# Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 07:38 PM EDT

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|---|---|---|
| PDB ID | : | 1NFV |
| Title | : | X-ray structure of Desulfovibrio desulfuricans bacterioferritin: the diiron centre in different catalytic states (as-isolated structure) |
| Authors | : | Macedo, S.; Romao, C.V.; Mitchell, E.; Matias, P.M.; Liu, M.Y.; Xavier, A.V.; LeGall, J.; Teixeira, M.; Lindley, P.; Carrondo, M.A. |
| Deposited on | : | 2002-12-16 |
| Resolution | : | 1.95 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

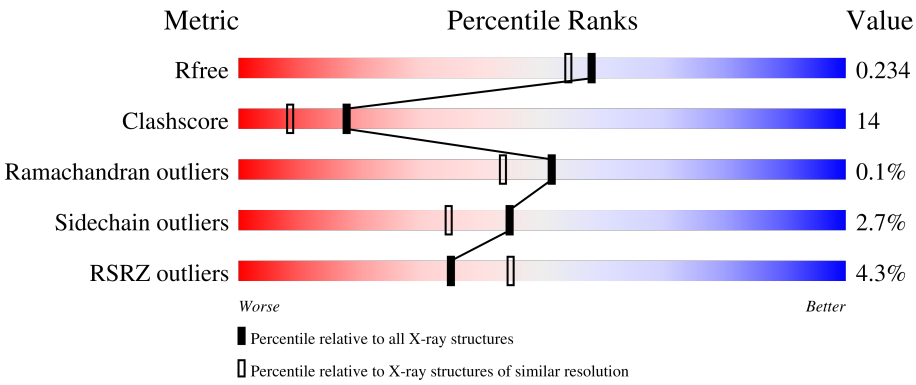
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.1 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2580 (1.96-1.96) |
| Clashscore | 141614 | 2705 (1.96-1.96) |
| Ramachandran outliers | 138981 | 2678 (1.96-1.96) |
| Sidechain outliers | 138945 | 2678 (1.96-1.96) |
| RSRZ outliers | 127900 | 2539 (1.96-1.96) |

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 179 | 6% 75% 17% • 6% |
| 1 | B | 179 | 5% 78% 15% • 5% |
| 1 | C | 179 | 4% 72% 20% • 5% |
| 1 | D | 179 | 5% 75% 17% • • 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 179 | 5% 78% 17% 5% |
| 1 | F | 179 | 4% 77% 17% 5% |
| 1 | G | 179 | 2% 81% 13% 6% |
| 1 | H | 179 | 7% 78% 16% 5% |
| 1 | I | 179 | 3% 78% 16% 5% |
| 1 | J | 179 | 5% 82% 12% 5% |
| 1 | K | 179 | 2% 83% 11% 5% |
| 1 | L | 179 | 2% 77% 17% 5% |
| 1 | M | 179 | 4% 82% 13% 5% |
| 1 | N | 179 | 3% 79% 15% 5% |
| 1 | O | 179 | 3% 78% 16% 6% |
| 1 | P | 179 | 4% 74% 20% 5% |

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 |
|---|---|---|---|---|---|---|---|
| 3 | SO4 | A | 1004 | - | - | - | X |
| 3 | SO4 | A | 1105 | - | - | X | - |
| 3 | SO4 | F | 1502 | - | - | X | - |
| 3 | SO4 | G | 1603 | - | - | - | X |
| 3 | SO4 | H | 1703 | - | - | - | X |
| 3 | SO4 | I | 1802 | - | - | X | - |
| 3 | SO4 | J | 1906 | - | - | X | - |
| 3 | SO4 | L | 2102 | - | - | X | - |
| 3 | SO4 | M | 2206 | - | - | X | - |
| 3 | SO4 | O | 2409 | - | - | - | X |
| 4 | GOL | A | 1010 | - | X | - | - |
| 4 | GOL | B | 1011 | - | X | - | - |
| 4 | GOL | B | 1110 | - | X | - | - |
| 4 | GOL | C | 1210 | - | X | - | - |
| 4 | GOL | D | 1211 | - | X | X | - |
| 4 | GOL | E | 1410 | - | X | X | - |
| 4 | GOL | E | 1411 | - | X | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 4 | GOL | F | 1510 | - | X | - | - |
| 4 | GOL | F | 1512 | - | X | - | - |
| 4 | GOL | G | 1610 | - | X | - | - |
| 4 | GOL | G | 1611 | - | X | - | - |
| 4 | GOL | H | 1710 | - | X | - | - |
| 4 | GOL | H | 1814 | - | X | - | - |
| 4 | GOL | I | 1713 | - | X | - | - |
| 4 | GOL | I | 1810 | - | X | X | - |
| 4 | GOL | J | 1811 | - | X | - | - |
| 4 | GOL | J | 1910 | - | X | X | - |
| 4 | GOL | K | 2011 | - | X | - | - |
| 4 | GOL | M | 2210 | - | X | X | - |
| 4 | GOL | M | 2211 | - | X | - | - |
| 4 | GOL | N | 2310 | - | X | - | - |
| 4 | GOL | O | 2410 | - | X | - | - |
| 4 | GOL | O | 2411 | - | X | - | - |
| 4 | GOL | P | 2510 | - | X | - | - |
| 6 | 3PY | D | 1310 | - | X | - | - |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25080 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.

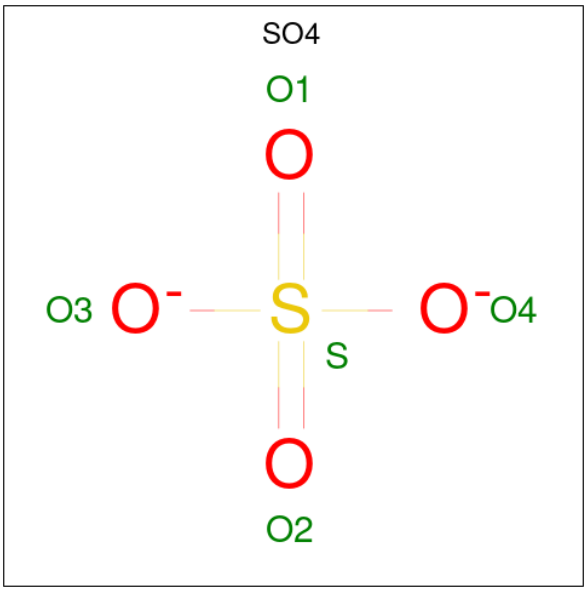
- Molecule 1 is a protein called bacterioferritin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 169 | 1365 | 848 | 239 | 272 | 6 | 0 | 4 | 0 |
| 1 | B | 170 | 1378 | 856 | 242 | 274 | 6 | 0 | 5 | 0 |
| 1 | C | 170 | 1361 | 845 | 236 | 274 | 6 | 0 | 4 | 0 |
| 1 | D | 170 | 1383 | 858 | 243 | 276 | 6 | 0 | 6 | 0 |
| 1 | E | 170 | 1374 | 852 | 240 | 276 | 6 | 0 | 5 | 0 |
| 1 | F | 170 | 1365 | 848 | 240 | 271 | 6 | 0 | 4 | 0 |
| 1 | G | 169 | 1380 | 856 | 243 | 275 | 6 | 0 | 6 | 0 |
| 1 | H | 170 | 1374 | 853 | 241 | 274 | 6 | 0 | 5 | 0 |
| 1 | I | 170 | 1382 | 858 | 242 | 276 | 6 | 0 | 5 | 0 |
| 1 | J | 170 | 1369 | 851 | 241 | 271 | 6 | 0 | 4 | 0 |
| 1 | K | 170 | 1378 | 855 | 241 | 276 | 6 | 0 | 5 | 0 |
| 1 | L | 170 | 1374 | 853 | 242 | 273 | 6 | 0 | 5 | 0 |
| 1 | M | 170 | 1373 | 853 | 241 | 273 | 6 | 0 | 4 | 0 |
| 1 | N | 170 | 1369 | 850 | 240 | 273 | 6 | 0 | 4 | 0 |
| 1 | O | 169 | 1366 | 847 | 239 | 274 | 6 | 0 | 5 | 0 |
| 1 | P | 170 | 1378 | 855 | 241 | 276 | 6 | 0 | 5 | 0 |

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | | |
| 2 | A | 2 | 2 | 2 | 0 | 0 |
| 2 | B | 2 | 2 | 2 | 0 | 0 |
| 2 | C | 2 | 2 | 2 | 0 | 0 |
| 2 | D | 2 | 2 | 2 | 0 | 0 |
| 2 | E | 2 | 2 | 2 | 0 | 0 |
| 2 | F | 2 | 2 | 2 | 0 | 0 |
| 2 | G | 2 | 2 | 2 | 0 | 0 |
| 2 | H | 2 | 2 | 2 | 0 | 0 |
| 2 | I | 2 | 2 | 2 | 0 | 0 |
| 2 | J | 2 | 2 | 2 | 0 | 0 |
| 2 | K | 2 | 2 | 2 | 0 | 0 |
| 2 | L | 2 | 2 | 2 | 0 | 0 |
| 2 | M | 2 | 2 | 2 | 0 | 0 |
| 2 | N | 2 | 2 | 2 | 0 | 0 |
| 2 | O | 2 | 2 | 2 | 0 | 0 |
| 2 | P | 2 | 2 | 2 | 0 | 0 |

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: $O_4S$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | O | S | | | |
| 3 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | C | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | C | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | C | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | D | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 3 | D | 1 | 5 | 4 | 1 | | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | E | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | E | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | E | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | F | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | F | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | F | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | G | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | G | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | G | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | H | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | H | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | H | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | I | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | I | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | I | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | I | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | J | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | J | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | J | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | K | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | K | 1 | Total O S<br>5 4 1 | 0 | 0 |

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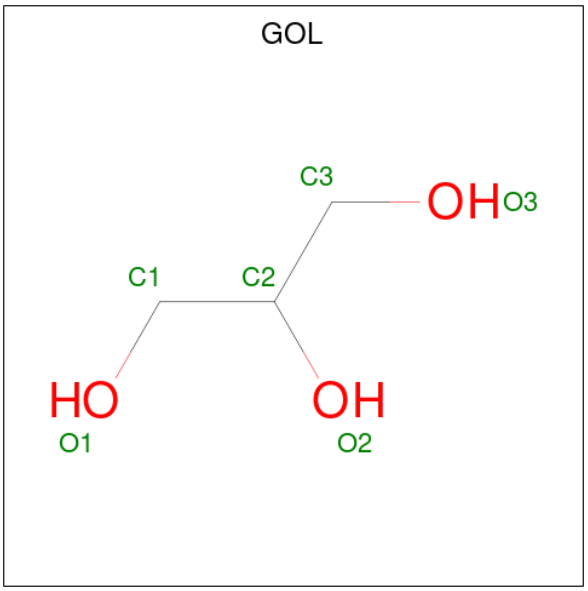
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | O | S | | |
| 3 | K | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | K | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | L | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | L | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | L | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | L | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | M | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | M | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | N | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | N | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | N | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | O | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | O | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | P | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | P | 1 | 5 | 4 | 1 | 0 | 0 |
| | | | Total | O | S | | |
| 3 | P | 1 | 5 | 4 | 1 | 0 | 0 |

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 4 | A | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | B | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | B | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | C | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | D | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | E | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | E | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | F | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | F | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | G | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | G | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | H | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | H | 1 | 6 | 3 | 3 | 0 | 0 |
| 4 | I | 1 | 6 | 3 | 3 | 0 | 0 |

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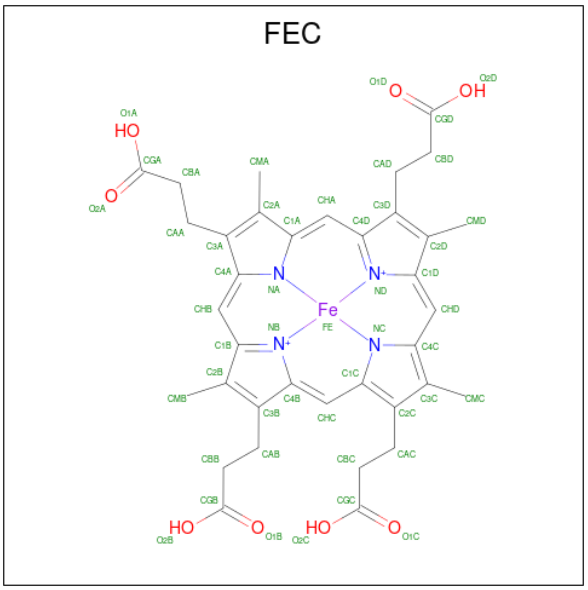
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | | |
| 4 | I | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | J | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | J | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | K | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | M | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | M | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | N | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | O | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | O | 1 | 6 | 3 | 3 | | 0 | 0 |
| | | | Total | C | O | | | |
| 4 | P | 1 | 6 | 3 | 3 | | 0 | 0 |

- Molecule 5 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (three-letter code: FEC) (formula: $C_{36}H_{36}FeN_4O_8$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | | |
| 5 | B | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |

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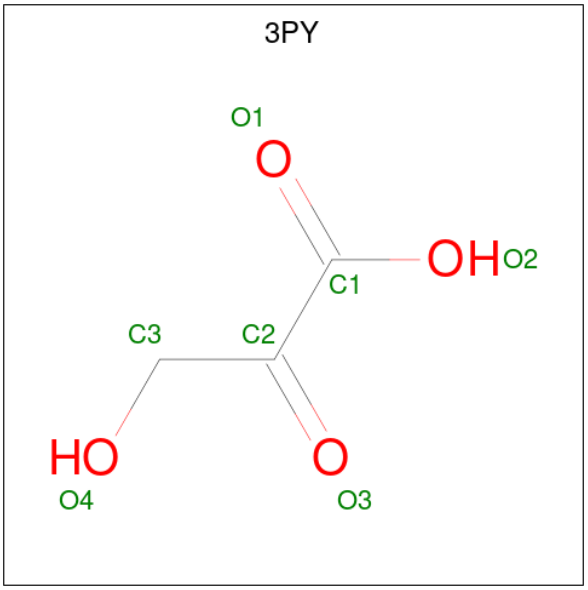
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | | |
| 5 | D | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |
| 5 | F | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |
| 5 | G | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |
| 5 | I | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |
| 5 | L | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |
| 5 | M | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |
| 5 | P | 1 | 98 | 72 | 2 | 8 | 16 | 0 | 1 |

- Molecule 6 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: $C_3H_4O_4$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 6 | D | 1 | 6 | 3 | 3 | 0 | 0 |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 7 | A | 131 | 131 | 131 | 0 | 0 |

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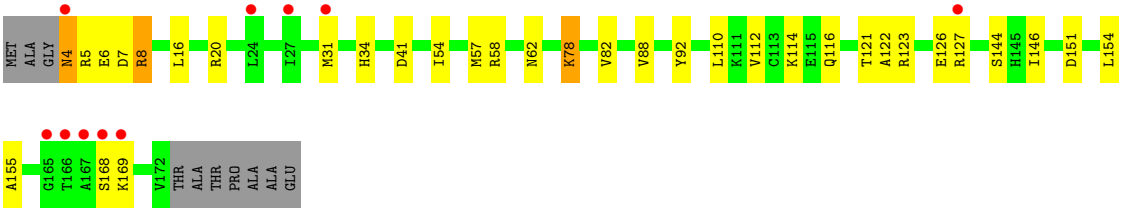
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 7 | B | 142 | 142 | 142 | 0 | 0 |
| | | | Total | O | | |
| 7 | C | 117 | 117 | 117 | 0 | 0 |
| | | | Total | O | | |
| 7 | D | 99 | 99 | 99 | 0 | 0 |
| | | | Total | O | | |
| 7 | E | 101 | 101 | 101 | 0 | 0 |
| | | | Total | O | | |
| 7 | F | 103 | 103 | 103 | 0 | 0 |
| | | | Total | O | | |
| 7 | G | 146 | 146 | 146 | 0 | 0 |
| | | | Total | O | | |
| 7 | H | 91 | 91 | 91 | 0 | 0 |
| | | | Total | O | | |
| 7 | I | 131 | 131 | 131 | 0 | 0 |
| | | | Total | O | | |
| 7 | J | 99 | 99 | 99 | 0 | 0 |
| | | | Total | O | | |
| 7 | K | 130 | 130 | 130 | 0 | 0 |
| | | | Total | O | | |
| 7 | L | 134 | 134 | 134 | 0 | 0 |
| | | | Total | O | | |
| 7 | M | 122 | 122 | 122 | 0 | 0 |
| | | | Total | O | | |
| 7 | N | 124 | 124 | 124 | 0 | 0 |
| | | | Total | O | | |
| 7 | O | 105 | 105 | 105 | 0 | 0 |
| | | | Total | O | | |
| 7 | P | 115 | 115 | 115 | 0 | 0 |

# 3 Residue-property plots (i)

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

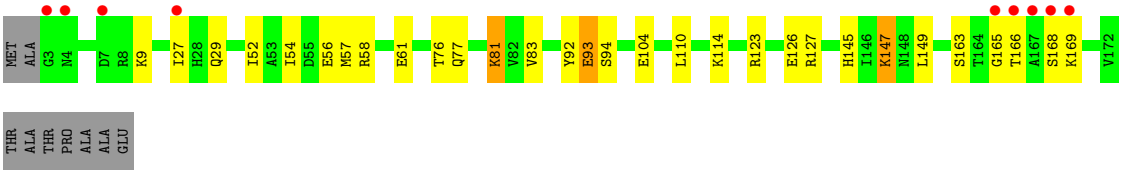
• Molecule 1: bacterioferritin

Chain A:



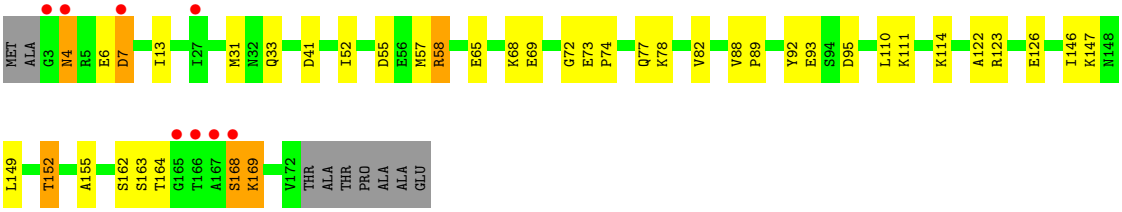

• Molecule 1: bacterioferritin

Chain B:



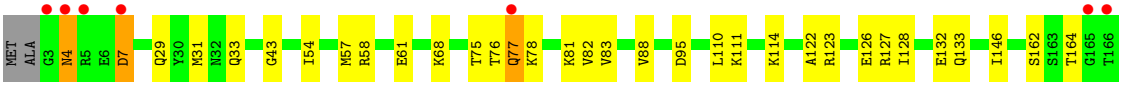

• Molecule 1: bacterioferritin

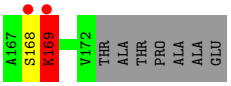
Chain C:




• Molecule 1: bacterioferritin

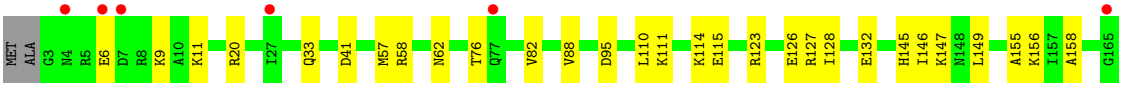
Chain D:

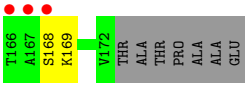





- Molecule 1: bacterioferritin

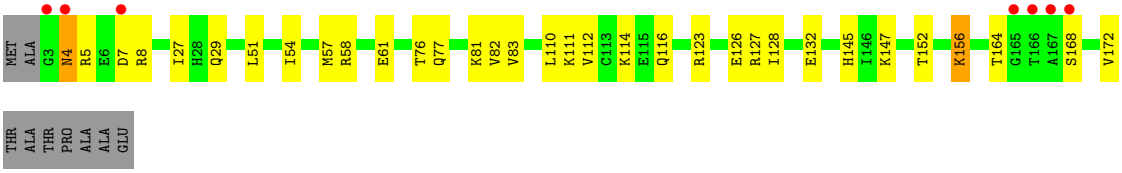
Chain E:



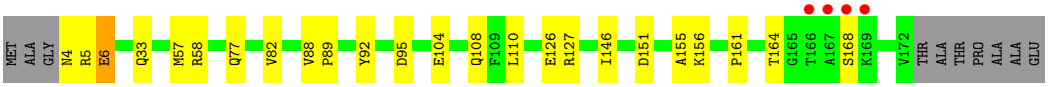

- Molecule 1: bacterioferritin

Chain F:



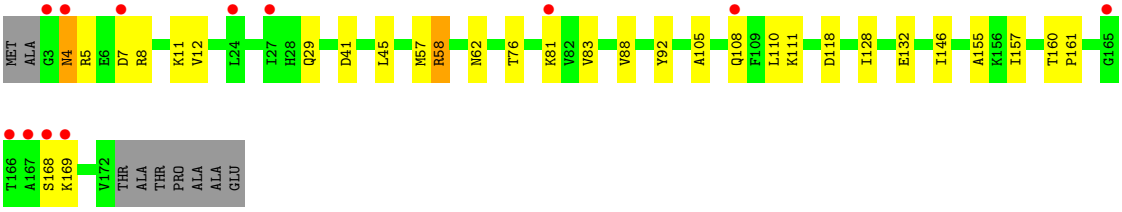

- Molecule 1: bacterioferritin

Chain G:



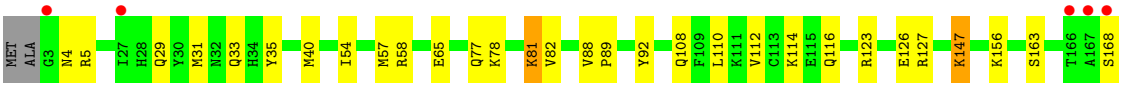

- Molecule 1: bacterioferritin

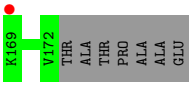
Chain H:




- Molecule 1: bacterioferritin

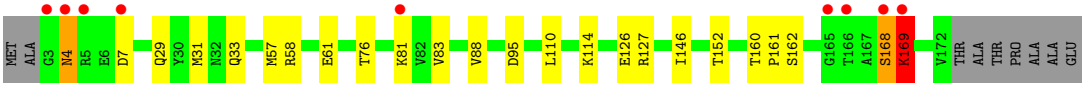
Chain I:





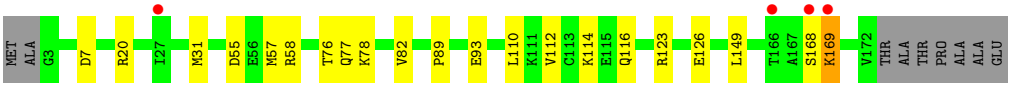

• Molecule 1: bacterioferritin

Chain J:



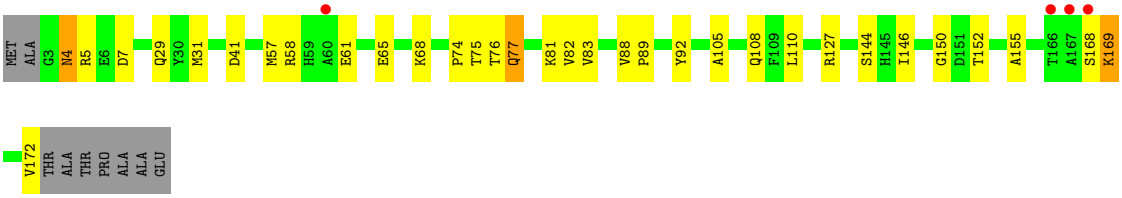

• Molecule 1: bacterioferritin

Chain K:



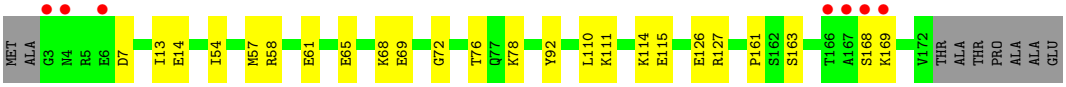

• Molecule 1: bacterioferritin

Chain L:



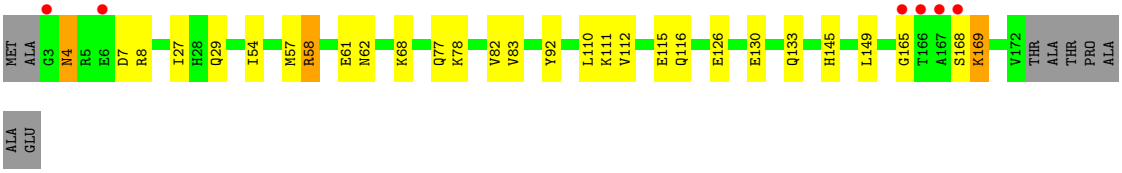

• Molecule 1: bacterioferritin

Chain M:



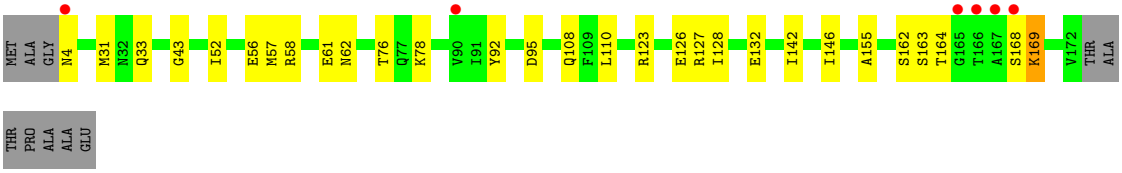

• Molecule 1: bacterioferritin

Chain N:



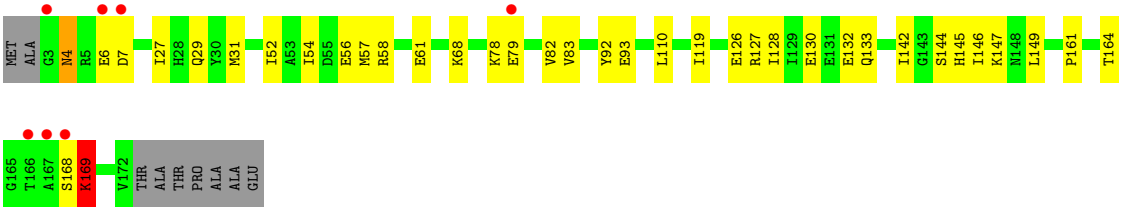

• Molecule 1: bacterioferritin

Chain O:




- Molecule 1: bacterioferritin

Chain P:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 3 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 225.30Å 225.30Å 225.30Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 1.95<br>29.84 – 1.95 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.9 (30.00-1.95)<br>99.2 (29.84-1.95) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.25 (at 1.95Å) | Xtriage |
| Refinement program | SHELXL-97 | Depositor |
| R, $R_{free}$ | 0.214 , 0.254<br>0.185 , 0.234 | Depositor<br>DCC |
| $R_{free}$ test set | 5260 reflections (1.94%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 27.1 | Xtriage |
| Anisotropy | 0.000 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.36 , 60.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.017 for l,-k,h | Xtriage |
| $F_o$,$F_c$ correlation | 0.96 | EDS |
| Total number of atoms | 25080 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 28.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FEC, 3PY, GOL, FE, SO4

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.31 | 0/1385 | 0.93 | 3/1864 (0.2%) |
| 1 | B | 0.31 | 0/1398 | 0.84 | 1/1880 (0.1%) |
| 1 | C | 0.32 | 0/1381 | 0.89 | 3/1861 (0.2%) |
| 1 | D | 0.51 | 2/1407 (0.1%) | 0.86 | 0/1892 |
| 1 | E | 0.31 | 0/1398 | 0.84 | 1/1881 (0.1%) |
| 1 | F | 0.31 | 0/1389 | 0.83 | 0/1868 |
| 1 | G | 0.44 | 2/1405 (0.1%) | 0.91 | 1/1890 (0.1%) |
| 1 | H | 0.32 | 0/1394 | 0.85 | 1/1876 (0.1%) |
| 1 | I | 0.31 | 0/1402 | 0.86 | 1/1885 (0.1%) |
| 1 | J | 0.34 | 0/1389 | 0.86 | 2/1868 (0.1%) |
| 1 | K | 0.32 | 0/1398 | 0.88 | 3/1881 (0.2%) |
| 1 | L | 1.07 | 2/1398 (0.1%) | 0.90 | 3/1880 (0.2%) |
| 1 | M | 0.31 | 0/1393 | 0.84 | 1/1873 (0.1%) |
| 1 | N | 0.30 | 0/1389 | 0.80 | 1/1869 (0.1%) |
| 1 | O | 0.77 | 2/1390 (0.1%) | 0.92 | 3/1872 (0.2%) |
| 1 | P | 0.60 | 2/1402 (0.1%) | 0.85 | 3/1885 (0.2%) |
| All | All | 0.48 | 10/22318 (0.0%) | 0.87 | 27/30025 (0.1%) |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | L | 169[A] | LYS | CB-CG | 27.00 | 2.25 | 1.52 |
| 1 | L | 169[B] | LYS | CB-CG | 27.00 | 2.25 | 1.52 |
| 1 | O | 169[A] | LYS | CB-CG | 18.20 | 2.01 | 1.52 |
| 1 | O | 169[B] | LYS | CB-CG | 18.20 | 2.01 | 1.52 |
| 1 | P | 169[A] | LYS | CB-CG | 13.45 | 1.88 | 1.52 |
| 1 | P | 169[B] | LYS | CB-CG | 13.45 | 1.88 | 1.52 |
| 1 | D | 169[A] | LYS | CB-CG | 10.65 | 1.81 | 1.52 |
| 1 | D | 169[B] | LYS | CB-CG | 10.65 | 1.81 | 1.52 |
| 1 | G | 6[A] | GLU | CD-OE1 | 5.97 | 1.32 | 1.25 |
| 1 | G | 6[B] | GLU | CD-OE1 | 5.97 | 1.32 | 1.25 |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | L | 169[A] | LYS | CA-CB-CG | -9.37 | 92.78 | 113.40 |
| 1 | L | 169[B] | LYS | CA-CB-CG | -9.37 | 92.78 | 113.40 |
| 1 | O | 169[A] | LYS | CA-CB-CG | -7.31 | 97.32 | 113.40 |
| 1 | O | 169[B] | LYS | CA-CB-CG | -7.31 | 97.32 | 113.40 |
| 1 | C | 58[A] | ARG | NE-CZ-NH2 | -6.23 | 117.18 | 120.30 |
| 1 | C | 58[B] | ARG | NE-CZ-NH2 | -6.23 | 117.18 | 120.30 |
| 1 | K | 20 | ARG | NE-CZ-NH2 | -6.19 | 117.21 | 120.30 |
| 1 | E | 123 | ARG | NE-CZ-NH1 | 5.93 | 123.26 | 120.30 |
| 1 | L | 92 | TYR | CA-CB-CG | -5.88 | 102.24 | 113.40 |
| 1 | A | 20 | ARG | NE-CZ-NH1 | 5.79 | 123.20 | 120.30 |
| 1 | O | 92 | TYR | CA-CB-CG | -5.71 | 102.54 | 113.40 |
| 1 | P | 169[A] | LYS | CA-CB-CG | -5.62 | 101.04 | 113.40 |
| 1 | P | 169[B] | LYS | CA-CB-CG | -5.62 | 101.04 | 113.40 |
| 1 | I | 92 | TYR | CA-CB-CG | -5.57 | 102.81 | 113.40 |
| 1 | H | 92 | TYR | CA-CB-CG | -5.56 | 102.83 | 113.40 |
| 1 | M | 92 | TYR | CA-CB-CG | -5.44 | 103.06 | 113.40 |
| 1 | N | 92 | TYR | CA-CB-CG | -5.37 | 103.20 | 113.40 |
| 1 | J | 169[A] | LYS | C-N-CA | 5.33 | 133.48 | 122.30 |
| 1 | J | 169[B] | LYS | C-N-CA | 5.33 | 133.48 | 122.30 |
| 1 | G | 92 | TYR | CA-CB-CG | -5.20 | 103.53 | 113.40 |
| 1 | A | 92 | TYR | CA-CB-CG | -5.19 | 103.54 | 113.40 |
| 1 | C | 92 | TYR | CA-CB-CG | -5.19 | 103.54 | 113.40 |
| 1 | K | 123 | ARG | CD-NE-CZ | 5.17 | 130.85 | 123.60 |
| 1 | K | 123 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | A | 8 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | P | 92 | TYR | CA-CB-CG | -5.03 | 103.84 | 113.40 |
| 1 | B | 92 | TYR | CA-CB-CG | -5.03 | 103.85 | 113.40 |

