | C4B-CHC-C1C | 2.28 | 130.47 | 127.47 |
| 15 | B | 1208 | CLA | C4D-C3D-CAD | 2.28 | 110.86 | 108.05 |
| 15 | B | 1202 | CLA | C4B-CHC-C1C | 2.28 | 130.47 | 127.47 |
| 15 | A | 1137 | CLA | C4B-CHC-C1C | 2.28 | 130.47 | 127.47 |
| 14 | A | 4012 | BCR | C33-C5-C4 | 2.28 | 117.71 | 113.39 |
| 15 | B | 1226 | CLA | C3A-C4A-CHB | -2.28 | 119.59 | 124.33 |
| 15 | B | 1021 | CLA | CMA-C3A-C2A | -2.28 | 104.34 | 114.45 |
| 15 | A | 1130 | CLA | C4D-C3D-CAD | 2.28 | 110.85 | 108.05 |
| 15 | B | 1212 | CLA | CMB-C2B-C3B | 2.28 | 129.45 | 125.16 |
| 15 | F | 1139 | CLA | O2D-CGD-O1D | -2.28 | 119.22 | 123.79 |
| 15 | B | 1230 | CLA | C3A-C4A-CHB | -2.28 | 119.60 | 124.33 |
| 15 | B | 1237 | CLA | C3A-C4A-CHB | -2.28 | 119.60 | 124.33 |
| 14 | A | 4001 | BCR | C23-C22-C21 | 2.28 | 122.48 | 118.98 |
| 15 | A | 1128 | CLA | C1-C2-C3 | -2.27 | 122.28 | 126.23 |
| 12 | A | 5001 | LHG | O8-C23-C24 | 2.27 | 118.86 | 111.90 |
| 16 | B | 1301 | LMU | C1B-O1B-C4' | -2.27 | 112.22 | 118.00 |
| 15 | B | 1232 | CLA | C3A-C4A-CHB | -2.27 | 119.60 | 124.33 |
| 14 | A | 4012 | BCR | C8-C7-C6 | -2.27 | 120.52 | 127.23 |
| 15 | A | 1133 | CLA | C4B-CHC-C1C | 2.27 | 130.46 | 127.47 |
| 15 | A | 1111 | CLA | C4B-CHC-C1C | 2.27 | 130.46 | 127.47 |
| 15 | A | 1112 | CLA | C2B-C1B-CHB | -2.27 | 121.69 | 126.00 |
| 15 | B | 1215 | CLA | C4B-CHC-C1C | 2.27 | 130.46 | 127.47 |
| 15 | A | 1801 | CLA | C4A-NA-C1A | 2.27 | 109.58 | 106.38 |
| 15 | B | 1234 | CLA | C4D-C3D-CAD | 2.27 | 110.84 | 108.05 |
| 15 | B | 1221 | CLA | C4D-C3D-CAD | 2.27 | 110.84 | 108.05 |
| 15 | A | 1012 | CLA | C4D-C3D-CAD | 2.27 | 110.84 | 108.05 |
| 15 | B | 1228 | CLA | O2D-CGD-O1D | -2.27 | 119.23 | 123.79 |
| 15 | A | 1109 | CLA | CMB-C2B-C3B | 2.27 | 129.44 | 125.16 |
| 15 | B | 1232 | CLA | OBD-CAD-C3D | -2.27 | 123.56 | 128.15 |
| 14 | F | 4015 | BCR | C19-C18-C17 | 2.27 | 122.47 | 118.98 |
| 15 | B | 1227 | CLA | C2A-C1A-NA | 2.27 | 114.23 | 111.33 |
| 15 | A | 1112 | CLA | CMB-C2B-C3B | 2.27 | 129.43 | 125.16 |
| 14 | B | 4004 | BCR | C15-C14-C13 | -2.26 | 124.02 | 127.29 |
| 15 | A | 1127 | CLA | C4B-NB-C1B | 2.26 | 109.30 | 107.12 |
| 15 | A | 1121 | CLA | C4B-CHC-C1C | 2.26 | 130.45 | 127.47 |
| 15 | A | 1123 | CLA | C2A-C1A-NA | 2.26 | 114.23 | 111.33 |
| 15 | F | 1139 | CLA | C2A-C1A-NA | 2.26 | 114.23 | 111.33 |
| 15 | K | 1401 | CLA | O2D-CGD-O1D | -2.26 | 119.25 | 123.79 |
| 15 | B | 1210 | CLA | C3A-C4A-NA | 2.26 | 113.54 | 110.81 |
| 15 | B | 1224 | CLA | C2B-C1B-CHB | -2.26 | 121.72 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1216 | CLA | C4D-C3D-CAD | 2.26 | 110.83 | 108.05 |
| 14 | A | 4007 | BCR | C30-C25-C26 | -2.26 | 119.32 | 122.59 |
| 14 | F | 4015 | BCR | C33-C5-C4 | 2.26 | 117.67 | 113.39 |
| 15 | B | 1239 | CLA | C4A-NA-C1A | 2.26 | 109.56 | 106.38 |
| 15 | B | 1206 | CLA | CMB-C2B-C3B | 2.26 | 129.41 | 125.16 |
| 15 | B | 1023 | CLA | C2A-C1A-NA | 2.26 | 114.22 | 111.33 |
| 15 | B | 1013 | CLA | C4D-C3D-CAD | 2.26 | 110.83 | 108.05 |
| 14 | A | 4002 | BCR | C23-C24-C25 | -2.25 | 120.58 | 127.23 |
| 15 | A | 1012 | CLA | C4A-NA-C1A | 2.25 | 109.56 | 106.38 |
| 15 | B | 1223 | CLA | C3A-C4A-NA | 2.26 | 113.54 | 110.81 |
| 14 | F | 4015 | BCR | C8-C7-C6 | -2.25 | 120.58 | 127.23 |
| 15 | B | 1228 | CLA | C3B-CAB-CBB | -2.25 | 121.28 | 125.95 |
| 14 | J | 4013 | BCR | C19-C18-C17 | 2.25 | 122.44 | 118.98 |
| 15 | A | 1113 | CLA | C2B-C1B-CHB | -2.25 | 121.73 | 126.00 |
| 15 | A | 1022 | CLA | CMB-C2B-C3B | 2.25 | 129.40 | 125.16 |
| 15 | A | 1134 | CLA | C3A-C4A-NA | 2.25 | 113.53 | 110.81 |
| 15 | A | 1104 | CLA | C4B-CHC-C1C | 2.25 | 130.43 | 127.47 |
| 15 | A | 1801 | CLA | CMB-C2B-C3B | 2.25 | 129.40 | 125.16 |
| 15 | A | 1102 | CLA | C4B-CHC-C1C | 2.25 | 130.43 | 127.47 |
| 15 | A | 1133 | CLA | C2A-C1A-NA | 2.25 | 114.21 | 111.33 |
| 15 | A | 1112 | CLA | C3A-C4A-NA | 2.25 | 113.53 | 110.81 |
| 15 | A | 1132 | CLA | C4B-CHC-C1C | 2.25 | 130.43 | 127.47 |
| 15 | F | 1139 | CLA | C3A-C4A-CHB | -2.25 | 119.66 | 124.33 |
| 15 | B | 1231 | CLA | C3A-C4A-CHB | -2.25 | 119.66 | 124.33 |
| 13 | A | 1108 | CL0 | CED-O2D-CGD | 2.25 | 121.35 | 116.00 |
| 15 | A | 1109 | CLA | C2B-C1B-CHB | -2.25 | 121.74 | 126.00 |
| 15 | K | 1402 | CLA | C3A-C4A-CHB | -2.25 | 119.66 | 124.33 |
| 10 | B | 2002 | PQN | C2M-C2-C3 | -2.24 | 119.91 | 124.36 |
| 15 | B | 1218 | CLA | C3A-C4A-NA | 2.24 | 113.52 | 110.81 |
| 13 | A | 1108 | CL0 | CHB-C4A-NA | 2.24 | 127.51 | 124.38 |
| 15 | A | 1103 | CLA | CAA-C2A-C1A | -2.24 | 106.57 | 112.51 |
| 15 | B | 1201 | CLA | C3A-C4A-NA | 2.24 | 113.52 | 110.81 |
| 15 | A | 1111 | CLA | O2D-CGD-O1D | -2.24 | 119.29 | 123.79 |
| 15 | B | 1220 | CLA | C4B-CHC-C1C | 2.24 | 130.41 | 127.47 |
| 15 | B | 1205 | CLA | CAA-C2A-C3A | -2.24 | 107.72 | 113.32 |
| 15 | A | 1110 | CLA | CMB-C2B-C3B | 2.24 | 129.37 | 125.16 |
| 15 | A | 1126 | CLA | C3C-C4C-NC | 2.24 | 112.84 | 110.15 |
| 15 | B | 1212 | CLA | C3A-C4A-CHB | -2.24 | 119.68 | 124.33 |
| 15 | A | 1136 | CLA | C4-C3-C2 | -2.23 | 119.07 | 123.52 |
| 15 | B | 1226 | CLA | CMB-C2B-C3B | 2.23 | 129.37 | 125.16 |
| 15 | A | 1103 | CLA | C3C-C4C-NC | 2.23 | 112.84 | 110.15 |
| 15 | B | 1235 | CLA | CMB-C2B-C3B | 2.23 | 129.37 | 125.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | K | 1401 | CLA | CHB-C4A-NA | 2.23 | 127.49 | 124.38 |
| 15 | B | 1221 | CLA | CHB-C4A-NA | 2.23 | 127.49 | 124.38 |
| 15 | B | 1237 | CLA | CMB-C2B-C3B | 2.23 | 129.36 | 125.16 |
| 15 | B | 1207 | CLA | C4B-CHC-C1C | 2.23 | 130.41 | 127.47 |
| 15 | B | 1235 | CLA | C2B-C1B-CHB | -2.23 | 121.78 | 126.00 |
| 15 | A | 1125 | CLA | C4B-CHC-C1C | 2.23 | 130.40 | 127.47 |
