



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 08:37 am GMT

PDB ID : 1FE1
Title : CRYSTAL STRUCTURE PHOTOSYSTEM II
Authors : Zouni, A.; Witt, H.-T.; Kern, J.; Fromme, P.; Krauss, N.; Saenger, W.; Orth, P.
Deposited on : 2000-07-20
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

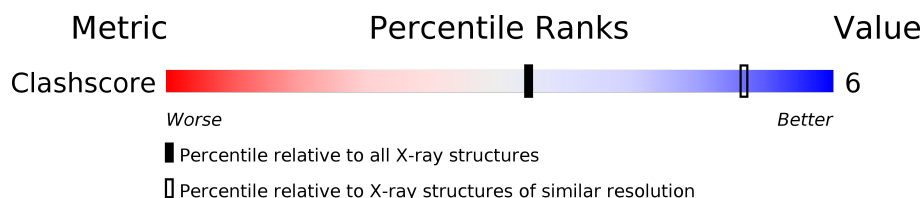
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

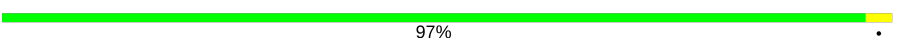
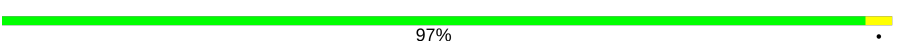
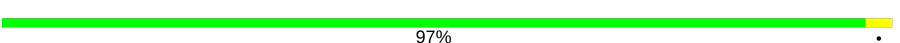
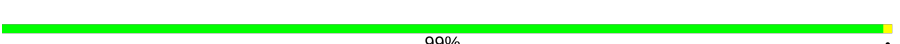
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 122078 | 1061 (4.00-3.60) |









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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 169 |  97% . |
| 1 | J | 169 |  97% . |
| 2 | B | 174 |  97% . |
| 2 | K | 174 |  97% . |
| 3 | C | 156 |  99% . |
| 3 | L | 156 |  99% . |
| 4 | D | 155 |  100% |
| 4 | M | 155 |  100% |
| 5 | E | 40 |  100% |
| 5 | N | 40 |  100% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 6 | F | 30 |  100% |
| 6 | O | 30 |  100% |
| 7 | G | 312 |  100% |
| 7 | P | 312 |  100% |
| 8 | H | 115 |  100% |
| 8 | Q | 115 |  100% |
| 9 | I | 87 |  100% |
| 9 | R | 87 |  100% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 12 | CLA | A | 175 | X | - | - | - |
| 12 | CLA | A | 176 | X | - | - | - |
| 12 | CLA | A | 177 | X | - | - | - |
| 12 | CLA | A | 179 | X | - | - | - |
| 12 | CLA | B | 177 | X | - | - | - |
| 12 | CLA | B | 179 | X | - | - | - |
| 12 | CLA | C | 157 | X | - | - | - |
| 12 | CLA | C | 158 | X | - | - | - |
| 12 | CLA | C | 159 | X | - | - | - |
| 12 | CLA | C | 160 | X | - | - | - |
| 12 | CLA | C | 161 | X | - | - | - |
| 12 | CLA | C | 162 | X | - | - | - |
| 12 | CLA | C | 163 | X | - | - | - |
| 12 | CLA | C | 164 | X | - | - | - |
| 12 | CLA | C | 165 | X | - | - | - |
| 12 | CLA | C | 166 | X | - | - | - |
| 12 | CLA | C | 167 | X | - | - | - |
| 12 | CLA | C | 168 | X | - | - | - |
| 12 | CLA | D | 156 | X | - | - | - |
| 12 | CLA | D | 157 | X | - | - | - |
| 12 | CLA | D | 158 | X | - | - | - |
| 12 | CLA | D | 159 | X | - | - | - |
| 12 | CLA | D | 160 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 12 | CLA | D | 161 | X | - | - | - |
| 12 | CLA | D | 162 | X | - | - | - |
| 12 | CLA | D | 163 | X | - | - | - |
| 12 | CLA | D | 164 | X | - | - | - |
| 12 | CLA | D | 165 | X | - | - | - |
| 12 | CLA | D | 166 | X | - | - | - |
| 12 | CLA | D | 167 | X | - | - | - |
| 12 | CLA | D | 168 | X | - | - | - |
| 12 | CLA | G | 313 | X | - | - | - |
| 12 | CLA | J | 175 | X | - | - | - |
| 12 | CLA | J | 176 | X | - | - | - |
| 12 | CLA | J | 177 | X | - | - | - |
| 12 | CLA | J | 179 | X | - | - | - |
| 12 | CLA | K | 177 | X | - | - | - |
| 12 | CLA | K | 179 | X | - | - | - |
| 12 | CLA | L | 157 | X | - | - | - |
| 12 | CLA | L | 158 | X | - | - | - |
| 12 | CLA | L | 159 | X | - | - | - |
| 12 | CLA | L | 160 | X | - | - | - |
| 12 | CLA | L | 161 | X | - | - | - |
| 12 | CLA | L | 162 | X | - | - | - |
| 12 | CLA | L | 163 | X | - | - | - |
| 12 | CLA | L | 164 | X | - | - | - |
| 12 | CLA | L | 165 | X | - | - | - |
| 12 | CLA | L | 166 | X | - | - | - |
| 12 | CLA | L | 167 | X | - | - | - |
| 12 | CLA | L | 168 | X | - | - | - |
| 12 | CLA | M | 156 | X | - | - | - |
| 12 | CLA | M | 157 | X | - | - | - |
| 12 | CLA | M | 158 | X | - | - | - |
| 12 | CLA | M | 159 | X | - | - | - |
| 12 | CLA | M | 160 | X | - | - | - |
| 12 | CLA | M | 161 | X | - | - | - |
| 12 | CLA | M | 162 | X | - | - | - |
| 12 | CLA | M | 163 | X | - | - | - |
| 12 | CLA | M | 164 | X | - | - | - |
| 12 | CLA | M | 165 | X | - | - | - |
| 12 | CLA | M | 166 | X | - | - | - |
| 12 | CLA | M | 167 | X | - | - | - |
| 12 | CLA | M | 168 | X | - | - | - |
| 12 | CLA | P | 313 | X | - | - | - |

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 4328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 1 | A | 169 | Total | C | 0 | 0 | 169 |
| | | | 169 | 169 | | | |
| 1 | J | 169 | Total | C | 0 | 0 | 169 |
| | | | 169 | 169 | | | |

- Molecule 2 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBD).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 2 | B | 174 | Total | C | 0 | 0 | 174 |
| | | | 174 | 174 | | | |
| 2 | K | 174 | Total | C | 0 | 0 | 174 |
| | | | 174 | 174 | | | |

- Molecule 3 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 3 | C | 156 | Total | C | 0 | 0 | 156 |
| | | | 156 | 156 | | | |
| 3 | L | 156 | Total | C | 0 | 0 | 156 |
| | | | 156 | 156 | | | |

- Molecule 4 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBB).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 4 | D | 155 | Total | C | 0 | 0 | 155 |
| | | | 155 | 155 | | | |
| 4 | M | 155 | Total | C | 0 | 0 | 155 |
| | | | 155 | 155 | | | |

- Molecule 5 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBE).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 5 | E | 40 | Total C 40 40 | 0 | 0 | 40 |
| 5 | N | 40 | Total C 40 40 | 0 | 0 | 40 |

- Molecule 6 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBF).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 6 | F | 30 | Total C 30 30 | 0 | 0 | 30 |
| 6 | O | 30 | Total C 30 30 | 0 | 0 | 30 |

- Molecule 7 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT UNKNOWN).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 7 | G | 312 | Total C 312 312 | 0 | 0 | 312 |
| 7 | P | 312 | Total C 312 312 | 0 | 0 | 312 |

- Molecule 8 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBO).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 8 | H | 115 | Total C 115 115 | 0 | 0 | 115 |
| 8 | Q | 115 | Total C 115 115 | 0 | 0 | 115 |

- Molecule 9 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBV).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 9 | I | 87 | Total C 87 87 | 0 | 0 | 87 |
| 9 | R | 87 | Total C 87 87 | 0 | 0 | 87 |

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

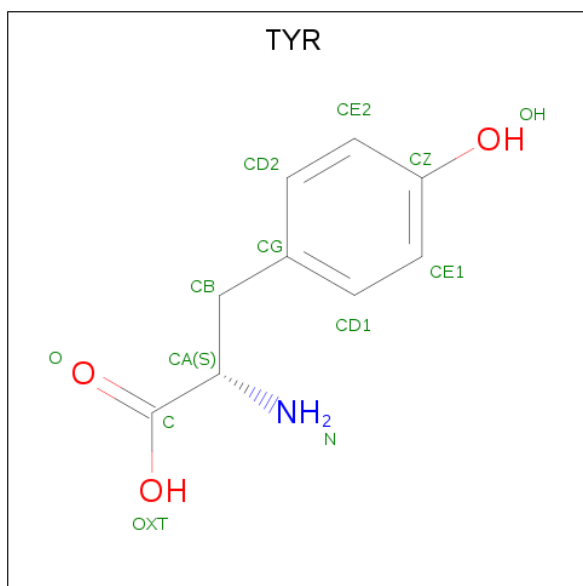
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 10 | J | 4 | Total Mn 4 4 | 0 | 0 |

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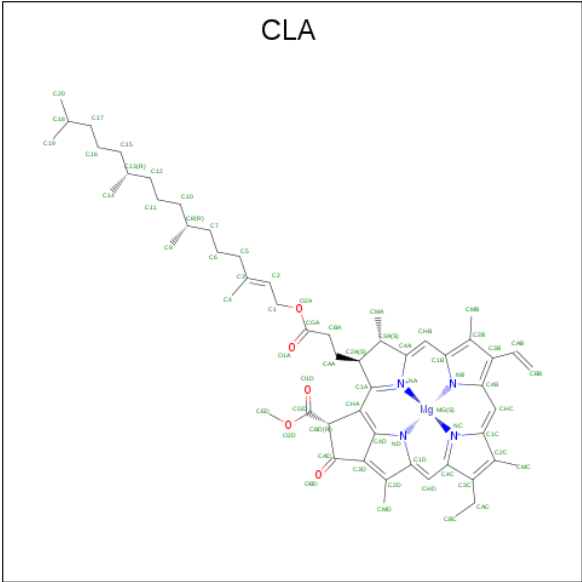
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 10 | A | 4 | Total | Mn | 0 | 0 |
| | | | 4 | 4 | | |

- Molecule 11 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 11 | A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 7 | 1 | | |
| 11 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 7 | 1 | | |
| 11 | J | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 7 | 1 | | |
| 11 | K | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 7 | 1 | | |

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12 | A | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | A | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | A | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | A | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | B | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | B | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | C | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|
| 12 | C | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | C | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | C | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | C | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | D | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | G | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | J | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | J | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |
| 12 | J | 1 | Total 25 | C 20 | Mg 1 | N 4 | 0 | 0 |

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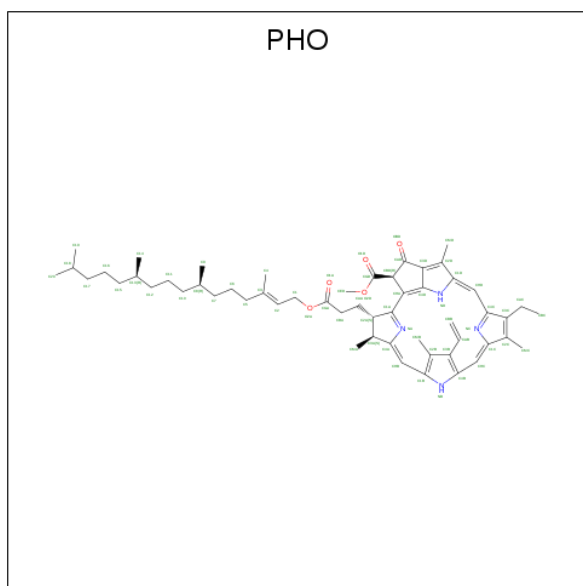
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12 | J | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | K | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | K | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | L | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | M | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |
| 12 | P | 1 | Total | C | Mg | N | 0 | 0 |
| | | | 25 | 20 | 1 | 4 | | |

- Molecule 13 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|--|---------|---------|
| 13 | A | 1 | Total | C | N | | 0 | 0 |
| | | | 24 | 20 | 4 | | | |
| 13 | B | 1 | Total | C | N | | 0 | 0 |
| | | | 24 | 20 | 4 | | | |
| 13 | J | 1 | Total | C | N | | 0 | 0 |
| | | | 24 | 20 | 4 | | | |

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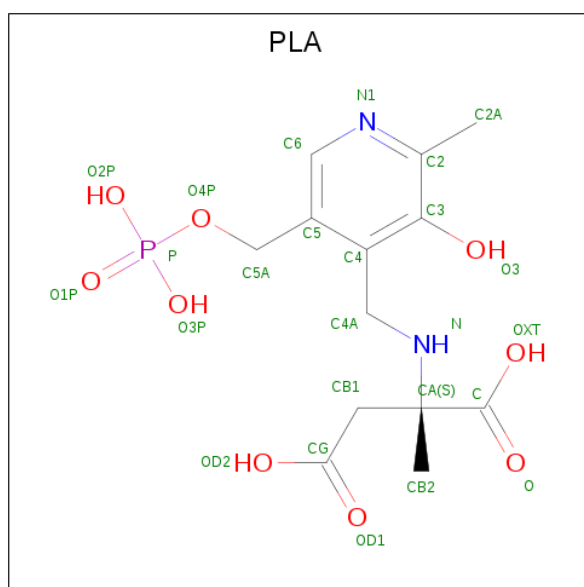
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 13 | K | 1 | Total | C | N | 0 | 0 |
| | | | 24 | 20 | 4 | | |

- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|--|---------|---------|
| 14 | B | 1 | Total | Fe | | 0 | 0 |
| | | | 1 | 1 | | | |
| 14 | K | 1 | Total | Fe | | 0 | 0 |
| | | | 1 | 1 | | | |

- Molecule 15 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: C₁₃H₁₉N₂O₉P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 15 | B | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 5 | 1 | | |
| 15 | K | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 5 | 1 | | |

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|
| 16 | F | 1 | Total 25 | C 20 | Fe 1 | N 4 | 0 | 0 |
| 16 | I | 1 | Total 25 | C 20 | Fe 1 | N 4 | 0 | 0 |
| 16 | O | 1 | Total 25 | C 20 | Fe 1 | N 4 | 0 | 0 |
| 16 | R | 1 | Total 25 | C 20 | Fe 1 | N 4 | 0 | 0 |

- Molecule 17 is CADMIUM ION (three-letter code: CD) (formula: Cd).