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 | 1365 | 0 | 1325 | 44 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 1378 | 0 | 1343 | 43 | 0 |
| 1 | C | 1361 | 0 | 1312 | 51 | 0 |
| 1 | D | 1383 | 0 | 1341 | 55 | 0 |
| 1 | E | 1374 | 0 | 1326 | 37 | 0 |
| 1 | F | 1365 | 0 | 1328 | 37 | 0 |
| 1 | G | 1380 | 0 | 1340 | 43 | 0 |
| 1 | H | 1374 | 0 | 1332 | 35 | 0 |
| 1 | I | 1382 | 0 | 1348 | 53 | 0 |
| 1 | J | 1369 | 0 | 1335 | 34 | 0 |
| 1 | K | 1378 | 0 | 1335 | 32 | 0 |
| 1 | L | 1374 | 0 | 1335 | 35 | 0 |
| 1 | M | 1373 | 0 | 1341 | 54 | 0 |
| 1 | N | 1369 | 0 | 1329 | 56 | 0 |
| 1 | O | 1366 | 0 | 1312 | 46 | 0 |
| 1 | P | 1378 | 0 | 1338 | 47 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 2 | 0 | 0 | 0 | 0 |
| 2 | D | 2 | 0 | 0 | 0 | 0 |
| 2 | E | 2 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 2 | G | 2 | 0 | 0 | 0 | 0 |
| 2 | H | 2 | 0 | 0 | 0 | 0 |
| 2 | I | 2 | 0 | 0 | 0 | 0 |
| 2 | J | 2 | 0 | 0 | 0 | 0 |
| 2 | K | 2 | 0 | 0 | 0 | 0 |
| 2 | L | 2 | 0 | 0 | 0 | 0 |
| 2 | M | 2 | 0 | 0 | 0 | 0 |
| 2 | N | 2 | 0 | 0 | 0 | 0 |
| 2 | O | 2 | 0 | 0 | 0 | 0 |
| 2 | P | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 25 | 0 | 0 | 3 | 0 |
| 3 | B | 20 | 0 | 0 | 3 | 0 |
| 3 | C | 15 | 0 | 0 | 2 | 0 |
| 3 | D | 10 | 0 | 0 | 0 | 0 |
| 3 | E | 15 | 0 | 0 | 1 | 0 |
| 3 | F | 15 | 0 | 0 | 3 | 0 |
| 3 | G | 15 | 0 | 0 | 1 | 0 |
| 3 | H | 15 | 0 | 0 | 0 | 0 |
| 3 | I | 20 | 0 | 0 | 2 | 7 |
| 3 | J | 15 | 0 | 0 | 4 | 0 |
| 3 | K | 20 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | L | 20 | 0 | 0 | 3 | 7 |
| 3 | M | 10 | 0 | 0 | 2 | 0 |
| 3 | N | 15 | 0 | 0 | 0 | 0 |
| 3 | O | 10 | 0 | 0 | 2 | 0 |
| 3 | P | 15 | 0 | 0 | 2 | 0 |
| 4 | A | 6 | 0 | 4 | 1 | 0 |
| 4 | B | 12 | 0 | 8 | 3 | 0 |
| 4 | C | 6 | 0 | 5 | 0 | 0 |
| 4 | D | 6 | 0 | 4 | 5 | 0 |
| 4 | E | 12 | 0 | 8 | 6 | 0 |
| 4 | F | 12 | 0 | 8 | 3 | 0 |
| 4 | G | 12 | 0 | 9 | 3 | 0 |
| 4 | H | 12 | 0 | 8 | 1 | 0 |
| 4 | I | 12 | 0 | 8 | 16 | 0 |
| 4 | J | 12 | 0 | 8 | 5 | 0 |
| 4 | K | 6 | 0 | 4 | 1 | 0 |
| 4 | M | 12 | 0 | 8 | 8 | 0 |
| 4 | N | 6 | 0 | 4 | 1 | 0 |
| 4 | O | 12 | 0 | 8 | 4 | 0 |
| 4 | P | 6 | 0 | 4 | 2 | 0 |
| 5 | B | 98 | 0 | 64 | 17 | 0 |
| 5 | D | 98 | 0 | 64 | 22 | 0 |
| 5 | F | 98 | 0 | 64 | 17 | 0 |
| 5 | G | 98 | 0 | 64 | 15 | 0 |
| 5 | I | 98 | 0 | 64 | 18 | 0 |
| 5 | L | 98 | 0 | 64 | 23 | 0 |
| 5 | M | 98 | 0 | 64 | 18 | 0 |
| 5 | P | 98 | 0 | 64 | 21 | 0 |
| 6 | D | 6 | 0 | 1 | 1 | 0 |
| 7 | A | 131 | 0 | 0 | 6 | 0 |
| 7 | B | 142 | 0 | 0 | 5 | 0 |
| 7 | C | 117 | 0 | 0 | 0 | 0 |
| 7 | D | 99 | 0 | 0 | 9 | 0 |
| 7 | E | 101 | 0 | 0 | 2 | 0 |
| 7 | F | 103 | 0 | 0 | 2 | 0 |
| 7 | G | 146 | 0 | 0 | 5 | 0 |
| 7 | H | 91 | 0 | 0 | 0 | 0 |
| 7 | I | 131 | 0 | 0 | 5 | 0 |
| 7 | J | 99 | 0 | 0 | 5 | 0 |
| 7 | K | 130 | 0 | 0 | 4 | 0 |
| 7 | L | 134 | 0 | 0 | 5 | 0 |
| 7 | M | 122 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 7 | N | 124 | 0 | 0 | 1 | 0 |
| 7 | O | 105 | 0 | 0 | 5 | 0 |
| 7 | P | 115 | 0 | 0 | 5 | 0 |
| All | All | 25080 | 0 | 21931 | 603 | 7 |

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 14.