| 15 | A | 1102 | CLA | CHB-C4A-NA | 2.23 | 127.49 | 124.38 |
| 15 | B | 1237 | CLA | C3A-C4A-NA | 2.23 | 113.50 | 110.81 |
| 15 | A | 1114 | CLA | C3B-CAB-CBB | -2.23 | 121.34 | 125.95 |
| 15 | B | 1201 | CLA | C2B-C1B-CHB | -2.23 | 121.78 | 126.00 |
| 15 | A | 1012 | CLA | C2B-C1B-CHB | -2.23 | 121.78 | 126.00 |
| 15 | B | 1225 | CLA | C2B-C1B-CHB | -2.22 | 121.78 | 126.00 |
| 15 | B | 1231 | CLA | C4B-CHC-C1C | 2.22 | 130.40 | 127.47 |
| 14 | F | 4015 | BCR | C30-C25-C26 | -2.22 | 119.37 | 122.59 |
| 15 | A | 1117 | CLA | C4D-C3D-CAD | 2.22 | 110.78 | 108.05 |
| 15 | A | 1131 | CLA | C3A-C4A-CHB | -2.22 | 119.71 | 124.33 |
| 15 | B | 1203 | CLA | C1-C2-C3 | -2.22 | 122.38 | 126.23 |
| 15 | B | 1238 | CLA | C3A-C4A-NA | 2.22 | 113.49 | 110.81 |
| 15 | A | 1127 | CLA | C3B-CAB-CBB | -2.22 | 121.35 | 125.95 |
| 15 | A | 1131 | CLA | CAC-C3C-C4C | 2.22 | 128.18 | 124.85 |
| 15 | B | 1231 | CLA | C2B-C1B-CHB | -2.22 | 121.79 | 126.00 |
| 15 | B | 1213 | CLA | CMB-C2B-C3B | 2.22 | 129.34 | 125.16 |
| 15 | B | 1230 | CLA | C4B-NB-C1B | 2.22 | 109.25 | 107.12 |
| 15 | B | 1206 | CLA | O2D-CGD-O1D | -2.22 | 119.34 | 123.79 |
| 15 | A | 1105 | CLA | C3A-C4A-NA | 2.22 | 113.49 | 110.81 |
| 15 | A | 1126 | CLA | O1D-CGD-CBD | -2.22 | 119.92 | 124.45 |
| 15 | A | 1104 | CLA | C4D-C3D-CAD | 2.22 | 110.78 | 108.05 |
| 15 | A | 1133 | CLA | CHD-C4C-NC | -2.22 | 122.73 | 124.28 |
| 15 | B | 1226 | CLA | C2A-C1A-NA | 2.22 | 114.17 | 111.33 |
| 15 | A | 1129 | CLA | CMD-C2D-C3D | -2.22 | 120.98 | 125.16 |
| 15 | A | 1132 | CLA | C4A-NA-C1A | 2.22 | 109.50 | 106.38 |
| 15 | B | 1204 | CLA | C3A-C4A-CHB | -2.21 | 119.73 | 124.33 |
| 15 | B | 1207 | CLA | CHB-C4A-NA | 2.21 | 127.47 | 124.38 |
| 15 | B | 1234 | CLA | C4A-NA-C1A | 2.21 | 109.50 | 106.38 |
| 15 | B | 1208 | CLA | C4B-CHC-C1C | 2.21 | 130.38 | 127.47 |
| 15 | A | 1103 | CLA | C4B-CHC-C1C | 2.21 | 130.38 | 127.47 |
| 15 | B | 1220 | CLA | C4D-C3D-CAD | 2.21 | 110.77 | 108.05 |
| 15 | A | 1113 | CLA | O2D-CGD-O1D | -2.21 | 119.35 | 123.79 |
| 15 | B | 1238 | CLA | C4D-C3D-CAD | 2.21 | 110.77 | 108.05 |
| 15 | B | 1211 | CLA | C3B-CAB-CBB | -2.21 | 121.37 | 125.95 |
| 15 | A | 1132 | CLA | C3A-C4A-CHB | -2.21 | 119.73 | 124.33 |
| 15 | B | 1206 | CLA | C3A-C4A-NA | 2.21 | 113.48 | 110.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1022 | CLA | C3A-C4A-CHB | -2.21 | 119.74 | 124.33 |
| 15 | A | 1801 | CLA | C3A-C4A-NA | 2.21 | 113.48 | 110.81 |
| 13 | A | 1108 | CL0 | C4A-NA-C1A | 2.21 | 109.49 | 106.38 |
| 15 | A | 1140 | CLA | C4B-CHC-C1C | 2.21 | 130.38 | 127.47 |
| 15 | B | 1235 | CLA | C4D-C3D-CAD | 2.21 | 110.77 | 108.05 |
| 15 | A | 1135 | CLA | C1-O2A-CGA | 2.21 | 123.41 | 117.00 |
| 15 | A | 1133 | CLA | C3A-C4A-NA | 2.21 | 113.48 | 110.81 |
| 15 | K | 1402 | CLA | C4A-NA-C1A | 2.21 | 109.49 | 106.38 |
| 15 | F | 1410 | CLA | C4B-CHC-C1C | 2.21 | 130.37 | 127.47 |
| 15 | A | 1119 | CLA | C2A-C1A-NA | 2.20 | 114.15 | 111.33 |
| 15 | K | 1401 | CLA | C3A-C4A-NA | 2.20 | 113.47 | 110.81 |
| 15 | A | 1121 | CLA | C3A-C4A-CHB | -2.20 | 119.75 | 124.33 |
| 15 | J | 1302 | CLA | C3A-C4A-NA | 2.20 | 113.47 | 110.81 |
| 15 | A | 1124 | CLA | O2D-CGD-O1D | -2.20 | 119.37 | 123.79 |
| 15 | A | 1115 | CLA | C4A-NA-C1A | 2.20 | 109.48 | 106.38 |
| 15 | B | 1224 | CLA | CAA-C2A-C1A | -2.20 | 106.68 | 112.51 |
| 15 | B | 1206 | CLA | CHB-C4A-NA | 2.20 | 127.45 | 124.38 |
| 15 | A | 1111 | CLA | C2B-C1B-CHB | -2.20 | 121.83 | 126.00 |
| 15 | B | 1226 | CLA | C4A-NA-C1A | 2.20 | 109.48 | 106.38 |
| 15 | B | 1237 | CLA | C2A-C1A-NA | 2.20 | 114.15 | 111.33 |
| 15 | A | 1118 | CLA | CHB-C4A-NA | 2.20 | 127.45 | 124.38 |
| 15 | B | 1224 | CLA | C3A-C4A-NA | 2.20 | 113.47 | 110.81 |
| 10 | B | 2002 | PQN | C11-C12-C13 | -2.20 | 123.05 | 126.76 |
| 15 | A | 1126 | CLA | CHB-C4A-NA | 2.20 | 127.44 | 124.38 |
| 15 | K | 1402 | CLA | O2D-CGD-O1D | -2.20 | 119.38 | 123.79 |
| 14 | B | 4006 | BCR | C23-C24-C25 | -2.20 | 120.76 | 127.23 |
| 15 | A | 1129 | CLA | C3B-CAB-CBB | -2.20 | 121.41 | 125.95 |
| 15 | A | 1101 | CLA | O1D-CGD-CBD | -2.19 | 119.97 | 124.45 |
| 15 | B | 1216 | CLA | C3A-C4A-CHB | -2.19 | 119.77 | 124.33 |
| 15 | A | 1126 | CLA | C4B-CHC-C1C | 2.19 | 130.36 | 127.47 |
| 14 | B | 4006 | BCR | C38-C26-C27 | 2.19 | 117.55 | 113.39 |
| 15 | B | 1208 | CLA | C2B-C1B-CHB | -2.19 | 121.84 | 126.00 |
| 15 | A | 1109 | CLA | C3A-C4A-CHB | -2.19 | 119.77 | 124.33 |
| 15 | B | 1240 | CLA | O2D-CGD-O1D | -2.19 | 119.39 | 123.79 |
| 15 | B | 1232 | CLA | O2D-CGD-O1D | -2.19 | 119.39 | 123.79 |
| 15 | A | 1138 | CLA | C1-O2A-CGA | 2.19 | 123.37 | 117.00 |
| 15 | B | 1235 | CLA | C4A-NA-C1A | 2.19 | 109.47 | 106.38 |
| 15 | A | 1113 | CLA | CMB-C2B-C3B | 2.19 | 129.29 | 125.16 |
| 15 | B | 1206 | CLA | C2B-C1B-CHB | -2.19 | 121.85 | 126.00 |
| 15 | B | 1203 | CLA | C1-O2A-CGA | 2.19 | 123.36 | 117.00 |
| 15 | A | 1113 | CLA | C3A-C4A-NA | 2.19 | 113.45 | 110.81 |
| 15 | B | 1013 | CLA | C4A-NA-C1A | 2.19 | 109.46 | 106.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | F | 4015 | BCR | C37-C22-C21 | -2.19 | 119.80 | 122.92 |
| 15 | B | 1213 | CLA | C2B-C1B-CHB | -2.18 | 121.86 | 126.00 |
| 15 | B | 1234 | CLA | C1-O2A-CGA | 2.18 | 123.35 | 117.00 |
| 15 | B | 1218 | CLA | OBD-CAD-C3D | -2.18 | 123.74 | 128.15 |
| 15 | A | 1138 | CLA | O2D-CGD-O1D | -2.18 | 119.41 | 123.79 |
| 15 | A | 1127 | CLA | OBD-CAD-CBD | -2.18 | 122.64 | 125.94 |
| 15 | A | 1107 | CLA | CMD-C2D-C3D | -2.18 | 121.04 | 125.16 |
| 15 | A | 1105 | CLA | C4B-CHC-C1C | 2.18 | 130.34 | 127.47 |
| 15 | F | 1139 | CLA | C4A-NA-C1A | 2.18 | 109.46 | 106.38 |
| 14 | A | 4007 | BCR | C34-C9-C8 | 2.18 | 121.61 | 118.09 |