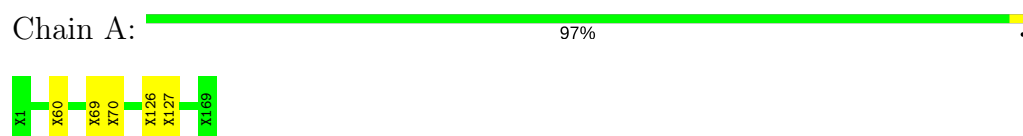
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 17 | H | 1 | Total Cd 1 1 | 0 | 0 |
| 17 | Q | 1 | Total Cd 1 1 | 0 | 0 |

3 Residue-property plots

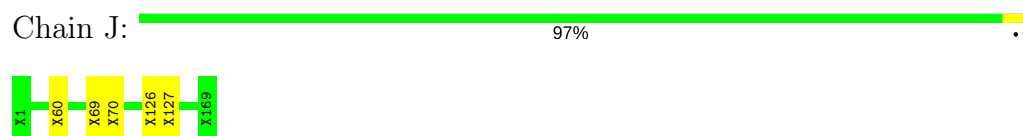
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

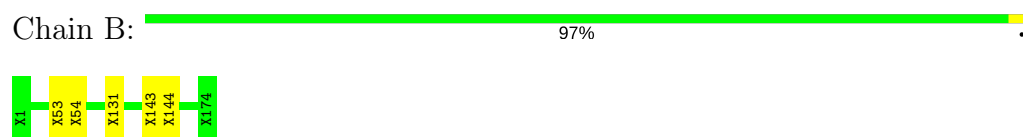
- Molecule 1: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA)



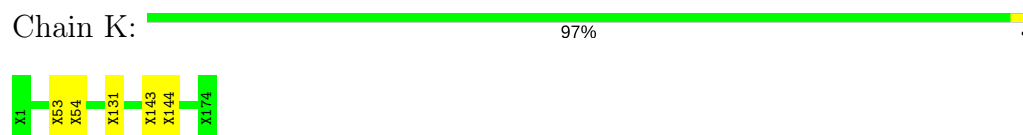
- Molecule 1: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA)



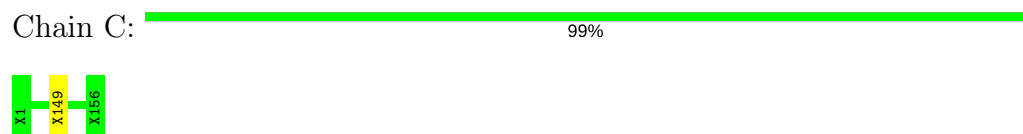
- Molecule 2: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBD)



- Molecule 2: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBD)

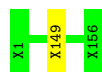


- Molecule 3: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC)



- Molecule 3: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC)

Chain L:  99%



- Molecule 4: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBB)

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBB)

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBE)

Chain E:  100%


There are no outlier residues recorded for this chain.

- Molecule 5: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBE)

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBF)

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBF)

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PROTEIN (PHOTOSYSTEM II: SUBUNIT UNKNOWN)

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PROTEIN (PHOTOSYSTEM II: SUBUNIT UNKNOWN)

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBO)

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBO)

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBV)

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBV)

Chain R:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 130.01Å 226.72Å 308.29Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.80 | Depositor |
| % Data completeness (in resolution range) | (Not available) (20.00-3.80) | Depositor |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | | Depositor |
| R, R_{free} | (Not available) , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 4328 | wwPDB-VP |
| Average B, all atoms (Å ²) | 28.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, MN, CLA, CD, FE, PLA, HEM

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 169 | 0 | 0 | 4 | 0 |
| 1 | J | 169 | 0 | 0 | 4 | 0 |
| 2 | B | 174 | 0 | 0 | 4 | 0 |
| 2 | K | 174 | 0 | 0 | 4 | 0 |
| 3 | C | 156 | 0 | 0 | 2 | 0 |
| 3 | L | 156 | 0 | 0 | 2 | 0 |
| 4 | D | 155 | 0 | 0 | 0 | 0 |
| 4 | M | 155 | 0 | 0 | 0 | 0 |
| 5 | E | 40 | 0 | 0 | 0 | 0 |
| 5 | N | 40 | 0 | 0 | 0 | 0 |
| 6 | F | 30 | 0 | 0 | 0 | 0 |
| 6 | O | 30 | 0 | 0 | 0 | 0 |
| 7 | G | 312 | 0 | 0 | 0 | 0 |
| 7 | P | 312 | 0 | 0 | 0 | 0 |
| 8 | H | 115 | 0 | 0 | 0 | 0 |
| 8 | Q | 115 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | I | 87 | 0 | 0 | 0 | 0 |
| 9 | R | 87 | 0 | 0 | 0 | 0 |
| 10 | A | 4 | 0 | 0 | 0 | 0 |
| 10 | J | 4 | 0 | 0 | 0 | 0 |
| 11 | A | 8 | 0 | 5 | 0 | 0 |
| 11 | B | 8 | 0 | 5 | 0 | 0 |
| 11 | J | 8 | 0 | 5 | 0 | 0 |
| 11 | K | 8 | 0 | 5 | 0 | 0 |
| 12 | A | 100 | 0 | 12 | 0 | 0 |
| 12 | B | 50 | 0 | 6 | 0 | 0 |
| 12 | C | 300 | 0 | 36 | 2 | 0 |
| 12 | D | 325 | 0 | 39 | 6 | 0 |
| 12 | G | 25 | 0 | 3 | 0 | 0 |
| 12 | J | 100 | 0 | 12 | 0 | 0 |
| 12 | K | 50 | 0 | 6 | 0 | 0 |
| 12 | L | 300 | 0 | 36 | 2 | 0 |
| 12 | M | 325 | 0 | 39 | 6 | 0 |
| 12 | P | 25 | 0 | 3 | 0 | 0 |
| 13 | A | 24 | 0 | 5 | 0 | 0 |
| 13 | B | 24 | 0 | 5 | 0 | 0 |
| 13 | J | 24 | 0 | 5 | 0 | 0 |
| 13 | K | 24 | 0 | 5 | 0 | 0 |
| 14 | B | 1 | 0 | 0 | 0 | 0 |
| 14 | K | 1 | 0 | 0 | 0 | 0 |
| 15 | B | 6 | 0 | 1 | 0 | 0 |
| 15 | K | 6 | 0 | 1 | 0 | 0 |
| 16 | F | 25 | 0 | 4 | 0 | 0 |
| 16 | I | 25 | 0 | 4 | 0 | 0 |
| 16 | O | 25 | 0 | 4 | 0 | 0 |
| 16 | R | 25 | 0 | 4 | 0 | 0 |
| 17 | H | 1 | 0 | 0 | 0 | 0 |
| 17 | Q | 1 | 0 | 0 | 0 | 0 |
| All | All | 4328 | 0 | 250 | 26 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:J:127:UNK:CA | 2:K:53:UNK:CA | 1.88 | 1.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:UNK:CA | 2:B:53:UNK:CA | 1.88 | 1.49 |
| 1:A:60:UNK:CA | 2:B:131:UNK:CA | 1.95 | 1.45 |
| 1:J:60:UNK:CA | 2:K:131:UNK:CA | 1.95 | 1.44 |
| 3:L:149:UNK:CA | 12:L:166:CLA:C2A | 2.23 | 1.17 |
| 3:C:149:UNK:CA | 12:C:166:CLA:C2A | 2.23 | 1.15 |
| 12:D:159:CLA:HHB | 12:D:162:CLA:CHD | 1.81 | 1.10 |
| 12:M:159:CLA:HHB | 12:M:162:CLA:CHD | 1.81 | 1.08 |
| 12:M:159:CLA:HHB | 12:M:162:CLA:HHD | 1.01 | 1.01 |
| 12:M:159:CLA:CHB | 12:M:162:CLA:HHD | 1.92 | 1.00 |
| 12:D:159:CLA:CHB | 12:D:162:CLA:HHD | 1.92 | 0.98 |
| 12:D:159:CLA:HHB | 12:D:162:CLA:HHD | 1.02 | 0.97 |
| 1:J:126:UNK:CA | 2:K:54:UNK:CA | 2.66 | 0.74 |
| 1:A:126:UNK:CA | 2:B:54:UNK:CA | 2.66 | 0.73 |
| 3:C:149:UNK:CA | 12:C:166:CLA:C3A | 2.69 | 0.70 |
| 3:L:149:UNK:CA | 12:L:166:CLA:C3A | 2.69 | 0.70 |
| 1:A:69:UNK:CA | 1:A:70:UNK:CA | 2.76 | 0.64 |
| 1:J:69:UNK:CA | 1:J:70:UNK:CA | 2.76 | 0.63 |
| 12:M:159:CLA:HHB | 12:M:162:CLA:C1D | 2.35 | 0.56 |
| 12:D:159:CLA:HHB | 12:D:162:CLA:C1D | 2.35 | 0.53 |
| 12:D:159:CLA:HHB | 12:D:162:CLA:C2D | 2.42 | 0.50 |
| 12:M:159:CLA:HHB | 12:M:162:CLA:C2D | 2.42 | 0.49 |
| 2:B:143:UNK:CA | 2:B:144:UNK:CA | 2.91 | 0.48 |
| 2:K:143:UNK:CA | 2:K:144:UNK:CA | 2.91 | 0.48 |
| 12:D:159:CLA:CHB | 12:D:162:CLA:C2D | 2.97 | 0.43 |
| 12:M:159:CLA:CHB | 12:M:162:CLA:C2D | 2.97 | 0.43 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 90 ligands modelled in this entry, 12 are monoatomic - leaving 78 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$ |
| 11 | TYR | A | 174 | 1 | 8,8,13 | 0.37 | 0 | 10,10,17 | 0.18 | 0 |
| 12 | CLA | A | 175 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.93 | 6 (25%) |
| 12 | CLA | A | 176 | - | 19,32,73 | 2.71 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | A | 177 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.94 | 6 (25%) |
| 13 | PHO | A | 178 | - | 18,28,69 | 1.14 | 0 | 7,40,99 | 1.91 | 3 (42%) |
| 12 | CLA | A | 179 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 11 | TYR | B | 176 | 2 | 8,8,13 | 0.38 | 0 | 10,10,17 | 0.17 | 0 |
| 12 | CLA | B | 177 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 13 | PHO | B | 178 | - | 18,28,69 | 1.14 | 0 | 7,40,99 | 1.91 | 3 (42%) |
| 12 | CLA | B | 179 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 15 | PLA | B | 180 | - | 6,6,25 | 2.96 | 5 (83%) | 6,6,37 | 0.88 | 0 |
| 12 | CLA | C | 157 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | C | 158 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | C | 159 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | C | 160 | - | 19,32,73 | 2.65 | 4 (21%) | 24,54,113 | 2.93 | 6 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CLA | C | 161 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | C | 162 | - | 19,32,73 | 2.72 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | C | 163 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | C | 164 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | C | 165 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | C | 166 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | C | 167 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | C | 168 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | D | 156 | - | 19,32,73 | 2.71 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | D | 157 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | D | 158 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | D | 159 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | D | 160 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | D | 161 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.91 | 7 (29%) |
| 12 | CLA | D | 162 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | D | 163 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | D | 164 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | D | 165 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | D | 166 | - | 19,32,73 | 2.71 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | D | 167 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | D | 168 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 16 | HEM | F | 31 | - | 12,32,50 | 3.15 | 2 (16%) | 23,54,82 | 3.66 | 11 (47%) |
| 12 | CLA | G | 313 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 16 | HEM | I | 88 | - | 12,32,50 | 3.16 | 2 (16%) | 23,54,82 | 3.68 | 11 (47%) |
| 11 | TYR | J | 174 | 1 | 8,8,13 | 0.37 | 0 | 10,10,17 | 0.18 | 0 |
| 12 | CLA | J | 175 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | J | 176 | - | 19,32,73 | 2.71 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | J | 177 | - | 19,32,73 | 2.65 | 4 (21%) | 24,54,113 | 2.95 | 6 (25%) |
| 13 | PHO | J | 178 | - | 18,28,69 | 1.14 | 0 | 7,40,99 | 1.90 | 3 (42%) |
| 12 | CLA | J | 179 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 11 | TYR | K | 176 | 2 | 8,8,13 | 0.38 | 0 | 10,10,17 | 0.17 | 0 |
| 12 | CLA | K | 177 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.88 | 6 (25%) |
| 13 | PHO | K | 178 | - | 18,28,69 | 1.14 | 0 | 7,40,99 | 1.89 | 3 (42%) |
| 12 | CLA | K | 179 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 15 | PLA | K | 180 | - | 6,6,25 | 2.95 | 5 (83%) | 6,6,37 | 0.88 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CLA | L | 157 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | L | 158 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | L | 159 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.93 | 6 (25%) |
| 12 | CLA | L | 160 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.93 | 6 (25%) |
| 12 | CLA | L | 161 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | L | 162 | - | 19,32,73 | 2.72 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | L | 163 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | L | 164 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | L | 165 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.91 | 7 (29%) |
| 12 | CLA | L | 166 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | L | 167 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | L | 168 | - | 19,32,73 | 2.66 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | M | 156 | - | 19,32,73 | 2.71 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | M | 157 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | M | 158 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | M | 159 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | M | 160 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.92 | 6 (25%) |
| 12 | CLA | M | 161 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | M | 162 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | M | 163 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | M | 164 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | M | 165 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.89 | 6 (25%) |
| 12 | CLA | M | 166 | - | 19,32,73 | 2.70 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 12 | CLA | M | 167 | - | 19,32,73 | 2.69 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 12 | CLA | M | 168 | - | 19,32,73 | 2.67 | 4 (21%) | 24,54,113 | 2.90 | 6 (25%) |
| 16 | HEM | O | 58 | - | 12,32,50 | 3.16 | 2 (16%) | 23,54,82 | 3.64 | 10 (43%) |
| 12 | CLA | P | 313 | - | 19,32,73 | 2.68 | 4 (21%) | 24,54,113 | 2.91 | 6 (25%) |
| 16 | HEM | R | 88 | - | 12,32,50 | 3.17 | 2 (16%) | 23,54,82 | 3.69 | 10 (43%) |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 11 | TYR | A | 174 | 1 | - | 0/0/0/8 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|----------|------------|---------|
| 12 | CLA | A | 175 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | A | 176 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | A | 177 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 13 | PHO | A | 178 | - | - | 0/2/34/103 | 0/4/5/6 |
| 12 | CLA | A | 179 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 11 | TYR | B | 176 | 2 | - | 0/0/0/8 | 0/1/1/1 |
| 12 | CLA | B | 177 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 13 | PHO | B | 178 | - | - | 0/2/34/103 | 0/4/5/6 |
| 12 | CLA | B | 179 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 15 | PLA | B | 180 | - | - | 0/0/0/23 | 0/1/1/1 |
| 12 | CLA | C | 157 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 158 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 159 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 160 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 161 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 162 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 163 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 164 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 165 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 166 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 167 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | C | 168 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 156 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 157 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 158 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 159 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 160 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 161 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 162 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 163 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 164 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 165 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 166 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 167 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | D | 168 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|----------|------------|---------|
| 16 | HEM | F | 31 | - | - | 0/0/40/54 | 0/0/8/8 |
| 12 | CLA | G | 313 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 16 | HEM | I | 88 | - | - | 0/0/40/54 | 0/0/8/8 |
| 11 | TYR | J | 174 | 1 | - | 0/0/0/8 | 0/1/1/1 |
| 12 | CLA | J | 175 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | J | 176 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | J | 177 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 13 | PHO | J | 178 | - | - | 0/2/34/103 | 0/4/5/6 |
| 12 | CLA | J | 179 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 11 | TYR | K | 176 | 2 | - | 0/0/0/8 | 0/1/1/1 |
| 12 | CLA | K | 177 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 13 | PHO | K | 178 | - | - | 0/2/34/103 | 0/4/5/6 |
| 12 | CLA | K | 179 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 15 | PLA | K | 180 | - | - | 0/0/0/23 | 0/1/1/1 |
| 12 | CLA | L | 157 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 158 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 159 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 160 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 161 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 162 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 163 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 164 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 165 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 166 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 167 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | L | 168 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 156 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 157 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 158 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 159 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 160 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 161 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 162 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 163 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 164 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|----------|------------|---------|
| 12 | CLA | M | 165 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 166 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 167 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 12 | CLA | M | 168 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 16 | HEM | O | 58 | - | - | 0/0/40/54 | 0/0/8/8 |
| 12 | CLA | P | 313 | - | 3/3/7/25 | 0/0/66/135 | 0/0/8/9 |
| 16 | HEM | R | 88 | - | - | 0/0/40/54 | 0/0/8/8 |