All (603) 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:M:168[A]:SER:CB | 1:N:58[A]:ARG:HH22 | 1.00 | 1.53 |
| 1:G:168[A]:SER:CB | 1:H:58[A]:ARG:HH22 | 1.23 | 1.49 |
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:H | 1.15 | 1.44 |
| 1:M:168[A]:SER:HB2 | 1:N:58[A]:ARG:NH2 | 1.32 | 1.44 |
| 1:G:168[A]:SER:HB2 | 1:H:58[A]:ARG:NH2 | 1.12 | 1.41 |
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:N | 1.66 | 1.40 |
| 1:M:168[A]:SER:CB | 1:N:58[A]:ARG:NH2 | 1.81 | 1.35 |
| 1:I:127[A]:ARG:HD3 | 4:I:1810:GOL:O1 | 1.15 | 1.29 |
| 1:L:168[A]:SER:HA | 5:L:2108[A]:FEC:O2C | 1.21 | 1.28 |
| 1:G:168[A]:SER:CB | 1:H:58[A]:ARG:NH2 | 1.88 | 1.20 |
| 1:K:168[B]:SER:HA | 5:L:2108[B]:FEC:O2C | 1.42 | 1.16 |
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:CA | 2.10 | 1.15 |
| 1:G:6[A]:GLU:OE1 | 7:G:1620:HOH:O | 1.61 | 1.14 |
| 1:I:127[B]:ARG:HG2 | 4:I:1810:GOL:O1 | 1.47 | 1.11 |
| 1:K:168[A]:SER:O | 1:L:58[A]:ARG:NH2 | 1.86 | 1.09 |
| 1:O:168[A]:SER:O | 1:P:58[A]:ARG:NH2 | 1.84 | 1.09 |
| 1:E:168[B]:SER:O | 1:F:58[B]:ARG:NH2 | 1.87 | 1.07 |
| 5:M:2207[B]:FEC:HBC1 | 1:N:168[B]:SER:OG | 0.88 | 1.06 |
| 1:C:168[A]:SER:O | 1:D:58[A]:ARG:NH2 | 1.91 | 1.03 |
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:CB | 2.23 | 1.00 |
| 1:I:127[A]:ARG:CD | 4:I:1810:GOL:HO1 | 1.71 | 0.99 |
| 1:A:78:LYS:HE2 | 3:A:1105:SO4:O3 | 1.63 | 0.98 |
| 1:I:127[B]:ARG:CD | 4:I:1810:GOL:O1 | 2.11 | 0.98 |
| 1:O:168[B]:SER:HA | 5:P:2507[B]:FEC:O2C | 0.80 | 0.97 |
| 1:G:168[A]:SER:CA | 1:H:58[A]:ARG:NH2 | 2.30 | 0.95 |
| 1:N:110:LEU:HD11 | 1:N:126:GLU:HG3 | 1.49 | 0.95 |
| 1:M:168[A]:SER:CA | 1:N:58[A]:ARG:HH22 | 1.78 | 0.94 |
| 1:E:168[B]:SER:C | 1:F:58[B]:ARG:NH2 | 2.21 | 0.94 |
| 1:C:58[B]:ARG:NH2 | 1:D:168[B]:SER:CB | 2.30 | 0.94 |
| 1:I:127[A]:ARG:HB3 | 4:I:1810:GOL:O1 | 1.67 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:168[B]:SER:CB | 5:L:2108[B]:FEC:O2C | 2.17 | 0.93 |
| 1:L:168[A]:SER:HB3 | 5:L:2108[A]:FEC:O2C | 1.69 | 0.90 |
| 1:H:29:GLN:HE22 | 1:H:83:VAL:H | 1.20 | 0.90 |
| 1:L:168[A]:SER:HA | 5:L:2108[A]:FEC:CGC | 2.03 | 0.89 |
| 1:C:58[B]:ARG:NH2 | 1:D:168[B]:SER:HB2 | 1.88 | 0.89 |
| 1:C:58[B]:ARG:NH2 | 1:D:168[B]:SER:CA | 2.35 | 0.89 |
| 1:G:168[A]:SER:CA | 1:H:58[A]:ARG:HH21 | 1.86 | 0.88 |
| 1:O:168[A]:SER:HB2 | 1:P:58[A]:ARG:HH12 | 1.38 | 0.88 |
| 1:J:110:LEU:HD11 | 1:J:126:GLU:HG3 | 1.56 | 0.87 |
| 1:M:168[A]:SER:CA | 1:N:58[A]:ARG:NH2 | 2.37 | 0.87 |
| 5:G:1608[B]:FEC:HBC2 | 5:G:1608[B]:FEC:HHC | 1.58 | 0.86 |
| 1:I:127[A]:ARG:CB | 4:I:1810:GOL:O1 | 2.24 | 0.86 |
| 1:C:147:LYS:NZ | 3:C:1203:SO4:O4 | 2.08 | 0.86 |
| 1:D:29:GLN:HE22 | 1:D:83:VAL:H | 1.20 | 0.86 |
| 5:D:1311[A]:FEC:HBC2 | 5:D:1311[A]:FEC:HHC | 1.56 | 0.85 |
| 1:M:168[A]:SER:HB3 | 1:N:58[A]:ARG:NH2 | 1.91 | 0.85 |
| 5:B:1107[A]:FEC:HBC2 | 5:B:1107[A]:FEC:HHC | 1.58 | 0.84 |
| 1:J:161:PRO:HA | 3:J:1906:SO4:O1 | 1.77 | 0.84 |
| 1:K:169[B]:LYS:HB3 | 7:K:9227:HOH:O | 1.79 | 0.82 |
| 3:F:1501:SO4:O2 | 7:F:660:HOH:O | 1.97 | 0.82 |
| 1:D:110:LEU:HD11 | 1:D:126:GLU:HG2 | 1.63 | 0.81 |
| 1:G:168[A]:SER:N | 1:H:58[A]:ARG:HH21 | 1.78 | 0.81 |
| 1:C:149:LEU:O | 1:C:152[B]:THR:HG22 | 1.81 | 0.80 |
| 1:I:163:SER:HB3 | 7:I:9021:HOH:O | 1.81 | 0.80 |
| 1:G:156:LYS:HD2 | 7:M:898:HOH:O | 1.80 | 0.80 |
| 1:O:123:ARG:NH2 | 3:O:2409:SO4:O1 | 2.15 | 0.80 |
| 5:M:2207[B]:FEC:HBC1 | 1:N:168[B]:SER:CB | 2.09 | 0.80 |
| 1:B:149:LEU:HD13 | 1:H:155:ALA:HA | 1.64 | 0.80 |
| 1:J:168[B]:SER:HA | 7:J:9964:HOH:O | 1.81 | 0.79 |
| 1:M:168[A]:SER:HB2 | 1:N:58[A]:ARG:CZ | 2.13 | 0.79 |
| 5:L:2108[A]:FEC:HHC | 5:L:2108[A]:FEC:HBC2 | 1.63 | 0.79 |
| 1:M:168[A]:SER:HB2 | 1:N:58[A]:ARG:HH22 | 0.63 | 0.79 |
| 1:I:81:LYS:HE3 | 1:I:82:VAL:H | 1.47 | 0.79 |
| 1:D:168[B]:SER:OG | 5:D:1311[B]:FEC:CGC | 2.30 | 0.79 |
| 1:C:58[B]:ARG:HH21 | 1:D:168[B]:SER:C | 1.86 | 0.78 |
| 1:G:164:THR:HA | 7:G:1691:HOH:O | 1.82 | 0.78 |
| 1:D:168[B]:SER:OG | 5:D:1311[B]:FEC:CBC | 2.33 | 0.77 |
| 1:G:168[A]:SER:HB3 | 5:G:1608[A]:FEC:HBC1 | 1.67 | 0.77 |
| 1:F:29:GLN:HE22 | 1:F:83:VAL:H | 1.29 | 0.77 |
| 1:H:105:ALA:HA | 1:H:108:GLN:OE1 | 1.84 | 0.76 |
| 1:P:29:GLN:HE22 | 1:P:83:VAL:H | 1.34 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:4:ASN:ND2 | 1:D:7:ASP:HB2 | 2.01 | 0.76 |
| 1:I:110:LEU:HD23 | 1:I:114:LYS:HD2 | 1.66 | 0.76 |
| 3:F:1502:SO4:O2 | 7:F:680:HOH:O | 2.03 | 0.75 |
| 1:I:127[A]:ARG:HD3 | 4:I:1810:GOL:HO1 | 0.94 | 0.75 |
| 1:J:169[A]:LYS:HB3 | 7:J:9004:HOH:O | 1.87 | 0.75 |
| 1:L:168[B]:SER:OG | 5:L:2108[B]:FEC:HAC2 | 1.86 | 0.74 |
| 1:O:168[A]:SER:OG | 5:P:2507[A]:FEC:HAC2 | 1.87 | 0.74 |
| 1:E:127[B]:ARG:HB3 | 4:E:1410:GOL:O3 | 1.88 | 0.74 |
| 1:B:29:GLN:HE22 | 1:B:83:VAL:H | 1.35 | 0.74 |
| 1:F:4:ASN:ND2 | 1:F:7:ASP:H | 1.86 | 0.74 |
| 1:J:4:ASN:ND2 | 1:J:7:ASP:H | 1.86 | 0.74 |
| 1:M:111:LYS:O | 1:M:115:GLU:HG3 | 1.88 | 0.74 |
| 1:N:29:GLN:HE22 | 1:N:83:VAL:H | 1.33 | 0.73 |
| 1:J:127[B]:ARG:HB3 | 4:J:1910:GOL:O3 | 1.88 | 0.73 |
| 1:C:58[B]:ARG:NH2 | 1:D:168[B]:SER:C | 2.42 | 0.73 |
| 1:A:168[A]:SER:CB | 1:B:58[A]:ARG:HH22 | 1.93 | 0.73 |
| 1:B:81:LYS:HE2 | 3:B:1005:SO4:O1 | 1.88 | 0.73 |
| 1:G:168[A]:SER:OG | 5:G:1608[A]:FEC:HAC2 | 1.88 | 0.73 |
| 5:M:2207[A]:FEC:HBB2 | 1:N:168[A]:SER:HB3 | 1.70 | 0.73 |
| 1:L:75:THR:OG1 | 1:L:77[B]:GLN:HG3 | 1.89 | 0.73 |
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:HB3 | 2.01 | 0.73 |
| 1:I:127[B]:ARG:CB | 4:I:1810:GOL:O1 | 2.25 | 0.72 |
| 1:J:29:GLN:HE22 | 1:J:83:VAL:H | 1.35 | 0.72 |
| 1:K:114:LYS:HE2 | 3:K:1504:SO4:O1 | 1.90 | 0.72 |
| 1:B:168[B]:SER:OG | 5:B:1107[B]:FEC:HAC2 | 1.90 | 0.71 |
| 1:E:127[A]:ARG:HB3 | 4:E:1410:GOL:O3 | 1.90 | 0.71 |
| 1:A:58[B]:ARG:NH2 | 1:B:168[B]:SER:HB3 | 2.05 | 0.71 |
| 1:P:4:ASN:ND2 | 1:P:7:ASP:H | 1.88 | 0.71 |
| 1:C:58[B]:ARG:NH2 | 1:D:168[B]:SER:N | 2.38 | 0.71 |
| 1:C:147:LYS:HD2 | 1:G:5[A]:ARG:NH1 | 2.05 | 0.71 |
| 1:M:127[B]:ARG:NH2 | 4:M:2210:GOL:O1 | 2.23 | 0.71 |
| 1:B:93[B]:GLU:OE2 | 1:B:147:LYS:NZ | 2.23 | 0.71 |
| 1:I:127[B]:ARG:HD2 | 4:I:1810:GOL:O1 | 1.91 | 0.71 |
| 1:C:78:LYS:NZ | 4:D:1211:GOL:H12 | 2.06 | 0.71 |
| 1:J:127[A]:ARG:HB3 | 4:J:1910:GOL:O3 | 1.90 | 0.71 |
| 1:D:168[B]:SER:CB | 5:D:1311[B]:FEC:HBC1 | 2.21 | 0.70 |
| 5:I:1807[A]:FEC:HHC | 5:I:1807[A]:FEC:HBC2 | 1.72 | 0.70 |
| 1:D:123:ARG:O | 1:D:127[B]:ARG:HG2 | 1.91 | 0.70 |
| 1:G:168[A]:SER:HB2 | 1:H:58[A]:ARG:CZ | 2.15 | 0.69 |
| 1:O:162:SER:N | 3:O:2406:SO4:O3 | 2.25 | 0.69 |
| 1:B:127[A]:ARG:HD2 | 4:B:1110:GOL:O1 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:168[A]:SER:H | 1:N:58[A]:ARG:NH1 | 1.91 | 0.69 |
| 1:M:169[B]:LYS:NZ | 1:N:165:GLY:HA3 | 2.06 | 0.69 |
| 1:L:29:GLN:HE22 | 1:L:83:VAL:H | 1.40 | 0.69 |
| 1:D:169[B]:LYS:CE | 7:D:9732:HOH:O | 2.41 | 0.69 |
| 4:M:2211:GOL:H12 | 1:N:78:LYS:NZ | 2.08 | 0.68 |
| 1:E:110:LEU:HD11 | 1:E:126:GLU:HG3 | 1.76 | 0.68 |
| 1:G:168[A]:SER:N | 1:H:58[A]:ARG:NH2 | 2.38 | 0.68 |
| 5:L:2108[B]:FEC:HBC2 | 5:L:2108[B]:FEC:HHC | 1.75 | 0.68 |
| 1:M:127[A]:ARG:HD2 | 4:M:2210:GOL:O1 | 1.93 | 0.68 |
| 5:M:2207[B]:FEC:HAC2 | 1:N:168[B]:SER:HB2 | 1.76 | 0.68 |
| 1:K:168[A]:SER:HB3 | 5:L:2108[A]:FEC:HBC1 | 1.76 | 0.68 |
| 1:L:168[B]:SER:HB3 | 5:L:2108[B]:FEC:HBC1 | 1.74 | 0.68 |
| 1:O:164:THR:HA | 7:O:2485:HOH:O | 1.94 | 0.68 |
| 1:D:122:ALA:O | 1:D:126:GLU:HG3 | 1.95 | 0.67 |
| 1:C:58[B]:ARG:NH2 | 1:D:168[B]:SER:O | 2.28 | 0.66 |
| 1:E:110:LEU:HD23 | 1:E:114:LYS:HD2 | 1.78 | 0.66 |
| 1:D:4:ASN:HD22 | 1:D:7:ASP:HB2 | 1.60 | 0.66 |
| 1:O:31:MET:HG3 | 5:P:2507[A]:FEC:HBD1 | 1.76 | 0.66 |
| 1:F:127[A]:ARG:HD3 | 4:F:1510:GOL:O1 | 1.96 | 0.66 |
| 1:I:123:ARG:HB3 | 1:I:127[B]:ARG:NH2 | 2.11 | 0.66 |
| 1:M:168[A]:SER:OG | 5:M:2207[A]:FEC:HAC2 | 1.96 | 0.66 |
| 1:D:75:THR:OG1 | 1:D:77[A]:GLN:HG2 | 1.97 | 0.65 |
| 5:D:1311[B]:FEC:HBC2 | 5:D:1311[B]:FEC:HHC | 1.78 | 0.65 |
| 5:G:1608[A]:FEC:HBC2 | 5:G:1608[A]:FEC:HHC | 1.78 | 0.65 |
| 1:P:168[B]:SER:OG | 5:P:2507[B]:FEC:HAC2 | 1.97 | 0.65 |
| 1:C:162:SER:N | 3:C:1206:SO4:O3 | 2.31 | 0.64 |
| 1:G:156:LYS:HE3 | 7:G:1708:HOH:O | 1.98 | 0.64 |
| 1:A:168[A]:SER:OG | 5:B:1107[A]:FEC:HAC2 | 1.98 | 0.63 |
| 1:I:168[A]:SER:OG | 5:I:1807[A]:FEC:HAC2 | 1.97 | 0.63 |
| 1:C:168[A]:SER:C | 1:D:58[A]:ARG:HH22 | 2.01 | 0.63 |
| 1:I:127[B]:ARG:HB3 | 4:I:1810:GOL:O1 | 1.97 | 0.63 |
| 1:K:168[A]:SER:OG | 5:L:2108[A]:FEC:HAC2 | 1.99 | 0.63 |
| 1:D:168[B]:SER:OG | 5:D:1311[B]:FEC:HBC1 | 1.99 | 0.62 |
| 5:B:1107[B]:FEC:HBC1 | 5:B:1107[B]:FEC:HHC | 1.82 | 0.62 |
| 1:E:155:ALA:HA | 1:P:149:LEU:HD13 | 1.81 | 0.62 |
| 1:K:31:MET:HG3 | 5:L:2108[A]:FEC:HBD1 | 1.81 | 0.62 |
| 1:O:168[B]:SER:CB | 5:P:2507[B]:FEC:O2C | 2.46 | 0.62 |
| 1:C:164:THR:O | 1:D:169[B]:LYS:HD2 | 1.99 | 0.62 |
| 1:J:4:ASN:HD22 | 1:J:7:ASP:H | 1.45 | 0.62 |
| 1:P:31:MET:HG3 | 5:P:2507[B]:FEC:HBD1 | 1.82 | 0.62 |
| 1:P:110:LEU:HD11 | 1:P:126:GLU:HG2 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:73:GLU:OE1 | 1:C:74:PRO:HD2 | 1.98 | 0.62 |
| 1:M:58[B]:ARG:HH12 | 1:N:168[B]:SER:HB3 | 1.64 | 0.62 |
| 1:L:5:ARG:HG2 | 3:L:2102:SO4:O1 | 1.99 | 0.62 |
| 1:L:168[A]:SER:OG | 5:L:2108[A]:FEC:O2B | 2.18 | 0.62 |
| 4:M:2211:GOL:H12 | 1:N:78:LYS:HZ3 | 1.65 | 0.62 |
| 1:A:62:ASN:OD1 | 4:A:1010:GOL:H12 | 2.00 | 0.61 |
| 1:B:145:HIS:HE1 | 1:H:41:ASP:OD2 | 1.82 | 0.61 |
| 1:O:110:LEU:HD11 | 1:O:126:GLU:HG3 | 1.81 | 0.61 |
| 1:E:168[B]:SER:HB3 | 5:F:1507[B]:FEC:HBB2 | 1.81 | 0.61 |
| 1:J:110:LEU:CD2 | 1:J:114:LYS:HE2 | 2.31 | 0.61 |
| 1:E:169[A]:LYS:O | 1:E:169[A]:LYS:HG3 | 2.00 | 0.61 |
| 1:M:168[A]:SER:C | 1:N:58[A]:ARG:NH2 | 2.54 | 0.61 |
| 1:K:169[B]:LYS:HD2 | 1:K:169[B]:LYS:N | 2.16 | 0.61 |
| 4:K:2011:GOL:O1 | 1:L:77[A]:GLN:HB3 | 2.00 | 0.61 |
| 1:O:168[A]:SER:CB | 1:P:58[A]:ARG:HH12 | 2.13 | 0.61 |
| 1:C:169[B]:LYS:HD3 | 1:C:169[B]:LYS:H | 1.66 | 0.60 |
| 1:B:110:LEU:HD21 | 1:B:114:LYS:HE3 | 1.83 | 0.60 |
| 1:D:169[B]:LYS:HE3 | 7:D:9732:HOH:O | 2.00 | 0.59 |
| 1:I:110:LEU:CD2 | 1:I:114:LYS:HD2 | 2.32 | 0.59 |
| 1:E:127[B]:ARG:HD2 | 4:E:1410:GOL:O3 | 2.01 | 0.59 |
| 1:O:168[A]:SER:HB2 | 1:P:58[A]:ARG:NH1 | 2.15 | 0.59 |
| 1:P:168[B]:SER:CB | 5:P:2507[B]:FEC:HAC2 | 2.32 | 0.59 |
| 3:P:2501:SO4:O3 | 7:P:9918:HOH:O | 2.17 | 0.59 |
| 1:G:58[B]:ARG:NH1 | 1:H:168[B]:SER:H | 2.01 | 0.59 |
| 1:M:169[B]:LYS:HZ1 | 1:N:165:GLY:HA3 | 1.68 | 0.59 |
| 1:P:169[B]:LYS:O | 1:P:169[B]:LYS:HG3 | 2.03 | 0.59 |
| 1:I:108:GLN:HG2 | 7:I:9786:HOH:O | 2.01 | 0.59 |
| 1:E:82:VAL:HG11 | 1:F:76:THR:HG21 | 1.85 | 0.58 |
| 1:K:58[B]:ARG:HG3 | 1:K:58[B]:ARG:HH11 | 1.67 | 0.58 |
| 1:M:168[A]:SER:HB3 | 5:M:2207[A]:FEC:HBC1 | 1.85 | 0.58 |
| 1:D:169[B]:LYS:NZ | 7:D:9732:HOH:O | 2.36 | 0.58 |
| 1:O:62:ASN:OD1 | 4:O:2410:GOL:H12 | 2.03 | 0.58 |
| 5:I:1807[A]:FEC:HBB2 | 1:J:168[A]:SER:OG | 2.03 | 0.58 |
| 1:D:168[B]:SER:HB3 | 5:D:1311[B]:FEC:HBC1 | 1.84 | 0.57 |
| 1:J:127[B]:ARG:HD2 | 4:J:1910:GOL:O3 | 2.04 | 0.57 |
| 1:A:58[B]:ARG:NH2 | 1:B:168[B]:SER:CB | 2.67 | 0.57 |
| 1:C:168[A]:SER:OG | 5:D:1311[A]:FEC:HAC2 | 2.05 | 0.57 |
| 1:F:168[B]:SER:CB | 5:F:1507[B]:FEC:HAC2 | 2.34 | 0.57 |
| 5:M:2207[B]:FEC:HAC2 | 1:N:168[B]:SER:CB | 2.34 | 0.57 |
| 1:J:88:VAL:HG23 | 7:J:955:HOH:O | 2.03 | 0.57 |
| 1:O:169[B]:LYS:HD2 | 1:P:164:THR:O | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:168[B]:SER:HA | 5:I:1807[B]:FEC:O2C | 2.05 | 0.57 |
| 1:C:78:LYS:HZ3 | 4:D:1211:GOL:H12 | 1.69 | 0.57 |
| 1:C:82:VAL:HG11 | 1:D:76:THR:HG21 | 1.87 | 0.57 |
| 1:C:168[A]:SER:CB | 5:D:1311[A]:FEC:HAC2 | 2.34 | 0.57 |
| 1:C:168[B]:SER:HB3 | 5:D:1311[B]:FEC:HBB2 | 1.87 | 0.57 |
| 1:M:58[B]:ARG:NH1 | 1:N:168[B]:SER:HB3 | 2.20 | 0.57 |
| 1:O:57:MET:HB3 | 5:P:2507[B]:FEC:C1D | 2.34 | 0.57 |
| 1:B:163:SER:HB2 | 3:B:1106:SO4:O2 | 2.05 | 0.57 |
| 1:J:162:SER:N | 3:J:1906:SO4:O1 | 2.37 | 0.57 |
| 1:P:110:LEU:HD11 | 1:P:126:GLU:CG | 2.34 | 0.57 |
| 1:A:5:ARG:HD2 | 1:A:8:ARG:NH1 | 2.19 | 0.56 |
| 1:B:57:MET:HB3 | 5:B:1107[A]:FEC:C1D | 2.35 | 0.56 |
| 1:F:145:HIS:HE1 | 1:L:41:ASP:OD2 | 1.88 | 0.56 |
| 1:A:110:LEU:CD2 | 1:A:114:LYS:HE3 | 2.35 | 0.56 |
| 1:M:54:ILE:HG21 | 1:N:169[B]:LYS:O | 2.04 | 0.56 |
| 1:P:57:MET:HB3 | 5:P:2507[A]:FEC:C1D | 2.36 | 0.56 |
| 1:A:41:ASP:OD2 | 1:N:145:HIS:HE1 | 1.89 | 0.56 |
| 1:F:168[B]:SER:HB2 | 5:F:1507[B]:FEC:HAC2 | 1.86 | 0.56 |
| 1:M:110:LEU:HD23 | 1:M:114:LYS:HD2 | 1.88 | 0.56 |
| 5:P:2507[A]:FEC:HBC2 | 5:P:2507[A]:FEC:HHC | 1.87 | 0.56 |
| 1:K:76:THR:HG21 | 1:L:82:VAL:HG11 | 1.87 | 0.56 |
| 1:O:128:ILE:O | 1:O:132:GLU:HG2 | 2.05 | 0.56 |
| 1:O:168[B]:SER:OG | 5:P:2507[B]:FEC:O2B | 2.24 | 0.56 |
| 1:C:4:ASN:OD1 | 1:C:7:ASP:HB2 | 2.06 | 0.56 |
| 1:E:110:LEU:HD11 | 1:E:126:GLU:CG | 2.35 | 0.56 |
| 5:I:1807[A]:FEC:C1D | 1:J:57:MET:HB3 | 2.35 | 0.55 |
| 1:E:41:ASP:OD2 | 1:P:145:HIS:HE1 | 1.89 | 0.55 |
| 5:G:1608[A]:FEC:O2C | 1:H:168[A]:SER:HB3 | 2.05 | 0.55 |
| 1:E:114:LYS:NZ | 3:E:1304:SO4:O3 | 2.31 | 0.55 |
| 5:M:2207[A]:FEC:HBC2 | 5:M:2207[A]:FEC:HHC | 1.88 | 0.55 |
| 1:B:147:LYS:HE3 | 7:B:1149:HOH:O | 2.07 | 0.55 |
| 1:M:169[A]:LYS:O | 1:N:54:ILE:HG21 | 2.06 | 0.55 |
| 5:M:2207[A]:FEC:O2C | 1:N:168[A]:SER:HB3 | 2.07 | 0.55 |
| 1:D:57:MET:HB3 | 5:D:1311[B]:FEC:C1B | 2.36 | 0.55 |
| 1:D:127[B]:ARG:HD3 | 7:D:9685:HOH:O | 2.05 | 0.55 |
| 1:M:127[B]:ARG:NE | 4:M:2210:GOL:C1 | 2.70 | 0.55 |
| 1:B:168[B]:SER:CB | 5:B:1107[B]:FEC:HAC2 | 2.37 | 0.54 |
| 1:M:57:MET:HB3 | 5:M:2207[A]:FEC:C1B | 2.37 | 0.54 |
| 1:K:110:LEU:HD11 | 1:K:126:GLU:CG | 2.38 | 0.54 |
| 1:L:144:SER:CB | 3:L:2103:SO4:O1 | 2.55 | 0.54 |
| 1:I:58[B]:ARG:NH2 | 1:J:168[B]:SER:HB3 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:93:GLU:CD | 1:G:4:ASN:HB2 | 2.28 | 0.54 |
| 1:A:110:LEU:HD11 | 1:A:126:GLU:HG2 | 1.88 | 0.54 |
| 1:E:20:ARG:HH22 | 5:F:1507[B]:FEC:CGD | 2.20 | 0.54 |
| 1:G:110:LEU:HD11 | 1:G:126:GLU:CG | 2.38 | 0.54 |
| 1:I:57:MET:HB3 | 5:I:1807[A]:FEC:C1B | 2.38 | 0.54 |
| 1:P:27:ILE:HD11 | 1:P:57:MET:HA | 1.90 | 0.54 |
| 1:F:57:MET:HB3 | 5:F:1507[A]:FEC:C1D | 2.37 | 0.54 |
| 1:A:110:LEU:HD11 | 1:A:126:GLU:CG | 2.38 | 0.53 |
| 1:C:4:ASN:ND2 | 1:C:6:GLU:H | 2.06 | 0.53 |
| 1:C:155:ALA:O | 1:E:156:LYS:HE2 | 2.08 | 0.53 |
| 1:B:114:LYS:HD3 | 3:B:1104:SO4:O2 | 2.08 | 0.53 |
| 1:P:57:MET:HB3 | 5:P:2507[B]:FEC:C1B | 2.39 | 0.53 |
| 1:I:127[A]:ARG:CG | 4:I:1810:GOL:O1 | 2.45 | 0.53 |
| 1:C:57:MET:HB3 | 5:D:1311[B]:FEC:C1D | 2.38 | 0.53 |
| 1:F:110:LEU:HD22 | 1:F:114:LYS:HE2 | 1.90 | 0.53 |
| 1:A:168[A]:SER:H | 1:B:58[A]:ARG:HH12 | 1.56 | 0.53 |
| 1:B:110:LEU:HD11 | 1:B:126:GLU:HG3 | 1.91 | 0.53 |
| 1:D:88:VAL:HG12 | 1:D:146:ILE:HD13 | 1.90 | 0.53 |
| 1:E:158:ALA:HB1 | 1:P:145:HIS:CD2 | 2.43 | 0.53 |
| 1:H:88:VAL:HG12 | 1:H:146:ILE:HD13 | 1.91 | 0.53 |
| 1:J:114:LYS:NZ | 3:J:1904:SO4:O2 | 2.25 | 0.53 |
| 1:C:78:LYS:HZ1 | 4:D:1211:GOL:H12 | 1.72 | 0.53 |
| 1:M:169[B]:LYS:HZ3 | 1:N:165:GLY:HA3 | 1.74 | 0.53 |
| 1:I:127[A]:ARG:HD2 | 7:I:9733:HOH:O | 2.08 | 0.52 |
| 1:M:58[B]:ARG:HH12 | 1:N:168[B]:SER:H | 1.56 | 0.52 |
| 1:C:169[A]:LYS:O | 1:D:54:ILE:HG21 | 2.09 | 0.52 |
| 1:D:78:LYS:HZ3 | 4:D:1211:GOL:C2 | 2.23 | 0.52 |
| 1:G:168[A]:SER:C | 1:H:58[A]:ARG:HH21 | 2.12 | 0.52 |
| 1:K:110:LEU:HD23 | 1:K:114:LYS:HD2 | 1.90 | 0.52 |
| 1:A:54:ILE:HG21 | 1:B:169[B]:LYS:O | 2.08 | 0.52 |
| 1:B:110:LEU:CD2 | 1:B:114:LYS:HE3 | 2.40 | 0.52 |
| 1:C:31:MET:HG3 | 5:D:1311[A]:FEC:HBD1 | 1.90 | 0.52 |
| 1:F:127[A]:ARG:HB3 | 4:F:1510:GOL:O1 | 2.09 | 0.52 |
| 1:K:110:LEU:HD11 | 1:K:126:GLU:HG3 | 1.92 | 0.52 |
| 1:K:149:LEU:HD13 | 1:O:155:ALA:HA | 1.90 | 0.52 |
| 1:M:127[B]:ARG:HB3 | 4:M:2210:GOL:H12 | 1.92 | 0.52 |
| 1:K:169[A]:LYS:HB2 | 7:K:9227:HOH:O | 2.10 | 0.52 |
| 5:G:1608[B]:FEC:O1C | 1:H:168[B]:SER:OG | 2.28 | 0.52 |
| 5:P:2507[B]:FEC:HBC1 | 5:P:2507[B]:FEC:HHC | 1.92 | 0.52 |
| 1:M:168[A]:SER:CB | 5:M:2207[A]:FEC:HBC1 | 2.39 | 0.52 |
| 3:A:1105:SO4:O4 | 1:B:77:GLN:HG2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:168[A]:SER:O | 1:D:58[A]:ARG:CZ | 2.57 | 0.52 |
| 1:D:164:THR:HA | 7:D:9672:HOH:O | 2.09 | 0.52 |
| 1:E:58[A]:ARG:HG2 | 4:E:1410:GOL:O1 | 2.10 | 0.52 |
| 1:K:93[B]:GLU:OE1 | 7:K:9178:HOH:O | 2.18 | 0.52 |
| 1:A:169[A]:LYS:O | 1:B:54:ILE:HG21 | 2.10 | 0.52 |
| 1:M:163:SER:HB2 | 3:M:2206:SO4:O4 | 2.10 | 0.52 |
| 1:P:58[B]:ARG:HG2 | 4:P:2510:GOL:O3 | 2.10 | 0.52 |
| 1:D:57:MET:HB3 | 5:D:1311[A]:FEC:C1D | 2.40 | 0.52 |
| 5:G:1608[A]:FEC:O2B | 1:H:168[A]:SER:OG | 2.27 | 0.52 |
| 5:I:1807[B]:FEC:O1C | 1:J:168[B]:SER:OG | 2.27 | 0.52 |
| 1:M:127[B]:ARG:HE | 4:M:2210:GOL:C1 | 2.22 | 0.51 |
| 1:D:31:MET:HG3 | 5:D:1311[B]:FEC:HBD1 | 1.93 | 0.51 |
| 5:M:2207[B]:FEC:CAC | 1:N:168[B]:SER:OG | 2.54 | 0.51 |
| 1:A:151:ASP:OD1 | 1:A:154:LEU:HD12 | 2.10 | 0.51 |
| 1:E:111:LYS:HG2 | 1:E:115:GLU:OE2 | 2.09 | 0.51 |
| 1:M:57:MET:HB3 | 5:M:2207[B]:FEC:C1D | 2.40 | 0.51 |
| 1:N:4:ASN:HD22 | 1:N:7:ASP:H | 1.59 | 0.51 |
| 1:C:89:PRO:CB | 1:G:6[A]:GLU:HG3 | 2.40 | 0.51 |
| 1:E:58[A]:ARG:HG2 | 4:E:1410:GOL:HO1 | 1.75 | 0.51 |
| 1:E:168[B]:SER:OG | 5:F:1507[B]:FEC:O2B | 2.28 | 0.51 |
| 1:G:110:LEU:HD11 | 1:G:126:GLU:HG3 | 1.93 | 0.51 |
| 1:A:123:ARG:HB3 | 1:A:127[B]:ARG:NH2 | 2.26 | 0.51 |
| 1:E:128:ILE:O | 1:E:132:GLU:HG2 | 2.10 | 0.51 |
| 5:M:2207[A]:FEC:O2B | 1:N:168[A]:SER:OG | 2.29 | 0.51 |
| 1:K:55:ASP:OD2 | 1:L:172:VAL:HG13 | 2.10 | 0.51 |
| 1:O:33:GLN:NE2 | 1:O:95:ASP:OD2 | 2.43 | 0.51 |
| 1:B:110:LEU:HD11 | 1:B:126:GLU:CG | 2.40 | 0.51 |
| 1:K:57:MET:HB3 | 5:L:2108[B]:FEC:C1D | 2.41 | 0.51 |
| 1:E:57:MET:HB3 | 5:F:1507[A]:FEC:C1B | 2.41 | 0.50 |
| 1:I:127[B]:ARG:CD | 4:I:1810:GOL:HO1 | 2.23 | 0.50 |
| 1:O:78:LYS:HZ1 | 4:O:2411:GOL:H12 | 1.76 | 0.50 |
| 1:G:127[B]:ARG:NE | 4:G:1610:GOL:O1 | 2.44 | 0.50 |
| 1:A:168[A]:SER:OG | 5:B:1107[A]:FEC:O1C | 2.30 | 0.50 |
| 1:L:31:MET:HG3 | 5:L:2108[B]:FEC:HBD1 | 1.94 | 0.50 |
| 1:G:88:VAL:HG12 | 1:G:146:ILE:HD13 | 1.94 | 0.50 |
| 1:I:127[B]:ARG:CB | 4:I:1810:GOL:HO1 | 2.25 | 0.50 |
| 1:G:168[A]:SER:HB2 | 1:H:58[A]:ARG:HH22 | 0.39 | 0.50 |
| 1:M:110:LEU:HD11 | 1:M:126:GLU:CG | 2.41 | 0.50 |
| 7:A:1167:HOH:O | 1:N:145:HIS:HD2 | 1.94 | 0.50 |
| 1:F:58[B]:ARG:HD3 | 5:F:1507[B]:FEC:O2B | 2.11 | 0.50 |
| 1:O:58[B]:ARG:CZ | 1:P:168[B]:SER:H | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:168[A]:SER:HB2 | 1:J:58[A]:ARG:NH1 | 2.27 | 0.50 |
| 1:E:168[A]:SER:OG | 5:F:1507[A]:FEC:HAC2 | 2.11 | 0.49 |
| 1:O:110:LEU:HD11 | 1:O:126:GLU:CG | 2.42 | 0.49 |
| 1:C:155:ALA:HA | 1:E:149:LEU:HD13 | 1.94 | 0.49 |
| 1:F:145:HIS:HD2 | 7:L:2192:HOH:O | 1.95 | 0.49 |
| 1:F:156:LYS:HE2 | 1:L:155:ALA:O | 2.12 | 0.49 |
| 1:H:4:ASN:HD22 | 1:H:7:ASP:HB2 | 1.77 | 0.49 |
| 1:J:168[B]:SER:OG | 1:J:169[B]:LYS:N | 2.45 | 0.49 |
| 1:G:168[A]:SER:C | 1:H:58[A]:ARG:NH2 | 2.65 | 0.49 |
| 1:I:65:GLU:HG2 | 7:J:8968:HOH:O | 2.12 | 0.49 |
| 1:I:127[B]:ARG:HD3 | 4:I:1713:GOL:C3 | 2.42 | 0.49 |
| 1:C:89:PRO:HB2 | 1:G:6[A]:GLU:HG3 | 1.93 | 0.49 |
| 1:B:165:GLY:HA3 | 7:B:1250:HOH:O | 2.12 | 0.49 |
| 1:I:78:LYS:NZ | 4:J:1811:GOL:H12 | 2.27 | 0.49 |
| 1:J:127[B]:ARG:NH2 | 7:J:8922:HOH:O | 2.44 | 0.49 |
| 1:K:58[B]:ARG:HG3 | 1:K:58[B]:ARG:NH1 | 2.28 | 0.49 |
| 1:M:127[B]:ARG:HG3 | 1:M:127[B]:ARG:HH11 | 1.78 | 0.49 |
| 1:F:4:ASN:HD22 | 1:F:7:ASP:H | 1.59 | 0.49 |
| 1:I:81:LYS:HE3 | 1:I:82:VAL:N | 2.24 | 0.49 |
| 1:K:168[B]:SER:HA | 5:L:2108[B]:FEC:CGC | 2.34 | 0.49 |
| 1:O:168[B]:SER:HB2 | 5:P:2507[B]:FEC:HBC2 | 1.93 | 0.49 |
| 1:I:35:TYR:OH | 5:I:1807[B]:FEC:O2A | 2.29 | 0.49 |
| 1:D:128:ILE:O | 1:D:132:GLU:HG2 | 2.12 | 0.48 |
| 1:I:88:VAL:HB | 1:I:89:PRO:HD3 | 1.95 | 0.48 |
| 1:K:168[B]:SER:OG | 5:L:2108[B]:FEC:O2B | 2.30 | 0.48 |
| 1:L:88:VAL:HG12 | 1:L:146:ILE:HD13 | 1.95 | 0.48 |
| 1:B:127[A]:ARG:HH22 | 1:N:130:GLU:CD | 2.17 | 0.48 |
| 1:P:79:GLU:HG2 | 7:P:9558:HOH:O | 2.12 | 0.48 |
| 1:E:88:VAL:HG12 | 1:E:146:ILE:HD13 | 1.95 | 0.48 |
| 1:I:168[B]:SER:HA | 5:I:1807[B]:FEC:CGC | 2.43 | 0.48 |
| 1:C:33:GLN:NE2 | 1:C:95:ASP:OD2 | 2.44 | 0.48 |
| 1:K:89:PRO:O | 1:K:93[B]:GLU:HG3 | 2.12 | 0.48 |
| 1:O:127[B]:ARG:NE | 7:O:2414:HOH:O | 2.42 | 0.48 |
| 1:E:62:ASN:ND2 | 7:E:9906:HOH:O | 2.47 | 0.48 |
| 1:C:110:LEU:HD11 | 1:C:126:GLU:HG2 | 1.95 | 0.48 |
| 1:F:51:LEU:HD21 | 1:F:164:THR:HB | 1.96 | 0.48 |
| 1:I:40:MET:HE1 | 7:I:996:HOH:O | 2.12 | 0.48 |
| 1:L:169[B]:LYS:NZ | 7:L:2166:HOH:O | 2.47 | 0.48 |
| 1:M:127[B]:ARG:NH1 | 7:M:823:HOH:O | 2.47 | 0.48 |
| 1:O:52:ILE:O | 1:O:56:GLU:HG2 | 2.13 | 0.48 |
| 1:L:4:ASN:ND2 | 1:L:7:ASP:H | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:168[A]:SER:N | 1:B:58[A]:ARG:NH2 | 2.60 | 0.48 |
| 1:D:132:GLU:OE1 | 1:D:132:GLU:HA | 2.14 | 0.48 |
| 1:G:57:MET:HB3 | 5:G:1608[B]:FEC:C1D | 2.43 | 0.48 |
| 1:I:127[B]:ARG:HE | 1:I:127[B]:ARG:HB2 | 1.37 | 0.48 |
| 1:F:128:ILE:O | 1:F:132:GLU:HG2 | 2.14 | 0.47 |
| 1:I:57:MET:HB3 | 5:I:1807[B]:FEC:C1D | 2.44 | 0.47 |
| 1:I:81:LYS:HD2 | 1:I:81:LYS:HA | 1.44 | 0.47 |
| 1:M:169[A]:LYS:O | 1:M:169[A]:LYS:HG3 | 2.13 | 0.47 |
| 1:A:57:MET:HB3 | 5:B:1107[A]:FEC:C1B | 2.44 | 0.47 |
| 1:C:57:MET:HB3 | 5:D:1311[A]:FEC:C1B | 2.44 | 0.47 |
| 1:M:14:GLU:O | 1:M:14:GLU:HG2 | 2.14 | 0.47 |
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:C | 2.65 | 0.47 |
| 1:M:169[B]:LYS:HB2 | 1:M:169[B]:LYS:HE3 | 1.64 | 0.47 |
| 1:A:127[B]:ARG:NE | 7:A:1195:HOH:O | 2.47 | 0.47 |
| 1:C:13:ILE:HD13 | 1:C:72:GLY:HA3 | 1.95 | 0.47 |
| 5:F:1507[B]:FEC:HHC | 5:F:1507[B]:FEC:CBC | 2.44 | 0.47 |
| 1:P:133:GLN:NE2 | 7:P:676:HOH:O | 2.47 | 0.47 |
| 1:L:88:VAL:HB | 1:L:89:PRO:HD3 | 1.97 | 0.47 |
| 5:M:2207[B]:FEC:HHC | 5:M:2207[B]:FEC:HBC2 | 1.96 | 0.47 |
| 1:A:168[A]:SER:HB2 | 1:B:58[A]:ARG:HH22 | 1.75 | 0.47 |
| 1:K:168[B]:SER:HB2 | 5:L:2108[B]:FEC:O2C | 2.12 | 0.47 |
| 5:P:2507[B]:FEC:HHC | 5:P:2507[B]:FEC:CBC | 2.45 | 0.47 |
| 1:B:147:LYS:HE2 | 7:B:1230:HOH:O | 2.14 | 0.47 |
| 1:F:58[B]:ARG:HH11 | 5:F:1507[B]:FEC:HBB2 | 1.80 | 0.47 |
| 5:G:1608[B]:FEC:HBC1 | 1:H:168[B]:SER:OG | 2.15 | 0.47 |
| 1:J:161:PRO:CA | 3:J:1906:SO4:O1 | 2.54 | 0.47 |
| 1:G:33:GLN:NE2 | 1:G:95:ASP:OD2 | 2.46 | 0.47 |
| 1:I:168[A]:SER:HB3 | 5:I:1807[A]:FEC:HBC1 | 1.97 | 0.47 |
| 1:P:31:MET:HG3 | 5:P:2507[A]:FEC:HBA2 | 1.97 | 0.47 |
| 1:D:127[B]:ARG:NH1 | 7:D:9685:HOH:O | 2.48 | 0.47 |
| 1:D:168[B]:SER:HG | 5:D:1311[B]:FEC:CGC | 2.10 | 0.47 |
| 5:I:1807[B]:FEC:HBD1 | 1:J:31:MET:HG3 | 1.97 | 0.47 |
| 1:N:4:ASN:ND2 | 1:N:7:ASP:H | 2.13 | 0.47 |
| 1:C:147:LYS:HD2 | 1:G:5[A]:ARG:HH12 | 1.79 | 0.46 |
| 1:M:65:GLU:O | 1:M:69:GLU:HG3 | 2.15 | 0.46 |
| 1:A:127[B]:ARG:NH2 | 7:A:1195:HOH:O | 2.48 | 0.46 |
| 1:C:31:MET:HG3 | 5:D:1311[B]:FEC:HBA2 | 1.97 | 0.46 |
| 1:D:88:VAL:CG1 | 1:D:146:ILE:HD13 | 2.46 | 0.46 |
| 1:D:111:LYS:HD2 | 7:D:526:HOH:O | 2.15 | 0.46 |
| 1:E:33:GLN:NE2 | 1:E:95:ASP:OD2 | 2.48 | 0.46 |
| 1:H:29:GLN:NE2 | 1:H:83:VAL:H | 2.00 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:127[B]:ARG:HG2 | 4:I:1810:GOL:C1 | 2.45 | 0.46 |
| 1:E:169[A]:LYS:O | 1:F:54:ILE:HG21 | 2.14 | 0.46 |
| 1:F:4:ASN:HB2 | 3:F:1502:SO4:O2 | 2.15 | 0.46 |
| 1:I:123:ARG:HB3 | 1:I:127[B]:ARG:HH22 | 1.81 | 0.46 |
| 1:A:88:VAL:HG12 | 1:A:146:ILE:HD13 | 1.97 | 0.46 |
| 1:E:11:LYS:NZ | 7:E:713:HOH:O | 2.49 | 0.46 |
| 1:G:88:VAL:HB | 1:G:89:PRO:HD3 | 1.97 | 0.46 |
| 1:M:58[B]:ARG:NH1 | 1:N:168[B]:SER:H | 2.12 | 0.46 |
| 1:G:77:GLN:HB3 | 4:G:1611:GOL:O1 | 2.15 | 0.46 |
| 1:F:127[A]:ARG:NH1 | 1:P:130:GLU:OE2 | 2.48 | 0.46 |
| 1:H:45:LEU:HG | 1:H:157:ILE:HG21 | 1.97 | 0.46 |
| 1:H:62:ASN:ND2 | 4:H:1710:GOL:O3 | 2.49 | 0.46 |
| 1:O:169[B]:LYS:O | 1:P:54:ILE:HG21 | 2.15 | 0.46 |
| 1:O:142:ILE:HG22 | 1:O:146:ILE:HD12 | 1.98 | 0.46 |
| 1:G:168[A]:SER:O | 1:H:58[A]:ARG:NH2 | 2.48 | 0.46 |
| 5:M:2207[A]:FEC:CGC | 1:N:168[A]:SER:HA | 2.46 | 0.46 |
| 5:I:1807[A]:FEC:CMD | 1:J:61:GLU:HB2 | 2.46 | 0.46 |
| 1:M:168[A]:SER:O | 1:N:58[A]:ARG:NH2 | 2.49 | 0.46 |
| 1:B:27:ILE:HD11 | 1:B:57:MET:HA | 1.97 | 0.45 |
| 1:B:127[A]:ARG:HD2 | 4:B:1110:GOL:HO1 | 1.77 | 0.45 |
| 1:E:58[B]:ARG:NH2 | 1:F:168[B]:SER:O | 2.47 | 0.45 |
| 1:F:123:ARG:NH1 | 1:F:126:GLU:OE2 | 2.50 | 0.45 |
| 1:L:68:LYS:HD3 | 1:L:74:PRO:HD3 | 1.98 | 0.45 |
| 1:F:127[B]:ARG:HB3 | 4:F:1510:GOL:O1 | 2.17 | 0.45 |
| 1:O:108[A]:GLN:NE2 | 7:O:2478:HOH:O | 2.49 | 0.45 |
| 1:C:88:VAL:HG12 | 1:C:146:ILE:HD13 | 1.99 | 0.45 |
| 1:D:133:GLN:NE2 | 7:D:499:HOH:O | 2.49 | 0.45 |
| 5:I:1807[B]:FEC:HHC | 5:I:1807[B]:FEC:CBC | 2.47 | 0.45 |
| 1:L:4:ASN:HD22 | 1:L:7:ASP:H | 1.64 | 0.45 |
| 1:L:61:GLU:O | 1:L:65:GLU:HG3 | 2.16 | 0.45 |
| 1:M:127[B]:ARG:HG3 | 1:M:127[B]:ARG:NH1 | 2.30 | 0.45 |
| 1:P:58[A]:ARG:NH2 | 7:P:9899:HOH:O | 2.49 | 0.45 |
| 1:P:61:GLU:HB2 | 5:P:2507[A]:FEC:CMD | 2.47 | 0.45 |
| 1:A:57:MET:HB3 | 5:B:1107[B]:FEC:C1D | 2.46 | 0.45 |
| 1:G:104:GLU:OE2 | 1:N:8[B]:ARG:NH2 | 2.49 | 0.45 |
| 1:I:110:LEU:HD11 | 1:I:126:GLU:CG | 2.46 | 0.45 |
| 1:N:111:LYS:O | 1:N:115:GLU:HG3 | 2.17 | 0.45 |
| 1:A:82:VAL:HG11 | 1:B:76:THR:HG21 | 1.99 | 0.45 |
| 1:A:169[A]:LYS:HD2 | 7:B:1250:HOH:O | 2.17 | 0.45 |
| 1:F:61:GLU:HB2 | 5:F:1507[A]:FEC:CMD | 2.46 | 0.45 |
| 1:L:127[B]:ARG:NH2 | 7:L:2109:HOH:O | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:58[B]:ARG:NH2 | 1:P:168[B]:SER:O | 2.49 | 0.45 |
| 1:A:4:ASN:ND2 | 7:A:1208:HOH:O | 2.49 | 0.45 |
| 1:F:112:VAL:O | 1:F:116:GLN:HG2 | 2.16 | 0.45 |
| 1:I:147:LYS:NZ | 3:I:1803:SO4:O3 | 2.50 | 0.45 |
| 1:M:58[B]:ARG:NH2 | 1:N:168[B]:SER:CB | 2.78 | 0.45 |
| 1:I:110:LEU:HD11 | 1:I:126:GLU:HG2 | 1.98 | 0.45 |
| 1:P:168[B]:SER:OG | 5:P:2507[B]:FEC:O1C | 2.29 | 0.45 |
| 1:M:76:THR:HG21 | 1:N:82:VAL:HG11 | 1.99 | 0.45 |
| 1:N:133:GLN:NE2 | 7:N:2315:HOH:O | 2.50 | 0.45 |
| 1:O:43:GLY:HA2 | 1:O:162:SER:HB3 | 1.99 | 0.45 |
| 1:P:127[B]:ARG:NE | 4:P:2510:GOL:O1 | 2.50 | 0.45 |
| 1:M:161:PRO:HB3 | 3:M:2206:SO4:O2 | 2.17 | 0.45 |
| 1:C:168[B]:SER:OG | 5:D:1311[B]:FEC:O2B | 2.35 | 0.44 |
| 1:G:151:ASP:HB2 | 7:G:1676:HOH:O | 2.17 | 0.44 |
| 1:B:61:GLU:HB2 | 5:B:1107[A]:FEC:CMD | 2.47 | 0.44 |
| 1:F:58[B]:ARG:HH11 | 5:F:1507[B]:FEC:CBB | 2.30 | 0.44 |
| 1:J:33:GLN:OE1 | 1:J:95:ASP:OD2 | 2.35 | 0.44 |
| 1:J:110:LEU:HD11 | 1:J:126:GLU:CG | 2.38 | 0.44 |
| 1:L:57:MET:HB3 | 5:L:2108[A]:FEC:C1D | 2.47 | 0.44 |
| 1:L:150:GLY:HA3 | 3:L:2107:SO4:O2 | 2.16 | 0.44 |
| 1:M:127[B]:ARG:NH2 | 7:M:823:HOH:O | 2.49 | 0.44 |
| 1:O:127[B]:ARG:HG3 | 1:O:127[B]:ARG:HH11 | 1.83 | 0.44 |
| 1:A:122:ALA:O | 1:A:126:GLU:HG3 | 2.18 | 0.44 |
| 1:A:168[B]:SER:HB2 | 5:B:1107[B]:FEC:HBC2 | 1.31 | 0.44 |
| 1:F:152:THR:CG2 | 1:L:152:THR:HA | 2.48 | 0.44 |
| 1:H:160:THR:HB | 1:H:161:PRO:HD2 | 1.99 | 0.44 |
| 1:I:112:VAL:O | 1:I:116:GLN:HG2 | 2.18 | 0.44 |
| 1:B:57:MET:HB3 | 5:B:1107[B]:FEC:C1B | 2.48 | 0.44 |
| 1:D:168[A]:SER:OG | 5:D:1311[A]:FEC:HBB2 | 2.18 | 0.44 |
| 1:F:5:ARG:HD2 | 1:F:8:ARG:NH1 | 2.33 | 0.44 |
| 1:G:82:VAL:HG11 | 1:H:76:THR:HG21 | 1.99 | 0.44 |
| 1:L:127[A]:ARG:HD2 | 7:L:2162:HOH:O | 2.18 | 0.44 |
| 1:D:169[B]:LYS:HG2 | 7:D:9732:HOH:O | 2.18 | 0.44 |
| 1:E:6:GLU:OE2 | 1:E:9:LYS:HD2 | 2.17 | 0.44 |
| 1:I:29:GLN:O | 1:I:33:GLN:HG3 | 2.17 | 0.44 |
| 1:M:110:LEU:HD11 | 1:M:126:GLU:HG2 | 1.99 | 0.44 |
| 5:M:2207[A]:FEC:HMD2 | 1:N:61:GLU:HB2 | 1.99 | 0.44 |
| 1:O:76:THR:HG21 | 1:P:82:VAL:HG11 | 2.00 | 0.44 |
| 1:A:78:LYS:HE2 | 3:A:1105:SO4:S | 2.55 | 0.44 |
| 1:L:168[B]:SER:OG | 5:L:2108[B]:FEC:HMC1 | 2.18 | 0.44 |
| 1:B:169[B]:LYS:O | 1:B:169[B]:LYS:HG3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:127[A]:ARG:HD3 | 4:E:1410:GOL:O3 | 2.18 | 0.44 |
| 5:I:1807[A]:FEC:O1C | 1:J:168[A]:SER:HA | 2.16 | 0.44 |
| 1:K:82:VAL:HG11 | 1:L:76:THR:HG21 | 2.00 | 0.44 |
| 1:L:105:ALA:O | 1:L:108:GLN:HB2 | 2.18 | 0.44 |
| 1:P:4:ASN:HD22 | 1:P:7:ASP:H | 1.60 | 0.43 |
| 1:B:127[B]:ARG:HB3 | 4:B:1110:GOL:O1 | 2.17 | 0.43 |
| 1:I:54:ILE:HG21 | 1:J:169[B]:LYS:O | 2.19 | 0.43 |
| 1:A:7:ASP:OD1 | 1:O:4:ASN:ND2 | 2.51 | 0.43 |
| 1:D:33:GLN:OE1 | 1:D:95:ASP:OD2 | 2.35 | 0.43 |
| 1:D:127[A]:ARG:HD2 | 6:D:1310:3PY:O1 | 2.17 | 0.43 |
| 1:M:110:LEU:HD11 | 1:M:126:GLU:HG3 | 2.00 | 0.43 |
| 1:I:82:VAL:HG11 | 1:J:76:THR:HG21 | 2.00 | 0.43 |
| 1:O:127[B]:ARG:NH2 | 7:O:2437:HOH:O | 2.51 | 0.43 |
| 1:C:110:LEU:HD11 | 1:C:126:GLU:CG | 2.48 | 0.43 |
| 1:M:78:LYS:HE2 | 4:M:2211:GOL:O2 | 2.18 | 0.43 |
| 1:A:110:LEU:HD21 | 1:A:114:LYS:HE3 | 1.98 | 0.43 |
| 1:C:41:ASP:HB3 | 1:E:145:HIS:CE1 | 2.54 | 0.43 |
| 1:C:122:ALA:O | 1:C:126:GLU:HG3 | 2.19 | 0.43 |
| 1:H:12:VAL:HG11 | 1:H:118:ASP:OD2 | 2.19 | 0.43 |
| 1:M:13:ILE:HD13 | 1:M:72:GLY:HA3 | 2.00 | 0.43 |
| 1:P:142:ILE:O | 1:P:146:ILE:HG12 | 2.19 | 0.43 |
| 1:P:161:PRO:HA | 3:P:2506:SO4:O4 | 2.18 | 0.43 |
| 1:C:123:ARG:NH2 | 1:C:126:GLU:OE2 | 2.49 | 0.43 |
| 1:D:110:LEU:O | 1:D:114:LYS:HG3 | 2.18 | 0.43 |
| 1:G:155:ALA:O | 1:I:156:LYS:HD3 | 2.19 | 0.43 |
| 1:D:78:LYS:NZ | 4:D:1211:GOL:O2 | 2.49 | 0.43 |
| 1:F:58[B]:ARG:NH1 | 5:F:1507[B]:FEC:HBB2 | 2.34 | 0.43 |
| 1:G:110:LEU:HD11 | 1:G:126:GLU:HG2 | 2.00 | 0.43 |
| 1:O:78:LYS:HZ1 | 4:O:2411:GOL:C1 | 2.31 | 0.43 |
| 1:O:127[B]:ARG:NH2 | 7:O:2414:HOH:O | 2.50 | 0.43 |
| 1:E:76:THR:HG21 | 1:F:82:VAL:HG11 | 2.01 | 0.43 |
| 1:O:61:GLU:HB2 | 5:P:2507[B]:FEC:CMD | 2.48 | 0.43 |
| 1:D:43:GLY:HA2 | 1:D:162:SER:HB3 | 2.00 | 0.43 |
| 1:K:110:LEU:HD11 | 1:K:126:GLU:HG2 | 2.01 | 0.43 |
| 1:L:77[B]:GLN:NE2 | 7:L:2203:HOH:O | 2.52 | 0.43 |
| 1:B:93[A]:GLU:HG2 | 1:B:94:SER:N | 2.33 | 0.42 |
| 5:I:1807[B]:FEC:HHC | 5:I:1807[B]:FEC:HBC2 | 2.01 | 0.42 |
| 1:N:27:ILE:HD11 | 1:N:57:MET:HA | 2.00 | 0.42 |
| 1:F:58[B]:ARG:HG2 | 5:F:1507[B]:FEC:HBB1 | 2.01 | 0.42 |
| 1:G:161:PRO:HA | 3:G:1606:SO4:O3 | 2.19 | 0.42 |
| 1:K:78:LYS:NZ | 7:K:9116:HOH:O | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:F:1507[B]:FEC:HHC | 5:F:1507[B]:FEC:HBC1 | 2.00 | 0.42 |
| 5:G:1608[A]:FEC:C1D | 1:H:57:MET:HB3 | 2.48 | 0.42 |
| 1:A:34:HIS:HE1 | 7:A:1152:HOH:O | 2.02 | 0.42 |
| 1:C:68:LYS:HD2 | 1:C:68:LYS:HA | 1.86 | 0.42 |
| 1:P:128:ILE:O | 1:P:132:GLU:HG2 | 2.19 | 0.42 |
| 5:G:1608[B]:FEC:HAC2 | 1:H:168[B]:SER:CB | 2.49 | 0.42 |
| 1:B:123:ARG:HD3 | 1:N:126:GLU:OE2 | 2.19 | 0.42 |
| 1:B:127[A]:ARG:NH2 | 1:N:130:GLU:OE1 | 2.53 | 0.42 |
| 1:C:168[B]:SER:HA | 5:D:1311[B]:FEC:O2C | 2.19 | 0.42 |
| 1:G:127[B]:ARG:NH2 | 7:G:1638:HOH:O | 2.49 | 0.42 |
| 1:H:5:ARG:HD2 | 1:H:8:ARG:NH1 | 2.35 | 0.42 |
| 1:M:68:LYS:HA | 1:M:68:LYS:HD2 | 1.89 | 0.42 |
| 1:N:62:ASN:ND2 | 4:N:2310:GOL:O1 | 2.52 | 0.42 |
| 1:N:169[B]:LYS:O | 1:N:169[B]:LYS:HG3 | 2.18 | 0.42 |
| 1:C:52:ILE:O | 1:C:55:ASP:HB2 | 2.19 | 0.42 |
| 1:E:58[A]:ARG:HH22 | 1:F:172:VAL:HG22 | 1.85 | 0.42 |
| 1:H:58[A]:ARG:NH1 | 1:H:58[A]:ARG:HG3 | 2.35 | 0.42 |
| 5:I:1807[B]:FEC:HAC2 | 1:J:168[B]:SER:CB | 2.49 | 0.42 |
| 1:K:57:MET:HB3 | 5:L:2108[A]:FEC:C1B | 2.50 | 0.42 |
| 1:D:61:GLU:HB2 | 5:D:1311[A]:FEC:CMD | 2.49 | 0.42 |
| 1:I:81:LYS:CE | 1:I:82:VAL:H | 2.26 | 0.42 |
| 1:J:110:LEU:HD23 | 1:J:114:LYS:HE2 | 2.02 | 0.42 |
| 5:P:2507[A]:FEC:HHC | 5:P:2507[A]:FEC:CBC | 2.50 | 0.42 |
| 1:A:155:ALA:HA | 1:N:149:LEU:HD13 | 2.02 | 0.41 |
| 1:A:168[A]:SER:HB3 | 5:B:1107[A]:FEC:HBC1 | 2.00 | 0.41 |
| 1:B:9:LYS:HA | 7:B:1142:HOH:O | 2.20 | 0.41 |
| 1:E:58[B]:ARG:NH2 | 1:F:168[B]:SER:N | 2.68 | 0.41 |
| 1:G:57:MET:HB3 | 5:G:1608[A]:FEC:C1B | 2.49 | 0.41 |
| 1:L:61:GLU:HB2 | 5:L:2108[A]:FEC:HMD2 | 2.02 | 0.41 |
| 1:A:31:MET:HG3 | 5:B:1107[A]:FEC:HBD1 | 2.02 | 0.41 |
| 1:B:61:GLU:HB2 | 5:B:1107[A]:FEC:HMD2 | 2.02 | 0.41 |
| 1:D:4:ASN:ND2 | 1:D:7:ASP:H | 2.18 | 0.41 |
| 5:G:1608[B]:FEC:C1B | 1:H:57:MET:HB3 | 2.51 | 0.41 |
| 1:A:58[B]:ARG:NH1 | 1:B:168[B]:SER:H | 2.18 | 0.41 |
| 1:A:123:ARG:NH1 | 1:A:127[B]:ARG:NH1 | 2.69 | 0.41 |
| 1:P:78:LYS:NZ | 7:P:9538:HOH:O | 2.53 | 0.41 |
| 1:I:127[A]:ARG:CB | 4:I:1810:GOL:HO1 | 2.24 | 0.41 |
| 1:K:110:LEU:CD2 | 1:K:114:LYS:HD2 | 2.49 | 0.41 |
| 1:M:61:GLU:HB2 | 5:M:2207[B]:FEC:CMD | 2.50 | 0.41 |
| 1:P:147:LYS:HA | 1:P:147:LYS:HD3 | 1.85 | 0.41 |
| 1:B:168[A]:SER:OG | 5:B:1107[A]:FEC:HBB2 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:29:GLN:HA | 1:D:82:VAL:HG13 | 2.03 | 0.41 |
| 1:F:57:MET:HB3 | 5:F:1507[B]:FEC:C1B | 2.50 | 0.41 |
| 1:J:58[B]:ARG:NE | 4:J:1910:GOL:O1 | 2.48 | 0.41 |
| 1:A:112:VAL:O | 1:A:116:GLN:HG2 | 2.21 | 0.41 |
| 1:G:104:GLU:OE1 | 1:N:8[A]:ARG:NH2 | 2.53 | 0.41 |
| 1:I:58[B]:ARG:NH2 | 1:J:168[B]:SER:N | 2.68 | 0.41 |
| 1:O:57:MET:HB3 | 5:P:2507[A]:FEC:C1B | 2.50 | 0.41 |
| 1:P:52:ILE:O | 1:P:56:GLU:HG2 | 2.21 | 0.41 |
| 1:P:68:LYS:HD2 | 1:P:68:LYS:HA | 1.89 | 0.41 |
| 1:C:65:GLU:O | 1:C:69:GLU:HG3 | 2.21 | 0.41 |
| 1:G:58[A]:ARG:NE | 4:G:1610:GOL:O3 | 2.48 | 0.41 |
| 5:G:1608[A]:FEC:HBC2 | 5:G:1608[A]:FEC:CHC | 2.49 | 0.41 |
| 1:K:110:LEU:HD13 | 1:P:119:ILE:HG13 | 2.02 | 0.41 |
| 1:M:58[B]:ARG:NH2 | 1:N:168[B]:SER:N | 2.64 | 0.41 |
| 1:A:168[B]:SER:OG | 5:B:1107[B]:FEC:O2B | 2.39 | 0.41 |
| 1:D:29:GLN:HE22 | 1:D:83:VAL:N | 2.01 | 0.41 |
| 1:I:5:ARG:HG2 | 3:I:1802:SO4:O4 | 2.20 | 0.41 |
| 1:I:127[B]:ARG:NH2 | 7:I:9733:HOH:O | 2.54 | 0.41 |
| 1:M:58[B]:ARG:HH12 | 1:N:168[B]:SER:CB | 2.32 | 0.41 |
| 1:O:127[B]:ARG:NE | 4:O:2410:GOL:O3 | 2.50 | 0.41 |
| 1:A:16:LEU:HD21 | 1:A:121:THR:HG23 | 2.02 | 0.41 |
| 1:N:68:LYS:HD2 | 1:N:68:LYS:HA | 1.84 | 0.41 |
| 1:N:112:VAL:O | 1:N:116:GLN:HG2 | 2.21 | 0.41 |
| 1:A:4:ASN:O | 1:A:7:ASP:HB3 | 2.21 | 0.40 |
| 1:A:6:GLU:HB2 | 7:A:1208:HOH:O | 2.20 | 0.40 |
| 1:D:68:LYS:HD2 | 1:D:68:LYS:HA | 1.91 | 0.40 |
| 5:G:1608[A]:FEC:HBA2 | 5:G:1608[A]:FEC:HHB | 2.03 | 0.40 |
| 1:I:31:MET:HG3 | 5:I:1807[A]:FEC:HBD1 | 2.03 | 0.40 |
| 1:K:112:VAL:O | 1:K:116:GLN:HG2 | 2.22 | 0.40 |
| 1:F:27:ILE:HD11 | 1:F:57:MET:HA | 2.03 | 0.40 |
| 1:J:160:THR:HB | 1:J:161:PRO:HD2 | 2.03 | 0.40 |
| 1:A:7:ASP:CG | 1:O:4:ASN:HD21 | 2.23 | 0.40 |
| 1:B:52:ILE:O | 1:B:56:GLU:HG2 | 2.22 | 0.40 |
| 1:C:73:GLU:HA | 1:C:74:PRO:HD3 | 1.97 | 0.40 |
| 1:D:29:GLN:NE2 | 1:D:83:VAL:H | 2.02 | 0.40 |
| 1:H:128:ILE:O | 1:H:132:GLU:HG2 | 2.22 | 0.40 |
| 1:K:168[B]:SER:HB3 | 5:L:2108[B]:FEC:O2C | 2.11 | 0.40 |
| 1:L:75:THR:HG1 | 1:L:77[B]:GLN:HG3 | 1.86 | 0.40 |
| 1:M:58[B]:ARG:NH2 | 1:N:168[B]:SER:HB3 | 2.37 | 0.40 |