| 15 | A | 1123 | CLA | C4A-NA-C1A | 2.18 | 109.45 | 106.38 |
| 14 | B | 4004 | BCR | C30-C25-C26 | -2.18 | 119.44 | 122.59 |
| 15 | A | 1123 | CLA | C3A-C4A-NA | 2.18 | 113.45 | 110.81 |
| 15 | B | 1231 | CLA | CMB-C2B-C3B | 2.18 | 129.27 | 125.16 |
| 15 | B | 1212 | CLA | O1D-CGD-CBD | -2.18 | 120.00 | 124.45 |
| 15 | B | 1023 | CLA | CHB-C4A-NA | 2.18 | 127.42 | 124.38 |
| 15 | B | 1211 | CLA | CMB-C2B-C3B | 2.18 | 129.26 | 125.16 |
| 15 | B | 1220 | CLA | C4-C3-C5 | 2.18 | 118.69 | 115.39 |
| 15 | B | 1201 | CLA | C4B-CHC-C1C | 2.18 | 130.33 | 127.47 |
| 15 | B | 1235 | CLA | CHB-C4A-NA | 2.18 | 127.42 | 124.38 |
| 15 | A | 1106 | CLA | C2B-C1B-CHB | -2.17 | 121.88 | 126.00 |
| 15 | A | 1106 | CLA | CMB-C2B-C3B | 2.17 | 129.26 | 125.16 |
| 15 | A | 1130 | CLA | C4B-CHC-C1C | 2.18 | 130.33 | 127.47 |
| 15 | B | 1238 | CLA | CMB-C2B-C3B | 2.17 | 129.25 | 125.16 |
| 15 | A | 1140 | CLA | C2A-C1A-NA | 2.17 | 114.11 | 111.33 |
| 15 | A | 1128 | CLA | C4A-NA-C1A | 2.17 | 109.44 | 106.38 |
| 15 | B | 1226 | CLA | C4-C3-C2 | -2.17 | 119.20 | 123.52 |
| 15 | B | 1231 | CLA | C4A-NA-C1A | 2.17 | 109.44 | 106.38 |
| 15 | B | 1222 | CLA | CMB-C2B-C3B | 2.17 | 129.25 | 125.16 |
| 15 | B | 1237 | CLA | C2B-C1B-CHB | -2.17 | 121.89 | 126.00 |
| 14 | B | 4011 | BCR | C4-C5-C6 | -2.17 | 120.00 | 122.86 |
| 15 | B | 1234 | CLA | CMB-C2B-C3B | 2.17 | 129.24 | 125.16 |
| 14 | F | 4015 | BCR | C32-C1-C6 | -2.17 | 106.74 | 110.33 |
| 15 | A | 1125 | CLA | C3A-C4A-NA | 2.17 | 113.43 | 110.81 |
| 15 | B | 1230 | CLA | C4B-CHC-C1C | 2.17 | 130.32 | 127.47 |
| 15 | A | 1112 | CLA | C4B-CHC-C1C | 2.17 | 130.32 | 127.47 |
| 14 | A | 4007 | BCR | C37-C22-C21 | -2.17 | 119.83 | 122.92 |
| 15 | B | 1215 | CLA | C3A-C4A-CHB | -2.17 | 119.83 | 124.33 |
| 15 | B | 1209 | CLA | CHB-C4A-NA | 2.16 | 127.40 | 124.38 |
| 15 | B | 1201 | CLA | C4A-NA-C1A | 2.16 | 109.43 | 106.38 |
| 15 | B | 1237 | CLA | C4B-CHC-C1C | 2.16 | 130.32 | 127.47 |
| 15 | A | 1110 | CLA | C4D-C3D-CAD | 2.16 | 110.71 | 108.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1235 | CLA | CAA-C2A-C3A | -2.16 | 107.91 | 113.32 |
| 15 | B | 1213 | CLA | C1-O2A-CGA | 2.16 | 123.28 | 117.00 |
| 14 | A | 4003 | BCR | C8-C9-C10 | 2.16 | 122.30 | 118.98 |
| 14 | F | 4016 | BCR | C7-C8-C9 | -2.16 | 122.99 | 126.22 |
| 15 | B | 1232 | CLA | C3A-C4A-NA | 2.16 | 113.42 | 110.81 |
| 15 | B | 1214 | CLA | CHB-C4A-NA | 2.16 | 127.39 | 124.38 |
| 13 | A | 1108 | CL0 | CGD-CBD-CAD | -2.15 | 103.55 | 110.79 |
| 15 | B | 1202 | CLA | CMB-C2B-C3B | 2.15 | 129.22 | 125.16 |
| 15 | A | 1118 | CLA | C2A-C1A-NA | 2.15 | 114.09 | 111.33 |
| 15 | A | 1120 | CLA | C4A-NA-C1A | 2.15 | 109.41 | 106.38 |
| 15 | B | 1231 | CLA | O2D-CGD-O1D | -2.15 | 119.47 | 123.79 |
| 15 | A | 1103 | CLA | C1-O2A-CGA | 2.15 | 123.26 | 117.00 |
| 13 | A | 1011 | CL0 | CMA-C3A-C4A | -2.15 | 105.52 | 112.40 |
| 15 | A | 1104 | CLA | CMB-C2B-C3B | 2.15 | 129.21 | 125.16 |
| 15 | B | 1217 | CLA | C2B-C1B-CHB | -2.15 | 121.92 | 126.00 |
| 14 | B | 4006 | BCR | C15-C14-C13 | -2.15 | 124.18 | 127.29 |
| 14 | A | 4001 | BCR | C31-C1-C6 | -2.15 | 106.77 | 110.33 |
| 15 | B | 1209 | CLA | C4A-NA-C1A | 2.15 | 109.40 | 106.38 |
| 15 | B | 1209 | CLA | C2B-C1B-CHB | -2.15 | 121.93 | 126.00 |
| 15 | A | 1123 | CLA | C4B-CHC-C1C | 2.14 | 130.29 | 127.47 |
| 15 | B | 1238 | CLA | C3A-C4A-CHB | -2.14 | 119.87 | 124.33 |
| 15 | B | 1218 | CLA | C2B-C1B-CHB | -2.14 | 121.94 | 126.00 |
| 15 | A | 1106 | CLA | C3A-C4A-NA | 2.14 | 113.40 | 110.81 |
| 15 | A | 1124 | CLA | C1-C2-C3 | -2.14 | 122.51 | 126.23 |
| 15 | B | 1238 | CLA | C4B-CHC-C1C | 2.14 | 130.29 | 127.47 |
| 15 | A | 1140 | CLA | C4A-NA-C1A | 2.14 | 109.40 | 106.38 |
| 14 | F | 4015 | BCR | C23-C24-C25 | -2.14 | 120.92 | 127.23 |
| 15 | A | 1137 | CLA | C4A-NA-C1A | 2.14 | 109.40 | 106.38 |
| 15 | A | 1117 | CLA | C1-C2-C3 | -2.14 | 122.52 | 126.23 |
| 14 | B | 4004 | BCR | C35-C13-C14 | -2.14 | 119.87 | 122.92 |
| 15 | A | 1104 | CLA | C4-C3-C2 | -2.14 | 119.26 | 123.52 |
| 15 | B | 1202 | CLA | C4-C3-C2 | -2.14 | 119.26 | 123.52 |
| 15 | B | 1203 | CLA | C3A-C4A-CHB | -2.14 | 119.89 | 124.33 |
| 16 | B | 1301 | LMU | O5'-C5'-C4' | 2.14 | 114.19 | 109.71 |
| 15 | B | 1212 | CLA | C4A-NA-C1A | 2.14 | 109.39 | 106.38 |
| 15 | B | 1238 | CLA | C2B-C1B-CHB | -2.14 | 121.95 | 126.00 |
| 15 | A | 1135 | CLA | O2D-CGD-O1D | -2.14 | 119.50 | 123.79 |
| 15 | B | 1221 | CLA | C4B-CHC-C1C | 2.14 | 130.28 | 127.47 |
| 15 | A | 1125 | CLA | O1D-CGD-CBD | -2.14 | 120.08 | 124.45 |
| 15 | J | 1303 | CLA | C4A-NA-C1A | 2.14 | 109.39 | 106.38 |
| 15 | A | 1801 | CLA | C2B-C1B-CHB | -2.13 | 121.95 | 126.00 |
| 15 | A | 1122 | CLA | CMB-C2B-C3B | 2.13 | 129.18 | 125.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | A | 1136 | CLA | C3A-C4A-CHB | -2.13 | 119.89 | 124.33 |
| 15 | A | 1133 | CLA | CAC-C3C-C4C | 2.13 | 128.05 | 124.85 |
| 15 | A | 1140 | CLA | C1-C2-C3 | -2.13 | 122.53 | 126.23 |
| 15 | B | 1217 | CLA | CMB-C2B-C3B | 2.13 | 129.17 | 125.16 |
| 15 | B | 1238 | CLA | O2D-CGD-O1D | -2.13 | 119.51 | 123.79 |
| 15 | B | 1219 | CLA | C2B-C1B-CHB | -2.13 | 121.96 | 126.00 |
| 15 | B | 1203 | CLA | C4B-CHC-C1C | 2.13 | 130.27 | 127.47 |
| 15 | B | 1023 | CLA | C4B-CHC-C1C | 2.13 | 130.27 | 127.47 |
| 15 | A | 1123 | CLA | CMB-C2B-C3B | 2.13 | 129.17 | 125.16 |
| 15 | B | 1023 | CLA | C4A-NA-C1A | 2.13 | 109.38 | 106.38 |
| 15 | B | 1207 | CLA | C4A-NA-C1A | 2.13 | 109.38 | 106.38 |
| 15 | A | 1114 | CLA | CMB-C2B-C3B | 2.13 | 129.17 | 125.16 |
| 15 | A | 1128 | CLA | CHB-C4A-NA | 2.13 | 127.35 | 124.38 |
| 15 | B | 1023 | CLA | C2B-C1B-CHB | -2.13 | 121.97 | 126.00 |