All (274) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 15 | K | 180 | PLA | C4-C3 | 2.51 | 1.44 | 1.38 |
| 15 | B | 180 | PLA | C4-C3 | 2.53 | 1.44 | 1.38 |
| 15 | K | 180 | PLA | C5-C6 | 2.85 | 1.46 | 1.37 |
| 15 | B | 180 | PLA | C5-C6 | 2.86 | 1.46 | 1.37 |
| 15 | K | 180 | PLA | C5-C4 | 2.95 | 1.45 | 1.38 |
| 15 | B | 180 | PLA | C5-C4 | 2.95 | 1.45 | 1.38 |
| 15 | K | 180 | PLA | C2-N1 | 3.45 | 1.44 | 1.33 |
| 15 | B | 180 | PLA | C2-N1 | 3.46 | 1.44 | 1.33 |
| 15 | B | 180 | PLA | C6-N1 | 3.66 | 1.44 | 1.33 |
| 15 | K | 180 | PLA | C6-N1 | 3.66 | 1.44 | 1.33 |
| 12 | K | 177 | CLA | C2C-C1C | 3.99 | 1.52 | 1.43 |
| 12 | L | 157 | CLA | C2C-C1C | 4.00 | 1.52 | 1.43 |
| 12 | B | 177 | CLA | C2C-C1C | 4.01 | 1.52 | 1.43 |
| 12 | G | 313 | CLA | C2C-C1C | 4.01 | 1.52 | 1.43 |
| 12 | C | 157 | CLA | C2C-C1C | 4.02 | 1.52 | 1.43 |
| 12 | D | 159 | CLA | C2C-C1C | 4.02 | 1.52 | 1.43 |
| 12 | P | 313 | CLA | C2C-C1C | 4.02 | 1.52 | 1.43 |
| 12 | M | 163 | CLA | C2C-C1C | 4.02 | 1.52 | 1.43 |
| 12 | D | 160 | CLA | C2C-C1C | 4.02 | 1.52 | 1.43 |
| 12 | D | 156 | CLA | C2C-C1C | 4.02 | 1.52 | 1.43 |
| 12 | D | 163 | CLA | C2C-C1C | 4.03 | 1.52 | 1.43 |
| 12 | M | 156 | CLA | C2C-C1C | 4.03 | 1.52 | 1.43 |
| 12 | D | 161 | CLA | C2C-C1C | 4.03 | 1.52 | 1.43 |
| 12 | M | 157 | CLA | C2C-C1C | 4.03 | 1.52 | 1.43 |
| 12 | L | 166 | CLA | C2C-C1C | 4.03 | 1.52 | 1.43 |
| 12 | M | 161 | CLA | C2C-C1C | 4.03 | 1.52 | 1.43 |
| 12 | M | 158 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | D | 164 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | J | 177 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | D | 158 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | D | 157 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | M | 168 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | C | 166 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | M | 159 | CLA | C2C-C1C | 4.04 | 1.52 | 1.43 |
| 12 | M | 162 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | J | 176 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | L | 158 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | A | 177 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | M | 160 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | L | 159 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | C | 161 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | M | 165 | CLA | C2C-C1C | 4.05 | 1.52 | 1.43 |
| 12 | D | 166 | CLA | C2C-C1C | 4.06 | 1.52 | 1.43 |
| 12 | C | 164 | CLA | C2C-C1C | 4.06 | 1.52 | 1.43 |
| 12 | C | 167 | CLA | C2C-C1C | 4.06 | 1.52 | 1.43 |
| 12 | M | 166 | CLA | C2C-C1C | 4.06 | 1.52 | 1.43 |
| 12 | C | 158 | CLA | C2C-C1C | 4.06 | 1.52 | 1.43 |
| 12 | C | 159 | CLA | C2C-C1C | 4.06 | 1.52 | 1.43 |
| 12 | L | 163 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | M | 164 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | L | 161 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | L | 162 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | C | 162 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | B | 179 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | L | 164 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | D | 165 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | D | 168 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | A | 175 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | D | 167 | CLA | C2C-C1C | 4.07 | 1.52 | 1.43 |
| 12 | L | 167 | CLA | C2C-C1C | 4.08 | 1.52 | 1.43 |
| 12 | A | 176 | CLA | C2C-C1C | 4.08 | 1.52 | 1.43 |
| 12 | C | 168 | CLA | C2C-C1C | 4.08 | 1.52 | 1.43 |
| 12 | J | 175 | CLA | C2C-C1C | 4.08 | 1.52 | 1.43 |
| 12 | D | 162 | CLA | C2C-C1C | 4.09 | 1.52 | 1.43 |
| 12 | C | 160 | CLA | C2C-C1C | 4.09 | 1.52 | 1.43 |
| 12 | C | 163 | CLA | C2C-C1C | 4.09 | 1.52 | 1.43 |
| 12 | K | 179 | CLA | C2C-C1C | 4.09 | 1.52 | 1.43 |
| 12 | L | 168 | CLA | C2C-C1C | 4.09 | 1.52 | 1.43 |
| 12 | M | 167 | CLA | C2C-C1C | 4.09 | 1.52 | 1.43 |
| 12 | J | 179 | CLA | C2C-C1C | 4.10 | 1.52 | 1.43 |
| 12 | C | 165 | CLA | C2C-C1C | 4.10 | 1.52 | 1.43 |
| 12 | L | 165 | CLA | C2C-C1C | 4.10 | 1.52 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | A | 179 | CLA | C2C-C1C | 4.11 | 1.52 | 1.43 |
| 12 | L | 160 | CLA | C2C-C1C | 4.12 | 1.52 | 1.43 |
| 12 | M | 161 | CLA | C3C-C4C | 4.33 | 1.53 | 1.43 |
| 12 | A | 177 | CLA | C3C-C4C | 4.34 | 1.53 | 1.43 |
| 12 | J | 177 | CLA | C3C-C4C | 4.36 | 1.53 | 1.43 |
| 12 | D | 160 | CLA | C3C-C4C | 4.36 | 1.53 | 1.43 |
| 12 | L | 167 | CLA | C3C-C4C | 4.36 | 1.53 | 1.43 |
| 12 | C | 160 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | C | 163 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | D | 161 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | P | 313 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | L | 161 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | D | 164 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | M | 168 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | M | 167 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | L | 166 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | L | 160 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | C | 166 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | L | 163 | CLA | C3C-C4C | 4.37 | 1.53 | 1.43 |
| 12 | M | 159 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | L | 157 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | L | 168 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | D | 168 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | C | 161 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | M | 164 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | D | 167 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | D | 159 | CLA | C3C-C4C | 4.38 | 1.53 | 1.43 |
| 12 | M | 165 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | G | 313 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | K | 179 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | B | 179 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | D | 156 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | C | 164 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | L | 162 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | M | 160 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | L | 165 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | D | 163 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | M | 163 | CLA | C3C-C4C | 4.39 | 1.53 | 1.43 |
| 12 | C | 168 | CLA | C3C-C4C | 4.40 | 1.53 | 1.43 |
| 12 | D | 165 | CLA | C3C-C4C | 4.40 | 1.53 | 1.43 |
| 12 | A | 176 | CLA | C3C-C4C | 4.40 | 1.53 | 1.43 |
| 12 | C | 167 | CLA | C3C-C4C | 4.40 | 1.53 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | M | 156 | CLA | C3C-C4C | 4.40 | 1.53 | 1.43 |
| 12 | L | 164 | CLA | C3C-C4C | 4.41 | 1.53 | 1.43 |
| 12 | C | 157 | CLA | C3C-C4C | 4.41 | 1.53 | 1.43 |
| 12 | M | 158 | CLA | C3C-C4C | 4.41 | 1.53 | 1.43 |
| 12 | J | 179 | CLA | C3C-C4C | 4.41 | 1.53 | 1.43 |
| 12 | C | 165 | CLA | C3C-C4C | 4.41 | 1.53 | 1.43 |
| 12 | A | 179 | CLA | C3C-C4C | 4.41 | 1.53 | 1.43 |
| 12 | L | 159 | CLA | C3C-C4C | 4.42 | 1.53 | 1.43 |
| 12 | C | 159 | CLA | C3C-C4C | 4.42 | 1.53 | 1.43 |
| 12 | D | 158 | CLA | C3C-C4C | 4.42 | 1.53 | 1.43 |
| 12 | M | 166 | CLA | C3C-C4C | 4.42 | 1.53 | 1.43 |
| 12 | D | 162 | CLA | C3C-C4C | 4.42 | 1.53 | 1.43 |
| 12 | C | 162 | CLA | C3C-C4C | 4.42 | 1.53 | 1.43 |
| 12 | A | 175 | CLA | C3C-C4C | 4.43 | 1.53 | 1.43 |
| 12 | J | 175 | CLA | C3C-C4C | 4.43 | 1.53 | 1.43 |
| 12 | D | 157 | CLA | C3C-C4C | 4.43 | 1.53 | 1.43 |
| 12 | M | 157 | CLA | C3C-C4C | 4.43 | 1.53 | 1.43 |
| 12 | J | 176 | CLA | C3C-C4C | 4.43 | 1.53 | 1.43 |
| 12 | B | 177 | CLA | C3C-C4C | 4.44 | 1.53 | 1.43 |
| 12 | C | 158 | CLA | C3C-C4C | 4.45 | 1.53 | 1.43 |
| 12 | M | 162 | CLA | C3C-C4C | 4.45 | 1.53 | 1.43 |
| 12 | D | 166 | CLA | C3C-C4C | 4.45 | 1.53 | 1.43 |
| 12 | L | 158 | CLA | C3C-C4C | 4.45 | 1.53 | 1.43 |
| 12 | K | 177 | CLA | C3C-C4C | 4.46 | 1.53 | 1.43 |
| 12 | D | 160 | CLA | C3C-C2C | 5.90 | 1.48 | 1.35 |
| 12 | M | 160 | CLA | C3C-C2C | 5.91 | 1.48 | 1.35 |
| 12 | L | 164 | CLA | C3C-C2C | 5.92 | 1.48 | 1.35 |
| 12 | C | 164 | CLA | C3C-C2C | 5.92 | 1.48 | 1.35 |
| 12 | L | 167 | CLA | C3C-C2C | 5.92 | 1.48 | 1.35 |
| 12 | C | 167 | CLA | C3C-C2C | 5.93 | 1.48 | 1.35 |
| 12 | B | 179 | CLA | C3C-C2C | 5.94 | 1.48 | 1.35 |
| 12 | K | 179 | CLA | C3C-C2C | 5.94 | 1.48 | 1.35 |
| 12 | M | 167 | CLA | C3C-C2C | 5.94 | 1.48 | 1.35 |
| 12 | A | 179 | CLA | C3C-C2C | 5.94 | 1.48 | 1.35 |
| 12 | L | 161 | CLA | C3C-C2C | 5.94 | 1.48 | 1.35 |
| 12 | M | 159 | CLA | C3C-C2C | 5.94 | 1.48 | 1.35 |
| 12 | D | 167 | CLA | C3C-C2C | 5.95 | 1.48 | 1.35 |
| 12 | C | 160 | CLA | C3C-C2C | 5.95 | 1.48 | 1.35 |
| 12 | L | 158 | CLA | C3C-C2C | 5.95 | 1.48 | 1.35 |
| 12 | L | 160 | CLA | C3C-C2C | 5.95 | 1.48 | 1.35 |
| 12 | M | 168 | CLA | C3C-C2C | 5.95 | 1.48 | 1.35 |
| 12 | C | 162 | CLA | C3C-C2C | 5.96 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | D | 159 | CLA | C3C-C2C | 5.96 | 1.48 | 1.35 |
| 12 | D | 165 | CLA | C3C-C2C | 5.96 | 1.48 | 1.35 |
| 12 | J | 179 | CLA | C3C-C2C | 5.96 | 1.48 | 1.35 |
| 12 | L | 168 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | D | 168 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | C | 159 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | C | 161 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | M | 158 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | C | 168 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | D | 158 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | M | 165 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | B | 177 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | L | 162 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | C | 158 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | G | 313 | CLA | C3C-C2C | 5.97 | 1.48 | 1.35 |
| 12 | A | 176 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | L | 159 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | K | 177 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | M | 164 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | P | 313 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | J | 176 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | M | 156 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | C | 157 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | M | 166 | CLA | C3C-C2C | 5.98 | 1.48 | 1.35 |
| 12 | D | 156 | CLA | C3C-C2C | 5.99 | 1.48 | 1.35 |
| 12 | L | 166 | CLA | C3C-C2C | 5.99 | 1.48 | 1.35 |
| 12 | C | 166 | CLA | C3C-C2C | 5.99 | 1.48 | 1.35 |
| 12 | D | 157 | CLA | C3C-C2C | 5.99 | 1.48 | 1.35 |
| 12 | D | 166 | CLA | C3C-C2C | 6.00 | 1.48 | 1.35 |
| 12 | C | 163 | CLA | C3C-C2C | 6.00 | 1.48 | 1.35 |
| 12 | M | 157 | CLA | C3C-C2C | 6.00 | 1.48 | 1.35 |
| 12 | M | 161 | CLA | C3C-C2C | 6.00 | 1.48 | 1.35 |
| 12 | D | 161 | CLA | C3C-C2C | 6.00 | 1.48 | 1.35 |
| 12 | D | 164 | CLA | C3C-C2C | 6.00 | 1.48 | 1.35 |
| 12 | D | 162 | CLA | C3C-C2C | 6.01 | 1.48 | 1.35 |
| 12 | L | 157 | CLA | C3C-C2C | 6.01 | 1.48 | 1.35 |
| 12 | L | 165 | CLA | C3C-C2C | 6.01 | 1.48 | 1.35 |
| 12 | C | 165 | CLA | C3C-C2C | 6.01 | 1.48 | 1.35 |
| 12 | L | 163 | CLA | C3C-C2C | 6.02 | 1.48 | 1.35 |
| 12 | A | 177 | CLA | C3C-C2C | 6.03 | 1.48 | 1.35 |
| 12 | J | 175 | CLA | C3C-C2C | 6.03 | 1.48 | 1.35 |
| 12 | D | 163 | CLA | C3C-C2C | 6.04 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | M | 162 | CLA | C3C-C2C | 6.04 | 1.49 | 1.35 |
| 12 | A | 175 | CLA | C3C-C2C | 6.05 | 1.49 | 1.35 |
| 12 | J | 177 | CLA | C3C-C2C | 6.05 | 1.49 | 1.35 |
| 12 | M | 163 | CLA | C3C-C2C | 6.06 | 1.49 | 1.35 |
| 16 | F | 31 | HEM | C3A-C4A | 6.81 | 1.51 | 1.39 |
| 16 | I | 88 | HEM | C3A-C4A | 6.82 | 1.51 | 1.39 |
| 16 | R | 88 | HEM | C3A-C4A | 6.82 | 1.51 | 1.39 |
| 16 | O | 58 | HEM | C3A-C4A | 6.85 | 1.52 | 1.39 |
| 12 | J | 177 | CLA | CHB-C4A | 7.14 | 1.40 | 1.34 |
| 12 | D | 162 | CLA | CHB-C4A | 7.16 | 1.40 | 1.34 |
| 12 | L | 159 | CLA | CHB-C4A | 7.19 | 1.40 | 1.34 |
| 12 | M | 162 | CLA | CHB-C4A | 7.20 | 1.40 | 1.34 |
| 12 | C | 160 | CLA | CHB-C4A | 7.20 | 1.40 | 1.34 |
| 12 | A | 175 | CLA | CHB-C4A | 7.22 | 1.40 | 1.34 |
| 12 | A | 177 | CLA | CHB-C4A | 7.24 | 1.40 | 1.34 |
| 12 | L | 160 | CLA | CHB-C4A | 7.25 | 1.40 | 1.34 |
| 12 | J | 175 | CLA | CHB-C4A | 7.27 | 1.40 | 1.34 |
| 12 | L | 168 | CLA | CHB-C4A | 7.27 | 1.40 | 1.34 |
| 12 | C | 167 | CLA | CHB-C4A | 7.27 | 1.40 | 1.34 |
| 12 | D | 163 | CLA | CHB-C4A | 7.28 | 1.40 | 1.34 |
| 12 | L | 165 | CLA | CHB-C4A | 7.28 | 1.40 | 1.34 |
| 12 | L | 167 | CLA | CHB-C4A | 7.28 | 1.40 | 1.34 |
| 12 | D | 164 | CLA | CHB-C4A | 7.29 | 1.40 | 1.34 |
| 12 | M | 163 | CLA | CHB-C4A | 7.30 | 1.40 | 1.34 |
| 12 | G | 313 | CLA | CHB-C4A | 7.31 | 1.40 | 1.34 |
| 12 | M | 168 | CLA | CHB-C4A | 7.31 | 1.40 | 1.34 |
| 12 | C | 159 | CLA | CHB-C4A | 7.31 | 1.40 | 1.34 |
| 12 | C | 163 | CLA | CHB-C4A | 7.32 | 1.40 | 1.34 |
| 12 | L | 157 | CLA | CHB-C4A | 7.33 | 1.40 | 1.34 |
| 12 | C | 161 | CLA | CHB-C4A | 7.33 | 1.40 | 1.34 |
| 12 | C | 165 | CLA | CHB-C4A | 7.34 | 1.40 | 1.34 |
| 12 | D | 159 | CLA | CHB-C4A | 7.34 | 1.40 | 1.34 |
| 12 | J | 179 | CLA | CHB-C4A | 7.34 | 1.40 | 1.34 |
| 16 | F | 31 | HEM | C2A-C1A | 7.35 | 1.52 | 1.39 |
| 12 | B | 179 | CLA | CHB-C4A | 7.35 | 1.40 | 1.34 |
| 16 | O | 58 | HEM | C2A-C1A | 7.35 | 1.52 | 1.39 |
| 12 | L | 163 | CLA | CHB-C4A | 7.35 | 1.40 | 1.34 |
| 12 | M | 161 | CLA | CHB-C4A | 7.36 | 1.40 | 1.34 |
| 12 | K | 179 | CLA | CHB-C4A | 7.36 | 1.40 | 1.34 |
| 16 | I | 88 | HEM | C2A-C1A | 7.36 | 1.52 | 1.39 |
| 12 | D | 168 | CLA | CHB-C4A | 7.37 | 1.40 | 1.34 |
| 12 | L | 158 | CLA | CHB-C4A | 7.37 | 1.40 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 16 | R | 88 | HEM | C2A-C1A | 7.38 | 1.52 | 1.39 |
| 12 | C | 168 | CLA | CHB-C4A | 7.38 | 1.40 | 1.34 |
| 12 | D | 165 | CLA | CHB-C4A | 7.38 | 1.40 | 1.34 |
| 12 | L | 164 | CLA | CHB-C4A | 7.39 | 1.40 | 1.34 |
| 12 | A | 179 | CLA | CHB-C4A | 7.40 | 1.40 | 1.34 |
| 12 | P | 313 | CLA | CHB-C4A | 7.40 | 1.40 | 1.34 |
| 12 | M | 164 | CLA | CHB-C4A | 7.40 | 1.40 | 1.34 |
| 12 | C | 158 | CLA | CHB-C4A | 7.40 | 1.40 | 1.34 |
| 12 | L | 166 | CLA | CHB-C4A | 7.41 | 1.40 | 1.34 |
| 12 | M | 165 | CLA | CHB-C4A | 7.41 | 1.40 | 1.34 |
| 12 | M | 159 | CLA | CHB-C4A | 7.42 | 1.40 | 1.34 |
| 12 | C | 164 | CLA | CHB-C4A | 7.43 | 1.40 | 1.34 |
| 12 | C | 166 | CLA | CHB-C4A | 7.43 | 1.40 | 1.34 |
| 12 | L | 161 | CLA | CHB-C4A | 7.43 | 1.40 | 1.34 |
| 12 | D | 158 | CLA | CHB-C4A | 7.44 | 1.40 | 1.34 |
| 12 | M | 167 | CLA | CHB-C4A | 7.45 | 1.40 | 1.34 |
| 12 | M | 166 | CLA | CHB-C4A | 7.46 | 1.40 | 1.34 |
| 12 | M | 158 | CLA | CHB-C4A | 7.46 | 1.40 | 1.34 |
| 12 | C | 157 | CLA | CHB-C4A | 7.46 | 1.40 | 1.34 |
| 12 | D | 160 | CLA | CHB-C4A | 7.47 | 1.40 | 1.34 |
| 12 | B | 177 | CLA | CHB-C4A | 7.47 | 1.40 | 1.34 |
| 12 | D | 157 | CLA | CHB-C4A | 7.47 | 1.40 | 1.34 |
| 12 | D | 166 | CLA | CHB-C4A | 7.47 | 1.40 | 1.34 |
| 12 | D | 161 | CLA | CHB-C4A | 7.47 | 1.40 | 1.34 |
| 12 | D | 167 | CLA | CHB-C4A | 7.48 | 1.40 | 1.34 |
| 12 | M | 157 | CLA | CHB-C4A | 7.49 | 1.40 | 1.34 |
| 12 | K | 177 | CLA | CHB-C4A | 7.52 | 1.40 | 1.34 |
| 12 | J | 176 | CLA | CHB-C4A | 7.52 | 1.40 | 1.34 |
| 12 | D | 156 | CLA | CHB-C4A | 7.53 | 1.40 | 1.34 |
| 12 | A | 176 | CLA | CHB-C4A | 7.53 | 1.40 | 1.34 |
| 12 | M | 160 | CLA | CHB-C4A | 7.56 | 1.40 | 1.34 |
| 12 | M | 156 | CLA | CHB-C4A | 7.57 | 1.40 | 1.34 |
| 12 | L | 162 | CLA | CHB-C4A | 7.60 | 1.40 | 1.34 |
| 12 | C | 162 | CLA | CHB-C4A | 7.61 | 1.40 | 1.34 |