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:1802:SO4:S | 3:L:2102:SO4:S[9_465] | 0.16 | 2.04 |
| 3:I:1802:SO4:O1 | 3:L:2102:SO4:O3[9_465] | 0.22 | 1.98 |
| 3:I:1802:SO4:O4 | 3:L:2102:SO4:O2[9_465] | 0.35 | 1.85 |
| 3:I:1802:SO4:O2 | 3:L:2102:SO4:O4[9_465] | 0.37 | 1.83 |
| 3:I:1802:SO4:O3 | 3:L:2102:SO4:O1[9_465] | 0.49 | 1.71 |
| 3:I:1802:SO4:O3 | 3:L:2102:SO4:O2[9_465] | 2.14 | 0.06 |
| 3:I:1802:SO4:O2 | 3:L:2102:SO4:O1[9_465] | 2.18 | 0.02 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 171/179 (96%) | 170 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | B | 173/179 (97%) | 170 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | C | 172/179 (96%) | 169 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | D | 174/179 (97%) | 173 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | E | 173/179 (97%) | 170 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | F | 172/179 (96%) | 170 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | G | 173/179 (97%) | 171 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | H | 173/179 (97%) | 171 (99%) | 0 | 2 (1%) | 13 | 4 |
| 1 | I | 173/179 (97%) | 168 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | J | 172/179 (96%) | 169 (98%) | 1 (1%) | 2 (1%) | 13 | 4 |
| 1 | K | 173/179 (97%) | 169 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | L | 173/179 (97%) | 168 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | M | 172/179 (96%) | 170 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | N | 172/179 (96%) | 169 (98%) | 1 (1%) | 2 (1%) | 13 | 4 |
| 1 | O | 172/179 (96%) | 170 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | P | 173/179 (97%) | 168 (97%) | 3 (2%) | 2 (1%) | 13 | 4 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 2761/2864 (96%) | 2715 (98%) | 38 (1%) | 8 (0%) | 51 30 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 169[A] | LYS |
| 1 | H | 169[B] | LYS |
| 1 | J | 168[A] | SER |
| 1 | J | 168[B] | SER |
| 1 | N | 169[A] | LYS |
| 1 | N | 169[B] | LYS |
| 1 | P | 169[A] | LYS |
| 1 | P | 169[B] | LYS |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 143/145 (99%) | 140 (98%) | 3 (2%) | 53 46 |
| 1 | B | 144/145 (99%) | 138 (96%) | 6 (4%) | 30 17 |
| 1 | C | 142/145 (98%) | 130 (92%) | 12 (8%) | 10 3 |
| 1 | D | 145/145 (100%) | 138 (95%) | 7 (5%) | 25 12 |
| 1 | E | 144/145 (99%) | 143 (99%) | 1 (1%) | 84 82 |
| 1 | F | 143/145 (99%) | 137 (96%) | 6 (4%) | 30 17 |
| 1 | G | 145/145 (100%) | 144 (99%) | 1 (1%) | 84 82 |
| 1 | H | 143/145 (99%) | 136 (95%) | 7 (5%) | 25 12 |
| 1 | I | 145/145 (100%) | 141 (97%) | 4 (3%) | 43 33 |
| 1 | J | 143/145 (99%) | 137 (96%) | 6 (4%) | 30 17 |
| 1 | K | 144/145 (99%) | 140 (97%) | 4 (3%) | 43 33 |
| 1 | L | 144/145 (99%) | 139 (96%) | 5 (4%) | 36 24 |
| 1 | M | 144/145 (99%) | 143 (99%) | 1 (1%) | 84 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | N | 143/145 (99%) | 139 (97%) | 4 (3%) | 43 | 33 |
| 1 | O | 143/145 (99%) | 142 (99%) | 1 (1%) | 84 | 82 |
| 1 | P | 145/145 (100%) | 140 (97%) | 5 (3%) | 37 | 25 |
| All | All | 2300/2320 (99%) | 2227 (97%) | 73 (3%) | 44 | 27 |

All (73) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4 | ASN |
| 1 | A | 78 | LYS |
| 1 | A | 144 | SER |
| 1 | B | 81 | LYS |
| 1 | B | 93[A] | GLU |
| 1 | B | 93[B] | GLU |
| 1 | B | 104 | GLU |
| 1 | B | 147 | LYS |
| 1 | B | 166 | THR |
| 1 | C | 4 | ASN |
| 1 | C | 7 | ASP |
| 1 | C | 77 | GLN |
| 1 | C | 111 | LYS |
| 1 | C | 114 | LYS |
| 1 | C | 152[A] | THR |
| 1 | C | 152[B] | THR |
| 1 | C | 163 | SER |
| 1 | C | 168[A] | SER |
| 1 | C | 168[B] | SER |
| 1 | C | 169[A] | LYS |
| 1 | C | 169[B] | LYS |
| 1 | D | 4 | ASN |
| 1 | D | 7 | ASP |
| 1 | D | 77[A] | GLN |
| 1 | D | 77[B] | GLN |
| 1 | D | 81 | LYS |
| 1 | D | 169[A] | LYS |
| 1 | D | 169[B] | LYS |
| 1 | E | 147 | LYS |
| 1 | F | 4 | ASN |
| 1 | F | 77 | GLN |
| 1 | F | 81 | LYS |
| 1 | F | 111 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 147 | LYS |
| 1 | F | 156 | LYS |
| 1 | G | 108 | GLN |
| 1 | H | 4 | ASN |
| 1 | H | 11 | LYS |
| 1 | H | 58[A] | ARG |
| 1 | H | 58[B] | ARG |
| 1 | H | 81 | LYS |
| 1 | H | 110 | LEU |
| 1 | H | 111 | LYS |
| 1 | I | 4 | ASN |
| 1 | I | 77 | GLN |
| 1 | I | 81 | LYS |
| 1 | I | 147 | LYS |
| 1 | J | 4 | ASN |
| 1 | J | 81 | LYS |
| 1 | J | 146 | ILE |
| 1 | J | 152 | THR |
| 1 | J | 169[A] | LYS |
| 1 | J | 169[B] | LYS |
| 1 | K | 7 | ASP |
| 1 | K | 77 | GLN |
| 1 | K | 169[A] | LYS |
| 1 | K | 169[B] | LYS |
| 1 | L | 4 | ASN |
| 1 | L | 77[A] | GLN |
| 1 | L | 77[B] | GLN |
| 1 | L | 81 | LYS |
| 1 | L | 110 | LEU |
| 1 | M | 7 | ASP |
| 1 | N | 4 | ASN |
| 1 | N | 58[A] | ARG |
| 1 | N | 58[B] | ARG |
| 1 | N | 77 | GLN |
| 1 | O | 163 | SER |
| 1 | P | 4 | ASN |
| 1 | P | 6 | GLU |
| 1 | P | 93[A] | GLU |
| 1 | P | 93[B] | GLU |
| 1 | P | 144 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 33 | GLN |
| 1 | B | 4 | ASN |
| 1 | B | 29 | GLN |
| 1 | B | 62 | ASN |
| 1 | B | 133 | GLN |
| 1 | B | 145 | HIS |
| 1 | C | 32 | ASN |
| 1 | C | 33 | GLN |
| 1 | D | 4 | ASN |
| 1 | D | 29 | GLN |
| 1 | D | 62 | ASN |
| 1 | E | 32 | ASN |
| 1 | E | 33 | GLN |
| 1 | F | 4 | ASN |
| 1 | F | 29 | GLN |
| 1 | F | 62 | ASN |
| 1 | F | 133 | GLN |
| 1 | F | 145 | HIS |
| 1 | G | 4 | ASN |
| 1 | G | 32 | ASN |
| 1 | G | 33 | GLN |
| 1 | H | 4 | ASN |
| 1 | H | 29 | GLN |
| 1 | H | 62 | ASN |
| 1 | H | 133 | GLN |
| 1 | I | 32 | ASN |
| 1 | I | 33 | GLN |
| 1 | J | 4 | ASN |
| 1 | J | 29 | GLN |
| 1 | J | 62 | ASN |
| 1 | J | 133 | GLN |
| 1 | K | 32 | ASN |
| 1 | K | 33 | GLN |
| 1 | K | 77 | GLN |
| 1 | L | 4 | ASN |
| 1 | L | 29 | GLN |
| 1 | L | 148 | ASN |
| 1 | M | 4 | ASN |
| 1 | M | 32 | ASN |
| 1 | M | 33 | GLN |
| 1 | N | 4 | ASN |
| 1 | N | 29 | GLN |
| 1 | N | 62 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 133 | GLN |
| 1 | N | 145 | HIS |
| 1 | N | 148 | ASN |
| 1 | O | 32 | ASN |
| 1 | O | 33 | GLN |
| 1 | P | 4 | ASN |
| 1 | P | 29 | GLN |
| 1 | P | 62 | ASN |
| 1 | P | 98 | GLN |
| 1 | P | 133 | GLN |
| 1 | P | 145 | HIS |
| 1 | P | 148 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 124 ligands modelled in this entry, 32 are monoatomic - leaving 92 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 | $\#\|Z\| > 2$ |
| 3 | SO4 | H | 1706 | - | 4,4,4 | 0.46 | 0 | 6,6,6 | 0.87 | 0 |
| 4 | GOL | K | 2011 | - | 5,5,5 | 4.44 | 5 (100%) | 5,5,5 | 4.81 | 3 (60%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | SO4 | P | 2506 | - | 4,4,4 | 0.46 | 0 | 6,6,6 | 0.56 | 0 |
| 4 | GOL | G | 1611 | - | 5,5,5 | 4.39 | 5 (100%) | 5,5,5 | 4.39 | 3 (60%) |
| 3 | SO4 | P | 2501 | - | 4,4,4 | 1.91 | 1 (25%) | 6,6,6 | 0.91 | 0 |
| 3 | SO4 | G | 1603 | - | 4,4,4 | 2.02 | 1 (25%) | 6,6,6 | 0.89 | 0 |
| 4 | GOL | I | 1810 | 1 | 5,5,5 | 4.38 | 5 (100%) | 5,5,5 | 3.88 | 3 (60%) |
| 3 | SO4 | I | 1806 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.60 | 0 |
| 4 | GOL | E | 1411 | - | 5,5,5 | 4.45 | 5 (100%) | 5,5,5 | 4.19 | 3 (60%) |
| 4 | GOL | F | 1512 | - | 5,5,5 | 4.54 | 5 (100%) | 5,5,5 | 3.72 | 3 (60%) |
| 3 | SO4 | M | 2206 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.40 | 0 |
| 3 | SO4 | A | 1004 | - | 4,4,4 | 1.88 | 1 (25%) | 6,6,6 | 0.92 | 0 |
| 3 | SO4 | A | 1008 | - | 4,4,4 | 0.53 | 0 | 6,6,6 | 2.46 | 2 (33%) |
| 5 | FEC | I | 1807[B] | 1 | 40,56,56 | 1.21 | 4 (10%) | 42,90,90 | 2.03 | 12 (28%) |
| 3 | SO4 | L | 2102 | 3 | 4,4,4 | 1.95 | 1 (25%) | 6,6,6 | 0.86 | 0 |
| 4 | GOL | J | 1811 | - | 5,5,5 | 4.52 | 5 (100%) | 5,5,5 | 5.39 | 3 (60%) |
| 5 | FEC | L | 2108[B] | 1 | 40,56,56 | 1.26 | 4 (10%) | 42,90,90 | 1.78 | 9 (21%) |
| 3 | SO4 | K | 2001 | - | 4,4,4 | 1.93 | 1 (25%) | 6,6,6 | 0.95 | 0 |
| 5 | FEC | P | 2507[A] | 1 | 40,56,56 | 1.21 | 4 (10%) | 42,90,90 | 1.97 | 12 (28%) |
| 3 | SO4 | K | 1504 | - | 4,4,4 | 1.94 | 1 (25%) | 6,6,6 | 0.86 | 0 |
| 4 | GOL | B | 1110 | - | 5,5,5 | 4.51 | 5 (100%) | 5,5,5 | 4.49 | 3 (60%) |
| 4 | GOL | M | 2211 | - | 5,5,5 | 4.52 | 5 (100%) | 5,5,5 | 4.58 | 3 (60%) |
| 4 | GOL | P | 2510 | - | 5,5,5 | 4.46 | 5 (100%) | 5,5,5 | 4.69 | 3 (60%) |
| 5 | FEC | D | 1311[A] | 1 | 40,56,56 | 1.25 | 4 (10%) | 42,90,90 | 2.01 | 13 (30%) |
| 5 | FEC | M | 2207[B] | 1 | 40,56,56 | 1.28 | 4 (10%) | 42,90,90 | 1.69 | 14 (33%) |
| 3 | SO4 | B | 1005 | - | 4,4,4 | 0.53 | 0 | 6,6,6 | 2.46 | 2 (33%) |
| 4 | GOL | D | 1211 | - | 5,5,5 | 4.50 | 5 (100%) | 5,5,5 | 4.66 | 3 (60%) |
| 4 | GOL | I | 1713 | - | 5,5,5 | 4.48 | 5 (100%) | 5,5,5 | 5.59 | 3 (60%) |
| 3 | SO4 | B | 1106 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 1.50 | 0 |
| 4 | GOL | M | 2210 | 1 | 5,5,5 | 4.51 | 5 (100%) | 5,5,5 | 4.39 | 2 (40%) |
| 4 | GOL | H | 1710 | - | 5,5,5 | 4.53 | 5 (100%) | 5,5,5 | 5.65 | 3 (60%) |
| 3 | SO4 | L | 2107 | - | 4,4,4 | 1.94 | 1 (25%) | 6,6,6 | 0.86 | 0 |
| 3 | SO4 | O | 2406 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 1.07 | 0 |
| 4 | GOL | E | 1410 | - | 5,5,5 | 4.53 | 5 (100%) | 5,5,5 | 4.34 | 3 (60%) |
| 3 | SO4 | D | 1303 | - | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.60 | 0 |
| 4 | GOL | J | 1910 | - | 5,5,5 | 4.56 | 5 (100%) | 5,5,5 | 4.88 | 3 (60%) |
| 5 | FEC | L | 2108[A] | 1 | 40,56,56 | 1.25 | 3 (7%) | 42,90,90 | 1.84 | 11 (26%) |
| 4 | GOL | O | 2411 | - | 5,5,5 | 4.42 | 5 (100%) | 5,5,5 | 3.91 | 3 (60%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | SO4 | F | 1502 | - | 4,4,4 | 1.91 | 1 (25%) | 6,6,6 | 0.92 | 0 |
| 5 | FEC | F | 1507[B] | 1 | 40,56,56 | 1.25 | 4 (10%) | 42,90,90 | 1.91 | 10 (23%) |
| 3 | SO4 | A | 1105 | - | 4,4,4 | 0.53 | 0 | 6,6,6 | 2.46 | 2 (33%) |
| 3 | SO4 | C | 1201 | - | 4,4,4 | 1.93 | 1 (25%) | 6,6,6 | 0.93 | 0 |
| 3 | SO4 | H | 1703 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.58 | 0 |
| 6 | 3PY | D | 1310 | 1 | 5,5,6 | 12.83 | 5 (100%) | 5,5,7 | 7.82 | 5 (100%) |
| 3 | SO4 | N | 2303 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.81 | 0 |
| 3 | SO4 | F | 1501 | - | 4,4,4 | 2.02 | 1 (25%) | 6,6,6 | 0.84 | 0 |
| 3 | SO4 | N | 2306 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.76 | 0 |
| 3 | SO4 | B | 1104 | - | 4,4,4 | 2.02 | 1 (25%) | 6,6,6 | 0.89 | 0 |
| 3 | SO4 | D | 1301 | - | 4,4,4 | 1.99 | 1 (25%) | 6,6,6 | 0.88 | 0 |
| 3 | SO4 | O | 2409 | - | 4,4,4 | 0.46 | 0 | 6,6,6 | 0.56 | 0 |
| 3 | SO4 | P | 2503 | - | 4,4,4 | 0.20 | 0 | 6,6,6 | 0.92 | 0 |
| 3 | SO4 | F | 1506 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 1.31 | 1 (16%) |
| 3 | SO4 | A | 1001 | - | 4,4,4 | 1.80 | 1 (25%) | 6,6,6 | 0.94 | 0 |
| 3 | SO4 | I | 1801 | - | 4,4,4 | 1.93 | 1 (25%) | 6,6,6 | 0.92 | 0 |
| 3 | SO4 | L | 2101 | - | 4,4,4 | 1.91 | 1 (25%) | 6,6,6 | 0.92 | 0 |
| 5 | FEC | G | 1608[B] | 1 | 40,56,56 | 1.23 | 4 (10%) | 42,90,90 | 1.92 | 14 (33%) |
| 4 | GOL | F | 1510 | - | 5,5,5 | 4.45 | 5 (100%) | 5,5,5 | 4.78 | 3 (60%) |
| 3 | SO4 | C | 1206 | - | 4,4,4 | 0.34 | 0 | 6,6,6 | 0.63 | 0 |
| 3 | SO4 | B | 1101 | - | 4,4,4 | 1.88 | 1 (25%) | 6,6,6 | 0.92 | 0 |
| 3 | SO4 | J | 1904 | - | 4,4,4 | 1.93 | 1 (25%) | 6,6,6 | 0.91 | 0 |
| 5 | FEC | F | 1507[A] | 1 | 40,56,56 | 1.28 | 4 (10%) | 42,90,90 | 1.69 | 13 (30%) |
| 5 | FEC | I | 1807[A] | 1 | 40,56,56 | 1.22 | 4 (10%) | 42,90,90 | 1.93 | 13 (30%) |
| 3 | SO4 | G | 1606 | - | 4,4,4 | 0.24 | 0 | 6,6,6 | 0.71 | 0 |
| 3 | SO4 | E | 1304 | 1 | 4,4,4 | 1.92 | 1 (25%) | 6,6,6 | 0.93 | 0 |
| 3 | SO4 | H | 1701 | - | 4,4,4 | 1.84 | 1 (25%) | 6,6,6 | 0.84 | 0 |
| 3 | SO4 | L | 2103 | 1 | 4,4,4 | 1.94 | 1 (25%) | 6,6,6 | 0.86 | 0 |
| 3 | SO4 | J | 1906 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.95 | 0 |
| 5 | FEC | B | 1107[B] | 1 | 40,56,56 | 1.21 | 3 (7%) | 42,90,90 | 2.01 | 11 (26%) |
| 3 | SO4 | E | 1406 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 1.22 | 1 (16%) |
| 3 | SO4 | M | 2201 | - | 4,4,4 | 1.89 | 1 (25%) | 6,6,6 | 0.93 | 0 |
| 3 | SO4 | I | 1803 | - | 4,4,4 | 0.33 | 0 | 6,6,6 | 0.49 | 0 |
| 3 | SO4 | E | 1401 | - | 4,4,4 | 1.92 | 1 (25%) | 6,6,6 | 0.96 | 0 |
| 5 | FEC | M | 2207[A] | 1 | 40,56,56 | 1.26 | 4 (10%) | 42,90,90 | 1.74 | 10 (23%) |
| 4 | GOL | C | 1210 | - | 5,5,5 | 4.37 | 5 (100%) | 5,5,5 | 4.98 | 3 (60%) |
| 3 | SO4 | C | 1203 | - | 4,4,4 | 0.40 | 0 | 6,6,6 | 0.98 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | FEC | G | 1608[A] | 1 | 40,56,56 | 1.22 | 4 (10%) | 42,90,90 | 1.83 | 14 (33%) |
| 4 | GOL | G | 1610 | - | 5,5,5 | 4.53 | 5 (100%) | 5,5,5 | 5.68 | 3 (60%) |
| 3 | SO4 | A | 1006 | - | 4,4,4 | 0.24 | 0 | 6,6,6 | 1.10 | 0 |
| 4 | GOL | N | 2310 | - | 5,5,5 | 4.51 | 5 (100%) | 5,5,5 | 5.50 | 3 (60%) |
| 3 | SO4 | J | 1901 | - | 4,4,4 | 1.89 | 1 (25%) | 6,6,6 | 0.84 | 0 |
| 4 | GOL | B | 1011 | - | 5,5,5 | 4.62 | 5 (100%) | 5,5,5 | 4.00 | 3 (60%) |
| 3 | SO4 | K | 2006 | - | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.67 | 0 |
| 3 | SO4 | N | 2301 | - | 4,4,4 | 1.94 | 1 (25%) | 6,6,6 | 0.81 | 0 |
| 3 | SO4 | I | 1802 | 3 | 4,4,4 | 1.96 | 2 (50%) | 6,6,6 | 0.79 | 0 |
| 4 | GOL | O | 2410 | - | 5,5,5 | 4.40 | 5 (100%) | 5,5,5 | 4.82 | 3 (60%) |
| 4 | GOL | H | 1814 | - | 5,5,5 | 4.64 | 5 (100%) | 5,5,5 | 4.75 | 3 (60%) |
| 5 | FEC | P | 2507[B] | 1 | 40,56,56 | 1.19 | 4 (10%) | 42,90,90 | 2.08 | 13 (30%) |
| 3 | SO4 | K | 2003 | - | 4,4,4 | 1.91 | 1 (25%) | 6,6,6 | 0.92 | 0 |
| 5 | FEC | B | 1107[A] | 1 | 40,56,56 | 1.21 | 3 (7%) | 42,90,90 | 1.93 | 12 (28%) |
| 3 | SO4 | G | 1607 | - | 4,4,4 | 0.34 | 0 | 6,6,6 | 0.49 | 0 |
| 4 | GOL | A | 1010 | - | 5,5,5 | 4.64 | 5 (100%) | 5,5,5 | 5.84 | 3 (60%) |
| 5 | FEC | D | 1311[B] | 1 | 40,56,56 | 1.23 | 4 (10%) | 42,90,90 | 1.69 | 9 (21%) |

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 |
|---|---|---|---|---|---|---|---|
| 4 | GOL | K | 2011 | - | - | 2/4/4/4 | - |
| 5 | FEC | G | 1608[A] | 1 | - | 10/20/120/120 | - |
| 4 | GOL | D | 1211 | - | - | 3/4/4/4 | - |
| 4 | GOL | G | 1611 | - | - | 2/4/4/4 | - |
| 4 | GOL | G | 1610 | - | - | 3/4/4/4 | - |
| 4 | GOL | I | 1713 | - | - | 3/4/4/4 | - |
| 4 | GOL | I | 1810 | 1 | - | 3/4/4/4 | - |
| 5 | FEC | G | 1608[B] | 1 | - | 9/20/120/120 | - |
| 4 | GOL | N | 2310 | - | - | 4/4/4/4 | - |
| 4 | GOL | F | 1510 | - | - | 2/4/4/4 | - |
| 4 | GOL | F | 1512 | - | - | 2/4/4/4 | - |
| 4 | GOL | E | 1411 | - | - | 4/4/4/4 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | GOL | M | 2210 | 1 | - | 2/4/4/4 | - |
| 4 | GOL | H | 1710 | - | - | 2/4/4/4 | - |
| 4 | GOL | E | 1410 | - | - | 2/4/4/4 | - |
| 4 | GOL | B | 1011 | - | - | 2/4/4/4 | - |
| 5 | FEC | F | 1507[A] | 1 | - | 8/20/120/120 | - |
| 5 | FEC | I | 1807[A] | 1 | - | 10/20/120/120 | - |
| 4 | GOL | J | 1910 | - | - | 2/4/4/4 | - |
| 5 | FEC | I | 1807[B] | 1 | - | 13/20/120/120 | - |
| 5 | FEC | L | 2108[A] | 1 | - | 9/20/120/120 | - |
| 4 | GOL | O | 2411 | - | - | 4/4/4/4 | - |
| 5 | FEC | F | 1507[B] | 1 | - | 6/20/120/120 | - |
| 4 | GOL | J | 1811 | - | - | 3/4/4/4 | - |
| 5 | FEC | L | 2108[B] | 1 | - | 9/20/120/120 | - |
| 5 | FEC | P | 2507[A] | 1 | - | 8/20/120/120 | - |
| 4 | GOL | O | 2410 | - | - | 3/4/4/4 | - |
| 4 | GOL | H | 1814 | - | - | 3/4/4/4 | - |
| 5 | FEC | P | 2507[B] | 1 | - | 10/20/120/120 | - |
| 5 | FEC | B | 1107[A] | 1 | - | 9/20/120/120 | - |
| 4 | GOL | B | 1110 | - | - | 2/4/4/4 | - |
| 4 | GOL | M | 2211 | - | - | 2/4/4/4 | - |
| 4 | GOL | P | 2510 | - | - | 2/4/4/4 | - |
| 5 | FEC | B | 1107[B] | 1 | - | 8/20/120/120 | - |
| 5 | FEC | D | 1311[A] | 1 | - | 10/20/120/120 | - |
| 4 | GOL | A | 1010 | - | - | 2/4/4/4 | - |
| 6 | 3PY | D | 1310 | 1 | - | 0/1/4/6 | - |
| 5 | FEC | D | 1311[B] | 1 | - | 8/20/120/120 | - |
| 5 | FEC | M | 2207[A] | 1 | - | 10/20/120/120 | - |
| 5 | FEC | M | 2207[B] | 1 | - | 8/20/120/120 | - |
| 4 | GOL | C | 1210 | - | - | 2/4/4/4 | - |