| 15 | B | 1239 | CLA | C3A-C4A-CHB | -2.13 | 119.90 | 124.33 |
| 15 | A | 1801 | CLA | CHB-C4A-NA | 2.13 | 127.35 | 124.38 |
| 15 | B | 1237 | CLA | C4A-NA-C1A | 2.13 | 109.38 | 106.38 |
| 15 | B | 1223 | CLA | C4B-CHC-C1C | 2.12 | 130.27 | 127.47 |
| 15 | B | 1227 | CLA | C4A-NA-C1A | 2.12 | 109.37 | 106.38 |
| 15 | F | 1410 | CLA | C2B-C1B-CHB | -2.12 | 121.97 | 126.00 |
| 15 | A | 1116 | CLA | CHB-C4A-NA | 2.12 | 127.34 | 124.38 |
| 15 | A | 1113 | CLA | CHB-C4A-NA | 2.12 | 127.34 | 124.38 |
| 15 | B | 1204 | CLA | CHB-C4A-NA | 2.12 | 127.34 | 124.38 |
| 15 | B | 1232 | CLA | C2A-C1A-NA | 2.12 | 114.05 | 111.33 |
| 15 | A | 1116 | CLA | C1-O2A-CGA | 2.12 | 123.17 | 117.00 |
| 15 | A | 1135 | CLA | C3A-C4A-CHB | -2.12 | 119.92 | 124.33 |
| 15 | F | 1410 | CLA | O1D-CGD-CBD | -2.11 | 120.13 | 124.45 |
| 15 | A | 1110 | CLA | C4B-CHC-C1C | 2.12 | 130.25 | 127.47 |
| 15 | A | 1115 | CLA | C3A-C4A-CHB | -2.12 | 119.93 | 124.33 |
| 15 | A | 1133 | CLA | C4A-NA-C1A | 2.12 | 109.36 | 106.38 |
| 15 | A | 1116 | CLA | O1D-CGD-CBD | -2.12 | 120.13 | 124.45 |
| 13 | A | 1108 | CL0 | CAC-C3C-C4C | 2.12 | 128.03 | 124.85 |
| 15 | B | 1023 | CLA | C3A-C4A-NA | 2.11 | 113.37 | 110.81 |
| 14 | J | 4013 | BCR | C35-C13-C14 | -2.11 | 119.91 | 122.92 |
| 15 | B | 1230 | CLA | C4A-NA-C1A | 2.11 | 109.36 | 106.38 |
| 15 | A | 1133 | CLA | CMB-C2B-C3B | 2.11 | 129.14 | 125.16 |
| 14 | B | 4010 | BCR | C7-C8-C9 | -2.11 | 123.05 | 126.22 |
| 13 | A | 1011 | CL0 | C2A-C1A-NA | 2.11 | 114.04 | 111.33 |
| 14 | B | 4004 | BCR | C3-C4-C5 | -2.11 | 110.34 | 113.81 |
| 15 | B | 1205 | CLA | C3A-C4A-CHB | -2.11 | 119.94 | 124.33 |
| 15 | A | 1126 | CLA | C2A-C1A-NA | 2.11 | 114.04 | 111.33 |
| 15 | B | 1225 | CLA | C3A-C4A-CHB | -2.11 | 119.94 | 124.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1232 | CLA | C4A-NA-C1A | 2.11 | 109.35 | 106.38 |
| 15 | A | 1801 | CLA | CAC-C3C-C2C | 2.11 | 131.31 | 127.50 |
| 15 | J | 1303 | CLA | CHB-C4A-NA | 2.11 | 127.32 | 124.38 |
| 15 | A | 1109 | CLA | CAA-C2A-C1A | -2.11 | 106.92 | 112.51 |
| 15 | B | 1232 | CLA | C2B-C1B-CHB | -2.11 | 122.01 | 126.00 |
| 15 | B | 1224 | CLA | C1-O2A-CGA | 2.11 | 123.13 | 117.00 |
| 15 | A | 1801 | CLA | C4-C3-C5 | 2.11 | 118.59 | 115.39 |
| 15 | A | 1120 | CLA | CHB-C4A-NA | 2.11 | 127.32 | 124.38 |
| 14 | B | 4014 | BCR | C3-C4-C5 | -2.11 | 110.35 | 113.81 |
| 15 | A | 1127 | CLA | C4A-NA-C1A | 2.11 | 109.35 | 106.38 |
| 15 | B | 1021 | CLA | C2B-C1B-CHB | -2.11 | 122.01 | 126.00 |
| 15 | B | 1231 | CLA | C2A-C1A-NA | 2.11 | 114.03 | 111.33 |
| 15 | A | 1138 | CLA | CHB-C4A-NA | 2.10 | 127.32 | 124.38 |
| 15 | A | 1119 | CLA | CED-O2D-CGD | 2.11 | 121.01 | 116.00 |
| 15 | A | 1112 | CLA | O1D-CGD-CBD | -2.11 | 120.15 | 124.45 |
| 15 | A | 1103 | CLA | CED-O2D-CGD | 2.11 | 121.01 | 116.00 |
| 15 | A | 1106 | CLA | C4A-NA-C1A | 2.11 | 109.35 | 106.38 |
| 15 | B | 1230 | CLA | C3B-CAB-CBB | -2.10 | 121.60 | 125.95 |
| 15 | B | 1237 | CLA | CMD-C2D-C3D | -2.10 | 121.19 | 125.16 |
| 15 | B | 1227 | CLA | O1D-CGD-CBD | -2.10 | 120.16 | 124.45 |
| 15 | F | 1410 | CLA | CMB-C2B-C3B | 2.10 | 129.12 | 125.16 |
| 15 | A | 1120 | CLA | CMB-C2B-C3B | 2.10 | 129.12 | 125.16 |
| 15 | B | 1204 | CLA | C4B-CHC-C1C | 2.10 | 130.23 | 127.47 |
| 15 | B | 1204 | CLA | C4A-NA-C1A | 2.10 | 109.34 | 106.38 |
| 15 | B | 1227 | CLA | C2B-C1B-CHB | -2.10 | 122.02 | 126.00 |
| 15 | B | 1217 | CLA | C4B-CHC-C1C | 2.10 | 130.23 | 127.47 |
| 15 | B | 1219 | CLA | C4B-CHC-C1C | 2.10 | 130.23 | 127.47 |
| 15 | A | 1129 | CLA | CHB-C4A-NA | 2.10 | 127.31 | 124.38 |
| 15 | B | 1230 | CLA | C1-C2-C3 | -2.10 | 122.59 | 126.23 |
| 15 | B | 1202 | CLA | C4A-NA-C1A | 2.10 | 109.33 | 106.38 |
| 15 | A | 1102 | CLA | C3A-C4A-NA | 2.10 | 113.34 | 110.81 |
| 15 | B | 1021 | CLA | CED-O2D-CGD | 2.10 | 120.99 | 116.00 |
| 15 | B | 1204 | CLA | CMB-C2B-C3B | 2.09 | 129.11 | 125.16 |
| 15 | B | 1212 | CLA | C4B-CHC-C1C | 2.09 | 130.22 | 127.47 |
| 15 | B | 1219 | CLA | C3A-C4A-NA | 2.09 | 113.34 | 110.81 |
| 16 | B | 1301 | LMU | C1'-O5'-C5' | 2.09 | 117.78 | 113.73 |
| 15 | A | 1129 | CLA | C4B-CHC-C1C | 2.09 | 130.22 | 127.47 |
| 15 | B | 1203 | CLA | C4-C3-C5 | 2.09 | 118.56 | 115.39 |
| 15 | A | 1137 | CLA | O1D-CGD-CBD | -2.09 | 120.18 | 124.45 |
| 15 | B | 1214 | CLA | O1D-CGD-CBD | -2.09 | 120.18 | 124.45 |
| 15 | B | 1211 | CLA | O1D-CGD-CBD | -2.09 | 120.18 | 124.45 |
| 15 | A | 1109 | CLA | C4B-CHC-C1C | 2.09 | 130.22 | 127.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 4006 | BCR | C19-C18-C17 | 2.09 | 122.19 | 118.98 |
| 15 | A | 1111 | CLA | C3A-C4A-NA | 2.09 | 113.33 | 110.81 |
| 15 | B | 1240 | CLA | C4B-CHC-C1C | 2.09 | 130.22 | 127.47 |
| 15 | A | 1136 | CLA | CHB-C4A-NA | 2.09 | 127.29 | 124.38 |
| 15 | B | 1226 | CLA | CHB-C4A-NA | 2.09 | 127.29 | 124.38 |
| 15 | A | 1133 | CLA | C2B-C1B-CHB | -2.08 | 122.05 | 126.00 |
| 15 | J | 1302 | CLA | C4A-NA-C1A | 2.08 | 109.32 | 106.38 |
| 15 | A | 1012 | CLA | C3A-C4A-NA | 2.08 | 113.33 | 110.81 |
| 15 | A | 1106 | CLA | CHB-C4A-NA | 2.08 | 127.29 | 124.38 |
| 15 | A | 1102 | CLA | C4A-NA-C1A | 2.08 | 109.31 | 106.38 |
| 15 | A | 1130 | CLA | O1D-CGD-CBD | -2.08 | 120.20 | 124.45 |
| 15 | B | 1213 | CLA | C3A-C4A-CHB | -2.08 | 120.01 | 124.33 |
| 15 | A | 1128 | CLA | C1-O2A-CGA | 2.08 | 123.04 | 117.00 |
| 15 | B | 1234 | CLA | CHB-C4A-NA | 2.08 | 127.28 | 124.38 |
| 14 | B | 4005 | BCR | C23-C24-C25 | -2.08 | 121.10 | 127.23 |
| 15 | A | 1116 | CLA | C3A-C4A-NA | 2.08 | 113.32 | 110.81 |
| 15 | A | 1120 | CLA | C2A-C1A-NA | 2.08 | 113.99 | 111.33 |
| 15 | B | 1239 | CLA | C4B-CHC-C1C | 2.08 | 130.20 | 127.47 |
| 10 | A | 2001 | PQN | C2M-C2-C3 | -2.08 | 120.24 | 124.36 |