All (440) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | J | 177 | CLA | C2D-C3D-C4D | -8.84 | 98.68 | 106.30 |
| 12 | A | 177 | CLA | C2D-C3D-C4D | -8.80 | 98.72 | 106.30 |
| 12 | L | 160 | CLA | C2D-C3D-C4D | -8.78 | 98.73 | 106.30 |
| 12 | K | 179 | CLA | C2D-C3D-C4D | -8.77 | 98.75 | 106.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | M | 160 | CLA | C2D-C3D-C4D | -8.76 | 98.75 | 106.30 |
| 12 | M | 166 | CLA | C2D-C3D-C4D | -8.76 | 98.75 | 106.30 |
| 12 | A | 179 | CLA | C2D-C3D-C4D | -8.76 | 98.75 | 106.30 |
| 12 | C | 160 | CLA | C2D-C3D-C4D | -8.76 | 98.76 | 106.30 |
| 12 | D | 158 | CLA | C2D-C3D-C4D | -8.75 | 98.76 | 106.30 |
| 12 | D | 160 | CLA | C2D-C3D-C4D | -8.74 | 98.77 | 106.30 |
| 12 | L | 159 | CLA | C2D-C3D-C4D | -8.74 | 98.77 | 106.30 |
| 12 | C | 158 | CLA | C2D-C3D-C4D | -8.74 | 98.77 | 106.30 |
| 12 | D | 166 | CLA | C2D-C3D-C4D | -8.74 | 98.77 | 106.30 |
| 12 | A | 175 | CLA | C2D-C3D-C4D | -8.74 | 98.77 | 106.30 |
| 12 | C | 159 | CLA | C2D-C3D-C4D | -8.73 | 98.78 | 106.30 |
| 12 | B | 179 | CLA | C2D-C3D-C4D | -8.73 | 98.78 | 106.30 |
| 12 | L | 158 | CLA | C2D-C3D-C4D | -8.73 | 98.78 | 106.30 |
| 12 | M | 161 | CLA | C2D-C3D-C4D | -8.73 | 98.78 | 106.30 |
| 16 | I | 88 | HEM | C2D-C3D-C4D | -8.73 | 98.78 | 106.30 |
| 12 | C | 168 | CLA | C2D-C3D-C4D | -8.72 | 98.79 | 106.30 |
| 12 | J | 176 | CLA | C2D-C3D-C4D | -8.72 | 98.79 | 106.30 |
| 12 | C | 165 | CLA | C2D-C3D-C4D | -8.72 | 98.79 | 106.30 |
| 16 | R | 88 | HEM | C2D-C3D-C4D | -8.72 | 98.79 | 106.30 |
| 12 | J | 179 | CLA | C2D-C3D-C4D | -8.71 | 98.79 | 106.30 |
| 12 | J | 175 | CLA | C2D-C3D-C4D | -8.71 | 98.80 | 106.30 |
| 12 | A | 176 | CLA | C2D-C3D-C4D | -8.71 | 98.80 | 106.30 |
| 12 | D | 161 | CLA | C2D-C3D-C4D | -8.71 | 98.80 | 106.30 |
| 12 | M | 158 | CLA | C2D-C3D-C4D | -8.71 | 98.80 | 106.30 |
| 12 | L | 165 | CLA | C2D-C3D-C4D | -8.71 | 98.80 | 106.30 |
| 12 | D | 163 | CLA | C2D-C3D-C4D | -8.70 | 98.80 | 106.30 |
| 12 | L | 162 | CLA | C2D-C3D-C4D | -8.70 | 98.81 | 106.30 |
| 12 | M | 168 | CLA | C2D-C3D-C4D | -8.70 | 98.81 | 106.30 |
| 12 | L | 168 | CLA | C2D-C3D-C4D | -8.70 | 98.81 | 106.30 |
| 12 | M | 167 | CLA | C2D-C3D-C4D | -8.70 | 98.81 | 106.30 |
| 12 | L | 161 | CLA | C2D-C3D-C4D | -8.69 | 98.81 | 106.30 |
| 12 | L | 166 | CLA | C2D-C3D-C4D | -8.69 | 98.81 | 106.30 |
| 12 | M | 163 | CLA | C2D-C3D-C4D | -8.69 | 98.82 | 106.30 |
| 12 | C | 161 | CLA | C2D-C3D-C4D | -8.69 | 98.82 | 106.30 |
| 12 | C | 167 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | D | 164 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | C | 162 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | L | 167 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | M | 164 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | D | 162 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | C | 166 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | D | 165 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | C | 164 | CLA | C2D-C3D-C4D | -8.68 | 98.82 | 106.30 |
| 12 | L | 163 | CLA | C2D-C3D-C4D | -8.67 | 98.83 | 106.30 |
| 12 | G | 313 | CLA | C2D-C3D-C4D | -8.67 | 98.83 | 106.30 |
| 12 | D | 168 | CLA | C2D-C3D-C4D | -8.67 | 98.83 | 106.30 |
| 12 | M | 162 | CLA | C2D-C3D-C4D | -8.67 | 98.83 | 106.30 |
| 12 | D | 167 | CLA | C2D-C3D-C4D | -8.67 | 98.83 | 106.30 |
| 12 | C | 157 | CLA | C2D-C3D-C4D | -8.67 | 98.83 | 106.30 |
| 12 | P | 313 | CLA | C2D-C3D-C4D | -8.67 | 98.84 | 106.30 |
| 12 | L | 164 | CLA | C2D-C3D-C4D | -8.67 | 98.84 | 106.30 |
| 12 | M | 165 | CLA | C2D-C3D-C4D | -8.66 | 98.84 | 106.30 |
| 12 | K | 177 | CLA | C2D-C3D-C4D | -8.66 | 98.85 | 106.30 |
| 12 | C | 163 | CLA | C2D-C3D-C4D | -8.65 | 98.85 | 106.30 |
| 12 | D | 157 | CLA | C2D-C3D-C4D | -8.65 | 98.85 | 106.30 |
| 12 | M | 157 | CLA | C2D-C3D-C4D | -8.65 | 98.85 | 106.30 |
| 12 | B | 177 | CLA | C2D-C3D-C4D | -8.65 | 98.85 | 106.30 |
| 12 | M | 156 | CLA | C2D-C3D-C4D | -8.64 | 98.85 | 106.30 |
| 12 | L | 157 | CLA | C2D-C3D-C4D | -8.64 | 98.86 | 106.30 |
| 16 | F | 31 | HEM | C2D-C3D-C4D | -8.62 | 98.87 | 106.30 |
| 12 | D | 156 | CLA | C2D-C3D-C4D | -8.62 | 98.88 | 106.30 |
| 12 | D | 159 | CLA | C2D-C3D-C4D | -8.61 | 98.88 | 106.30 |
| 12 | M | 159 | CLA | C2D-C3D-C4D | -8.61 | 98.88 | 106.30 |
| 16 | O | 58 | HEM | C2D-C3D-C4D | -8.58 | 98.91 | 106.30 |
| 13 | A | 178 | PHO | CHA-C1A-NA | -2.97 | 121.79 | 125.89 |
| 13 | J | 178 | PHO | CHA-C1A-NA | -2.95 | 121.82 | 125.89 |
| 13 | B | 178 | PHO | CHA-C1A-NA | -2.95 | 121.82 | 125.89 |
| 13 | K | 178 | PHO | CHA-C1A-NA | -2.94 | 121.84 | 125.89 |
| 13 | B | 178 | PHO | C3C-C2C-C1C | -2.58 | 104.08 | 106.30 |
| 16 | F | 31 | HEM | C3C-C2C-C1C | -2.56 | 104.10 | 106.30 |
| 13 | K | 178 | PHO | C3C-C2C-C1C | -2.56 | 104.10 | 106.30 |
| 16 | R | 88 | HEM | C3C-C2C-C1C | -2.54 | 104.11 | 106.30 |
| 16 | O | 58 | HEM | C3C-C2C-C1C | -2.54 | 104.12 | 106.30 |
| 12 | J | 179 | CLA | C3C-C2C-C1C | -2.52 | 104.04 | 107.17 |
| 16 | I | 88 | HEM | C3C-C2C-C1C | -2.52 | 104.13 | 106.30 |
| 12 | A | 179 | CLA | C3C-C2C-C1C | -2.52 | 104.04 | 107.17 |
| 12 | M | 163 | CLA | C3C-C2C-C1C | -2.51 | 104.05 | 107.17 |
| 13 | J | 178 | PHO | C3C-C2C-C1C | -2.50 | 104.15 | 106.30 |
| 12 | D | 163 | CLA | C3C-C2C-C1C | -2.49 | 104.08 | 107.17 |
| 12 | J | 177 | CLA | C3C-C2C-C1C | -2.48 | 104.08 | 107.17 |
| 12 | C | 168 | CLA | C3C-C2C-C1C | -2.48 | 104.08 | 107.17 |
| 12 | D | 168 | CLA | C3C-C2C-C1C | -2.48 | 104.09 | 107.17 |
| 12 | L | 165 | CLA | C3C-C2C-C1C | -2.48 | 104.09 | 107.17 |
| 12 | L | 168 | CLA | C3C-C2C-C1C | -2.48 | 104.09 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | K | 179 | CLA | C3C-C2C-C1C | -2.48 | 104.09 | 107.17 |
| 12 | D | 157 | CLA | C3C-C2C-C1C | -2.48 | 104.09 | 107.17 |
| 12 | D | 162 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | D | 167 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | M | 164 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | M | 167 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | M | 168 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | D | 166 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | M | 162 | CLA | C3C-C2C-C1C | -2.47 | 104.10 | 107.17 |
| 12 | A | 177 | CLA | C3C-C2C-C1C | -2.47 | 104.11 | 107.17 |
| 12 | L | 166 | CLA | C3C-C2C-C1C | -2.46 | 104.11 | 107.17 |
| 12 | L | 159 | CLA | C3C-C2C-C1C | -2.46 | 104.11 | 107.17 |
| 12 | B | 179 | CLA | C3C-C2C-C1C | -2.46 | 104.11 | 107.17 |
| 13 | A | 178 | PHO | C3C-C2C-C1C | -2.46 | 104.18 | 106.30 |
| 12 | D | 164 | CLA | C3C-C2C-C1C | -2.46 | 104.12 | 107.17 |
| 12 | M | 166 | CLA | C3C-C2C-C1C | -2.46 | 104.12 | 107.17 |
| 12 | M | 157 | CLA | C3C-C2C-C1C | -2.46 | 104.12 | 107.17 |
| 12 | C | 165 | CLA | C3C-C2C-C1C | -2.46 | 104.12 | 107.17 |
| 12 | C | 159 | CLA | C3C-C2C-C1C | -2.45 | 104.12 | 107.17 |
| 12 | D | 161 | CLA | C3C-C2C-C1C | -2.45 | 104.12 | 107.17 |
| 12 | C | 158 | CLA | C3C-C2C-C1C | -2.45 | 104.13 | 107.17 |
| 12 | D | 165 | CLA | C3C-C2C-C1C | -2.45 | 104.13 | 107.17 |
| 12 | M | 161 | CLA | C3C-C2C-C1C | -2.45 | 104.13 | 107.17 |
| 12 | C | 166 | CLA | C3C-C2C-C1C | -2.45 | 104.13 | 107.17 |
| 12 | D | 158 | CLA | C3C-C2C-C1C | -2.44 | 104.13 | 107.17 |
| 12 | C | 157 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | M | 159 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | D | 159 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | D | 156 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | C | 160 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | M | 165 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | L | 162 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | L | 163 | CLA | C3C-C2C-C1C | -2.44 | 104.14 | 107.17 |
| 12 | C | 161 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | C | 163 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | G | 313 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | P | 313 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | M | 158 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | L | 157 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | L | 167 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | L | 160 | CLA | C3C-C2C-C1C | -2.43 | 104.15 | 107.17 |
| 12 | M | 156 | CLA | C3C-C2C-C1C | -2.43 | 104.16 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | B | 177 | CLA | C3C-C2C-C1C | -2.42 | 104.16 | 107.17 |
| 12 | A | 176 | CLA | C3C-C2C-C1C | -2.42 | 104.16 | 107.17 |
| 12 | C | 162 | CLA | C3C-C2C-C1C | -2.42 | 104.16 | 107.17 |
| 12 | D | 160 | CLA | C3C-C2C-C1C | -2.42 | 104.17 | 107.17 |
| 12 | C | 167 | CLA | C3C-C2C-C1C | -2.42 | 104.17 | 107.17 |
| 12 | C | 164 | CLA | C3C-C2C-C1C | -2.41 | 104.17 | 107.17 |
| 12 | L | 161 | CLA | C3C-C2C-C1C | -2.41 | 104.17 | 107.17 |
| 12 | L | 158 | CLA | C3C-C2C-C1C | -2.41 | 104.17 | 107.17 |
| 12 | M | 160 | CLA | C3C-C2C-C1C | -2.41 | 104.18 | 107.17 |
| 12 | J | 176 | CLA | C3C-C2C-C1C | -2.40 | 104.19 | 107.17 |
| 12 | L | 164 | CLA | C3C-C2C-C1C | -2.40 | 104.19 | 107.17 |
| 12 | K | 177 | CLA | C3C-C2C-C1C | -2.39 | 104.19 | 107.17 |
| 12 | A | 175 | CLA | C3C-C2C-C1C | -2.38 | 104.21 | 107.17 |
| 12 | J | 175 | CLA | C3C-C2C-C1C | -2.38 | 104.22 | 107.17 |
| 12 | A | 175 | CLA | C2C-C3C-C4C | -2.34 | 104.27 | 107.17 |
| 12 | J | 175 | CLA | C2C-C3C-C4C | -2.32 | 104.28 | 107.17 |