All (213) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | D | 1310 | 3PY | C3-C2 | -20.42 | 1.21 | 1.51 |
| 6 | D | 1310 | 3PY | O1-C1 | 17.86 | 1.63 | 1.22 |
| 4 | A | 1010 | GOL | C3-C2 | -7.61 | 1.20 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | H | 1710 | GOL | C3-C2 | -7.43 | 1.21 | 1.51 |
| 6 | D | 1310 | 3PY | O3-C2 | 7.39 | 1.35 | 1.23 |
| 4 | J | 1811 | GOL | C3-C2 | -7.38 | 1.21 | 1.51 |
| 4 | G | 1610 | GOL | C3-C2 | -7.35 | 1.21 | 1.51 |
| 4 | N | 2310 | GOL | C3-C2 | -7.31 | 1.21 | 1.51 |
| 4 | D | 1211 | GOL | C3-C2 | -7.28 | 1.21 | 1.51 |
| 4 | I | 1713 | GOL | C3-C2 | -7.26 | 1.21 | 1.51 |
| 4 | K | 2011 | GOL | C3-C2 | -7.25 | 1.21 | 1.51 |
| 4 | E | 1410 | GOL | C3-C2 | -7.22 | 1.22 | 1.51 |
| 4 | C | 1210 | GOL | C3-C2 | -7.22 | 1.22 | 1.51 |
| 4 | H | 1814 | GOL | C3-C2 | -7.22 | 1.22 | 1.51 |
| 4 | B | 1011 | GOL | C3-C2 | -7.21 | 1.22 | 1.51 |
| 4 | J | 1910 | GOL | C3-C2 | -7.20 | 1.22 | 1.51 |
| 4 | M | 2211 | GOL | C3-C2 | -7.20 | 1.22 | 1.51 |
| 4 | P | 2510 | GOL | C3-C2 | -7.18 | 1.22 | 1.51 |
| 4 | M | 2210 | GOL | C3-C2 | -7.17 | 1.22 | 1.51 |
| 4 | O | 2410 | GOL | C3-C2 | -7.17 | 1.22 | 1.51 |
| 4 | B | 1110 | GOL | C3-C2 | -7.15 | 1.22 | 1.51 |
| 4 | G | 1611 | GOL | C3-C2 | -7.08 | 1.22 | 1.51 |
| 4 | F | 1512 | GOL | C3-C2 | -7.08 | 1.22 | 1.51 |
| 4 | F | 1510 | GOL | C3-C2 | -7.02 | 1.22 | 1.51 |
| 4 | E | 1411 | GOL | C3-C2 | -7.01 | 1.22 | 1.51 |
| 4 | O | 2411 | GOL | C3-C2 | -6.88 | 1.23 | 1.51 |
| 4 | I | 1810 | GOL | C3-C2 | -6.86 | 1.23 | 1.51 |
| 6 | D | 1310 | 3PY | O4-C3 | 5.03 | 1.59 | 1.41 |
| 4 | B | 1011 | GOL | O1-C1 | 4.89 | 1.63 | 1.42 |
| 4 | F | 1510 | GOL | O1-C1 | 4.80 | 1.62 | 1.42 |
| 4 | A | 1010 | GOL | O1-C1 | 4.77 | 1.62 | 1.42 |
| 4 | N | 2310 | GOL | O1-C1 | 4.75 | 1.62 | 1.42 |
| 4 | O | 2411 | GOL | O1-C1 | 4.74 | 1.62 | 1.42 |
| 4 | H | 1710 | GOL | O1-C1 | 4.73 | 1.62 | 1.42 |
| 4 | H | 1814 | GOL | O1-C1 | 4.71 | 1.62 | 1.42 |
| 4 | M | 2210 | GOL | O1-C1 | 4.70 | 1.62 | 1.42 |
| 4 | E | 1411 | GOL | O1-C1 | 4.69 | 1.62 | 1.42 |
| 4 | D | 1211 | GOL | O1-C1 | 4.68 | 1.62 | 1.42 |
| 4 | J | 1811 | GOL | O1-C1 | 4.63 | 1.62 | 1.42 |
| 4 | M | 2211 | GOL | O1-C1 | 4.62 | 1.61 | 1.42 |
| 4 | G | 1611 | GOL | O1-C1 | 4.58 | 1.61 | 1.42 |
| 4 | F | 1512 | GOL | O1-C1 | 4.55 | 1.61 | 1.42 |
| 4 | J | 1910 | GOL | O1-C1 | 4.54 | 1.61 | 1.42 |
| 4 | I | 1810 | GOL | O1-C1 | 4.51 | 1.61 | 1.42 |
| 4 | G | 1610 | GOL | O1-C1 | 4.50 | 1.61 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 1410 | GOL | O1-C1 | 4.50 | 1.61 | 1.42 |
| 4 | B | 1110 | GOL | O1-C1 | 4.49 | 1.61 | 1.42 |
| 4 | K | 2011 | GOL | O1-C1 | 4.46 | 1.61 | 1.42 |
| 4 | P | 2510 | GOL | O1-C1 | 4.40 | 1.61 | 1.42 |
| 4 | I | 1713 | GOL | O1-C1 | 4.40 | 1.61 | 1.42 |
| 4 | O | 2410 | GOL | O1-C1 | 4.25 | 1.60 | 1.42 |
| 4 | C | 1210 | GOL | O1-C1 | 4.25 | 1.60 | 1.42 |
| 4 | E | 1410 | GOL | O3-C3 | 4.02 | 1.59 | 1.42 |
| 4 | G | 1611 | GOL | O3-C3 | 3.99 | 1.59 | 1.42 |
| 4 | J | 1910 | GOL | O3-C3 | 3.93 | 1.59 | 1.42 |
| 4 | I | 1810 | GOL | O3-C3 | 3.86 | 1.58 | 1.42 |
| 4 | F | 1512 | GOL | O3-C3 | 3.86 | 1.58 | 1.42 |
| 4 | E | 1411 | GOL | O3-C3 | 3.86 | 1.58 | 1.42 |
| 4 | M | 2210 | GOL | O3-C3 | 3.86 | 1.58 | 1.42 |
| 4 | H | 1814 | GOL | O3-C3 | 3.83 | 1.58 | 1.42 |
| 4 | B | 1011 | GOL | O3-C3 | 3.82 | 1.58 | 1.42 |
| 4 | B | 1110 | GOL | O3-C3 | 3.82 | 1.58 | 1.42 |
| 4 | O | 2411 | GOL | O3-C3 | 3.75 | 1.58 | 1.42 |
| 4 | I | 1713 | GOL | O3-C3 | 3.75 | 1.58 | 1.42 |
| 4 | M | 2211 | GOL | O3-C3 | 3.67 | 1.57 | 1.42 |
| 4 | O | 2410 | GOL | O3-C3 | 3.66 | 1.57 | 1.42 |
| 4 | P | 2510 | GOL | O3-C3 | 3.66 | 1.57 | 1.42 |
| 3 | B | 1104 | SO4 | O1-S | 3.65 | 1.65 | 1.46 |
| 3 | G | 1603 | SO4 | O1-S | 3.64 | 1.65 | 1.46 |
| 4 | K | 2011 | GOL | O3-C3 | 3.60 | 1.57 | 1.42 |
| 4 | A | 1010 | GOL | O3-C3 | 3.59 | 1.57 | 1.42 |
| 4 | F | 1510 | GOL | O3-C3 | 3.57 | 1.57 | 1.42 |
| 3 | F | 1501 | SO4 | O1-S | 3.56 | 1.65 | 1.46 |
| 4 | C | 1210 | GOL | O3-C3 | 3.54 | 1.57 | 1.42 |
| 4 | J | 1811 | GOL | O3-C3 | 3.53 | 1.57 | 1.42 |
| 3 | D | 1301 | SO4 | O1-S | 3.52 | 1.65 | 1.46 |
| 4 | D | 1211 | GOL | O3-C3 | 3.52 | 1.57 | 1.42 |
| 4 | N | 2310 | GOL | O3-C3 | 3.49 | 1.57 | 1.42 |
| 3 | L | 2102 | SO4 | O1-S | 3.48 | 1.64 | 1.46 |
| 3 | L | 2103 | SO4 | O1-S | 3.48 | 1.64 | 1.46 |
| 3 | K | 1504 | SO4 | O1-S | 3.47 | 1.64 | 1.46 |
| 4 | H | 1710 | GOL | O3-C3 | 3.47 | 1.57 | 1.42 |
| 3 | L | 2107 | SO4 | O1-S | 3.46 | 1.64 | 1.46 |
| 3 | N | 2301 | SO4 | O1-S | 3.45 | 1.64 | 1.46 |
| 3 | E | 1401 | SO4 | O1-S | 3.45 | 1.64 | 1.46 |
| 3 | C | 1201 | SO4 | O1-S | 3.45 | 1.64 | 1.46 |
| 3 | E | 1304 | SO4 | O1-S | 3.44 | 1.64 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | G | 1610 | GOL | O3-C3 | 3.41 | 1.56 | 1.42 |
| 3 | F | 1502 | SO4 | O1-S | 3.39 | 1.64 | 1.46 |
| 3 | P | 2501 | SO4 | O1-S | 3.39 | 1.64 | 1.46 |
| 3 | K | 2003 | SO4 | O1-S | 3.38 | 1.64 | 1.46 |
| 3 | K | 2001 | SO4 | O1-S | 3.38 | 1.64 | 1.46 |
| 3 | I | 1801 | SO4 | O1-S | 3.38 | 1.64 | 1.46 |
| 3 | J | 1904 | SO4 | O1-S | 3.37 | 1.64 | 1.46 |
| 3 | J | 1901 | SO4 | O1-S | 3.36 | 1.64 | 1.46 |
| 3 | L | 2101 | SO4 | O1-S | 3.36 | 1.64 | 1.46 |
| 3 | B | 1101 | SO4 | O1-S | 3.35 | 1.64 | 1.46 |
| 3 | A | 1004 | SO4 | O1-S | 3.34 | 1.64 | 1.46 |
| 3 | M | 2201 | SO4 | O1-S | 3.30 | 1.63 | 1.46 |
| 3 | I | 1802 | SO4 | O1-S | 3.30 | 1.63 | 1.46 |
| 3 | H | 1701 | SO4 | O1-S | 3.21 | 1.63 | 1.46 |
| 4 | H | 1814 | GOL | O2-C2 | -3.16 | 1.34 | 1.43 |
| 4 | B | 1011 | GOL | C1-C2 | -3.08 | 1.39 | 1.51 |
| 4 | F | 1512 | GOL | C1-C2 | -3.08 | 1.39 | 1.51 |
| 3 | A | 1001 | SO4 | O1-S | 3.07 | 1.62 | 1.46 |
| 4 | G | 1610 | GOL | C1-C2 | -2.96 | 1.39 | 1.51 |
| 4 | H | 1814 | GOL | C1-C2 | -2.96 | 1.39 | 1.51 |
| 4 | J | 1910 | GOL | C1-C2 | -2.95 | 1.39 | 1.51 |
| 4 | E | 1410 | GOL | C1-C2 | -2.93 | 1.39 | 1.51 |
| 4 | C | 1210 | GOL | C1-C2 | -2.90 | 1.39 | 1.51 |
| 4 | A | 1010 | GOL | C1-C2 | -2.88 | 1.39 | 1.51 |
| 4 | I | 1810 | GOL | C1-C2 | -2.88 | 1.39 | 1.51 |
| 5 | L | 2108[B] | FEC | CMB-C2B | 2.86 | 1.55 | 1.50 |
| 4 | O | 2411 | GOL | C1-C2 | -2.86 | 1.40 | 1.51 |
| 5 | M | 2207[B] | FEC | CMD-C2D | 2.86 | 1.55 | 1.50 |
| 4 | M | 2211 | GOL | C1-C2 | -2.85 | 1.40 | 1.51 |
| 4 | B | 1110 | GOL | O2-C2 | -2.83 | 1.34 | 1.43 |
| 4 | I | 1713 | GOL | C1-C2 | -2.82 | 1.40 | 1.51 |
| 5 | B | 1107[B] | FEC | CMD-C2D | 2.81 | 1.55 | 1.50 |
| 4 | G | 1610 | GOL | O2-C2 | -2.81 | 1.35 | 1.43 |
| 5 | M | 2207[A] | FEC | CMB-C2B | 2.80 | 1.55 | 1.50 |
| 4 | B | 1110 | GOL | C1-C2 | -2.78 | 1.40 | 1.51 |
| 4 | F | 1512 | GOL | O2-C2 | -2.78 | 1.35 | 1.43 |
| 4 | D | 1211 | GOL | C1-C2 | -2.77 | 1.40 | 1.51 |
| 4 | P | 2510 | GOL | O2-C2 | -2.76 | 1.35 | 1.43 |
| 4 | N | 2310 | GOL | C1-C2 | -2.76 | 1.40 | 1.51 |
| 4 | H | 1710 | GOL | O2-C2 | -2.76 | 1.35 | 1.43 |
| 4 | P | 2510 | GOL | C1-C2 | -2.75 | 1.40 | 1.51 |
| 4 | O | 2410 | GOL | C1-C2 | -2.73 | 1.40 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | L | 2108[A] | FEC | CMB-C2B | 2.72 | 1.55 | 1.50 |
| 5 | B | 1107[A] | FEC | CMD-C2D | 2.72 | 1.55 | 1.50 |
| 4 | J | 1910 | GOL | O2-C2 | -2.72 | 1.35 | 1.43 |
| 5 | G | 1608[B] | FEC | CMB-C2B | 2.72 | 1.55 | 1.50 |
| 5 | L | 2108[A] | FEC | CMD-C2D | 2.71 | 1.55 | 1.50 |
| 5 | P | 2507[A] | FEC | CMD-C2D | 2.71 | 1.55 | 1.50 |
| 4 | M | 2211 | GOL | O2-C2 | -2.70 | 1.35 | 1.43 |
| 4 | E | 1411 | GOL | O2-C2 | -2.70 | 1.35 | 1.43 |
| 4 | M | 2210 | GOL | C1-C2 | -2.68 | 1.40 | 1.51 |
| 4 | F | 1510 | GOL | C1-C2 | -2.68 | 1.40 | 1.51 |
| 5 | D | 1311[A] | FEC | CMD-C2D | 2.67 | 1.54 | 1.50 |
| 5 | D | 1311[B] | FEC | CMB-C2B | 2.66 | 1.54 | 1.50 |
| 5 | D | 1311[A] | FEC | CMB-C2B | 2.64 | 1.54 | 1.50 |
| 5 | F | 1507[A] | FEC | CMD-C2D | 2.63 | 1.54 | 1.50 |
| 5 | I | 1807[B] | FEC | CMB-C2B | 2.63 | 1.54 | 1.50 |
| 4 | J | 1811 | GOL | O2-C2 | -2.63 | 1.35 | 1.43 |
| 5 | G | 1608[A] | FEC | CMD-C2D | 2.63 | 1.54 | 1.50 |
| 4 | J | 1811 | GOL | C1-C2 | -2.61 | 1.41 | 1.51 |
| 5 | P | 2507[A] | FEC | CMB-C2B | 2.61 | 1.54 | 1.50 |
| 5 | L | 2108[B] | FEC | CMD-C2D | 2.59 | 1.54 | 1.50 |
| 6 | D | 1310 | 3PY | C1-C2 | -2.59 | 1.39 | 1.46 |
| 4 | F | 1510 | GOL | O2-C2 | -2.59 | 1.35 | 1.43 |
| 5 | I | 1807[A] | FEC | CMD-C2D | 2.59 | 1.54 | 1.50 |
| 4 | K | 2011 | GOL | O2-C2 | -2.57 | 1.35 | 1.43 |
| 5 | F | 1507[B] | FEC | CMD-C2D | 2.56 | 1.54 | 1.50 |
| 5 | I | 1807[B] | FEC | CMD-C2D | 2.55 | 1.54 | 1.50 |
| 4 | B | 1011 | GOL | O2-C2 | -2.55 | 1.35 | 1.43 |
| 5 | G | 1608[A] | FEC | CMB-C2B | 2.54 | 1.54 | 1.50 |
| 5 | D | 1311[B] | FEC | CMD-C2D | 2.54 | 1.54 | 1.50 |
| 5 | I | 1807[A] | FEC | CMB-C2B | 2.54 | 1.54 | 1.50 |
| 4 | I | 1713 | GOL | O2-C2 | -2.53 | 1.35 | 1.43 |
| 4 | K | 2011 | GOL | C1-C2 | -2.52 | 1.41 | 1.51 |
| 4 | D | 1211 | GOL | O2-C2 | -2.52 | 1.35 | 1.43 |
| 5 | B | 1107[A] | FEC | CMB-C2B | 2.50 | 1.54 | 1.50 |
| 4 | O | 2410 | GOL | O2-C2 | -2.49 | 1.35 | 1.43 |
| 4 | M | 2210 | GOL | O2-C2 | -2.47 | 1.36 | 1.43 |
| 5 | M | 2207[A] | FEC | CMD-C2D | 2.47 | 1.54 | 1.50 |
| 5 | G | 1608[B] | FEC | CMD-C2D | 2.46 | 1.54 | 1.50 |
| 5 | F | 1507[A] | FEC | CAD-C3D | 2.46 | 1.55 | 1.51 |
| 4 | N | 2310 | GOL | O2-C2 | -2.46 | 1.36 | 1.43 |
| 5 | F | 1507[A] | FEC | CMB-C2B | 2.43 | 1.54 | 1.50 |
| 5 | M | 2207[B] | FEC | CMB-C2B | 2.43 | 1.54 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 1411 | GOL | C1-C2 | -2.43 | 1.41 | 1.51 |
| 5 | B | 1107[B] | FEC | CMB-C2B | 2.43 | 1.54 | 1.50 |
| 5 | B | 1107[B] | FEC | CAB-C3B | 2.40 | 1.55 | 1.51 |
| 5 | D | 1311[A] | FEC | CAB-C3B | 2.39 | 1.55 | 1.51 |
| 4 | A | 1010 | GOL | O2-C2 | -2.39 | 1.36 | 1.43 |
| 5 | F | 1507[B] | FEC | CMB-C2B | 2.39 | 1.54 | 1.50 |
| 5 | F | 1507[A] | FEC | CAB-C3B | 2.38 | 1.55 | 1.51 |
| 5 | P | 2507[B] | FEC | CMD-C2D | 2.38 | 1.54 | 1.50 |
| 5 | M | 2207[B] | FEC | CAB-C3B | 2.36 | 1.55 | 1.51 |
| 5 | P | 2507[B] | FEC | CMB-C2B | 2.36 | 1.54 | 1.50 |
| 4 | H | 1710 | GOL | C1-C2 | -2.35 | 1.42 | 1.51 |
| 4 | E | 1410 | GOL | O2-C2 | -2.35 | 1.36 | 1.43 |
| 5 | L | 2108[B] | FEC | CAD-C3D | 2.34 | 1.55 | 1.51 |
| 5 | F | 1507[B] | FEC | CAD-C3D | 2.34 | 1.55 | 1.51 |
| 4 | O | 2411 | GOL | O2-C2 | -2.32 | 1.36 | 1.43 |
| 5 | M | 2207[A] | FEC | CAB-C3B | 2.29 | 1.55 | 1.51 |
| 5 | M | 2207[B] | FEC | CAD-C3D | 2.29 | 1.55 | 1.51 |
| 4 | I | 1810 | GOL | O2-C2 | -2.27 | 1.36 | 1.43 |
| 4 | G | 1611 | GOL | C1-C2 | -2.27 | 1.42 | 1.51 |
| 5 | L | 2108[B] | FEC | CAB-C3B | 2.27 | 1.55 | 1.51 |
| 5 | D | 1311[B] | FEC | CAB-C3B | 2.26 | 1.55 | 1.51 |
| 5 | G | 1608[B] | FEC | CAB-C3B | 2.25 | 1.55 | 1.51 |
| 5 | I | 1807[A] | FEC | CAB-C3B | 2.24 | 1.55 | 1.51 |
| 5 | D | 1311[A] | FEC | CAD-C3D | 2.23 | 1.55 | 1.51 |
| 5 | G | 1608[A] | FEC | CAB-C3B | 2.21 | 1.54 | 1.51 |
| 5 | I | 1807[A] | FEC | CAD-C3D | 2.21 | 1.54 | 1.51 |
| 5 | D | 1311[B] | FEC | CAD-C3D | 2.19 | 1.54 | 1.51 |
| 5 | P | 2507[A] | FEC | CAD-C3D | 2.18 | 1.54 | 1.51 |
| 5 | B | 1107[A] | FEC | CAD-C3D | 2.17 | 1.54 | 1.51 |
| 5 | L | 2108[A] | FEC | CAB-C3B | 2.17 | 1.54 | 1.51 |
| 5 | F | 1507[B] | FEC | CAB-C3B | 2.17 | 1.54 | 1.51 |
| 5 | P | 2507[B] | FEC | CAD-C3D | 2.15 | 1.54 | 1.51 |
| 5 | G | 1608[A] | FEC | CAD-C3D | 2.13 | 1.54 | 1.51 |
| 5 | I | 1807[B] | FEC | CAD-C3D | 2.09 | 1.54 | 1.51 |
| 5 | G | 1608[B] | FEC | CAD-C3D | 2.09 | 1.54 | 1.51 |
| 4 | C | 1210 | GOL | O2-C2 | -2.08 | 1.37 | 1.43 |
| 5 | P | 2507[B] | FEC | CAB-C3B | 2.07 | 1.54 | 1.51 |
| 5 | M | 2207[A] | FEC | CAD-C3D | 2.06 | 1.54 | 1.51 |
| 5 | P | 2507[A] | FEC | CAB-C3B | 2.05 | 1.54 | 1.51 |
| 4 | G | 1611 | GOL | O2-C2 | -2.04 | 1.37 | 1.43 |
| 5 | I | 1807[B] | FEC | CAB-C3B | 2.03 | 1.54 | 1.51 |
| 3 | I | 1802 | SO4 | O3-S | -2.03 | 1.31 | 1.47 |