| 15 | B | 1210 | CLA | C3B-CAB-CBB | -2.08 | 121.65 | 125.95 |
| 15 | A | 1114 | CLA | CAC-C3C-C4C | 2.07 | 127.96 | 124.85 |
| 15 | B | 1218 | CLA | C1-O2A-CGA | 2.07 | 123.03 | 117.00 |
| 14 | B | 4004 | BCR | C24-C23-C22 | -2.07 | 123.11 | 126.22 |
| 15 | B | 1209 | CLA | CHD-C4C-NC | -2.07 | 122.83 | 124.28 |
| 15 | K | 1401 | CLA | CMB-C2B-C3B | 2.07 | 129.07 | 125.16 |
| 15 | K | 1401 | CLA | C4A-NA-C1A | 2.07 | 109.30 | 106.38 |
| 15 | A | 1109 | CLA | C3A-C4A-NA | 2.07 | 113.32 | 110.81 |
| 15 | A | 1103 | CLA | C4-C3-C5 | 2.07 | 118.54 | 115.39 |
| 15 | A | 1104 | CLA | C3A-C4A-NA | 2.07 | 113.31 | 110.81 |
| 15 | A | 1123 | CLA | O1D-CGD-CBD | -2.07 | 120.22 | 124.45 |
| 14 | B | 4006 | BCR | C4-C5-C6 | -2.07 | 120.12 | 122.86 |
| 15 | B | 1209 | CLA | C4B-CHC-C1C | 2.07 | 130.19 | 127.47 |
| 15 | A | 1112 | CLA | C4A-NA-C1A | 2.07 | 109.30 | 106.38 |
| 15 | A | 1103 | CLA | CMB-C2B-C3B | 2.07 | 129.06 | 125.16 |
| 15 | J | 1303 | CLA | C3A-C4A-NA | 2.07 | 113.31 | 110.81 |
| 15 | A | 1129 | CLA | C4A-NA-C1A | 2.07 | 109.30 | 106.38 |
| 14 | B | 4004 | BCR | C30-C25-C24 | 2.07 | 121.42 | 115.69 |
| 15 | A | 1127 | CLA | CED-O2D-CGD | 2.07 | 120.92 | 116.00 |
| 15 | B | 1228 | CLA | CED-O2D-CGD | 2.07 | 120.92 | 116.00 |
| 15 | K | 1402 | CLA | CHB-C4A-NA | 2.07 | 127.26 | 124.38 |
| 14 | F | 4016 | BCR | C1-C6-C7 | 2.06 | 121.41 | 115.69 |
| 15 | A | 1131 | CLA | C4A-NA-C1A | 2.06 | 109.29 | 106.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1234 | CLA | C4B-CHC-C1C | 2.06 | 130.19 | 127.47 |
| 15 | B | 1234 | CLA | C3A-C4A-CHB | -2.06 | 120.04 | 124.33 |
| 15 | B | 1206 | CLA | C4B-CHC-C1C | 2.06 | 130.19 | 127.47 |
| 15 | A | 1120 | CLA | C4B-CHC-C1C | 2.06 | 130.18 | 127.47 |
| 15 | A | 1127 | CLA | C1-O2A-CGA | 2.06 | 122.99 | 117.00 |
| 15 | A | 1104 | CLA | CBC-CAC-C3C | -2.06 | 106.13 | 112.37 |
| 15 | B | 1235 | CLA | C4B-NB-C1B | 2.06 | 109.10 | 107.12 |
| 15 | B | 1013 | CLA | C2A-C1A-NA | 2.06 | 113.97 | 111.33 |
| 15 | F | 1410 | CLA | C3A-C4A-NA | 2.06 | 113.30 | 110.81 |
| 15 | A | 1133 | CLA | CHB-C4A-NA | 2.06 | 127.25 | 124.38 |
| 15 | A | 1131 | CLA | CHD-C4C-NC | -2.06 | 122.85 | 124.28 |
| 15 | A | 1132 | CLA | CHB-C4A-NA | 2.06 | 127.25 | 124.38 |
| 15 | B | 1229 | CLA | C3A-C4A-NA | 2.06 | 113.30 | 110.81 |
| 15 | A | 1105 | CLA | C2B-C1B-CHB | -2.06 | 122.10 | 126.00 |
| 15 | B | 1218 | CLA | CMB-C2B-C3B | 2.05 | 129.03 | 125.16 |
| 15 | A | 1126 | CLA | C4A-NA-C1A | 2.06 | 109.28 | 106.38 |
| 15 | A | 1103 | CLA | C4A-NA-C1A | 2.06 | 109.28 | 106.38 |
| 15 | A | 1119 | CLA | C4B-CHC-C1C | 2.05 | 130.18 | 127.47 |
| 15 | B | 1230 | CLA | O1D-CGD-CBD | -2.06 | 120.25 | 124.45 |
| 15 | B | 1236 | CLA | CHD-C4C-C3C | -2.05 | 121.82 | 124.97 |
| 15 | B | 1209 | CLA | C2A-C1A-NA | 2.05 | 113.96 | 111.33 |
| 15 | B | 1211 | CLA | C3A-C4A-CHB | -2.05 | 120.06 | 124.33 |
| 15 | B | 1215 | CLA | CMB-C2B-C3B | 2.05 | 129.03 | 125.16 |
| 15 | B | 1215 | CLA | C2B-C1B-CHB | -2.05 | 122.11 | 126.00 |
| 15 | A | 1128 | CLA | C2A-C1A-NA | 2.05 | 113.96 | 111.33 |
| 15 | B | 1203 | CLA | CHB-C4A-NA | 2.05 | 127.24 | 124.38 |
| 15 | B | 1238 | CLA | C3B-CAB-CBB | -2.05 | 121.71 | 125.95 |
| 15 | F | 1301 | CLA | C4B-CHC-C1C | 2.05 | 130.16 | 127.47 |
| 15 | A | 1801 | CLA | OBD-CAD-C3D | -2.04 | 124.02 | 128.15 |
| 13 | A | 1108 | CL0 | C4B-NB-C1B | 2.04 | 109.09 | 107.12 |
| 15 | A | 1102 | CLA | C4D-C3D-CAD | 2.04 | 110.56 | 108.05 |
| 15 | B | 1216 | CLA | C4B-CHC-C1C | 2.05 | 130.16 | 127.47 |
| 15 | B | 1217 | CLA | O1D-CGD-CBD | -2.04 | 120.28 | 124.45 |
| 15 | B | 1236 | CLA | C4-C3-C2 | -2.04 | 119.50 | 123.66 |
| 15 | B | 1235 | CLA | C3B-CAB-CBB | -2.04 | 121.72 | 125.95 |
| 15 | B | 1213 | CLA | C4B-CHC-C1C | 2.04 | 130.16 | 127.47 |
| 15 | B | 1202 | CLA | C3A-C4A-NA | 2.04 | 113.28 | 110.81 |
| 15 | A | 1114 | CLA | C3A-C4A-NA | 2.04 | 113.28 | 110.81 |
| 15 | B | 1021 | CLA | C3A-C4A-CHB | -2.04 | 120.09 | 124.33 |
| 15 | A | 1137 | CLA | CHD-C4C-NC | -2.04 | 122.86 | 124.28 |
| 15 | B | 1239 | CLA | CHC-C1C-C2C | -2.04 | 121.04 | 126.51 |
| 15 | B | 1224 | CLA | CHB-C4A-NA | 2.04 | 127.22 | 124.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1212 | CLA | C2B-C1B-CHB | -2.04 | 122.14 | 126.00 |
| 15 | A | 1105 | CLA | CAC-C3C-C4C | 2.03 | 127.91 | 124.85 |
| 14 | B | 4017 | BCR | C31-C1-C6 | -2.03 | 106.96 | 110.33 |
| 15 | F | 1139 | CLA | C2B-C1B-CHB | -2.03 | 122.15 | 126.00 |
| 15 | B | 1210 | CLA | C4B-CHC-C1C | 2.03 | 130.14 | 127.47 |
| 15 | A | 1123 | CLA | CHC-C1C-C2C | -2.03 | 121.06 | 126.51 |
| 15 | A | 1137 | CLA | CHB-C4A-NA | 2.03 | 127.21 | 124.38 |
| 15 | B | 1219 | CLA | C4A-NA-C1A | 2.03 | 109.24 | 106.38 |
| 14 | J | 4013 | BCR | C23-C22-C21 | 2.03 | 122.10 | 118.98 |
| 14 | B | 4004 | BCR | C23-C24-C25 | -2.03 | 121.25 | 127.23 |
| 15 | F | 1410 | CLA | CHB-C4A-NA | 2.03 | 127.21 | 124.38 |
| 15 | B | 1237 | CLA | CAC-C3C-C4C | 2.03 | 127.89 | 124.85 |
| 15 | F | 1410 | CLA | C6-C5-C3 | 2.02 | 117.24 | 112.62 |
| 15 | A | 1110 | CLA | CAC-C3C-C4C | 2.02 | 127.89 | 124.85 |
| 15 | B | 1225 | CLA | C4A-NA-C1A | 2.03 | 109.23 | 106.38 |
| 15 | A | 1128 | CLA | C4-C3-C5 | 2.03 | 118.47 | 115.39 |
| 14 | B | 4005 | BCR | C35-C13-C12 | 2.03 | 121.36 | 118.09 |
| 13 | A | 1108 | CL0 | O2D-CGD-O1D | -2.03 | 119.72 | 123.79 |
| 14 | B | 4011 | BCR | C1-C6-C7 | 2.02 | 121.30 | 115.69 |
| 15 | B | 1239 | CLA | CAC-C3C-C4C | 2.02 | 127.89 | 124.85 |
| 15 | B | 1230 | CLA | C2B-C1B-CHB | -2.02 | 122.16 | 126.00 |
| 15 | A | 1131 | CLA | C3A-C4A-NA | 2.02 | 113.25 | 110.81 |
| 15 | A | 1111 | CLA | C4A-NA-C1A | 2.02 | 109.23 | 106.38 |