| 12 | L | 163 | CLA | C2C-C3C-C4C | -2.32 | 104.29 | 107.17 |
| 12 | J | 176 | CLA | C2C-C3C-C4C | -2.28 | 104.33 | 107.17 |
| 12 | C | 163 | CLA | C2C-C3C-C4C | -2.28 | 104.34 | 107.17 |
| 12 | J | 177 | CLA | C2C-C3C-C4C | -2.27 | 104.35 | 107.17 |
| 12 | A | 177 | CLA | C2C-C3C-C4C | -2.27 | 104.35 | 107.17 |
| 12 | K | 177 | CLA | C2C-C3C-C4C | -2.27 | 104.36 | 107.17 |
| 12 | C | 165 | CLA | C2C-C3C-C4C | -2.27 | 104.36 | 107.17 |
| 12 | D | 164 | CLA | C2C-C3C-C4C | -2.25 | 104.38 | 107.17 |
| 12 | L | 165 | CLA | C2C-C3C-C4C | -2.25 | 104.38 | 107.17 |
| 12 | D | 161 | CLA | C2C-C3C-C4C | -2.25 | 104.38 | 107.17 |
| 12 | D | 159 | CLA | C2C-C3C-C4C | -2.25 | 104.38 | 107.17 |
| 12 | M | 157 | CLA | C2C-C3C-C4C | -2.24 | 104.38 | 107.17 |
| 12 | P | 313 | CLA | C2C-C3C-C4C | -2.24 | 104.38 | 107.17 |
| 12 | C | 167 | CLA | C2C-C3C-C4C | -2.24 | 104.38 | 107.17 |
| 12 | L | 164 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | M | 162 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | M | 163 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | G | 313 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 16 | F | 31 | HEM | C3A-C2A-C1A | -2.24 | 104.37 | 106.29 |
| 12 | M | 161 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | B | 177 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | L | 157 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 13 | A | 178 | PHO | C2C-C3C-C4C | -2.24 | 104.38 | 106.30 |
| 12 | A | 176 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | M | 164 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |
| 12 | M | 156 | CLA | C2C-C3C-C4C | -2.24 | 104.39 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | M | 159 | CLA | C2C-C3C-C4C | -2.23 | 104.40 | 107.17 |
| 12 | D | 157 | CLA | C2C-C3C-C4C | -2.23 | 104.40 | 107.17 |
| 12 | L | 167 | CLA | C2C-C3C-C4C | -2.23 | 104.40 | 107.17 |
| 12 | C | 159 | CLA | C2C-C3C-C4C | -2.23 | 104.40 | 107.17 |
| 16 | R | 88 | HEM | C3A-C2A-C1A | -2.23 | 104.38 | 106.29 |
| 12 | C | 166 | CLA | C2C-C3C-C4C | -2.23 | 104.41 | 107.17 |
| 12 | C | 164 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | D | 163 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | L | 160 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | D | 158 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | M | 158 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | C | 157 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | L | 159 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | M | 165 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | C | 162 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 12 | D | 156 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 13 | J | 178 | PHO | C2C-C3C-C4C | -2.22 | 104.39 | 106.30 |
| 12 | D | 162 | CLA | C2C-C3C-C4C | -2.22 | 104.41 | 107.17 |
| 16 | I | 88 | HEM | C3A-C2A-C1A | -2.22 | 104.39 | 106.29 |
| 12 | C | 161 | CLA | C2C-C3C-C4C | -2.22 | 104.42 | 107.17 |
| 16 | O | 58 | HEM | C3A-C2A-C1A | -2.21 | 104.39 | 106.29 |
| 12 | L | 162 | CLA | C2C-C3C-C4C | -2.21 | 104.42 | 107.17 |
| 12 | L | 166 | CLA | C2C-C3C-C4C | -2.21 | 104.42 | 107.17 |
| 12 | C | 160 | CLA | C2C-C3C-C4C | -2.21 | 104.42 | 107.17 |
| 12 | D | 165 | CLA | C2C-C3C-C4C | -2.21 | 104.42 | 107.17 |
| 12 | L | 158 | CLA | C2C-C3C-C4C | -2.21 | 104.42 | 107.17 |
| 12 | C | 168 | CLA | C2C-C3C-C4C | -2.21 | 104.43 | 107.17 |
| 12 | L | 168 | CLA | C2C-C3C-C4C | -2.21 | 104.43 | 107.17 |
| 12 | L | 161 | CLA | C2C-C3C-C4C | -2.20 | 104.44 | 107.17 |
| 16 | F | 31 | HEM | C2C-C3C-C4C | -2.20 | 104.41 | 106.30 |
| 12 | C | 158 | CLA | C2C-C3C-C4C | -2.20 | 104.44 | 107.17 |
| 12 | D | 166 | CLA | C2C-C3C-C4C | -2.19 | 104.44 | 107.17 |
| 16 | O | 58 | HEM | C2C-C3C-C4C | -2.19 | 104.41 | 106.30 |
| 12 | B | 179 | CLA | C2C-C3C-C4C | -2.19 | 104.44 | 107.17 |
| 12 | M | 160 | CLA | C2C-C3C-C4C | -2.19 | 104.45 | 107.17 |
| 16 | R | 88 | HEM | C2C-C3C-C4C | -2.19 | 104.41 | 106.30 |
| 12 | M | 166 | CLA | C2C-C3C-C4C | -2.19 | 104.45 | 107.17 |
| 12 | D | 168 | CLA | C2C-C3C-C4C | -2.19 | 104.45 | 107.17 |
| 16 | I | 88 | HEM | C2C-C3C-C4C | -2.19 | 104.42 | 106.30 |
| 12 | D | 167 | CLA | C2C-C3C-C4C | -2.19 | 104.45 | 107.17 |
| 12 | M | 168 | CLA | C2C-C3C-C4C | -2.18 | 104.46 | 107.17 |
| 12 | A | 179 | CLA | C2C-C3C-C4C | -2.18 | 104.46 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | K | 179 | CLA | C2C-C3C-C4C | -2.18 | 104.46 | 107.17 |
| 12 | D | 160 | CLA | C2C-C3C-C4C | -2.18 | 104.47 | 107.17 |
| 12 | J | 179 | CLA | C2C-C3C-C4C | -2.18 | 104.47 | 107.17 |
| 12 | M | 167 | CLA | C2C-C3C-C4C | -2.17 | 104.48 | 107.17 |
| 13 | B | 178 | PHO | C2C-C3C-C4C | -2.16 | 104.44 | 106.30 |
| 13 | K | 178 | PHO | C2C-C3C-C4C | -2.15 | 104.45 | 106.30 |
| 16 | F | 31 | HEM | C4D-CHA-C1A | -2.02 | 126.47 | 129.92 |
| 12 | D | 161 | CLA | C3A-C4A-CHB | -2.02 | 121.64 | 123.86 |
| 16 | I | 88 | HEM | C4D-CHA-C1A | -2.01 | 126.48 | 129.92 |
| 12 | L | 165 | CLA | C3A-C4A-CHB | -2.01 | 121.66 | 123.86 |
| 12 | L | 161 | CLA | C2A-C1A-CHA | 2.69 | 127.23 | 122.63 |
| 12 | C | 161 | CLA | C2A-C1A-CHA | 2.70 | 127.23 | 122.63 |
| 12 | J | 176 | CLA | C2A-C1A-CHA | 2.70 | 127.23 | 122.63 |
| 12 | J | 175 | CLA | C2A-C1A-CHA | 2.71 | 127.25 | 122.63 |
| 12 | K | 179 | CLA | C2A-C1A-CHA | 2.71 | 127.26 | 122.63 |
| 12 | M | 165 | CLA | C2A-C1A-CHA | 2.72 | 127.27 | 122.63 |
| 12 | J | 179 | CLA | C2A-C1A-CHA | 2.72 | 127.27 | 122.63 |
| 12 | A | 176 | CLA | C2A-C1A-CHA | 2.72 | 127.28 | 122.63 |
| 12 | L | 168 | CLA | C2A-C1A-CHA | 2.72 | 127.28 | 122.63 |
| 12 | M | 161 | CLA | C2A-C1A-CHA | 2.73 | 127.29 | 122.63 |
| 12 | M | 164 | CLA | C2A-C1A-CHA | 2.73 | 127.29 | 122.63 |
| 12 | A | 179 | CLA | C2A-C1A-CHA | 2.73 | 127.29 | 122.63 |
| 12 | M | 168 | CLA | C2A-C1A-CHA | 2.73 | 127.30 | 122.63 |
| 12 | A | 175 | CLA | C2A-C1A-CHA | 2.73 | 127.30 | 122.63 |
| 12 | D | 165 | CLA | C2A-C1A-CHA | 2.73 | 127.30 | 122.63 |
| 12 | L | 163 | CLA | C2A-C1A-CHA | 2.73 | 127.30 | 122.63 |
| 12 | B | 177 | CLA | C2A-C1A-CHA | 2.73 | 127.30 | 122.63 |
| 12 | M | 159 | CLA | C2A-C1A-CHA | 2.73 | 127.30 | 122.63 |
| 12 | D | 168 | CLA | C2A-C1A-CHA | 2.74 | 127.30 | 122.63 |
| 12 | L | 165 | CLA | C2A-C1A-CHA | 2.74 | 127.30 | 122.63 |
| 12 | B | 179 | CLA | C2A-C1A-CHA | 2.74 | 127.30 | 122.63 |
| 12 | D | 164 | CLA | C2A-C1A-CHA | 2.74 | 127.30 | 122.63 |
| 12 | C | 163 | CLA | C2A-C1A-CHA | 2.74 | 127.31 | 122.63 |
| 12 | C | 168 | CLA | C2A-C1A-CHA | 2.74 | 127.31 | 122.63 |
| 12 | C | 164 | CLA | C2A-C1A-CHA | 2.74 | 127.31 | 122.63 |
| 12 | D | 161 | CLA | C2A-C1A-CHA | 2.74 | 127.31 | 122.63 |
| 12 | L | 167 | CLA | C2A-C1A-CHA | 2.74 | 127.31 | 122.63 |
| 12 | C | 159 | CLA | C2A-C1A-CHA | 2.74 | 127.31 | 122.63 |
| 12 | D | 159 | CLA | C2A-C1A-CHA | 2.75 | 127.32 | 122.63 |
| 12 | K | 177 | CLA | C2A-C1A-CHA | 2.75 | 127.32 | 122.63 |
| 12 | D | 163 | CLA | C2A-C1A-CHA | 2.75 | 127.32 | 122.63 |
| 12 | C | 165 | CLA | C2A-C1A-CHA | 2.75 | 127.32 | 122.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 12 | C | 160 | CLA | C2A-C1A-CHA | 2.75 | 127.33 | 122.63 |
| 12 | M | 166 | CLA | C2A-C1A-CHA | 2.75 | 127.33 | 122.63 |
| 12 | C | 167 | CLA | C2A-C1A-CHA | 2.75 | 127.33 | 122.63 |
| 12 | L | 164 | CLA | C2A-C1A-CHA | 2.76 | 127.33 | 122.63 |
| 12 | A | 177 | CLA | C2A-C1A-CHA | 2.76 | 127.33 | 122.63 |
| 12 | L | 160 | CLA | C2A-C1A-CHA | 2.76 | 127.33 | 122.63 |
| 12 | L | 158 | CLA | C2A-C1A-CHA | 2.76 | 127.34 | 122.63 |
| 12 | G | 313 | CLA | C2A-C1A-CHA | 2.76 | 127.34 | 122.63 |
| 12 | J | 177 | CLA | C2A-C1A-CHA | 2.76 | 127.34 | 122.63 |
| 12 | M | 163 | CLA | C2A-C1A-CHA | 2.76 | 127.34 | 122.63 |
| 12 | C | 158 | CLA | C2A-C1A-CHA | 2.76 | 127.35 | 122.63 |
| 12 | D | 166 | CLA | C2A-C1A-CHA | 2.77 | 127.36 | 122.63 |
| 12 | P | 313 | CLA | C2A-C1A-CHA | 2.77 | 127.36 | 122.63 |
| 12 | D | 157 | CLA | C2A-C1A-CHA | 2.77 | 127.36 | 122.63 |
| 12 | M | 157 | CLA | C2A-C1A-CHA | 2.77 | 127.37 | 122.63 |
| 12 | L | 159 | CLA | C2A-C1A-CHA | 2.78 | 127.37 | 122.63 |
| 12 | L | 166 | CLA | C2A-C1A-CHA | 2.78 | 127.37 | 122.63 |
| 12 | D | 156 | CLA | C2A-C1A-CHA | 2.78 | 127.38 | 122.63 |
| 12 | L | 157 | CLA | C2A-C1A-CHA | 2.78 | 127.38 | 122.63 |
| 12 | C | 157 | CLA | C2A-C1A-CHA | 2.78 | 127.38 | 122.63 |
| 12 | D | 167 | CLA | C2A-C1A-CHA | 2.78 | 127.38 | 122.63 |
| 12 | M | 162 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | D | 160 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | D | 158 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | M | 160 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | C | 162 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | D | 162 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | M | 156 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | M | 167 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | L | 162 | CLA | C2A-C1A-CHA | 2.79 | 127.39 | 122.63 |
| 12 | C | 166 | CLA | C2A-C1A-CHA | 2.79 | 127.40 | 122.63 |
| 12 | M | 158 | CLA | C2A-C1A-CHA | 2.79 | 127.40 | 122.63 |
| 16 | R | 88 | HEM | C4C-NC-C1C | 3.42 | 108.36 | 105.79 |
| 16 | O | 58 | HEM | C4C-NC-C1C | 3.45 | 108.39 | 105.79 |
| 16 | I | 88 | HEM | C4C-NC-C1C | 3.45 | 108.39 | 105.79 |
| 16 | F | 31 | HEM | C4C-NC-C1C | 3.47 | 108.40 | 105.79 |