All (274) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | D | 1310 | 3PY | O4-C3-C2 | 12.04 | 145.08 | 112.66 |
| 4 | A | 1010 | GOL | O3-C3-C2 | 11.00 | 162.95 | 110.20 |
| 4 | I | 1713 | GOL | O3-C3-C2 | 10.39 | 160.02 | 110.20 |
| 4 | N | 2310 | GOL | O3-C3-C2 | 10.15 | 158.86 | 110.20 |
| 4 | J | 1811 | GOL | O3-C3-C2 | 10.09 | 158.60 | 110.20 |
| 4 | G | 1610 | GOL | O3-C3-C2 | 9.99 | 158.10 | 110.20 |
| 4 | H | 1710 | GOL | O3-C3-C2 | 9.89 | 157.64 | 110.20 |
| 6 | D | 1310 | 3PY | O3-C2-C3 | 8.84 | 140.63 | 116.92 |
| 4 | C | 1210 | GOL | O3-C3-C2 | 8.65 | 151.66 | 110.20 |
| 4 | J | 1910 | GOL | O3-C3-C2 | 8.56 | 151.24 | 110.20 |
| 4 | O | 2410 | GOL | O3-C3-C2 | 8.54 | 151.14 | 110.20 |
| 4 | K | 2011 | GOL | O3-C3-C2 | 8.43 | 150.63 | 110.20 |
| 4 | D | 1211 | GOL | O3-C3-C2 | 8.31 | 150.06 | 110.20 |
| 4 | F | 1510 | GOL | O3-C3-C2 | 8.12 | 149.16 | 110.20 |
| 6 | D | 1310 | 3PY | O3-C2-C1 | -8.09 | 108.23 | 123.20 |
| 4 | G | 1611 | GOL | O3-C3-C2 | 7.87 | 147.96 | 110.20 |
| 4 | M | 2211 | GOL | O3-C3-C2 | 7.85 | 147.84 | 110.20 |
| 5 | P | 2507[B] | FEC | CBC-CAC-C2C | 7.77 | 125.70 | 112.60 |
| 4 | H | 1814 | GOL | O3-C3-C2 | 7.72 | 147.22 | 110.20 |
| 4 | P | 2510 | GOL | O3-C3-C2 | 7.71 | 147.15 | 110.20 |
| 5 | P | 2507[A] | FEC | CBC-CAC-C2C | 7.70 | 125.58 | 112.60 |
| 4 | M | 2210 | GOL | O3-C3-C2 | 7.68 | 147.05 | 110.20 |
| 4 | E | 1410 | GOL | O3-C3-C2 | 7.56 | 146.43 | 110.20 |
| 5 | B | 1107[B] | FEC | CBC-CAC-C2C | 7.48 | 125.21 | 112.60 |
| 4 | B | 1110 | GOL | O3-C3-C2 | 7.45 | 145.90 | 110.20 |
| 5 | I | 1807[B] | FEC | CBC-CAC-C2C | 7.37 | 125.02 | 112.60 |
| 5 | D | 1311[A] | FEC | CBC-CAC-C2C | 7.30 | 124.91 | 112.60 |
| 4 | H | 1710 | GOL | O2-C2-C3 | 7.13 | 140.53 | 109.12 |
| 4 | G | 1610 | GOL | O2-C2-C3 | 7.08 | 140.32 | 109.12 |
| 4 | O | 2411 | GOL | O3-C3-C2 | 6.90 | 143.29 | 110.20 |
| 4 | E | 1411 | GOL | O3-C3-C2 | 6.86 | 143.11 | 110.20 |
| 4 | P | 2510 | GOL | O2-C2-C3 | 6.58 | 138.08 | 109.12 |
| 5 | I | 1807[A] | FEC | CBC-CAC-C2C | 6.55 | 123.65 | 112.60 |
| 4 | I | 1810 | GOL | O3-C3-C2 | 6.49 | 141.33 | 110.20 |
| 4 | F | 1510 | GOL | O2-C2-C3 | 6.44 | 137.49 | 109.12 |
| 5 | F | 1507[B] | FEC | CBC-CAC-C2C | 6.41 | 123.41 | 112.60 |
| 4 | H | 1814 | GOL | O2-C2-C3 | 6.40 | 137.33 | 109.12 |
| 5 | B | 1107[A] | FEC | CBC-CAC-C2C | 6.38 | 123.36 | 112.60 |
| 4 | B | 1011 | GOL | O3-C3-C2 | 6.35 | 140.64 | 110.20 |
| 5 | L | 2108[B] | FEC | CBC-CAC-C2C | 6.33 | 123.28 | 112.60 |
| 4 | B | 1110 | GOL | O2-C2-C3 | 6.18 | 136.36 | 109.12 |
| 4 | K | 2011 | GOL | O2-C2-C3 | 6.08 | 135.90 | 109.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | N | 2310 | GOL | O2-C2-C3 | 6.05 | 135.78 | 109.12 |
| 4 | I | 1713 | GOL | O2-C2-C3 | 6.03 | 135.68 | 109.12 |
| 4 | J | 1811 | GOL | O2-C2-C3 | 6.00 | 135.55 | 109.12 |
| 4 | A | 1010 | GOL | O2-C2-C3 | 5.99 | 135.51 | 109.12 |
| 4 | C | 1210 | GOL | O2-C2-C3 | 5.97 | 135.44 | 109.12 |
| 4 | M | 2211 | GOL | O2-C2-C3 | 5.95 | 135.34 | 109.12 |
| 5 | L | 2108[A] | FEC | CBC-CAC-C2C | 5.90 | 122.55 | 112.60 |
| 4 | E | 1411 | GOL | O2-C2-C3 | 5.88 | 135.01 | 109.12 |
| 4 | J | 1910 | GOL | O2-C2-C3 | 5.78 | 134.56 | 109.12 |
| 4 | B | 1011 | GOL | O2-C2-C3 | 5.74 | 134.38 | 109.12 |
| 4 | M | 2210 | GOL | O2-C2-C3 | 5.73 | 134.38 | 109.12 |
| 5 | G | 1608[B] | FEC | CBC-CAC-C2C | 5.73 | 122.26 | 112.60 |
| 4 | D | 1211 | GOL | O2-C2-C3 | 5.66 | 134.07 | 109.12 |
| 4 | F | 1512 | GOL | O3-C3-C2 | 5.66 | 137.32 | 110.20 |
| 4 | F | 1512 | GOL | O2-C2-C3 | 5.42 | 133.00 | 109.12 |
| 4 | O | 2410 | GOL | O2-C2-C3 | 5.35 | 132.70 | 109.12 |
| 4 | G | 1611 | GOL | O2-C2-C3 | 5.35 | 132.69 | 109.12 |
| 5 | G | 1608[A] | FEC | CBC-CAC-C2C | 5.21 | 121.38 | 112.60 |
| 4 | E | 1410 | GOL | O2-C2-C3 | 4.88 | 130.63 | 109.12 |
| 5 | F | 1507[A] | FEC | CBC-CAC-C2C | 4.68 | 120.50 | 112.60 |
| 4 | I | 1810 | GOL | O2-C2-C3 | 4.66 | 129.67 | 109.12 |
| 4 | O | 2411 | GOL | O2-C2-C3 | 4.65 | 129.60 | 109.12 |
| 5 | M | 2207[A] | FEC | CBC-CAC-C2C | 4.60 | 120.36 | 112.60 |
| 5 | M | 2207[B] | FEC | CBC-CAC-C2C | 4.58 | 120.32 | 112.60 |
| 3 | A | 1105 | SO4 | O4-S-O1 | 4.25 | 131.51 | 109.31 |
| 3 | A | 1008 | SO4 | O4-S-O1 | 4.25 | 131.48 | 109.31 |
| 3 | B | 1005 | SO4 | O4-S-O1 | 4.25 | 131.47 | 109.31 |
| 5 | D | 1311[B] | FEC | CBA-CAA-C3A | 4.13 | 119.56 | 112.60 |
| 5 | F | 1507[B] | FEC | C4B-CHC-C1C | 4.00 | 129.48 | 118.67 |
| 5 | D | 1311[B] | FEC | CBC-CAC-C2C | 3.96 | 119.28 | 112.60 |
| 5 | G | 1608[B] | FEC | C4B-CHC-C1C | 3.82 | 128.99 | 118.67 |
| 4 | A | 1010 | GOL | O1-C1-C2 | 3.59 | 127.40 | 110.20 |
| 4 | C | 1210 | GOL | O1-C1-C2 | 3.57 | 127.30 | 110.20 |
| 4 | E | 1410 | GOL | O1-C1-C2 | 3.53 | 127.14 | 110.20 |
| 5 | D | 1311[A] | FEC | C4B-CHC-C1C | 3.53 | 128.21 | 118.67 |
| 5 | B | 1107[B] | FEC | CAB-CBB-CGB | 3.51 | 121.16 | 113.60 |
| 6 | D | 1310 | 3PY | O1-C1-C2 | -3.44 | 116.42 | 124.09 |
| 4 | O | 2410 | GOL | O1-C1-C2 | 3.40 | 126.52 | 110.20 |
| 4 | I | 1713 | GOL | O1-C1-C2 | 3.38 | 126.41 | 110.20 |
| 4 | H | 1814 | GOL | O1-C1-C2 | 3.37 | 126.35 | 110.20 |
| 5 | P | 2507[B] | FEC | C4B-CHC-C1C | 3.37 | 127.78 | 118.67 |
| 3 | A | 1105 | SO4 | O4-S-O3 | -3.37 | 94.70 | 109.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | J | 1910 | GOL | O1-C1-C2 | 3.36 | 126.31 | 110.20 |
| 3 | B | 1005 | SO4 | O4-S-O3 | -3.36 | 94.73 | 109.06 |
| 3 | A | 1008 | SO4 | O4-S-O3 | -3.35 | 94.77 | 109.06 |
| 5 | I | 1807[A] | FEC | CBA-CAA-C3A | 3.30 | 118.17 | 112.60 |
| 4 | N | 2310 | GOL | O1-C1-C2 | 3.29 | 125.99 | 110.20 |
| 5 | I | 1807[B] | FEC | CBB-CAB-C3B | 3.27 | 121.63 | 112.62 |
| 5 | B | 1107[A] | FEC | CBA-CAA-C3A | 3.26 | 118.10 | 112.60 |
| 4 | I | 1810 | GOL | O1-C1-C2 | 3.24 | 125.73 | 110.20 |
| 4 | H | 1710 | GOL | O1-C1-C2 | 3.21 | 125.61 | 110.20 |
| 5 | L | 2108[A] | FEC | C4B-CHC-C1C | 3.21 | 127.36 | 118.67 |
| 5 | B | 1107[B] | FEC | C4B-CHC-C1C | 3.20 | 127.33 | 118.67 |
| 5 | B | 1107[A] | FEC | C4B-CHC-C1C | 3.17 | 127.24 | 118.67 |
| 5 | I | 1807[B] | FEC | C4B-CHC-C1C | 3.17 | 127.23 | 118.67 |
| 5 | P | 2507[B] | FEC | CBA-CAA-C3A | 3.15 | 117.91 | 112.60 |
| 4 | G | 1610 | GOL | O1-C1-C2 | 3.13 | 125.20 | 110.20 |
| 5 | G | 1608[A] | FEC | C4B-CHC-C1C | 3.12 | 127.11 | 118.67 |
| 5 | D | 1311[A] | FEC | CBB-CAB-C3B | 3.08 | 121.11 | 112.62 |
| 5 | M | 2207[A] | FEC | C4B-CHC-C1C | 3.02 | 126.83 | 118.67 |
| 5 | I | 1807[A] | FEC | C4B-CHC-C1C | 3.01 | 126.80 | 118.67 |
| 5 | I | 1807[B] | FEC | CBA-CAA-C3A | 2.92 | 117.52 | 112.60 |
| 5 | G | 1608[B] | FEC | CBB-CAB-C3B | 2.88 | 120.55 | 112.62 |
| 5 | B | 1107[A] | FEC | CBB-CAB-C3B | 2.87 | 120.53 | 112.62 |
| 5 | P | 2507[A] | FEC | C4B-CHC-C1C | 2.86 | 126.41 | 118.67 |
| 5 | P | 2507[A] | FEC | CBA-CAA-C3A | 2.86 | 117.42 | 112.60 |
| 5 | I | 1807[A] | FEC | CBB-CAB-C3B | 2.84 | 120.45 | 112.62 |
| 5 | P | 2507[B] | FEC | C3D-C4D-ND | -2.81 | 108.92 | 114.98 |
| 5 | P | 2507[A] | FEC | CBB-CAB-C3B | 2.81 | 120.36 | 112.62 |
| 5 | G | 1608[B] | FEC | CAB-CBB-CGB | 2.80 | 119.63 | 113.60 |
| 5 | L | 2108[B] | FEC | C4B-CHC-C1C | 2.76 | 126.12 | 118.67 |
| 5 | F | 1507[A] | FEC | C4B-CHC-C1C | 2.74 | 126.09 | 118.67 |
| 4 | F | 1512 | GOL | O1-C1-C2 | 2.72 | 123.22 | 110.20 |
| 5 | P | 2507[B] | FEC | CBB-CAB-C3B | 2.71 | 120.08 | 112.62 |
| 5 | I | 1807[B] | FEC | CAB-C3B-C2B | 2.71 | 132.92 | 127.88 |
| 5 | D | 1311[B] | FEC | C3D-C4D-ND | -2.70 | 109.15 | 114.98 |
| 5 | B | 1107[A] | FEC | CMC-C3C-C2C | 2.69 | 130.02 | 124.94 |
| 5 | B | 1107[B] | FEC | CBA-CAA-C3A | 2.68 | 117.13 | 112.60 |
| 4 | D | 1211 | GOL | O1-C1-C2 | 2.68 | 123.04 | 110.20 |
| 5 | M | 2207[A] | FEC | CBA-CAA-C3A | 2.68 | 117.12 | 112.60 |
| 5 | F | 1507[B] | FEC | CMA-C2A-C3A | 2.67 | 129.98 | 124.94 |
| 5 | D | 1311[A] | FEC | CMA-C2A-C3A | 2.67 | 129.97 | 124.94 |
| 4 | K | 2011 | GOL | O1-C1-C2 | 2.66 | 122.98 | 110.20 |
| 5 | L | 2108[A] | FEC | CBB-CAB-C3B | 2.66 | 119.96 | 112.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | F | 1506 | SO4 | O4-S-O1 | 2.66 | 123.20 | 109.31 |
| 5 | B | 1107[B] | FEC | C1D-CHD-C4C | 2.66 | 125.86 | 118.67 |
| 5 | G | 1608[B] | FEC | CMC-C3C-C2C | 2.65 | 129.94 | 124.94 |
| 4 | M | 2211 | GOL | O1-C1-C2 | 2.65 | 122.89 | 110.20 |
| 5 | L | 2108[A] | FEC | CMA-C2A-C3A | 2.64 | 129.93 | 124.94 |
| 4 | P | 2510 | GOL | O1-C1-C2 | 2.63 | 122.81 | 110.20 |
| 5 | M | 2207[B] | FEC | C4B-CHC-C1C | 2.62 | 125.76 | 118.67 |
| 5 | G | 1608[B] | FEC | CBA-CAA-C3A | 2.62 | 117.02 | 112.60 |
| 4 | J | 1811 | GOL | O1-C1-C2 | 2.62 | 122.75 | 110.20 |
| 5 | M | 2207[B] | FEC | C1D-CHD-C4C | 2.61 | 125.74 | 118.67 |
| 4 | O | 2411 | GOL | O1-C1-C2 | 2.60 | 122.66 | 110.20 |
| 5 | P | 2507[A] | FEC | C4D-CHA-C1A | 2.60 | 125.69 | 118.67 |
| 5 | P | 2507[A] | FEC | C1B-CHB-C4A | 2.59 | 125.66 | 118.67 |
| 5 | B | 1107[B] | FEC | C3D-C4D-ND | -2.58 | 109.42 | 114.98 |
| 5 | M | 2207[B] | FEC | C3B-C4B-NB | -2.57 | 109.44 | 114.98 |
| 5 | B | 1107[A] | FEC | C4D-CHA-C1A | 2.57 | 125.62 | 118.67 |
| 5 | P | 2507[B] | FEC | C4D-CHA-C1A | 2.57 | 125.61 | 118.67 |
| 5 | P | 2507[B] | FEC | CMA-C2A-C3A | 2.56 | 129.78 | 124.94 |
| 5 | B | 1107[B] | FEC | C1B-CHB-C4A | 2.56 | 125.60 | 118.67 |
| 5 | I | 1807[A] | FEC | C4D-CHA-C1A | 2.55 | 125.57 | 118.67 |
| 5 | D | 1311[B] | FEC | C4B-CHC-C1C | 2.54 | 125.55 | 118.67 |
| 5 | I | 1807[B] | FEC | C3D-C4D-ND | -2.54 | 109.50 | 114.98 |
| 5 | D | 1311[B] | FEC | C4D-CHA-C1A | 2.54 | 125.54 | 118.67 |
| 5 | L | 2108[A] | FEC | C3D-C4D-ND | -2.53 | 109.51 | 114.98 |
| 5 | L | 2108[B] | FEC | C3D-C4D-ND | -2.53 | 109.52 | 114.98 |
| 5 | F | 1507[A] | FEC | O1C-CGC-CBC | -2.52 | 114.98 | 123.08 |
| 5 | G | 1608[A] | FEC | CBA-CAA-C3A | 2.52 | 116.85 | 112.60 |
| 5 | F | 1507[B] | FEC | C4D-CHA-C1A | 2.52 | 125.47 | 118.67 |
| 4 | B | 1011 | GOL | O1-C1-C2 | 2.51 | 122.26 | 110.20 |
| 5 | I | 1807[B] | FEC | C4D-CHA-C1A | 2.51 | 125.47 | 118.67 |
| 5 | G | 1608[B] | FEC | CMA-C2A-C3A | 2.51 | 129.67 | 124.94 |
| 5 | I | 1807[A] | FEC | C3D-C4D-ND | -2.50 | 109.59 | 114.98 |
| 5 | L | 2108[B] | FEC | C1B-CHB-C4A | 2.49 | 125.41 | 118.67 |
| 5 | G | 1608[A] | FEC | C3D-C4D-ND | -2.49 | 109.61 | 114.98 |
| 5 | F | 1507[A] | FEC | C4D-CHA-C1A | 2.49 | 125.41 | 118.67 |
| 5 | M | 2207[A] | FEC | C3D-C4D-ND | -2.49 | 109.62 | 114.98 |
| 5 | I | 1807[A] | FEC | CAB-CBB-CGB | 2.48 | 118.94 | 113.60 |
| 5 | M | 2207[A] | FEC | CMA-C2A-C3A | 2.48 | 129.62 | 124.94 |
| 5 | F | 1507[B] | FEC | C3D-C4D-ND | -2.47 | 109.66 | 114.98 |
| 5 | M | 2207[A] | FEC | O1C-CGC-CBC | -2.46 | 115.17 | 123.08 |
| 5 | F | 1507[B] | FEC | CBB-CAB-C3B | 2.46 | 119.38 | 112.62 |
| 5 | F | 1507[A] | FEC | CMC-C3C-C2C | 2.45 | 129.56 | 124.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | M | 2207[B] | FEC | CMA-C2A-C3A | 2.44 | 129.53 | 124.94 |
| 4 | F | 1510 | GOL | O1-C1-C2 | 2.43 | 121.85 | 110.20 |
| 5 | D | 1311[B] | FEC | C1D-CHD-C4C | 2.43 | 125.23 | 118.67 |
| 5 | M | 2207[A] | FEC | C1D-CHD-C4C | 2.43 | 125.23 | 118.67 |
| 5 | P | 2507[B] | FEC | C1D-CHD-C4C | 2.42 | 125.22 | 118.67 |
| 4 | B | 1110 | GOL | O1-C1-C2 | 2.41 | 121.76 | 110.20 |
| 5 | D | 1311[A] | FEC | C4D-CHA-C1A | 2.41 | 125.19 | 118.67 |
| 3 | E | 1406 | SO4 | O3-S-O1 | -2.41 | 96.73 | 109.31 |
| 5 | G | 1608[B] | FEC | C3D-C4D-ND | -2.41 | 109.78 | 114.98 |
| 5 | P | 2507[B] | FEC | O1D-CGD-CBD | -2.40 | 115.37 | 123.08 |
| 5 | L | 2108[B] | FEC | C3B-C4B-NB | -2.40 | 109.81 | 114.98 |
| 5 | B | 1107[A] | FEC | CMA-C2A-C3A | 2.39 | 129.45 | 124.94 |
| 5 | M | 2207[A] | FEC | C1B-CHB-C4A | 2.39 | 125.13 | 118.67 |
| 5 | L | 2108[A] | FEC | CMC-C3C-C2C | 2.39 | 129.45 | 124.94 |
| 5 | B | 1107[A] | FEC | C3D-C4D-ND | -2.39 | 109.83 | 114.98 |
| 5 | M | 2207[B] | FEC | O1C-CGC-CBC | -2.39 | 115.41 | 123.08 |
| 5 | F | 1507[A] | FEC | C3D-C4D-ND | -2.37 | 109.86 | 114.98 |
| 5 | G | 1608[A] | FEC | CMC-C3C-C2C | 2.37 | 129.42 | 124.94 |
| 5 | I | 1807[B] | FEC | CMA-C2A-C3A | 2.37 | 129.42 | 124.94 |
| 5 | D | 1311[B] | FEC | O1C-CGC-CBC | -2.37 | 115.45 | 123.08 |
| 5 | P | 2507[A] | FEC | CMA-C2A-C3A | 2.37 | 129.41 | 124.94 |
| 5 | P | 2507[A] | FEC | C3D-C4D-ND | -2.37 | 109.87 | 114.98 |
| 5 | G | 1608[A] | FEC | O1D-CGD-CBD | -2.37 | 115.48 | 123.08 |
| 5 | L | 2108[A] | FEC | C4D-CHA-C1A | 2.36 | 125.05 | 118.67 |
| 5 | G | 1608[B] | FEC | C1B-CHB-C4A | 2.35 | 125.03 | 118.67 |
| 5 | P | 2507[B] | FEC | CAB-C3B-C2B | 2.35 | 132.25 | 127.88 |
| 5 | G | 1608[B] | FEC | O1C-CGC-CBC | -2.33 | 115.60 | 123.08 |
| 5 | L | 2108[A] | FEC | C1B-CHB-C4A | 2.33 | 124.97 | 118.67 |
| 5 | G | 1608[A] | FEC | O1C-CGC-CBC | -2.32 | 115.62 | 123.08 |
| 5 | L | 2108[B] | FEC | CMA-C2A-C3A | 2.30 | 129.28 | 124.94 |
| 4 | E | 1411 | GOL | O1-C1-C2 | 2.30 | 121.23 | 110.20 |
| 5 | D | 1311[B] | FEC | C3B-C4B-NB | -2.29 | 110.03 | 114.98 |
| 5 | M | 2207[A] | FEC | C4D-CHA-C1A | 2.29 | 124.86 | 118.67 |
| 5 | D | 1311[A] | FEC | C3D-C4D-ND | -2.29 | 110.05 | 114.98 |
| 5 | F | 1507[A] | FEC | CBA-CAA-C3A | 2.29 | 116.46 | 112.60 |
| 5 | I | 1807[A] | FEC | O1C-CGC-CBC | -2.28 | 115.75 | 123.08 |
| 5 | L | 2108[A] | FEC | O1C-CGC-CBC | -2.28 | 115.75 | 123.08 |
| 5 | D | 1311[A] | FEC | C1D-CHD-C4C | 2.28 | 124.83 | 118.67 |
| 5 | I | 1807[A] | FEC | CMA-C2A-C3A | 2.27 | 129.22 | 124.94 |
| 5 | F | 1507[B] | FEC | O1D-CGD-CBD | -2.27 | 115.79 | 123.08 |
| 5 | M | 2207[B] | FEC | O2A-CGA-CBA | -2.26 | 115.82 | 123.08 |
| 5 | B | 1107[A] | FEC | C1B-CHB-C4A | 2.26 | 124.78 | 118.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 1107[B] | FEC | C4D-CHA-C1A | 2.25 | 124.77 | 118.67 |
| 5 | M | 2207[A] | FEC | CBB-CAB-C3B | 2.25 | 118.83 | 112.62 |
| 5 | B | 1107[B] | FEC | CMA-C2A-C3A | 2.25 | 129.18 | 124.94 |
| 5 | F | 1507[B] | FEC | C1D-CHD-C4C | 2.25 | 124.75 | 118.67 |
| 5 | G | 1608[B] | FEC | C3B-C4B-NB | -2.24 | 110.14 | 114.98 |
| 5 | I | 1807[B] | FEC | C1B-CHB-C4A | 2.24 | 124.73 | 118.67 |
| 5 | P | 2507[B] | FEC | CAB-CBB-CGB | 2.24 | 118.42 | 113.60 |
| 5 | I | 1807[B] | FEC | C1D-CHD-C4C | 2.24 | 124.72 | 118.67 |
| 5 | G | 1608[A] | FEC | C4D-CHA-C1A | 2.24 | 124.72 | 118.67 |
| 5 | M | 2207[B] | FEC | C4D-CHA-C1A | 2.23 | 124.71 | 118.67 |
| 5 | L | 2108[B] | FEC | CBA-CAA-C3A | 2.23 | 116.37 | 112.60 |
| 5 | I | 1807[B] | FEC | O2A-CGA-CBA | -2.23 | 115.92 | 123.08 |
| 5 | F | 1507[A] | FEC | CMA-C2A-C3A | 2.23 | 129.14 | 124.94 |
| 5 | F | 1507[A] | FEC | C1B-CHB-C4A | 2.22 | 124.68 | 118.67 |
| 6 | D | 1310 | 3PY | C3-C2-C1 | -2.22 | 110.48 | 118.03 |
| 5 | L | 2108[A] | FEC | C3B-C4B-NB | -2.21 | 110.21 | 114.98 |
| 5 | F | 1507[A] | FEC | O2A-CGA-CBA | -2.21 | 115.97 | 123.08 |
| 5 | L | 2108[B] | FEC | C4D-CHA-C1A | 2.21 | 124.64 | 118.67 |
| 5 | P | 2507[B] | FEC | O2A-CGA-CBA | -2.21 | 116.00 | 123.08 |
| 5 | P | 2507[A] | FEC | CMC-C3C-C2C | 2.20 | 129.10 | 124.94 |
| 5 | G | 1608[B] | FEC | C4D-CHA-C1A | 2.20 | 124.63 | 118.67 |
| 5 | I | 1807[A] | FEC | C1B-CHB-C4A | 2.20 | 124.61 | 118.67 |
| 5 | D | 1311[B] | FEC | C1B-CHB-C4A | 2.19 | 124.60 | 118.67 |
| 5 | D | 1311[A] | FEC | O2A-CGA-CBA | -2.19 | 116.04 | 123.08 |
| 5 | G | 1608[B] | FEC | C1D-CHD-C4C | 2.19 | 124.59 | 118.67 |
| 5 | M | 2207[B] | FEC | CBD-CAD-C3D | 2.19 | 118.65 | 112.62 |
| 5 | D | 1311[A] | FEC | C3B-C4B-NB | -2.18 | 110.27 | 114.98 |
| 5 | F | 1507[B] | FEC | C1B-CHB-C4A | 2.18 | 124.57 | 118.67 |
| 5 | P | 2507[A] | FEC | C3B-C4B-NB | -2.18 | 110.28 | 114.98 |
| 5 | G | 1608[A] | FEC | O2C-CGC-O1C | 2.18 | 128.73 | 123.30 |
| 5 | B | 1107[B] | FEC | CBD-CAD-C3D | 2.18 | 118.61 | 112.62 |
| 5 | D | 1311[A] | FEC | O1C-CGC-CBC | -2.17 | 116.12 | 123.08 |
| 5 | I | 1807[A] | FEC | C1D-CHD-C4C | 2.15 | 124.50 | 118.67 |
| 5 | I | 1807[A] | FEC | CMC-C3C-C2C | 2.15 | 129.00 | 124.94 |
| 5 | D | 1311[A] | FEC | C1B-CHB-C4A | 2.15 | 124.49 | 118.67 |
| 5 | G | 1608[A] | FEC | CMA-C2A-C3A | 2.15 | 128.99 | 124.94 |
| 5 | M | 2207[B] | FEC | CAD-CBD-CGD | 2.14 | 118.21 | 113.60 |
| 5 | M | 2207[B] | FEC | CBB-CAB-C3B | 2.13 | 118.49 | 112.62 |
| 5 | M | 2207[B] | FEC | C3D-C4D-ND | -2.11 | 110.42 | 114.98 |
| 5 | G | 1608[A] | FEC | C1D-CHD-C4C | 2.11 | 124.38 | 118.67 |
| 5 | M | 2207[B] | FEC | C1B-CHB-C4A | 2.11 | 124.38 | 118.67 |
| 5 | L | 2108[B] | FEC | C1D-CHD-C4C | 2.11 | 124.36 | 118.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 1107[B] | FEC | O2A-CGA-CBA | -2.10 | 116.33 | 123.08 |
| 5 | L | 2108[A] | FEC | C1D-CHD-C4C | 2.10 | 124.35 | 118.67 |
| 5 | F | 1507[A] | FEC | C3B-C4B-NB | -2.10 | 110.45 | 114.98 |
| 5 | G | 1608[A] | FEC | O2A-CGA-CBA | -2.09 | 116.36 | 123.08 |
| 5 | F | 1507[B] | FEC | O1C-CGC-CBC | -2.09 | 116.37 | 123.08 |
| 5 | G | 1608[A] | FEC | C3B-C4B-NB | -2.07 | 110.51 | 114.98 |
| 5 | D | 1311[A] | FEC | O2C-CGC-O1C | 2.07 | 128.46 | 123.30 |
| 5 | F | 1507[A] | FEC | C1D-CHD-C4C | 2.06 | 124.25 | 118.67 |
| 5 | G | 1608[A] | FEC | CBB-CAB-C3B | 2.06 | 118.28 | 112.62 |
| 5 | B | 1107[A] | FEC | O1C-CGC-CBC | -2.04 | 116.53 | 123.08 |
| 5 | I | 1807[A] | FEC | C3B-C4B-NB | -2.04 | 110.59 | 114.98 |
| 5 | B | 1107[A] | FEC | O2A-CGA-CBA | -2.04 | 116.54 | 123.08 |
| 5 | D | 1311[A] | FEC | CMC-C3C-C2C | 2.03 | 128.78 | 124.94 |
| 5 | M | 2207[B] | FEC | O2C-CGC-O1C | 2.03 | 128.37 | 123.30 |
| 5 | P | 2507[B] | FEC | C1D-C2D-C3D | -2.03 | 106.92 | 108.61 |
| 5 | P | 2507[A] | FEC | CAB-C3B-C2B | 2.03 | 131.65 | 127.88 |
| 4 | G | 1611 | GOL | O1-C1-C2 | 2.02 | 119.87 | 110.20 |
| 5 | F | 1507[A] | FEC | CBB-CAB-C3B | 2.01 | 118.17 | 112.62 |
| 5 | G | 1608[B] | FEC | O1D-CGD-CBD | -2.01 | 116.61 | 123.08 |
| 5 | P | 2507[A] | FEC | O2A-CGA-CBA | -2.01 | 116.62 | 123.08 |
| 5 | I | 1807[B] | FEC | C3B-C4B-NB | -2.01 | 110.65 | 114.98 |
| 5 | B | 1107[A] | FEC | C1D-CHD-C4C | 2.00 | 124.08 | 118.67 |

There are no chirality outliers.

All (206) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 1010 | GOL | O1-C1-C2-C3 |
| 4 | C | 1210 | GOL | O1-C1-C2-C3 |
| 4 | E | 1410 | GOL | O1-C1-C2-C3 |
| 4 | E | 1411 | GOL | O1-C1-C2-C3 |
| 4 | G | 1611 | GOL | O1-C1-C2-C3 |
| 4 | H | 1814 | GOL | O1-C1-C2-C3 |
| 4 | I | 1810 | GOL | O1-C1-C2-C3 |
| 4 | J | 1811 | GOL | C1-C2-C3-O3 |
| 4 | J | 1910 | GOL | O1-C1-C2-C3 |
| 4 | N | 2310 | GOL | O1-C1-C2-C3 |
| 4 | N | 2310 | GOL | C1-C2-C3-O3 |
| 4 | O | 2410 | GOL | O1-C1-C2-C3 |
| 4 | O | 2410 | GOL | C1-C2-C3-O3 |
| 4 | O | 2411 | GOL | C1-C2-C3-O3 |
| 5 | B | 1107[A] | FEC | C3C-C2C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | B | 1107[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | B | 1107[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | B | 1107[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | D | 1311[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | D | 1311[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | D | 1311[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | D | 1311[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | F | 1507[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | F | 1507[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | F | 1507[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | F | 1507[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | G | 1608[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | G | 1608[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | G | 1608[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | G | 1608[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | I | 1807[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | I | 1807[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | I | 1807[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | I | 1807[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | I | 1807[B] | FEC | C4B-C3B-CAB-CBB |
| 5 | I | 1807[B] | FEC | C2B-C3B-CAB-CBB |
| 5 | L | 2108[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | L | 2108[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | L | 2108[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | L | 2108[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | M | 2207[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | M | 2207[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | M | 2207[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | M | 2207[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | P | 2507[A] | FEC | C3C-C2C-CAC-CBC |
| 5 | P | 2507[A] | FEC | C1C-C2C-CAC-CBC |
| 5 | P | 2507[B] | FEC | C3C-C2C-CAC-CBC |
| 5 | P | 2507[B] | FEC | C1C-C2C-CAC-CBC |
| 5 | P | 2507[B] | FEC | C4B-C3B-CAB-CBB |
| 5 | P | 2507[B] | FEC | C2B-C3B-CAB-CBB |
| 5 | D | 1311[A] | FEC | C2C-CAC-CBC-CGC |
| 5 | F | 1507[A] | FEC | C2C-CAC-CBC-CGC |
| 5 | M | 2207[B] | FEC | C2C-CAC-CBC-CGC |
| 4 | H | 1710 | GOL | O1-C1-C2-O2 |
| 4 | I | 1713 | GOL | O2-C2-C3-O3 |
| 4 | N | 2310 | GOL | O2-C2-C3-O3 |
| 4 | O | 2411 | GOL | O2-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | P | 2510 | GOL | O1-C1-C2-O2 |
| 4 | B | 1011 | GOL | O1-C1-C2-O2 |
| 4 | D | 1211 | GOL | O1-C1-C2-O2 |
| 4 | D | 1211 | GOL | O2-C2-C3-O3 |
| 4 | E | 1411 | GOL | O1-C1-C2-O2 |
| 4 | E | 1411 | GOL | O2-C2-C3-O3 |
| 4 | F | 1510 | GOL | O1-C1-C2-O2 |
| 4 | G | 1610 | GOL | O2-C2-C3-O3 |
| 4 | G | 1611 | GOL | O1-C1-C2-O2 |
| 4 | H | 1814 | GOL | O1-C1-C2-O2 |
| 4 | H | 1814 | GOL | O2-C2-C3-O3 |
| 4 | J | 1811 | GOL | O1-C1-C2-O2 |
| 4 | J | 1811 | GOL | O2-C2-C3-O3 |
| 4 | O | 2411 | GOL | O1-C1-C2-O2 |
| 4 | P | 2510 | GOL | O2-C2-C3-O3 |
| 5 | F | 1507[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | G | 1608[B] | FEC | C2C-CAC-CBC-CGC |
| 5 | M | 2207[A] | FEC | C2C-CAC-CBC-CGC |
| 4 | A | 1010 | GOL | O2-C2-C3-O3 |
| 4 | B | 1110 | GOL | O2-C2-C3-O3 |
| 4 | E | 1410 | GOL | O2-C2-C3-O3 |
| 4 | I | 1713 | GOL | O1-C1-C2-O2 |
| 4 | I | 1810 | GOL | O2-C2-C3-O3 |
| 4 | J | 1910 | GOL | O2-C2-C3-O3 |
| 4 | K | 2011 | GOL | O1-C1-C2-O2 |
| 4 | M | 2210 | GOL | O1-C1-C2-O2 |
| 4 | M | 2211 | GOL | O1-C1-C2-O2 |
| 4 | M | 2211 | GOL | O2-C2-C3-O3 |
| 4 | O | 2410 | GOL | O2-C2-C3-O3 |
| 4 | G | 1610 | GOL | O1-C1-C2-O2 |
| 4 | M | 2210 | GOL | O2-C2-C3-O3 |
| 4 | B | 1011 | GOL | O2-C2-C3-O3 |
| 4 | B | 1110 | GOL | O1-C1-C2-O2 |
| 4 | F | 1510 | GOL | O2-C2-C3-O3 |
| 4 | F | 1512 | GOL | O1-C1-C2-O2 |
| 4 | F | 1512 | GOL | O2-C2-C3-O3 |
| 4 | N | 2310 | GOL | O1-C1-C2-O2 |
| 4 | D | 1211 | GOL | C1-C2-C3-O3 |
| 4 | G | 1610 | GOL | O1-C1-C2-C3 |
| 4 | K | 2011 | GOL | C1-C2-C3-O3 |
| 5 | I | 1807[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | G | 1608[A] | FEC | C2C-CAC-CBC-CGC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | I | 1807[A] | FEC | C2C-CAC-CBC-CGC |
| 4 | H | 1710 | GOL | O2-C2-C3-O3 |
| 5 | M | 2207[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | M | 2207[B] | FEC | C3D-CAD-CBD-CGD |
| 5 | I | 1807[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | P | 2507[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | I | 1807[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | B | 1107[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | M | 2207[B] | FEC | CAC-CBC-CGC-O1C |
| 5 | P | 2507[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | D | 1311[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | G | 1608[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | L | 2108[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | L | 2108[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | M | 2207[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | B | 1107[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | D | 1311[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | L | 2108[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | F | 1507[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | G | 1608[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | L | 2108[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | F | 1507[A] | FEC | CAA-CBA-CGA-O2A |
| 5 | G | 1608[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | P | 2507[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | B | 1107[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | B | 1107[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | F | 1507[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | M | 2207[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | M | 2207[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | B | 1107[A] | FEC | C3D-CAD-CBD-CGD |
| 5 | B | 1107[B] | FEC | C3D-CAD-CBD-CGD |
| 5 | G | 1608[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | I | 1807[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | I | 1807[B] | FEC | CAD-CBD-CGD-O2D |
| 5 | P | 2507[B] | FEC | CAD-CBD-CGD-O2D |
| 5 | D | 1311[A] | FEC | CAA-CBA-CGA-O1A |
| 5 | M | 2207[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | L | 2108[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | L | 2108[B] | FEC | CAC-CBC-CGC-O2C |
| 5 | D | 1311[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | L | 2108[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | M | 2207[B] | FEC | CAC-CBC-CGC-O2C |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | D | 1311[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | P | 2507[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | F | 1507[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | D | 1311[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | G | 1608[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | I | 1807[A] | FEC | CAA-CBA-CGA-O1A |
| 4 | I | 1713 | GOL | C1-C2-C3-O3 |
| 4 | I | 1810 | GOL | C1-C2-C3-O3 |
| 4 | O | 2411 | GOL | O1-C1-C2-C3 |
| 5 | I | 1807[B] | FEC | C3D-CAD-CBD-CGD |
| 5 | G | 1608[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | I | 1807[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | G | 1608[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | B | 1107[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | F | 1507[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | L | 2108[B] | FEC | CAC-CBC-CGC-O1C |
| 5 | P | 2507[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | I | 1807[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | I | 1807[B] | FEC | CAC-CBC-CGC-O1C |
| 5 | F | 1507[A] | FEC | CAC-CBC-CGC-O2C |
| 5 | I | 1807[A] | FEC | CAC-CBC-CGC-O1C |
| 5 | I | 1807[B] | FEC | CAC-CBC-CGC-O2C |
| 5 | L | 2108[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | D | 1311[B] | FEC | CAC-CBC-CGC-O2C |
| 5 | G | 1608[B] | FEC | CAC-CBC-CGC-O2C |
| 5 | P | 2507[B] | FEC | CAA-CBA-CGA-O1A |
| 5 | D | 1311[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | I | 1807[B] | FEC | CAB-CBB-CGB-O2B |
| 5 | I | 1807[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | L | 2108[B] | FEC | CAD-CBD-CGD-O2D |
| 5 | L | 2108[B] | FEC | C2C-CAC-CBC-CGC |
| 5 | M | 2207[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | P | 2507[B] | FEC | CAB-CBB-CGB-O2B |
| 5 | B | 1107[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | D | 1311[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | L | 2108[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | I | 1807[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | D | 1311[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | D | 1311[B] | FEC | CAC-CBC-CGC-O1C |
| 5 | L | 2108[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | P | 2507[B] | FEC | CAB-CBB-CGB-O1B |
| 5 | G | 1608[A] | FEC | CAC-CBC-CGC-O1C |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | I | 1807[B] | FEC | CAB-CBB-CGB-O1B |
| 5 | M | 2207[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | B | 1107[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | P | 2507[B] | FEC | CAA-CBA-CGA-O2A |
| 5 | D | 1311[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | D | 1311[B] | FEC | CAD-CBD-CGD-O2D |
| 5 | G | 1608[B] | FEC | CAC-CBC-CGC-O1C |
| 5 | G | 1608[B] | FEC | CAD-CBD-CGD-O2D |
| 4 | C | 1210 | GOL | C1-C2-C3-O3 |
| 4 | E | 1411 | GOL | C1-C2-C3-O3 |
| 5 | P | 2507[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | B | 1107[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | B | 1107[B] | FEC | C2B-C3B-CAB-CBB |
| 5 | F | 1507[B] | FEC | CAC-CBC-CGC-O2C |
| 5 | L | 2108[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | P | 2507[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | B | 1107[B] | FEC | CAB-CBB-CGB-O2B |
| 5 | M | 2207[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | F | 1507[B] | FEC | CAD-CBD-CGD-O1D |
| 5 | G | 1608[A] | FEC | CAD-CBD-CGD-O1D |
| 5 | G | 1608[A] | FEC | CAD-CBD-CGD-O2D |
| 5 | M | 2207[B] | FEC | CAD-CBD-CGD-O2D |
| 5 | B | 1107[B] | FEC | CAB-CBB-CGB-O1B |

There are no ring outliers.