| 15 | B | 1229 | CLA | C4B-CHC-C1C | 2.02 | 130.13 | 127.47 |
| 15 | A | 1127 | CLA | C3A-C4A-CHB | -2.02 | 120.13 | 124.33 |
| 15 | B | 1213 | CLA | C3B-CAB-CBB | -2.02 | 121.77 | 125.95 |
| 15 | B | 1230 | CLA | C3A-C4A-NA | 2.02 | 113.25 | 110.81 |
| 14 | B | 4004 | BCR | C1-C6-C7 | 2.02 | 121.28 | 115.69 |
| 15 | A | 1125 | CLA | CHB-C4A-NA | 2.02 | 127.20 | 124.38 |
| 15 | B | 1223 | CLA | C4A-NA-C1A | 2.02 | 109.22 | 106.38 |
| 15 | B | 1210 | CLA | C4A-NA-C1A | 2.02 | 109.23 | 106.38 |
| 15 | K | 1401 | CLA | CED-O2D-CGD | 2.02 | 120.81 | 116.00 |
| 14 | A | 4003 | BCR | C23-C24-C25 | -2.02 | 121.28 | 127.23 |
| 15 | B | 1232 | CLA | CAA-C2A-C3A | -2.02 | 108.27 | 113.32 |
| 15 | B | 1226 | CLA | C4B-NB-C1B | 2.01 | 109.06 | 107.12 |
| 14 | B | 4010 | BCR | C30-C25-C24 | 2.02 | 121.27 | 115.69 |
| 15 | B | 1211 | CLA | C4A-NA-C1A | 2.02 | 109.22 | 106.38 |
| 15 | B | 1210 | CLA | C16-C15-C13 | -2.02 | 109.17 | 115.44 |
| 15 | A | 1134 | CLA | C4A-NA-C1A | 2.01 | 109.22 | 106.38 |
| 15 | B | 1021 | CLA | C11-C12-C13 | -2.01 | 109.17 | 115.44 |
| 14 | B | 4010 | BCR | C19-C18-C17 | 2.01 | 122.07 | 118.98 |
| 15 | A | 1106 | CLA | CBA-CAA-C2A | 2.01 | 118.87 | 113.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 1240 | CLA | C4A-NA-C1A | 2.01 | 109.21 | 106.38 |
| 15 | A | 1135 | CLA | C4A-NA-C1A | 2.01 | 109.21 | 106.38 |
| 15 | A | 1135 | CLA | CED-O2D-CGD | 2.01 | 120.79 | 116.00 |
| 15 | B | 1231 | CLA | CHB-C4A-NA | 2.01 | 127.19 | 124.38 |
| 15 | A | 1121 | CLA | C4A-NA-C1A | 2.01 | 109.21 | 106.38 |
| 15 | B | 1217 | CLA | C4A-NA-C1A | 2.01 | 109.21 | 106.38 |
| 15 | A | 1120 | CLA | CBA-CAA-C2A | 2.01 | 118.86 | 113.95 |
| 15 | B | 1208 | CLA | C3A-C4A-CHB | -2.01 | 120.15 | 124.33 |
| 15 | A | 1130 | CLA | C4-C3-C5 | 2.01 | 118.44 | 115.39 |
| 14 | A | 4008 | BCR | C37-C22-C21 | -2.01 | 120.06 | 122.92 |
| 15 | A | 1105 | CLA | O1D-CGD-CBD | -2.01 | 120.35 | 124.45 |
| 15 | B | 1209 | CLA | CHC-C1C-C2C | -2.01 | 121.12 | 126.51 |
| 15 | A | 1801 | CLA | C4B-CHC-C1C | 2.01 | 130.11 | 127.47 |
| 14 | J | 4013 | BCR | C35-C13-C12 | 2.01 | 121.33 | 118.09 |
| 15 | A | 1113 | CLA | CAC-C3C-C4C | 2.01 | 127.86 | 124.85 |
| 15 | A | 1125 | CLA | C4A-NA-C1A | 2.01 | 109.21 | 106.38 |
| 15 | A | 1116 | CLA | C4A-NA-C1A | 2.00 | 109.20 | 106.38 |
| 13 | A | 1011 | CL0 | C1-O2A-CGA | 2.01 | 122.83 | 117.00 |
| 15 | A | 1126 | CLA | CAA-C2A-C3A | -2.00 | 108.31 | 113.32 |
| 15 | A | 1012 | CLA | C4-C3-C2 | -2.00 | 119.53 | 123.52 |
| 15 | A | 1129 | CLA | CMB-C2B-C3B | 2.00 | 128.93 | 125.16 |
| 15 | B | 1229 | CLA | C2B-C1B-CHB | -2.00 | 122.20 | 126.00 |
| 15 | A | 1140 | CLA | C3A-C4A-CHB | -2.00 | 120.17 | 124.33 |
| 13 | A | 1011 | CL0 | C2B-C1B-CHB | -2.00 | 122.21 | 126.00 |
| 15 | B | 1210 | CLA | CHB-C4A-NA | 2.00 | 127.17 | 124.38 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 14 | B | 4009 | BCR | C11-C10-C9-C34 |
| 14 | B | 4009 | BCR | C11-C10-C9-C8 |

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 739/751 (98%) | 0.08 | 66 (8%) 10 8 | 43, 90, 141, 226 | 0 |
| 2 | B | 728/731 (99%) | -0.24 | 23 (3%) 45 46 | 53, 83, 126, 179 | 0 |
| 3 | C | 80/81 (98%) | -0.34 | 1 (1%) 74 75 | 60, 72, 95, 105 | 0 |
| 4 | D | 138/141 (97%) | 1.10 | 39 (28%) 1 1 | 72, 90, 125, 161 | 0 |
| 5 | E | 68/74 (91%) | 0.31 | 11 (16%) 2 2 | 59, 75, 109, 138 | 0 |
| 6 | F | 141/165 (85%) | -0.52 | 3 (2%) 60 61 | 64, 82, 111, 169 | 0 |
| 7 | J | 40/40 (100%) | -0.46 | 2 (5%) 28 28 | 66, 76, 124, 149 | 0 |
| 8 | K | 53/128 (41%) | 0.99 | 14 (26%) 1 1 | 134, 160, 207, 253 | 0 |
| 9 | M | 30/31 (96%) | 2.29 | 10 (33%) 1 1 | 109, 132, 158, 172 | 0 |
| All | All | 2017/2142 (94%) | 0.03 | 169 (8%) 11 9 | 43, 86, 145, 253 | 0 |

All (169) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | M | 2 | ALA | 26.8 |
| 9 | M | 3 | LEU | 15.6 |
| 4 | D | 113 | GLU | 10.8 |
| 1 | A | 260 | LEU | 8.7 |
| 1 | A | 751 | GLY | 7.8 |
| 9 | M | 4 | SER | 7.5 |
| 9 | M | 6 | THR | 7.0 |
| 4 | D | 114 | ALA | 6.8 |
| 1 | A | 257 | ALA | 6.3 |
| 4 | D | 10 | LYS | 6.3 |
| 5 | E | 31 | SER | 6.3 |
| 4 | D | 130 | THR | 6.1 |
| 4 | D | 58 | TYR | 6.1 |
| 2 | B | 92 | TRP | 6.0 |
| 1 | A | 511 | GLY | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | M | 5 | ASP | 5.3 |
| 1 | A | 300 | ILE | 5.3 |
| 4 | D | 49 | ILE | 5.1 |
| 4 | D | 140 | GLU | 5.1 |
| 4 | D | 126 | PRO | 5.1 |
| 1 | A | 238 | LEU | 4.9 |
| 1 | A | 623 | PRO | 4.9 |
| 4 | D | 37 | GLU | 4.9 |
| 2 | B | 111 | ASN | 4.8 |
| 4 | D | 127 | GLU | 4.8 |
| 1 | A | 488 | HIS | 4.8 |
| 8 | K | 127 | ILE | 4.7 |
| 2 | B | 96 | PHE | 4.7 |
| 1 | A | 622 | SER | 4.6 |
| 1 | A | 237 | PRO | 4.6 |
| 5 | E | 3 | LEU | 4.6 |
| 4 | D | 52 | GLU | 4.5 |
| 4 | D | 115 | GLN | 4.5 |
| 1 | A | 304 | PHE | 4.5 |
| 8 | K | 64 | MET | 4.5 |
| 1 | A | 236 | ILE | 4.4 |
| 4 | D | 139 | TYR | 4.4 |
| 5 | E | 30 | LYS | 4.3 |
| 1 | A | 235 | ASP | 4.3 |
| 1 | A | 496 | ALA | 4.3 |
| 1 | A | 361 | SER | 4.1 |
| 4 | D | 51 | ASN | 4.1 |
| 9 | M | 10 | ALA | 4.1 |
| 1 | A | 261 | THR | 4.0 |
| 4 | D | 4 | LEU | 4.0 |
| 1 | A | 299 | ALA | 4.0 |
| 4 | D | 100 | ALA | 3.9 |
| 2 | B | 110 | SER | 3.9 |
| 1 | A | 233 | PRO | 3.9 |
| 1 | A | 241 | GLU | 3.8 |
| 1 | A | 510 | GLY | 3.8 |
| 1 | A | 297 | HIS | 3.8 |
| 9 | M | 8 | ILE | 3.8 |
| 2 | B | 159 | PRO | 3.8 |
| 2 | B | 98 | GLU | 3.7 |
| 1 | A | 256 | PHE | 3.7 |
| 1 | A | 259 | GLY | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | D | 137 | ALA | 3.7 |
| 1 | A | 154 | ASP | 3.6 |
| 1 | A | 234 | LYS | 3.6 |
| 4 | D | 3 | GLU | 3.6 |
| 1 | A | 239 | PRO | 3.6 |
| 8 | K | 76 | TYR | 3.6 |
| 4 | D | 131 | ILE | 3.6 |