| 16 | O | 58 | HEM | C3C-C4C-NC | 3.61 | 111.13 | 108.27 |
| 16 | F | 31 | HEM | C3C-C4C-NC | 3.62 | 111.13 | 108.27 |
| 16 | I | 88 | HEM | C3C-C4C-NC | 3.63 | 111.13 | 108.27 |
| 16 | R | 88 | HEM | C3C-C4C-NC | 3.68 | 111.18 | 108.27 |
| 16 | O | 58 | HEM | C2B-C1B-NB | 3.87 | 111.33 | 108.27 |
| 16 | R | 88 | HEM | C2B-C1B-NB | 3.87 | 111.33 | 108.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 16 | I | 88 | HEM | C2B-C1B-NB | 3.88 | 111.33 | 108.27 |
| 16 | F | 31 | HEM | C2B-C1B-NB | 3.90 | 111.35 | 108.27 |
| 16 | I | 88 | HEM | C2C-C1C-NC | 4.63 | 111.92 | 108.27 |
| 16 | R | 88 | HEM | C2C-C1C-NC | 4.63 | 111.92 | 108.27 |
| 16 | O | 58 | HEM | C2C-C1C-NC | 4.66 | 111.95 | 108.27 |
| 16 | F | 31 | HEM | C2C-C1C-NC | 4.67 | 111.96 | 108.27 |
| 16 | O | 58 | HEM | C3D-C2D-C1D | 5.77 | 111.23 | 106.29 |
| 12 | L | 163 | CLA | C3D-C2D-C1D | 5.80 | 111.30 | 106.30 |
| 16 | F | 31 | HEM | C3D-C2D-C1D | 5.81 | 111.26 | 106.29 |
| 12 | D | 168 | CLA | C3D-C2D-C1D | 5.83 | 111.33 | 106.30 |
| 12 | C | 164 | CLA | C3D-C2D-C1D | 5.83 | 111.33 | 106.30 |
| 12 | C | 167 | CLA | C3D-C2D-C1D | 5.83 | 111.33 | 106.30 |
| 12 | P | 313 | CLA | C3D-C2D-C1D | 5.83 | 111.33 | 106.30 |
| 12 | G | 313 | CLA | C3D-C2D-C1D | 5.83 | 111.33 | 106.30 |
| 12 | M | 158 | CLA | C3D-C2D-C1D | 5.83 | 111.33 | 106.30 |
| 12 | L | 167 | CLA | C3D-C2D-C1D | 5.84 | 111.33 | 106.30 |
| 12 | J | 179 | CLA | C3D-C2D-C1D | 5.84 | 111.33 | 106.30 |
| 12 | B | 177 | CLA | C3D-C2D-C1D | 5.84 | 111.33 | 106.30 |
| 12 | L | 157 | CLA | C3D-C2D-C1D | 5.84 | 111.33 | 106.30 |
| 12 | K | 177 | CLA | C3D-C2D-C1D | 5.84 | 111.33 | 106.30 |
| 12 | C | 163 | CLA | C3D-C2D-C1D | 5.84 | 111.34 | 106.30 |
| 12 | M | 168 | CLA | C3D-C2D-C1D | 5.84 | 111.34 | 106.30 |
| 12 | D | 167 | CLA | C3D-C2D-C1D | 5.84 | 111.34 | 106.30 |
| 12 | D | 164 | CLA | C3D-C2D-C1D | 5.85 | 111.34 | 106.30 |
| 12 | L | 165 | CLA | C3D-C2D-C1D | 5.85 | 111.34 | 106.30 |
| 12 | L | 164 | CLA | C3D-C2D-C1D | 5.85 | 111.34 | 106.30 |
| 12 | M | 157 | CLA | C3D-C2D-C1D | 5.85 | 111.34 | 106.30 |
| 12 | M | 167 | CLA | C3D-C2D-C1D | 5.85 | 111.34 | 106.30 |
| 12 | C | 166 | CLA | C3D-C2D-C1D | 5.85 | 111.34 | 106.30 |
| 12 | L | 166 | CLA | C3D-C2D-C1D | 5.85 | 111.35 | 106.30 |
| 12 | D | 157 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | C | 162 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | A | 179 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | A | 176 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | D | 165 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | M | 159 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | M | 164 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | L | 162 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | D | 161 | CLA | C3D-C2D-C1D | 5.86 | 111.35 | 106.30 |
| 12 | C | 157 | CLA | C3D-C2D-C1D | 5.87 | 111.36 | 106.30 |
| 12 | D | 159 | CLA | C3D-C2D-C1D | 5.87 | 111.36 | 106.30 |
| 12 | M | 163 | CLA | C3D-C2D-C1D | 5.87 | 111.36 | 106.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 12 | L | 161 | CLA | C3D-C2D-C1D | 5.87 | 111.36 | 106.30 |
| 12 | D | 160 | CLA | C3D-C2D-C1D | 5.87 | 111.36 | 106.30 |
| 12 | D | 156 | CLA | C3D-C2D-C1D | 5.87 | 111.36 | 106.30 |
| 12 | J | 176 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | M | 160 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | M | 165 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | M | 161 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | C | 165 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | D | 162 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | D | 163 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | D | 158 | CLA | C3D-C2D-C1D | 5.88 | 111.37 | 106.30 |
| 12 | M | 166 | CLA | C3D-C2D-C1D | 5.89 | 111.37 | 106.30 |
| 12 | L | 158 | CLA | C3D-C2D-C1D | 5.89 | 111.38 | 106.30 |
| 12 | C | 161 | CLA | C3D-C2D-C1D | 5.89 | 111.38 | 106.30 |
| 12 | M | 162 | CLA | C3D-C2D-C1D | 5.90 | 111.38 | 106.30 |
| 12 | B | 179 | CLA | C3D-C2D-C1D | 5.90 | 111.39 | 106.30 |
| 12 | C | 168 | CLA | C3D-C2D-C1D | 5.91 | 111.39 | 106.30 |
| 12 | L | 168 | CLA | C3D-C2D-C1D | 5.91 | 111.39 | 106.30 |
| 12 | C | 158 | CLA | C3D-C2D-C1D | 5.92 | 111.40 | 106.30 |
| 12 | M | 156 | CLA | C3D-C2D-C1D | 5.92 | 111.41 | 106.30 |
| 12 | D | 166 | CLA | C3D-C2D-C1D | 5.93 | 111.42 | 106.30 |
| 12 | J | 175 | CLA | C3D-C2D-C1D | 5.94 | 111.42 | 106.30 |
| 12 | A | 177 | CLA | C3D-C2D-C1D | 5.94 | 111.42 | 106.30 |
| 12 | A | 175 | CLA | C3D-C2D-C1D | 5.95 | 111.42 | 106.30 |
| 12 | K | 179 | CLA | C3D-C2D-C1D | 5.96 | 111.43 | 106.30 |
| 12 | C | 160 | CLA | C3D-C2D-C1D | 5.96 | 111.44 | 106.30 |
| 16 | I | 88 | HEM | C3D-C2D-C1D | 5.97 | 111.40 | 106.29 |
| 12 | C | 159 | CLA | C3D-C2D-C1D | 5.98 | 111.45 | 106.30 |
| 12 | J | 177 | CLA | C3D-C2D-C1D | 5.98 | 111.45 | 106.30 |
| 16 | R | 88 | HEM | C3D-C2D-C1D | 5.98 | 111.41 | 106.29 |
| 12 | L | 160 | CLA | C3D-C2D-C1D | 6.00 | 111.47 | 106.30 |
| 12 | L | 159 | CLA | C3D-C2D-C1D | 6.01 | 111.48 | 106.30 |
| 12 | K | 177 | CLA | C3D-C4D-ND | 6.96 | 116.19 | 110.14 |
| 12 | D | 159 | CLA | C3D-C4D-ND | 6.97 | 116.20 | 110.14 |
| 12 | M | 159 | CLA | C3D-C4D-ND | 6.97 | 116.20 | 110.14 |
| 12 | M | 165 | CLA | C3D-C4D-ND | 6.99 | 116.21 | 110.14 |
| 12 | B | 177 | CLA | C3D-C4D-ND | 6.99 | 116.22 | 110.14 |
| 12 | C | 167 | CLA | C3D-C4D-ND | 6.99 | 116.22 | 110.14 |
| 12 | M | 162 | CLA | C3D-C4D-ND | 7.01 | 116.23 | 110.14 |
| 12 | L | 167 | CLA | C3D-C4D-ND | 7.01 | 116.23 | 110.14 |
| 12 | L | 164 | CLA | C3D-C4D-ND | 7.02 | 116.24 | 110.14 |
| 12 | D | 165 | CLA | C3D-C4D-ND | 7.02 | 116.24 | 110.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 12 | C | 161 | CLA | C3D-C4D-ND | 7.04 | 116.26 | 110.14 |
| 12 | D | 157 | CLA | C3D-C4D-ND | 7.05 | 116.26 | 110.14 |
| 12 | L | 157 | CLA | C3D-C4D-ND | 7.05 | 116.27 | 110.14 |
| 12 | M | 163 | CLA | C3D-C4D-ND | 7.05 | 116.27 | 110.14 |
| 12 | D | 162 | CLA | C3D-C4D-ND | 7.05 | 116.27 | 110.14 |
| 12 | K | 179 | CLA | C3D-C4D-ND | 7.05 | 116.27 | 110.14 |
| 12 | D | 163 | CLA | C3D-C4D-ND | 7.05 | 116.27 | 110.14 |
| 12 | C | 162 | CLA | C3D-C4D-ND | 7.05 | 116.27 | 110.14 |
| 12 | C | 164 | CLA | C3D-C4D-ND | 7.06 | 116.28 | 110.14 |
| 12 | D | 156 | CLA | C3D-C4D-ND | 7.06 | 116.28 | 110.14 |
| 12 | L | 168 | CLA | C3D-C4D-ND | 7.06 | 116.28 | 110.14 |
| 12 | C | 166 | CLA | C3D-C4D-ND | 7.07 | 116.28 | 110.14 |
| 12 | L | 161 | CLA | C3D-C4D-ND | 7.07 | 116.28 | 110.14 |
| 12 | C | 163 | CLA | C3D-C4D-ND | 7.08 | 116.29 | 110.14 |
| 12 | L | 162 | CLA | C3D-C4D-ND | 7.08 | 116.29 | 110.14 |
| 12 | L | 166 | CLA | C3D-C4D-ND | 7.08 | 116.29 | 110.14 |
| 12 | D | 166 | CLA | C3D-C4D-ND | 7.08 | 116.29 | 110.14 |
| 12 | M | 156 | CLA | C3D-C4D-ND | 7.08 | 116.30 | 110.14 |
| 12 | J | 179 | CLA | C3D-C4D-ND | 7.08 | 116.30 | 110.14 |
| 12 | D | 167 | CLA | C3D-C4D-ND | 7.09 | 116.30 | 110.14 |
| 12 | B | 179 | CLA | C3D-C4D-ND | 7.09 | 116.30 | 110.14 |
| 12 | C | 157 | CLA | C3D-C4D-ND | 7.09 | 116.30 | 110.14 |
| 12 | D | 161 | CLA | C3D-C4D-ND | 7.09 | 116.31 | 110.14 |
| 12 | M | 157 | CLA | C3D-C4D-ND | 7.09 | 116.31 | 110.14 |
| 12 | D | 168 | CLA | C3D-C4D-ND | 7.09 | 116.31 | 110.14 |
| 12 | C | 168 | CLA | C3D-C4D-ND | 7.10 | 116.31 | 110.14 |
| 12 | M | 167 | CLA | C3D-C4D-ND | 7.10 | 116.31 | 110.14 |
| 12 | L | 165 | CLA | C3D-C4D-ND | 7.10 | 116.31 | 110.14 |
| 12 | L | 163 | CLA | C3D-C4D-ND | 7.10 | 116.31 | 110.14 |
| 12 | C | 165 | CLA | C3D-C4D-ND | 7.11 | 116.32 | 110.14 |
| 12 | M | 168 | CLA | C3D-C4D-ND | 7.11 | 116.32 | 110.14 |
| 12 | G | 313 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | M | 161 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | L | 159 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | J | 176 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | C | 158 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | A | 177 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | M | 166 | CLA | C3D-C4D-ND | 7.12 | 116.33 | 110.14 |
| 12 | C | 160 | CLA | C3D-C4D-ND | 7.13 | 116.34 | 110.14 |
| 12 | D | 160 | CLA | C3D-C4D-ND | 7.13 | 116.34 | 110.14 |
| 12 | C | 159 | CLA | C3D-C4D-ND | 7.13 | 116.34 | 110.14 |
| 12 | L | 160 | CLA | C3D-C4D-ND | 7.13 | 116.34 | 110.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | A | 175 | CLA | C3D-C4D-ND | 7.14 | 116.34 | 110.14 |
| 12 | A | 176 | CLA | C3D-C4D-ND | 7.14 | 116.35 | 110.14 |
| 12 | A | 179 | CLA | C3D-C4D-ND | 7.14 | 116.35 | 110.14 |
| 12 | L | 158 | CLA | C3D-C4D-ND | 7.15 | 116.35 | 110.14 |
| 12 | M | 164 | CLA | C3D-C4D-ND | 7.15 | 116.36 | 110.14 |
| 12 | J | 177 | CLA | C3D-C4D-ND | 7.15 | 116.36 | 110.14 |
| 12 | D | 158 | CLA | C3D-C4D-ND | 7.16 | 116.36 | 110.14 |
| 12 | M | 158 | CLA | C3D-C4D-ND | 7.16 | 116.36 | 110.14 |
| 12 | J | 175 | CLA | C3D-C4D-ND | 7.16 | 116.37 | 110.14 |
| 12 | D | 164 | CLA | C3D-C4D-ND | 7.17 | 116.37 | 110.14 |
| 12 | P | 313 | CLA | C3D-C4D-ND | 7.17 | 116.37 | 110.14 |
| 12 | M | 160 | CLA | C3D-C4D-ND | 7.17 | 116.38 | 110.14 |
| 16 | O | 58 | HEM | C3D-C4D-ND | 10.04 | 116.20 | 108.27 |
| 16 | F | 31 | HEM | C3D-C4D-ND | 10.07 | 116.23 | 108.27 |
| 16 | I | 88 | HEM | C3D-C4D-ND | 10.17 | 116.30 | 108.27 |
| 16 | R | 88 | HEM | C3D-C4D-ND | 10.20 | 116.33 | 108.27 |