59 monomers are involved in 247 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | K | 2011 | GOL | 1 | 0 |
| 3 | P | 2506 | SO4 | 1 | 0 |
| 4 | G | 1611 | GOL | 1 | 0 |
| 3 | P | 2501 | SO4 | 1 | 0 |
| 4 | I | 1810 | GOL | 15 | 0 |
| 3 | M | 2206 | SO4 | 2 | 0 |
| 5 | I | 1807[B] | FEC | 9 | 0 |
| 3 | L | 2102 | SO4 | 1 | 7 |
| 4 | J | 1811 | GOL | 1 | 0 |
| 5 | L | 2108[B] | FEC | 12 | 0 |
| 5 | P | 2507[A] | FEC | 8 | 0 |
| 3 | K | 1504 | SO4 | 1 | 0 |
| 4 | B | 1110 | GOL | 3 | 0 |
| 4 | M | 2211 | GOL | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | P | 2510 | GOL | 2 | 0 |
| 5 | D | 1311[A] | FEC | 8 | 0 |
| 5 | M | 2207[B] | FEC | 8 | 0 |
| 3 | B | 1005 | SO4 | 1 | 0 |
| 4 | D | 1211 | GOL | 5 | 0 |
| 4 | I | 1713 | GOL | 1 | 0 |
| 3 | B | 1106 | SO4 | 1 | 0 |
| 4 | M | 2210 | GOL | 5 | 0 |
| 4 | H | 1710 | GOL | 1 | 0 |
| 3 | L | 2107 | SO4 | 1 | 0 |
| 3 | O | 2406 | SO4 | 1 | 0 |
| 4 | E | 1410 | GOL | 6 | 0 |
| 4 | J | 1910 | GOL | 4 | 0 |
| 5 | L | 2108[A] | FEC | 11 | 0 |
| 4 | O | 2411 | GOL | 2 | 0 |
| 3 | F | 1502 | SO4 | 2 | 0 |
| 5 | F | 1507[B] | FEC | 13 | 0 |
| 3 | A | 1105 | SO4 | 3 | 0 |
| 6 | D | 1310 | 3PY | 1 | 0 |
| 3 | F | 1501 | SO4 | 1 | 0 |
| 3 | B | 1104 | SO4 | 1 | 0 |
| 3 | O | 2409 | SO4 | 1 | 0 |
| 5 | G | 1608[B] | FEC | 6 | 0 |
| 4 | F | 1510 | GOL | 3 | 0 |
| 3 | C | 1206 | SO4 | 1 | 0 |
| 3 | J | 1904 | SO4 | 1 | 0 |
| 5 | F | 1507[A] | FEC | 4 | 0 |
| 5 | I | 1807[A] | FEC | 9 | 0 |
| 3 | G | 1606 | SO4 | 1 | 0 |
| 3 | E | 1304 | SO4 | 1 | 0 |
| 3 | L | 2103 | SO4 | 1 | 0 |
| 3 | J | 1906 | SO4 | 3 | 0 |
| 5 | B | 1107[B] | FEC | 7 | 0 |
| 3 | I | 1803 | SO4 | 1 | 0 |
| 5 | M | 2207[A] | FEC | 10 | 0 |
| 3 | C | 1203 | SO4 | 1 | 0 |
| 5 | G | 1608[A] | FEC | 9 | 0 |
| 4 | G | 1610 | GOL | 2 | 0 |
| 4 | N | 2310 | GOL | 1 | 0 |
| 3 | I | 1802 | SO4 | 1 | 7 |
| 4 | O | 2410 | GOL | 2 | 0 |
| 5 | P | 2507[B] | FEC | 13 | 0 |

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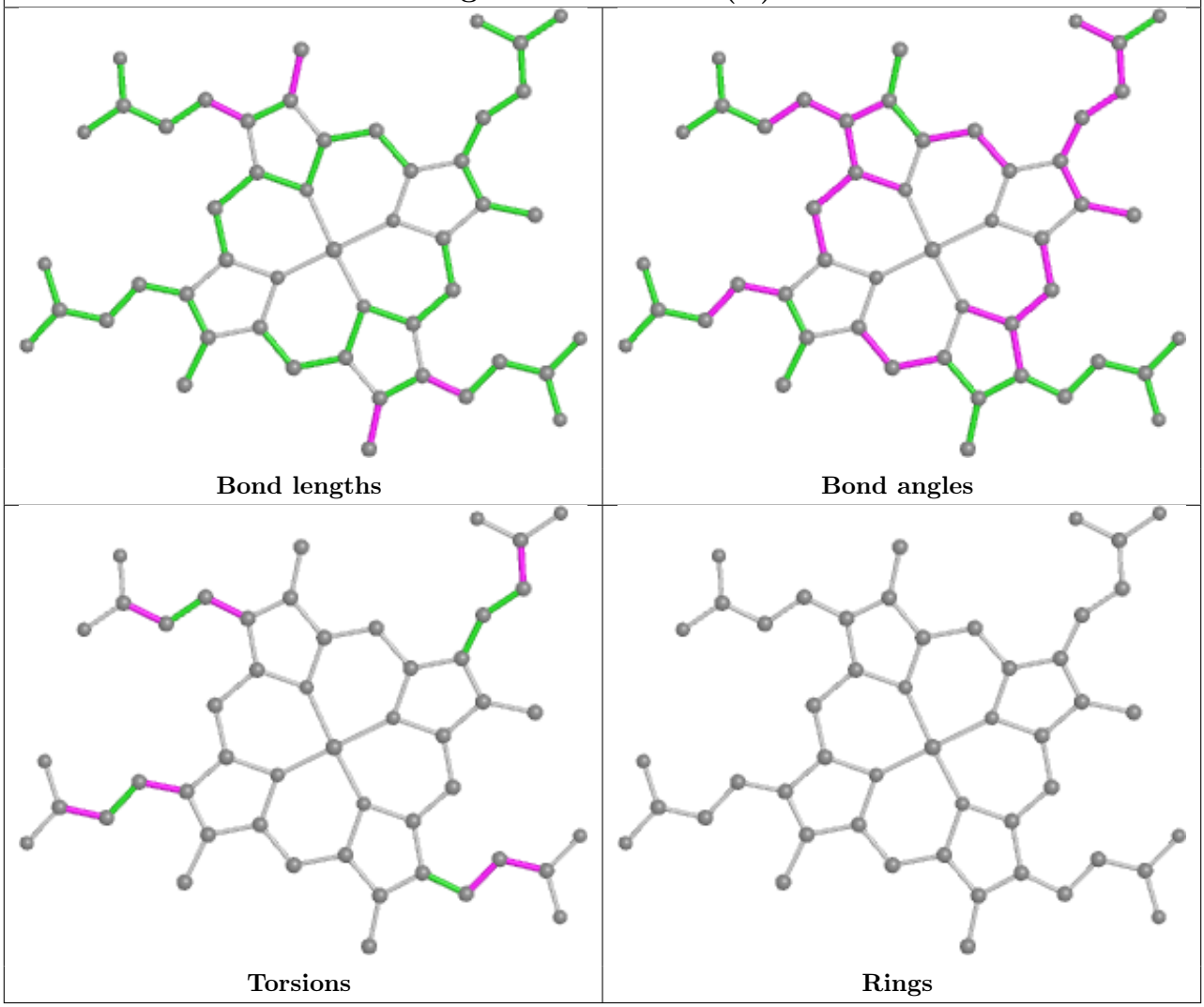
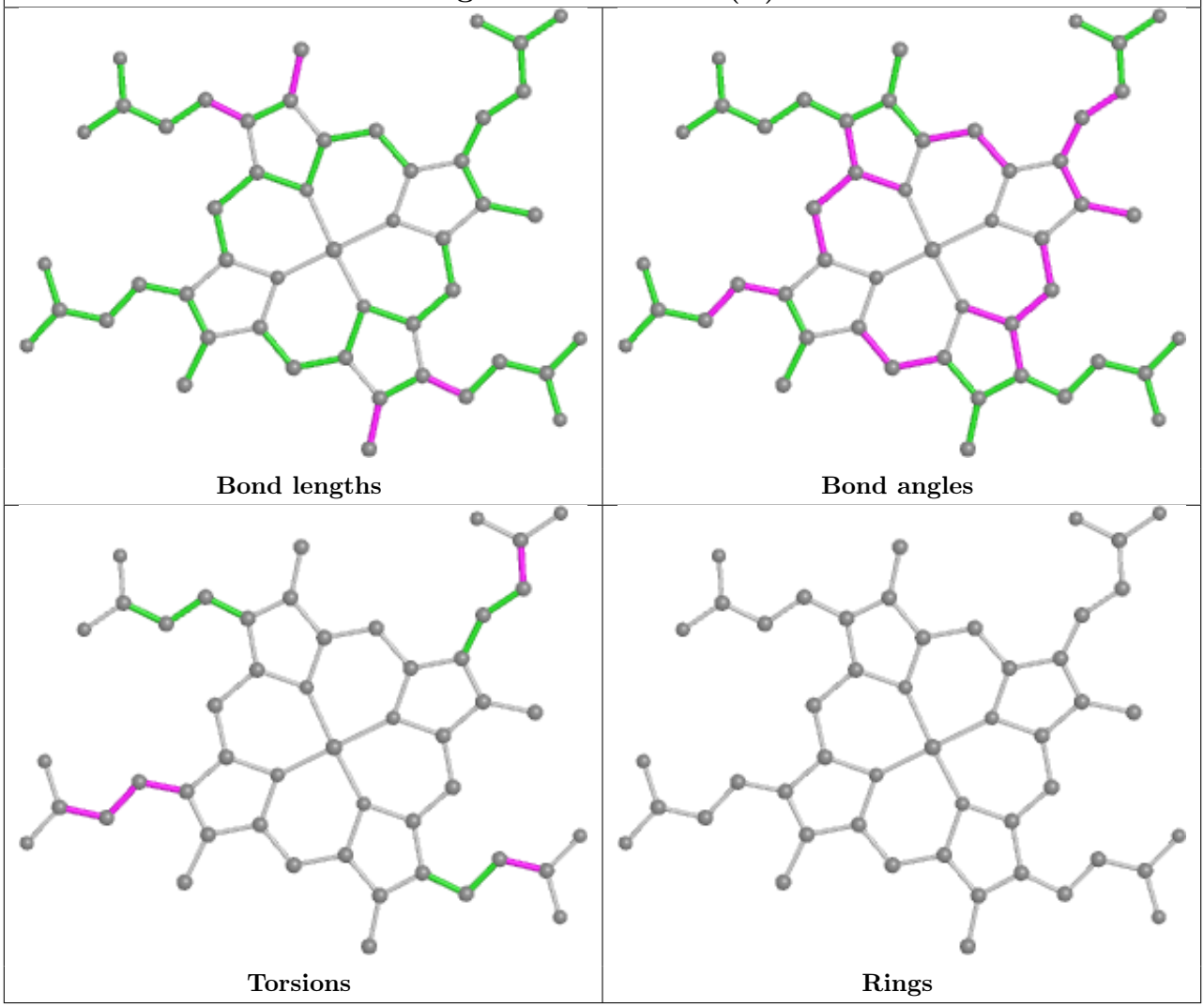
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | B | 1107[A] | FEC | 10 | 0 |
| 4 | A | 1010 | GOL | 1 | 0 |
| 5 | D | 1311[B] | FEC | 14 | 0 |