| 8 | K | 108 | MET | 3.6 |
| 5 | E | 7 | ASP | 3.5 |
| 1 | A | 251 | GLU | 3.5 |
| 1 | A | 296 | HIS | 3.5 |
| 2 | B | 248 | GLU | 3.4 |
| 1 | A | 363 | THR | 3.4 |
| 2 | B | 375 | TYR | 3.4 |
| 1 | A | 360 | GLY | 3.4 |
| 1 | A | 301 | ALA | 3.4 |
| 1 | A | 495 | GLY | 3.4 |
| 4 | D | 7 | GLN | 3.3 |
| 1 | A | 485 | TRP | 3.3 |
| 8 | K | 60 | VAL | 3.3 |
| 4 | D | 88 | VAL | 3.2 |
| 4 | D | 36 | SER | 3.2 |
| 9 | M | 7 | GLN | 3.2 |
| 4 | D | 77 | LYS | 3.2 |
| 1 | A | 365 | ILE | 3.2 |
| 8 | K | 100 | GLY | 3.2 |
| 1 | A | 252 | LEU | 3.1 |
| 1 | A | 303 | LEU | 3.1 |
| 7 | J | 2 | ASP | 2.9 |
| 4 | D | 11 | PHE | 2.9 |
| 4 | D | 134 | SER | 2.9 |
| 4 | D | 129 | VAL | 2.9 |
| 4 | D | 138 | PRO | 2.9 |
| 6 | F | 92 | GLU | 2.9 |
| 1 | A | 295 | HIS | 2.9 |
| 1 | A | 206 | GLY | 2.8 |
| 1 | A | 624 | ASP | 2.8 |
| 6 | F | 94 | LYS | 2.8 |
| 1 | A | 362 | LEU | 2.8 |
| 2 | B | 3 | THR | 2.8 |
| 2 | B | 584 | LEU | 2.8 |
| 4 | D | 54 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 688 | VAL | 2.7 |
| 1 | A | 298 | LEU | 2.7 |
| 1 | A | 209 | SER | 2.7 |
| 2 | B | 216 | PRO | 2.7 |
| 5 | E | 2 | ALA | 2.7 |
| 5 | E | 69 | VAL | 2.7 |
| 4 | D | 125 | ASN | 2.7 |
| 2 | B | 214 | SER | 2.7 |
| 5 | E | 4 | ASN | 2.6 |
| 1 | A | 36 | ARG | 2.6 |
| 8 | K | 62 | ILE | 2.6 |
| 1 | A | 364 | ILE | 2.6 |
| 1 | A | 489 | LEU | 2.6 |
| 4 | D | 133 | PHE | 2.6 |
| 2 | B | 347 | ALA | 2.6 |
| 1 | A | 205 | LEU | 2.6 |
| 5 | E | 32 | GLY | 2.6 |
| 3 | C | 47 | ASP | 2.5 |
| 4 | D | 50 | MET | 2.5 |
| 4 | D | 57 | LEU | 2.5 |
| 8 | K | 63 | ILE | 2.5 |
| 4 | D | 94 | VAL | 2.5 |
| 2 | B | 486 | THR | 2.5 |
| 1 | A | 355 | ASN | 2.5 |
| 1 | A | 258 | GLN | 2.5 |
| 1 | A | 156 | TYR | 2.5 |
| 2 | B | 343 | THR | 2.5 |
| 8 | K | 75 | GLY | 2.5 |
| 4 | D | 8 | PRO | 2.4 |
| 8 | K | 77 | PHE | 2.4 |
| 1 | A | 116 | VAL | 2.4 |
| 5 | E | 8 | LYS | 2.3 |
| 1 | A | 620 | THR | 2.3 |
| 2 | B | 580 | MET | 2.3 |
| 9 | M | 9 | LEU | 2.3 |
| 2 | B | 379 | PHE | 2.3 |
| 1 | A | 502 | LEU | 2.3 |
| 1 | A | 356 | LEU | 2.3 |
| 1 | A | 369 | HIS | 2.3 |
| 6 | F | 15 | ALA | 2.3 |
| 1 | A | 397 | GLY | 2.2 |
| 8 | K | 65 | CYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 230 | GLY | 2.2 |
| 4 | D | 101 | ASP | 2.2 |
| 4 | D | 116 | GLY | 2.2 |
| 7 | J | 1 | MET | 2.2 |
| 1 | A | 400 | LEU | 2.2 |
| 4 | D | 128 | PRO | 2.2 |
| 4 | D | 136 | LYS | 2.2 |
| 2 | B | 294 | ASN | 2.2 |
| 1 | A | 226 | LEU | 2.2 |
| 2 | B | 112 | PRO | 2.1 |
| 1 | A | 302 | VAL | 2.1 |
| 4 | D | 48 | ALA | 2.1 |
| 8 | K | 101 | LEU | 2.1 |
| 2 | B | 70 | TRP | 2.1 |
| 5 | E | 29 | GLU | 2.1 |
| 1 | A | 208 | GLY | 2.1 |
| 2 | B | 488 | ALA | 2.1 |
| 5 | E | 14 | THR | 2.1 |
| 1 | A | 625 | GLY | 2.1 |
| 9 | M | 11 | ALA | 2.1 |
| 8 | K | 59 | SER | 2.1 |
| 8 | K | 126 | GLY | 2.1 |
| 1 | A | 524 | PRO | 2.0 |
| 1 | A | 404 | ALA | 2.0 |
| 1 | A | 244 | LEU | 2.0 |
| 2 | B | 588 | THR | 2.0 |
| 1 | A | 359 | LEU | 2.0 |
| 1 | A | 492 | LEU | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 14 | BCR | B | 4009 | 40/40 | 0.39 | 9.83 | 72,103,147,151 | 0 |
| 15 | CLA | A | 1121 | 46/65 | 0.22 | 5.35 | 91,114,141,163 | 0 |
| 15 | CLA | J | 1303 | 46/65 | 0.33 | 5.28 | 94,114,141,159 | 0 |
| 11 | SF4 | C | 3003 | 8/8 | 0.22 | 4.80 | 60,67,100,115 | 0 |
| 15 | CLA | F | 1410 | 65/65 | 0.23 | 3.70 | 69,96,135,147 | 0 |
| 11 | SF4 | A | 3001 | 8/8 | 0.24 | 3.57 | 50,62,210,290 | 0 |
| 14 | BCR | A | 4007 | 40/40 | 0.36 | 3.48 | 69,86,137,139 | 0 |
| 15 | CLA | J | 1302 | 45/65 | 0.25 | 3.45 | 82,93,138,150 | 0 |
| 10 | PQN | B | 2002 | 33/33 | 0.28 | 3.40 | 59,79,99,105 | 0 |
| 15 | CLA | A | 1122 | 65/65 | 0.22 | 3.33 | 74,91,119,129 | 0 |
| 14 | BCR | A | 4003 | 40/40 | 0.40 | 3.11 | 69,111,146,146 | 0 |
| 15 | CLA | A | 1110 | 54/65 | 0.22 | 2.91 | 96,121,150,154 | 0 |
| 14 | BCR | B | 4017 | 40/40 | 0.20 | 2.71 | 70,87,101,104 | 0 |
| 14 | BCR | J | 4013 | 40/40 | 0.27 | 2.61 | 78,97,112,121 | 0 |
| 12 | LHG | A | 5003 | 49/49 | 0.33 | 2.40 | 91,121,142,143 | 0 |
| 15 | CLA | A | 1106 | 65/65 | 0.20 | 2.37 | 59,79,98,109 | 0 |
| 15 | CLA | A | 1801 | 52/65 | 0.35 | 2.30 | 100,122,154,158 | 0 |
| 14 | BCR | A | 4012 | 40/40 | 0.17 | 2.28 | 55,77,87,91 | 0 |
| 14 | BCR | B | 4006 | 40/40 | 0.24 | 2.10 | 86,109,141,142 | 0 |
| 14 | BCR | A | 4002 | 40/40 | 0.31 | 2.02 | 88,109,128,130 | 0 |
| 14 | BCR | B | 4005 | 40/40 | 0.29 | 1.98 | 73,93,125,128 | 0 |
| 15 | CLA | A | 1111 | 60/65 | 0.26 | 1.94 | 78,96,107,112 | 0 |
| 13 | CL0 | A | 1108 | 45/65 | 0.27 | 1.86 | 86,113,154,170 | 0 |
| 14 | BCR | F | 4015 | 40/40 | 0.21 | 1.79 | 52,73,107,111 | 0 |
| 14 | BCR | B | 4004 | 40/40 | 0.30 | 1.73 | 101,115,147,151 | 0 |
| 15 | CLA | B | 1240 | 45/65 | 0.28 | 1.69 | 71,83,124,151 | 0 |
| 15 | CLA | A | 1136 | 65/65 | 0.31 | 1.67 | 78,105,139,142 | 0 |
| 17 | LMG | B | 5002 | 55/55 | 0.27 | 1.38 | 71,101,130,137 | 0 |
| 15 | CLA | A | 1138 | 65/65 | 0.20 | 1.33 | 47,55,69,77 | 0 |
| 15 | CLA | B | 1229 | 65/65 | 0.18 | 1.32 | 50,62,86,107 | 0 |
| 15 | CLA | B | 1228 | 65/65 | 0.19 | 1.32 | 54,74,105,114 | 0 |
| 15 | CLA | A | 1101 | 65/65 | 0.18 | 1.32 | 55,73,89,96 | 0 |
| 15 | CLA | B | 1231 | 65/65 | 0.22 | 1.23 | 66,89,115,138 | 0 |
| 15 | CLA | B | 1214 | 65/65 | 0.23 | 1.21 | 72,89,119,133 | 0 |
| 15 | CLA | F | 1139 | 65/65 | 0.20 | 1.13 | 47,58,90,98 | 0 |
| 16 | LMU | J | 1304 | 35/35 | 0.32 | 1.13 | 91,159,172,173 | 0 |
| 15 | CLA | B | 1023 | 65/65 | 0.23 | 1.09 | 55,79,111,119 | 0 |
| 12 | LHG | B | 5004 | 49/49 | 0.21 | 1.08 | 59,88,99,106 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 15 | CLA | B | 1230 | 65/65 | 0.15 | 1.05 | 53,68,118,125 | 0 |