All (192) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12 | L | 160 | CLA | NC |
| 12 | L | 160 | CLA | ND |
| 12 | L | 160 | CLA | NA |
| 12 | D | 161 | CLA | NC |
| 12 | D | 161 | CLA | ND |
| 12 | D | 161 | CLA | NA |
| 12 | J | 177 | CLA | NC |
| 12 | J | 177 | CLA | ND |
| 12 | J | 177 | CLA | NA |
| 12 | D | 164 | CLA | NC |
| 12 | D | 164 | CLA | ND |
| 12 | D | 164 | CLA | NA |
| 12 | C | 168 | CLA | NC |
| 12 | C | 168 | CLA | ND |
| 12 | C | 168 | CLA | NA |
| 12 | C | 157 | CLA | NC |
| 12 | C | 157 | CLA | ND |
| 12 | C | 157 | CLA | NA |
| 12 | L | 164 | CLA | NC |
| 12 | L | 164 | CLA | ND |
| 12 | L | 164 | CLA | NA |
| 12 | B | 179 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12 | B | 179 | CLA | ND |
| 12 | B | 179 | CLA | NA |
| 12 | M | 166 | CLA | NC |
| 12 | M | 166 | CLA | ND |
| 12 | M | 166 | CLA | NA |
| 12 | M | 157 | CLA | NC |
| 12 | M | 157 | CLA | ND |
| 12 | M | 157 | CLA | NA |
| 12 | D | 162 | CLA | NC |
| 12 | D | 162 | CLA | ND |
| 12 | D | 162 | CLA | NA |
| 12 | P | 313 | CLA | NC |
| 12 | P | 313 | CLA | ND |
| 12 | P | 313 | CLA | NA |
| 12 | M | 161 | CLA | NC |
| 12 | M | 161 | CLA | ND |
| 12 | M | 161 | CLA | NA |
| 12 | D | 166 | CLA | NC |
| 12 | D | 166 | CLA | ND |
| 12 | D | 166 | CLA | NA |
| 12 | M | 156 | CLA | NC |
| 12 | M | 156 | CLA | ND |
| 12 | M | 156 | CLA | NA |
| 12 | D | 156 | CLA | NC |
| 12 | D | 156 | CLA | ND |
| 12 | D | 156 | CLA | NA |
| 12 | C | 163 | CLA | NC |
| 12 | C | 163 | CLA | ND |
| 12 | C | 163 | CLA | NA |
| 12 | B | 177 | CLA | NC |
| 12 | B | 177 | CLA | ND |
| 12 | B | 177 | CLA | NA |
| 12 | M | 162 | CLA | NC |
| 12 | M | 162 | CLA | ND |
| 12 | M | 162 | CLA | NA |
| 12 | L | 166 | CLA | NC |
| 12 | L | 166 | CLA | ND |
| 12 | L | 166 | CLA | NA |
| 12 | C | 158 | CLA | NC |
| 12 | C | 158 | CLA | ND |
| 12 | C | 158 | CLA | NA |
| 12 | L | 168 | CLA | NC |