| 15 | CLA | A | 1022 | 65/65 | 0.23 | 1.04 | 53,78,96,103 | 0 |
| 15 | CLA | A | 1127 | 65/65 | 0.36 | 1.04 | 67,79,100,106 | 0 |
| 15 | CLA | A | 1126 | 65/65 | 0.23 | 1.02 | 63,80,101,116 | 0 |
| 14 | BCR | F | 4016 | 40/40 | 0.15 | 1.01 | 59,72,89,94 | 0 |
| 11 | SF4 | C | 3002 | 8/8 | 0.21 | 1.01 | 60,88,151,152 | 0 |
| 15 | CLA | K | 1401 | 46/65 | 0.30 | 1.00 | 120,155,169,173 | 0 |
| 15 | CLA | B | 1234 | 65/65 | 0.25 | 0.98 | 56,73,108,120 | 0 |
| 15 | CLA | A | 1135 | 55/65 | 0.25 | 0.95 | 70,98,132,135 | 0 |
| 15 | CLA | A | 1012 | 65/65 | 0.23 | 0.94 | 47,60,86,93 | 0 |
| 10 | PQN | A | 2001 | 33/33 | 0.19 | 0.89 | 45,57,68,74 | 0 |
| 15 | CLA | A | 1132 | 62/65 | 0.15 | 0.85 | 74,105,153,156 | 0 |
| 14 | BCR | B | 4011 | 40/40 | 0.19 | 0.84 | 49,67,84,91 | 0 |
| 15 | CLA | K | 1402 | 46/65 | 0.32 | 0.77 | 163,187,214,221 | 0 |
| 15 | CLA | A | 1102 | 65/65 | 0.17 | 0.77 | 55,81,107,112 | 0 |
| 15 | CLA | B | 1219 | 55/65 | 0.17 | 0.75 | 74,86,119,142 | 0 |
| 15 | CLA | B | 1216 | 65/65 | 0.17 | 0.72 | 67,91,106,118 | 0 |
| 15 | CLA | A | 1116 | 54/65 | 0.37 | 0.69 | 84,113,130,141 | 0 |
| 15 | CLA | F | 1301 | 45/65 | 0.17 | 0.65 | 54,75,97,131 | 0 |
| 15 | CLA | B | 1224 | 65/65 | 0.27 | 0.63 | 60,78,98,108 | 0 |
| 15 | CLA | B | 1215 | 65/65 | 0.24 | 0.62 | 72,85,104,106 | 0 |
| 15 | CLA | A | 1105 | 65/65 | 0.19 | 0.50 | 70,96,111,120 | 0 |
| 15 | CLA | B | 1021 | 65/65 | 0.22 | 0.50 | 49,69,80,84 | 0 |
| 15 | CLA | B | 1218 | 51/65 | 0.19 | 0.50 | 86,98,125,159 | 0 |
| 15 | CLA | A | 1117 | 65/65 | 0.37 | 0.48 | 80,100,111,113 | 0 |
| 15 | CLA | B | 1210 | 65/65 | 0.20 | 0.47 | 75,95,108,120 | 0 |
| 15 | CLA | A | 1103 | 65/65 | 0.24 | 0.45 | 61,80,108,118 | 0 |
| 15 | CLA | A | 1140 | 65/65 | 0.18 | 0.44 | 52,73,103,116 | 0 |
| 15 | CLA | A | 1123 | 65/65 | 0.25 | 0.43 | 75,88,98,104 | 0 |
| 15 | CLA | A | 1130 | 55/65 | 0.15 | 0.39 | 82,106,133,139 | 0 |
| 12 | LHG | A | 5001 | 49/49 | 0.19 | 0.37 | 49,70,91,100 | 0 |
| 15 | CLA | B | 1217 | 47/65 | 0.19 | 0.30 | 96,114,132,157 | 0 |
| 13 | CL0 | A | 1011 | 65/65 | 0.18 | 0.27 | 51,69,81,99 | 0 |
| 15 | CLA | B | 1227 | 45/65 | 0.15 | 0.27 | 54,72,94,98 | 0 |
| 15 | CLA | B | 1013 | 65/65 | 0.20 | 0.27 | 46,53,77,89 | 0 |
| 14 | BCR | A | 4008 | 40/40 | 0.29 | 0.24 | 67,93,105,115 | 0 |
| 14 | BCR | B | 4014 | 40/40 | 0.17 | 0.24 | 46,62,88,89 | 0 |
| 15 | CLA | A | 1109 | 65/65 | 0.17 | 0.20 | 66,81,105,112 | 0 |
| 15 | CLA | B | 1220 | 56/65 | 0.14 | 0.18 | 61,77,111,119 | 0 |
| 15 | CLA | B | 1201 | 46/65 | 0.17 | 0.15 | 72,83,107,123 | 0 |
| 15 | CLA | A | 1133 | 46/65 | 0.25 | 0.13 | 86,103,118,128 | 0 |
| 15 | CLA | A | 1125 | 52/65 | 0.26 | 0.13 | 76,98,124,133 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 14 | BCR | B | 4010 | 40/40 | 0.17 | 0.12 | 55,74,102,113 | 0 |
| 15 | CLA | A | 1119 | 64/65 | 0.24 | 0.12 | 78,97,115,137 | 0 |
| 15 | CLA | A | 1118 | 46/65 | 0.17 | 0.11 | 99,113,135,154 | 0 |
| 15 | CLA | A | 1124 | 55/65 | 0.29 | 0.10 | 61,92,120,129 | 0 |
| 14 | BCR | A | 4001 | 40/40 | 0.25 | 0.09 | 111,127,138,140 | 0 |
| 15 | CLA | B | 1212 | 45/65 | 0.20 | 0.09 | 101,117,128,143 | 0 |
| 15 | CLA | B | 1208 | 45/65 | 0.17 | 0.09 | 88,114,130,140 | 0 |
| 15 | CLA | B | 1205 | 55/65 | 0.16 | 0.06 | 68,87,100,112 | 0 |
| 15 | CLA | A | 1128 | 65/65 | 0.20 | 0.06 | 54,74,90,101 | 0 |
| 15 | CLA | B | 1235 | 65/65 | 0.17 | 0.05 | 55,66,85,92 | 0 |
| 12 | LHG | A | 5005 | 36/49 | 0.21 | 0.03 | 103,143,182,188 | 0 |
| 15 | CLA | B | 1237 | 55/65 | 0.16 | -0.01 | 71,82,117,132 | 0 |
| 15 | CLA | A | 1131 | 55/65 | 0.16 | -0.01 | 78,107,126,140 | 0 |
| 15 | CLA | B | 1226 | 65/65 | 0.18 | -0.02 | 54,79,133,144 | 0 |
| 15 | CLA | B | 1223 | 65/65 | 0.22 | -0.02 | 59,77,94,98 | 0 |
| 15 | CLA | B | 1202 | 65/65 | 0.18 | -0.03 | 67,82,99,106 | 0 |
| 15 | CLA | B | 1213 | 50/65 | 0.16 | -0.06 | 89,104,128,136 | 0 |
| 15 | CLA | A | 1104 | 65/65 | 0.23 | -0.10 | 58,72,83,96 | 0 |
| 15 | CLA | B | 1203 | 65/65 | 0.21 | -0.16 | 62,83,99,104 | 0 |
| 15 | CLA | B | 1238 | 44/65 | 0.15 | -0.16 | 68,80,92,111 | 0 |
| 15 | CLA | B | 1211 | 46/65 | 0.15 | -0.16 | 90,106,116,133 | 0 |
| 15 | CLA | A | 1120 | 49/65 | 0.19 | -0.16 | 101,116,140,156 | 0 |
| 15 | CLA | B | 1225 | 65/65 | 0.21 | -0.19 | 66,80,100,104 | 0 |
| 15 | CLA | B | 1239 | 46/65 | 0.19 | -0.20 | 62,78,107,141 | 0 |
| 15 | CLA | B | 1236 | 50/65 | 0.18 | -0.21 | 52,72,106,114 | 0 |
| 15 | CLA | A | 1137 | 50/65 | 0.18 | -0.24 | 72,94,128,134 | 0 |
| 16 | LMU | B | 1301 | 35/35 | 0.20 | -0.28 | 120,136,148,154 | 0 |
| 15 | CLA | B | 1232 | 45/65 | 0.16 | -0.32 | 72,89,109,115 | 0 |
| 15 | CLA | B | 1221 | 65/65 | 0.17 | -0.36 | 68,79,105,125 | 0 |
| 15 | CLA | B | 1207 | 46/65 | 0.31 | -0.36 | 118,164,185,189 | 0 |
| 15 | CLA | A | 1113 | 45/65 | 0.24 | -0.38 | 112,129,158,162 | 0 |
| 15 | CLA | B | 1206 | 46/65 | 0.17 | -0.38 | 78,100,119,149 | 0 |
| 15 | CLA | A | 1134 | 46/65 | 0.22 | -0.42 | 109,127,151,186 | 0 |
| 15 | CLA | A | 1115 | 46/65 | 0.22 | -0.48 | 109,129,140,151 | 0 |
| 15 | CLA | A | 1129 | 46/65 | 0.16 | -0.51 | 76,92,115,151 | 0 |
| 15 | CLA | A | 1107 | 50/65 | 0.14 | -0.51 | 56,64,98,112 | 0 |
| 15 | CLA | A | 1112 | 45/65 | 0.16 | -0.62 | 89,115,127,130 | 0 |
| 15 | CLA | B | 1209 | 45/65 | 0.15 | -0.66 | 102,113,134,148 | 0 |
| 15 | CLA | B | 1204 | 46/65 | 0.16 | -0.69 | 79,96,115,137 | 0 |
| 15 | CLA | B | 1222 | 56/65 | 0.22 | -0.73 | 52,66,101,108 | 0 |
| 15 | CLA | A | 1114 | 49/65 | 0.20 | -0.85 | 98,124,137,150 | 0 |
| 18 | CL | B | 6000 | 1/1 | 0.09 | -1.70 | 82,82,82,82 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.