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Continued from previous page...

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12 | L | 168 | CLA | ND |
| 12 | L | 168 | CLA | NA |
| 12 | J | 176 | CLA | NC |
| 12 | J | 176 | CLA | ND |
| 12 | J | 176 | CLA | NA |
| 12 | J | 179 | CLA | NC |
| 12 | J | 179 | CLA | ND |
| 12 | J | 179 | CLA | NA |
| 12 | M | 168 | CLA | NC |
| 12 | M | 168 | CLA | ND |
| 12 | M | 168 | CLA | NA |
| 12 | A | 177 | CLA | NC |
| 12 | A | 177 | CLA | ND |
| 12 | A | 177 | CLA | NA |
| 12 | D | 168 | CLA | NC |
| 12 | D | 168 | CLA | ND |
| 12 | D | 168 | CLA | NA |
| 12 | D | 159 | CLA | NC |
| 12 | D | 159 | CLA | ND |
| 12 | D | 159 | CLA | NA |
| 12 | D | 158 | CLA | NC |
| 12 | D | 158 | CLA | ND |
| 12 | D | 158 | CLA | NA |
| 12 | D | 160 | CLA | NC |
| 12 | D | 160 | CLA | ND |
| 12 | D | 160 | CLA | NA |
| 12 | G | 313 | CLA | NC |
| 12 | G | 313 | CLA | ND |
| 12 | G | 313 | CLA | NA |
| 12 | L | 165 | CLA | NC |
| 12 | L | 165 | CLA | ND |
| 12 | L | 165 | CLA | NA |
| 12 | C | 164 | CLA | NC |
| 12 | C | 164 | CLA | ND |
| 12 | C | 164 | CLA | NA |
| 12 | L | 157 | CLA | NC |
| 12 | L | 157 | CLA | ND |
| 12 | L | 157 | CLA | NA |
| 12 | A | 175 | CLA | NC |
| 12 | A | 175 | CLA | ND |
| 12 | A | 175 | CLA | NA |
| 12 | M | 158 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12 | M | 158 | CLA | ND |
| 12 | M | 158 | CLA | NA |
| 12 | C | 166 | CLA | NC |
| 12 | C | 166 | CLA | ND |
| 12 | C | 166 | CLA | NA |
| 12 | M | 160 | CLA | NC |
| 12 | M | 160 | CLA | ND |
| 12 | M | 160 | CLA | NA |
| 12 | M | 165 | CLA | NC |
| 12 | M | 165 | CLA | ND |
| 12 | M | 165 | CLA | NA |
| 12 | C | 160 | CLA | NC |
| 12 | C | 160 | CLA | ND |
| 12 | C | 160 | CLA | NA |
| 12 | L | 159 | CLA | NC |
| 12 | L | 159 | CLA | ND |
| 12 | L | 159 | CLA | NA |
| 12 | L | 161 | CLA | NC |
| 12 | L | 161 | CLA | ND |
| 12 | L | 161 | CLA | NA |
| 12 | L | 167 | CLA | NC |
| 12 | L | 167 | CLA | ND |
| 12 | L | 167 | CLA | NA |
| 12 | A | 176 | CLA | NC |
| 12 | A | 176 | CLA | ND |
| 12 | A | 176 | CLA | NA |
| 12 | K | 179 | CLA | NC |
| 12 | K | 179 | CLA | ND |
| 12 | K | 179 | CLA | NA |
| 12 | D | 163 | CLA | NC |
| 12 | D | 163 | CLA | ND |
| 12 | D | 163 | CLA | NA |
| 12 | M | 163 | CLA | NC |
| 12 | M | 163 | CLA | ND |
| 12 | M | 163 | CLA | NA |
| 12 | C | 162 | CLA | NC |
| 12 | C | 162 | CLA | ND |
| 12 | C | 162 | CLA | NA |
| 12 | K | 177 | CLA | NC |
| 12 | K | 177 | CLA | ND |
| 12 | K | 177 | CLA | NA |
| 12 | D | 165 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12 | D | 165 | CLA | ND |
| 12 | D | 165 | CLA | NA |
| 12 | J | 175 | CLA | NC |
| 12 | J | 175 | CLA | ND |
| 12 | J | 175 | CLA | NA |
| 12 | C | 165 | CLA | NC |
| 12 | C | 165 | CLA | ND |
| 12 | C | 165 | CLA | NA |
| 12 | C | 161 | CLA | NC |
| 12 | C | 161 | CLA | ND |
| 12 | C | 161 | CLA | NA |
| 12 | C | 159 | CLA | NC |
| 12 | C | 159 | CLA | ND |
| 12 | C | 159 | CLA | NA |
| 12 | D | 157 | CLA | NC |
| 12 | D | 157 | CLA | ND |
| 12 | D | 157 | CLA | NA |
| 12 | A | 179 | CLA | NC |
| 12 | A | 179 | CLA | ND |
| 12 | A | 179 | CLA | NA |
| 12 | L | 162 | CLA | NC |
| 12 | L | 162 | CLA | ND |
| 12 | L | 162 | CLA | NA |
| 12 | M | 159 | CLA | NC |
| 12 | M | 159 | CLA | ND |
| 12 | M | 159 | CLA | NA |
| 12 | M | 164 | CLA | NC |
| 12 | M | 164 | CLA | ND |
| 12 | M | 164 | CLA | NA |
| 12 | L | 163 | CLA | NC |
| 12 | L | 163 | CLA | ND |
| 12 | L | 163 | CLA | NA |
| 12 | L | 158 | CLA | NC |
| 12 | L | 158 | CLA | ND |
| 12 | L | 158 | CLA | NA |
| 12 | M | 167 | CLA | NC |
| 12 | M | 167 | CLA | ND |
| 12 | M | 167 | CLA | NA |
| 12 | C | 167 | CLA | NC |
| 12 | C | 167 | CLA | ND |
| 12 | C | 167 | CLA | NA |
| 12 | D | 167 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12 | D | 167 | CLA | ND |
| 12 | D | 167 | CLA | NA |

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | C | 166 | CLA | 2 | 0 |
| 12 | D | 159 | CLA | 6 | 0 |
| 12 | D | 162 | CLA | 6 | 0 |
| 12 | L | 166 | CLA | 2 | 0 |
| 12 | M | 159 | CLA | 6 | 0 |
| 12 | M | 162 | CLA | 6 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.