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

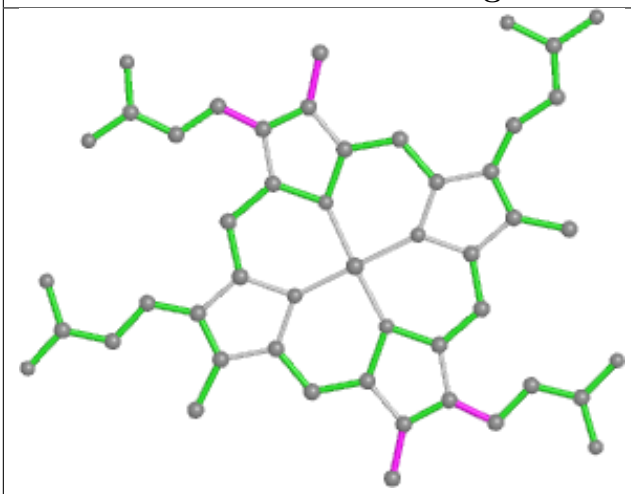
**Ligand FEC I 1807 (B)**



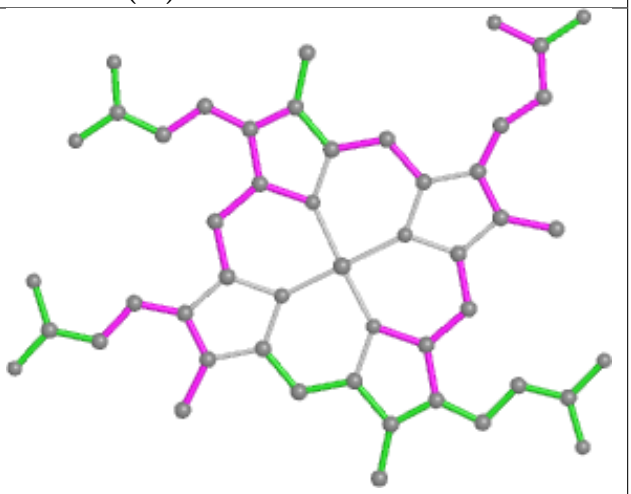
**Ligand FEC L 2108 (B)**



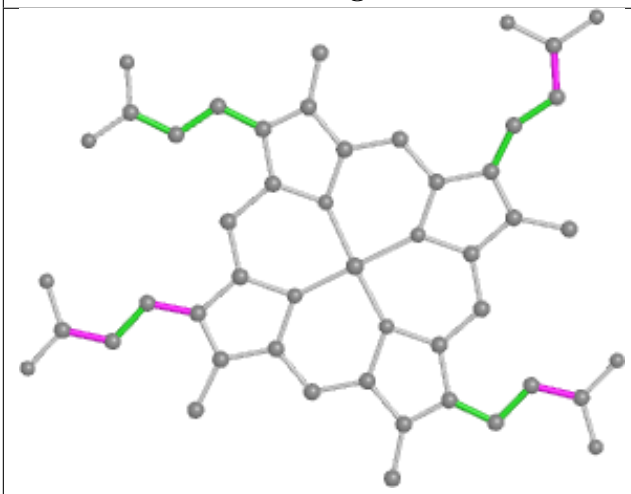
**Ligand FEC P 2507 (A)**



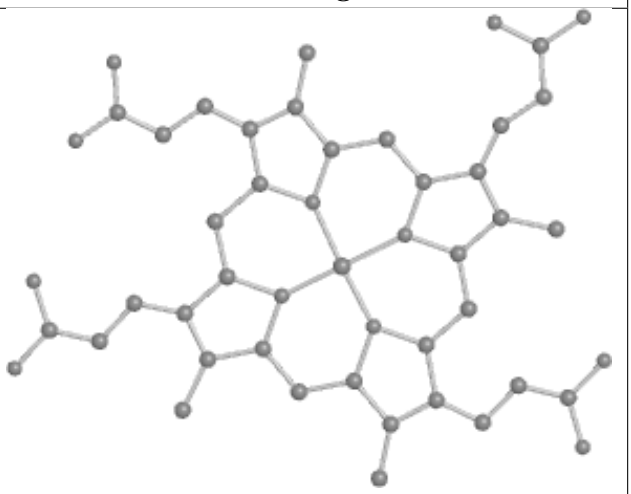
**Bond lengths**



**Bond angles**

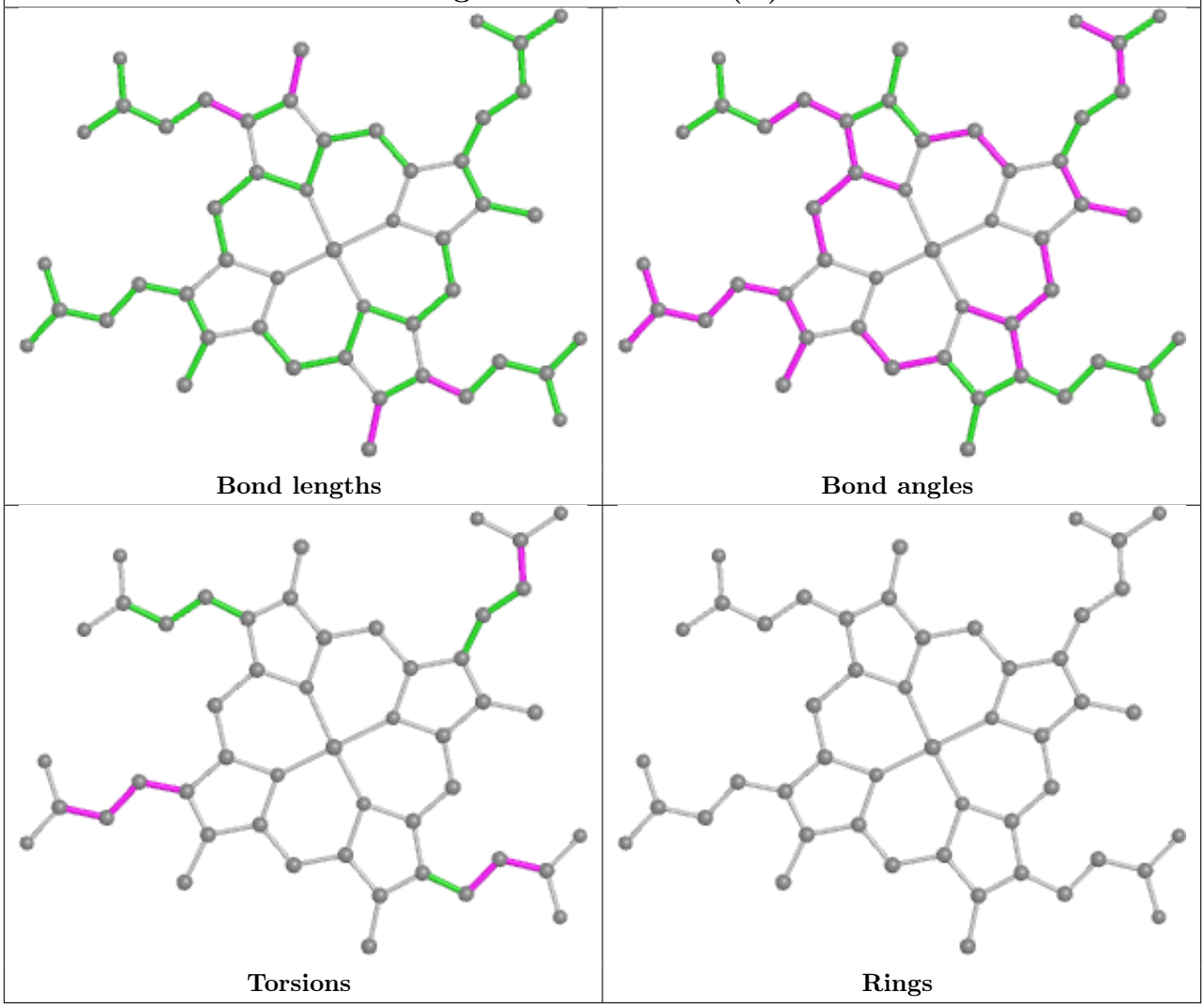


**Torsions**

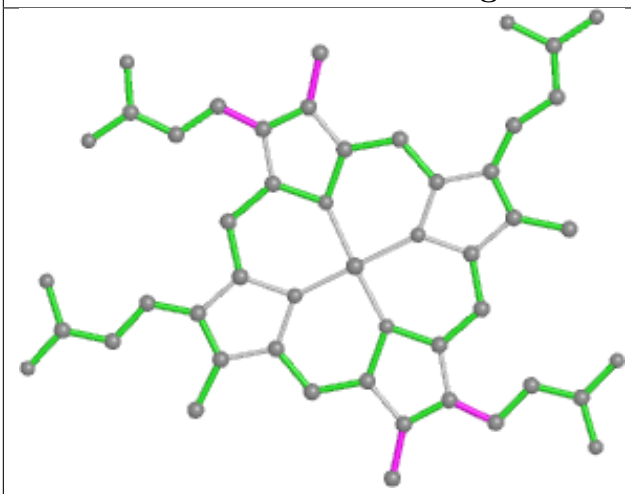


**Rings**

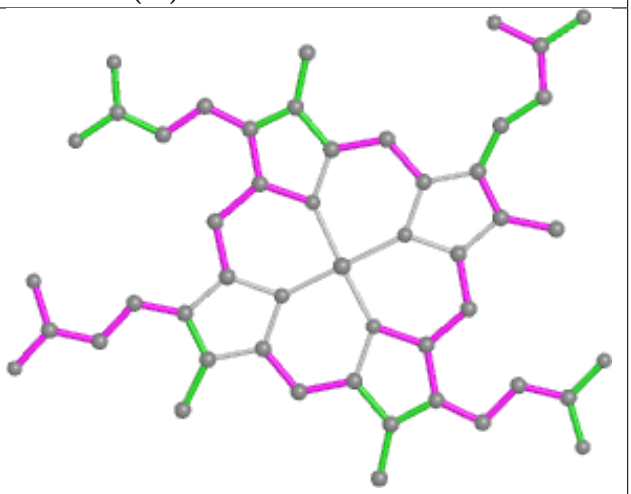
**Ligand FEC D 1311 (A)**



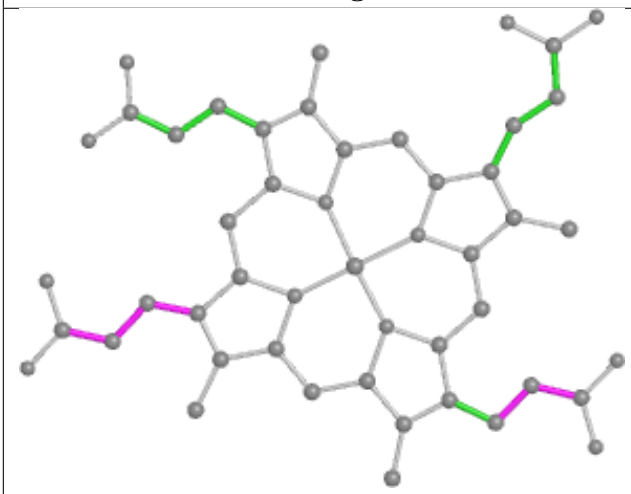
**Ligand FEC M 2207 (B)**



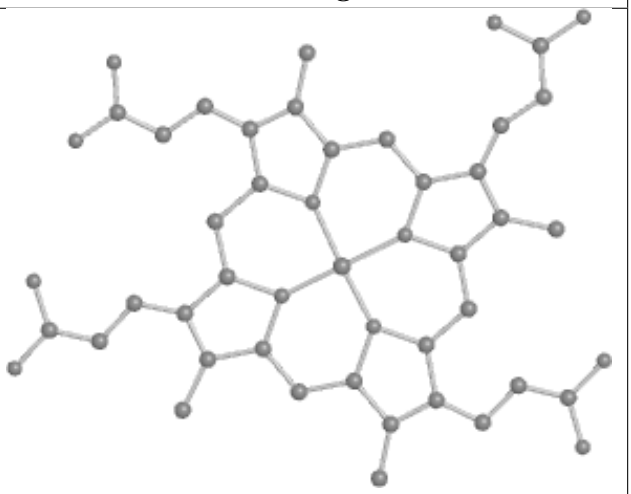
**Bond lengths**



**Bond angles**

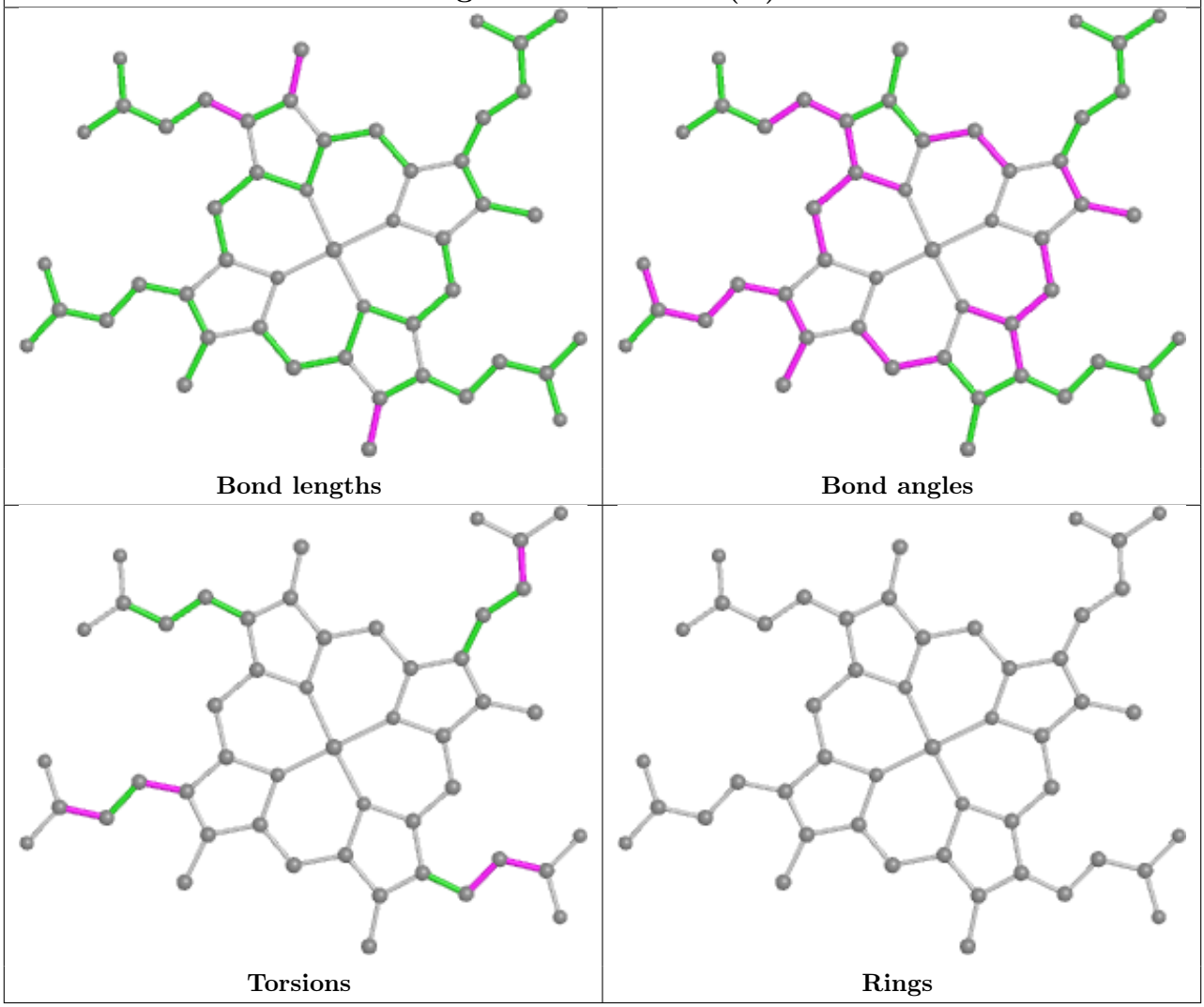


**Torsions**

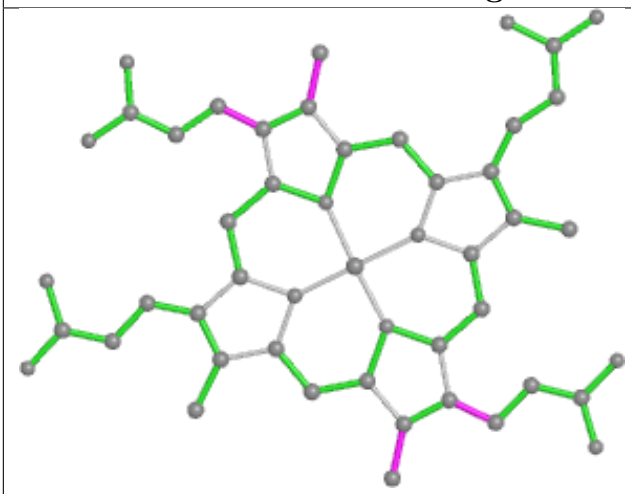


**Rings**

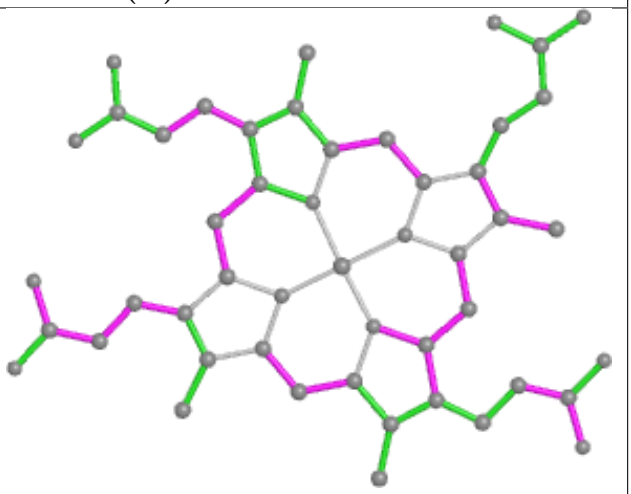
**Ligand FEC L 2108 (A)**



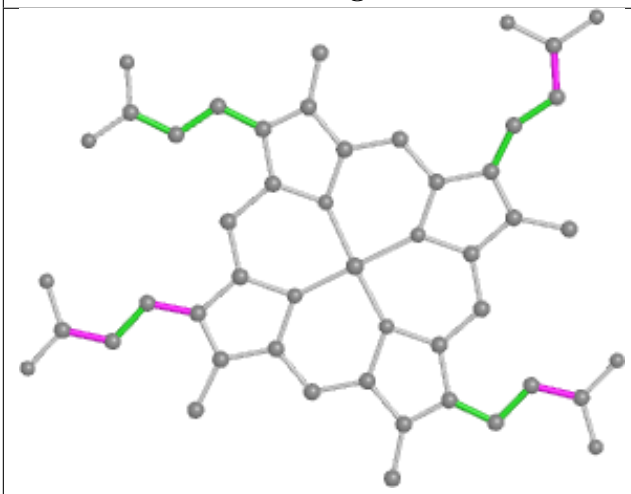
**Ligand FEC F 1507 (B)**



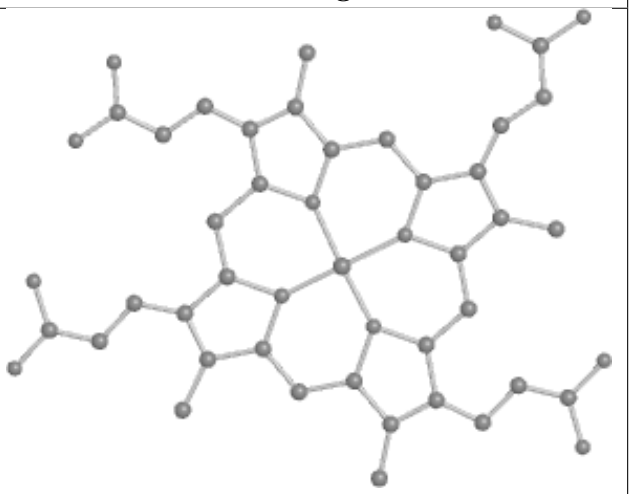
**Bond lengths**



**Bond angles**

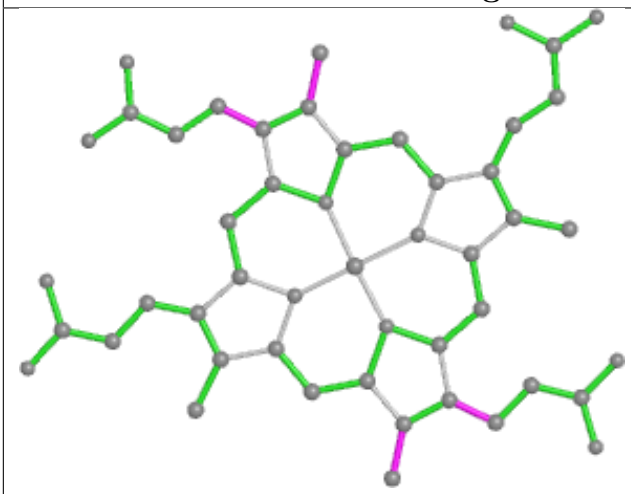


**Torsions**

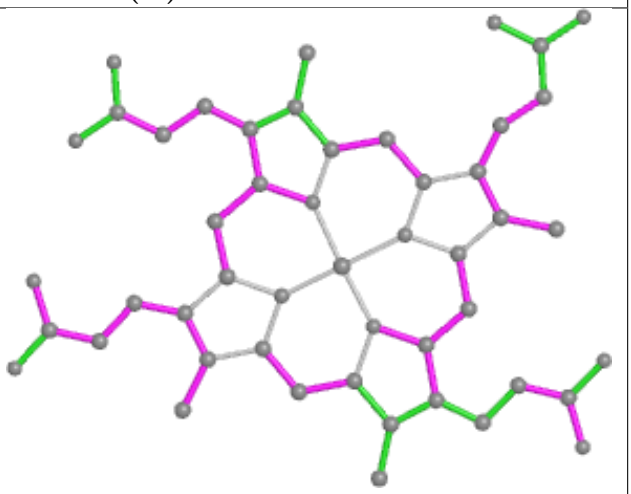


**Rings**

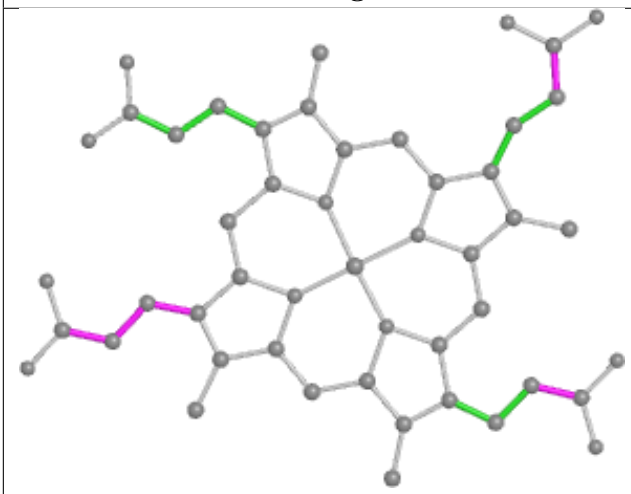
**Ligand FEC G 1608 (B)**



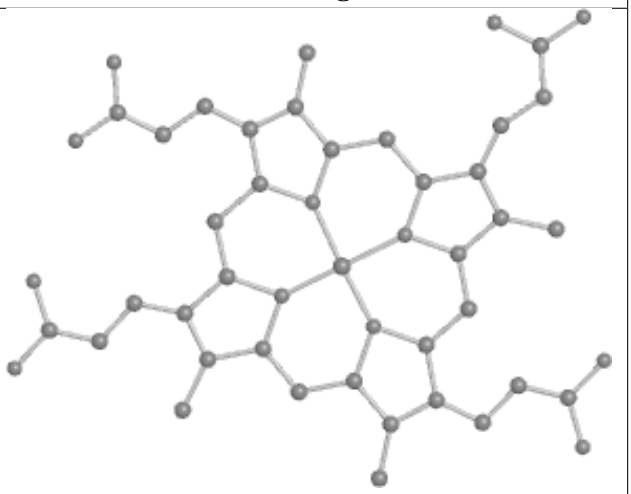
**Bond lengths**



**Bond angles**

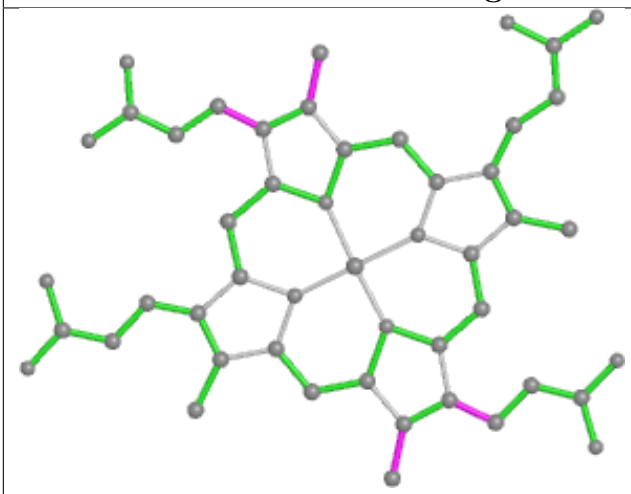


**Torsions**

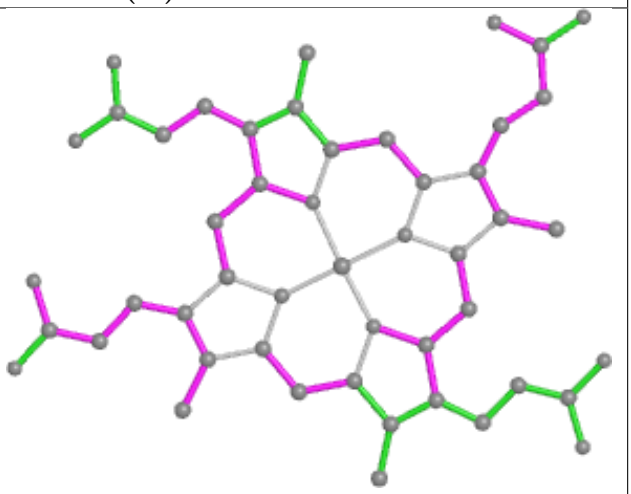


**Rings**

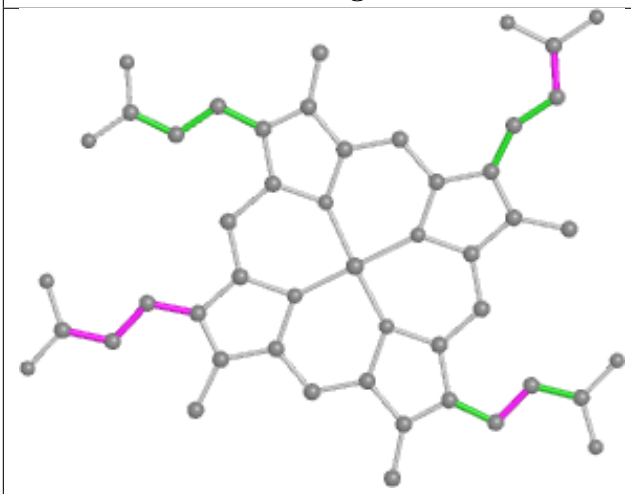
**Ligand FEC F 1507 (A)**



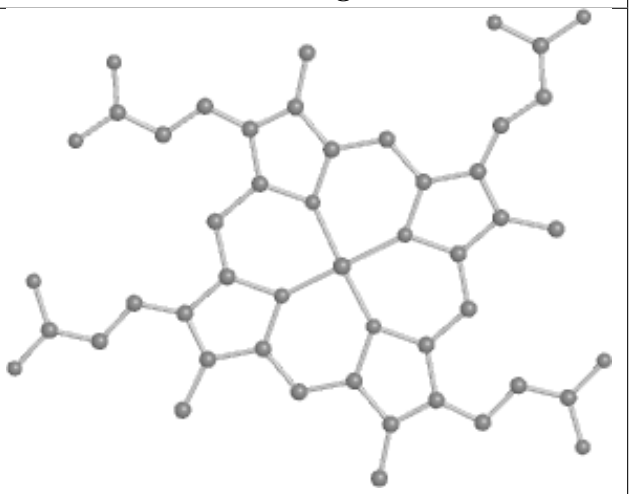
**Bond lengths**



**Bond angles**

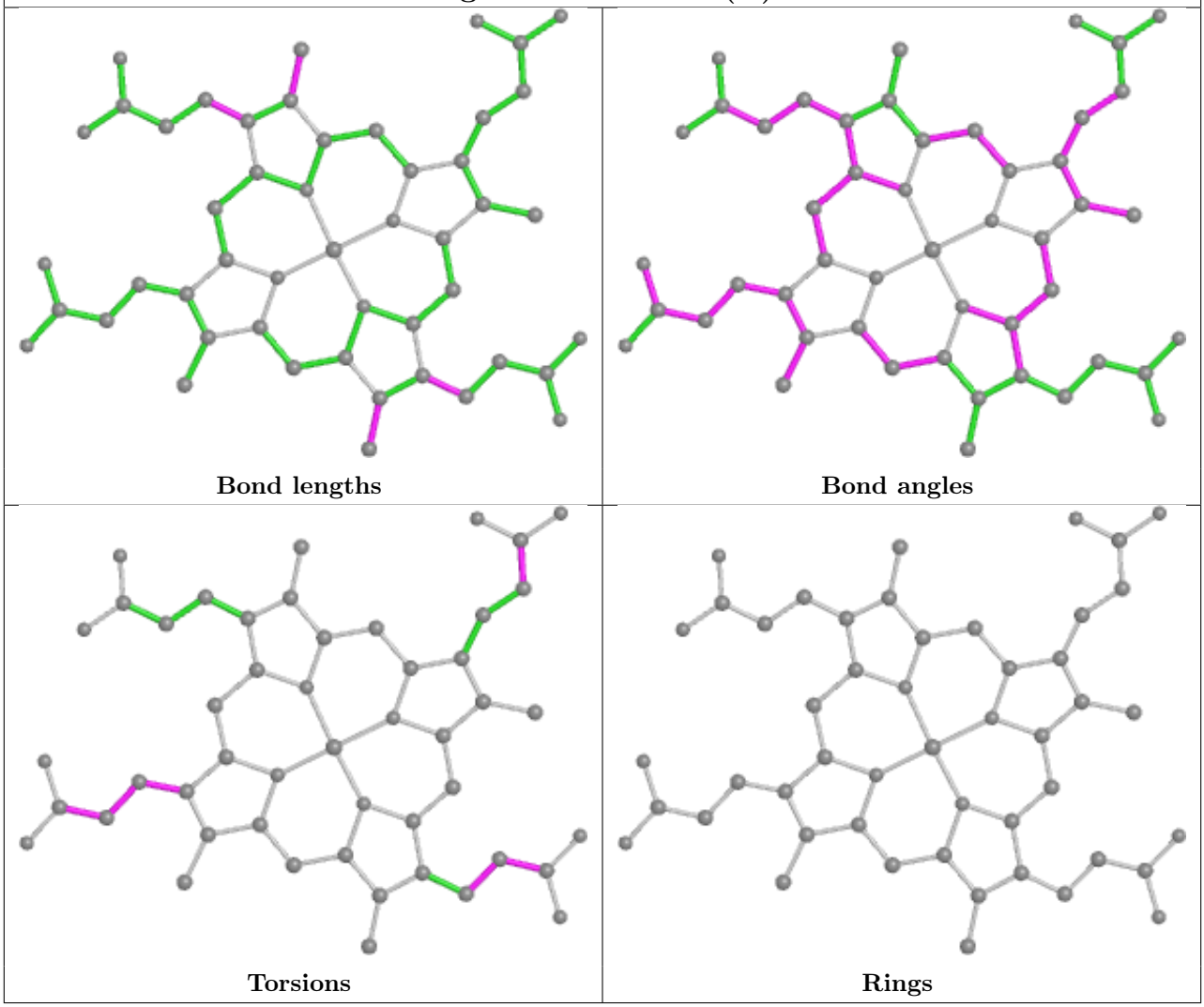


**Torsions**

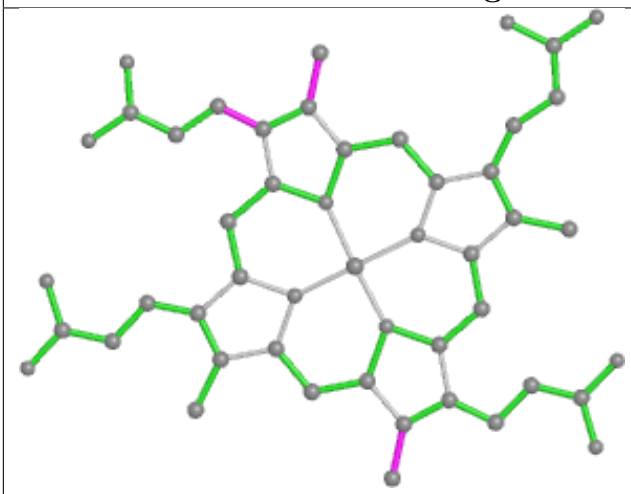


**Rings**

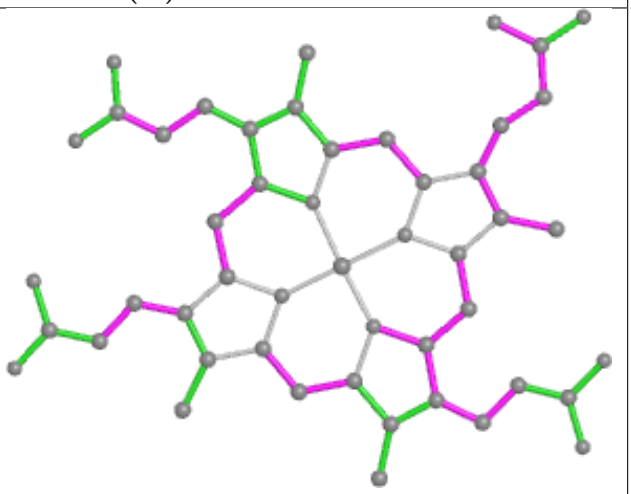
**Ligand FEC I 1807 (A)**



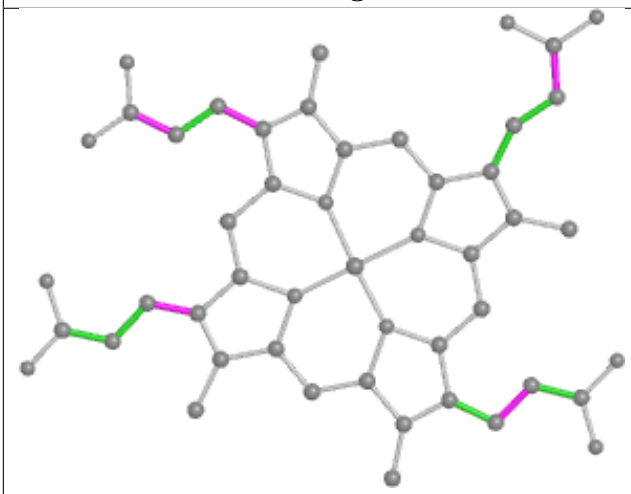
**Ligand FEC B 1107 (B)**



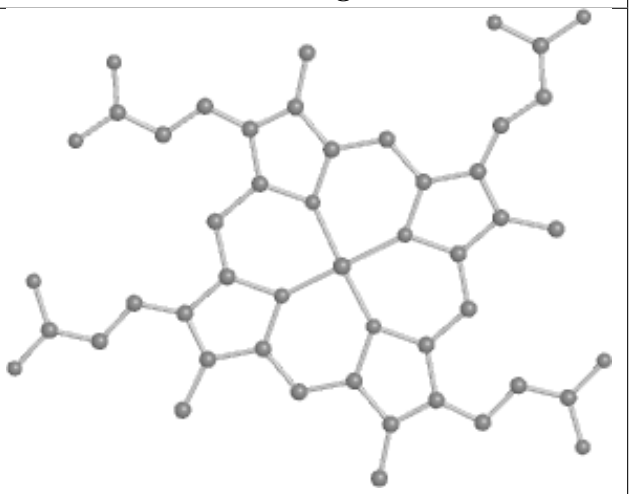
**Bond lengths**



**Bond angles**

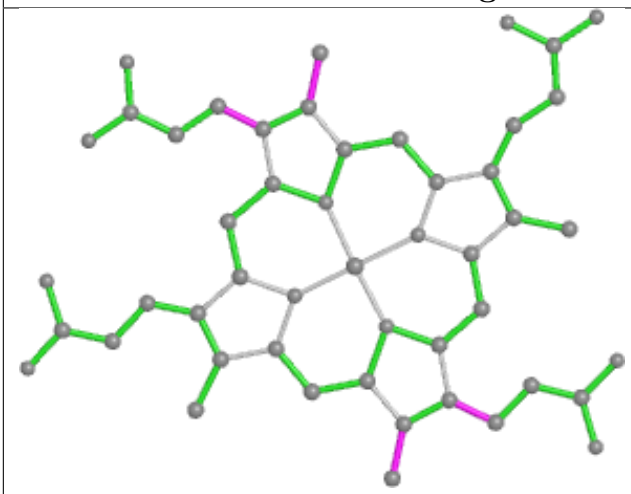


**Torsions**

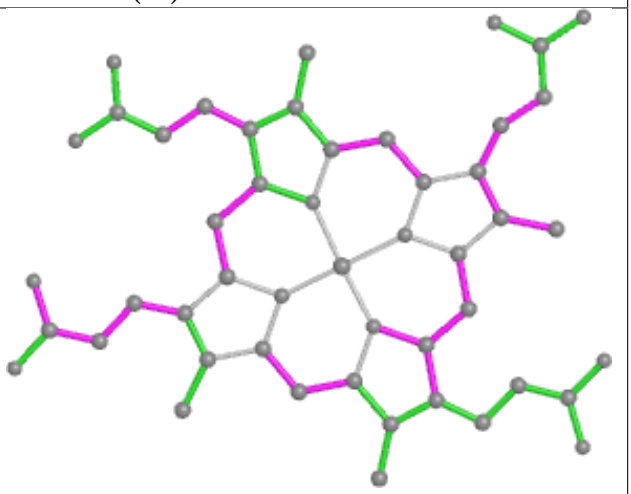


**Rings**

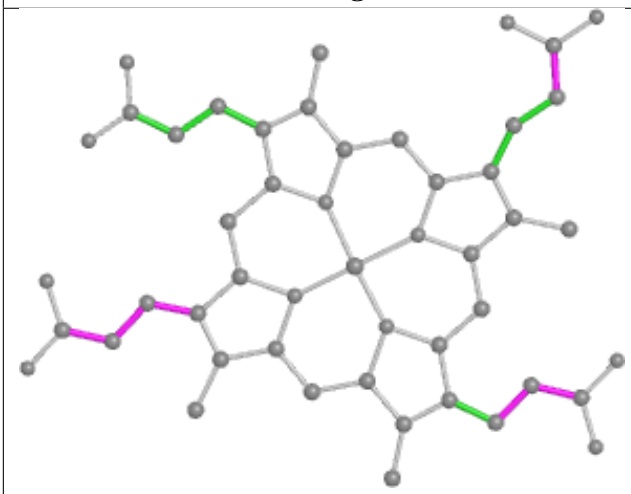
**Ligand FEC M 2207 (A)**



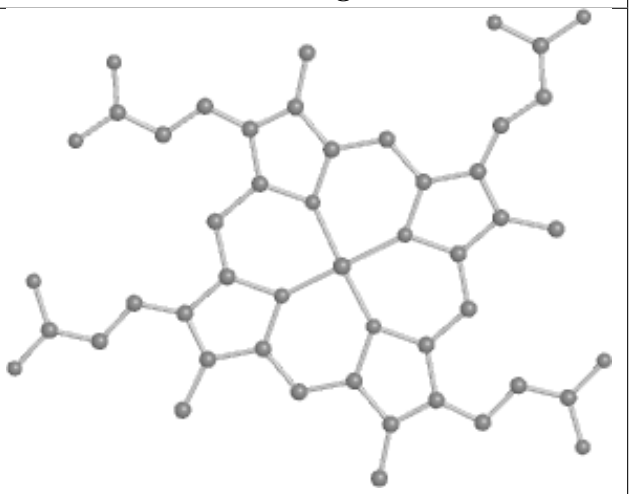
**Bond lengths**



**Bond angles**

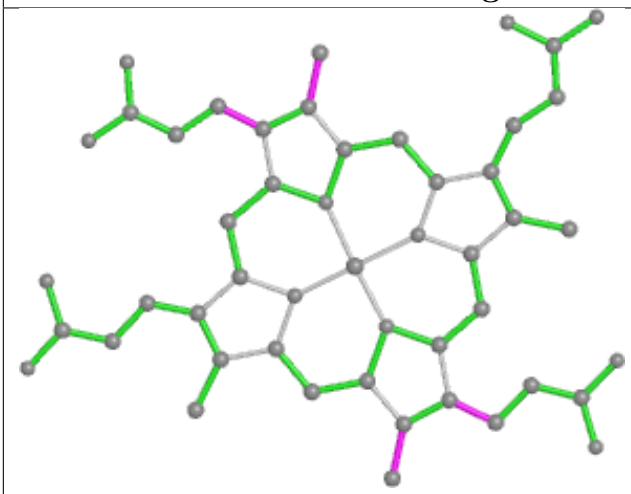


**Torsions**

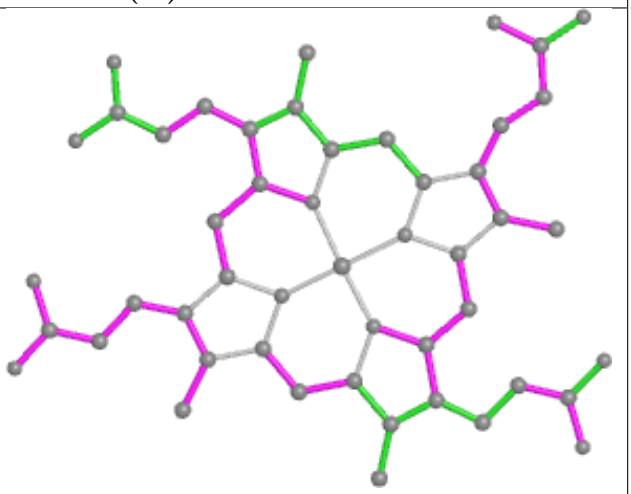


**Rings**

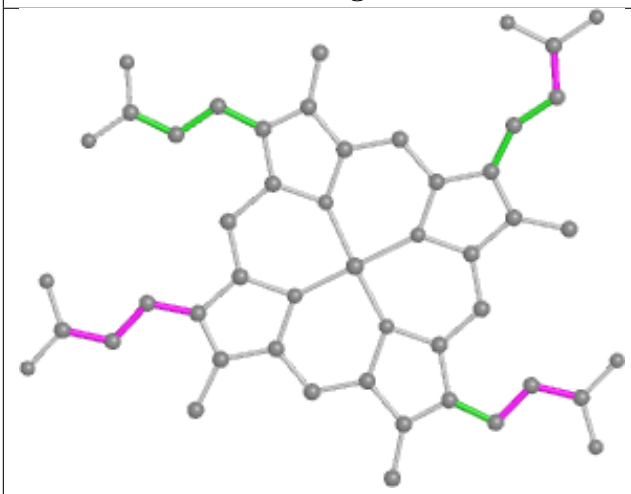
**Ligand FEC G 1608 (A)**



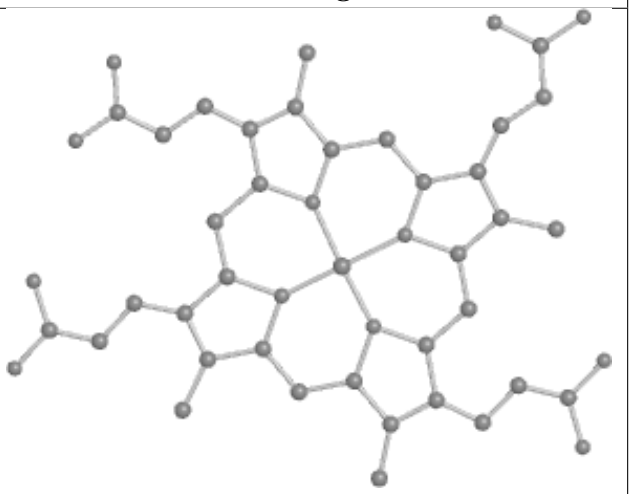
**Bond lengths**



**Bond angles**

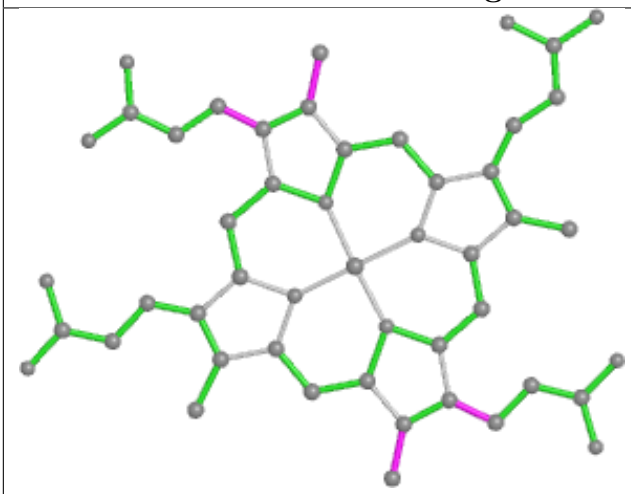


**Torsions**

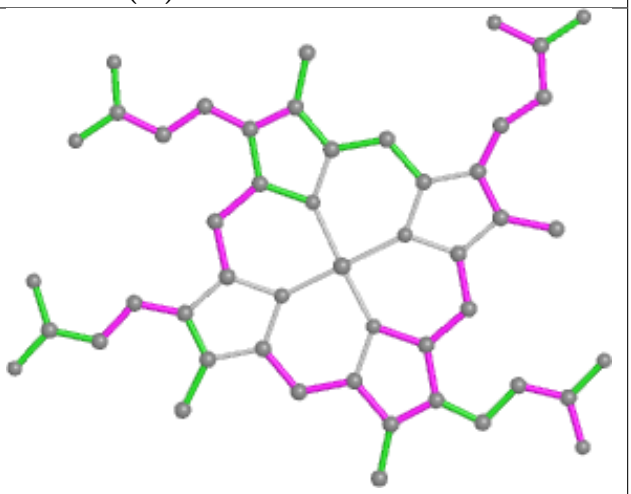


**Rings**

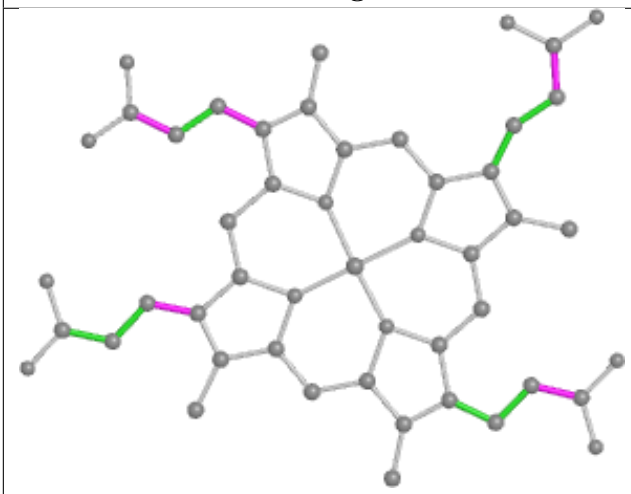
**Ligand FEC P 2507 (B)**



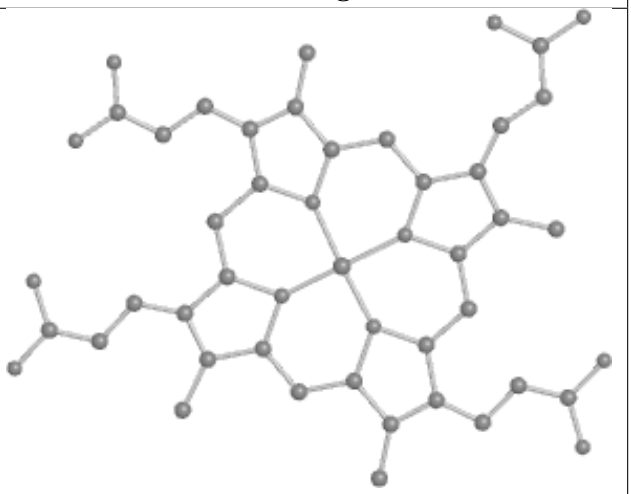
**Bond lengths**



**Bond angles**

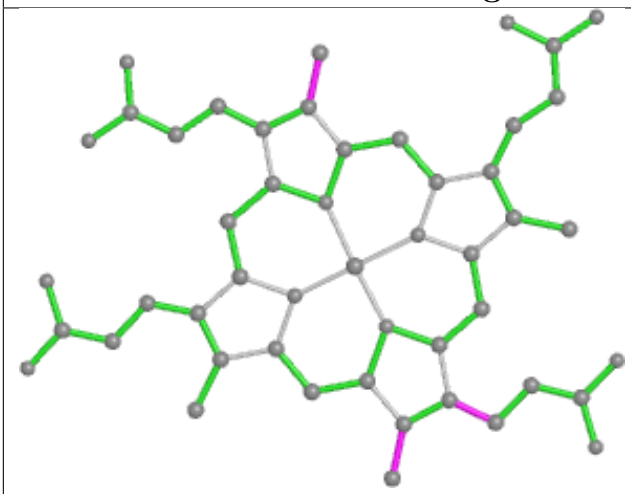


**Torsions**

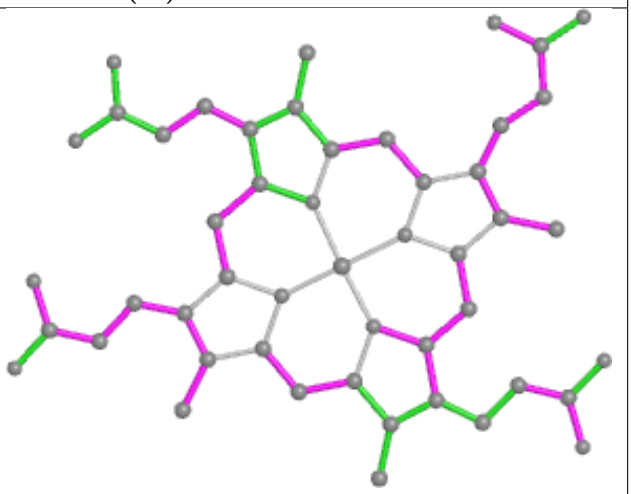


**Rings**

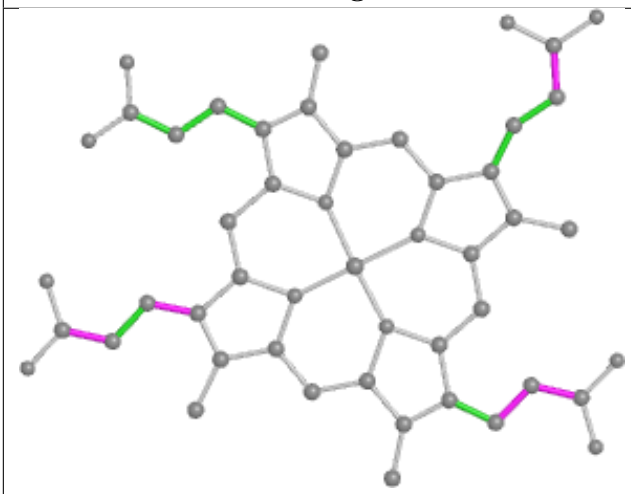
**Ligand FEC B 1107 (A)**



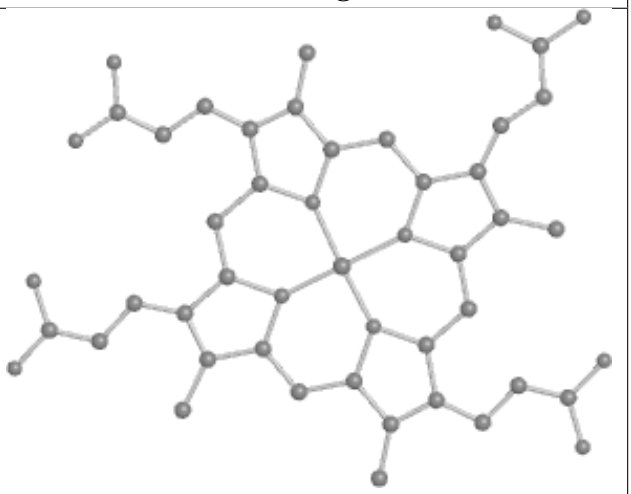
**Bond lengths**



**Bond angles**

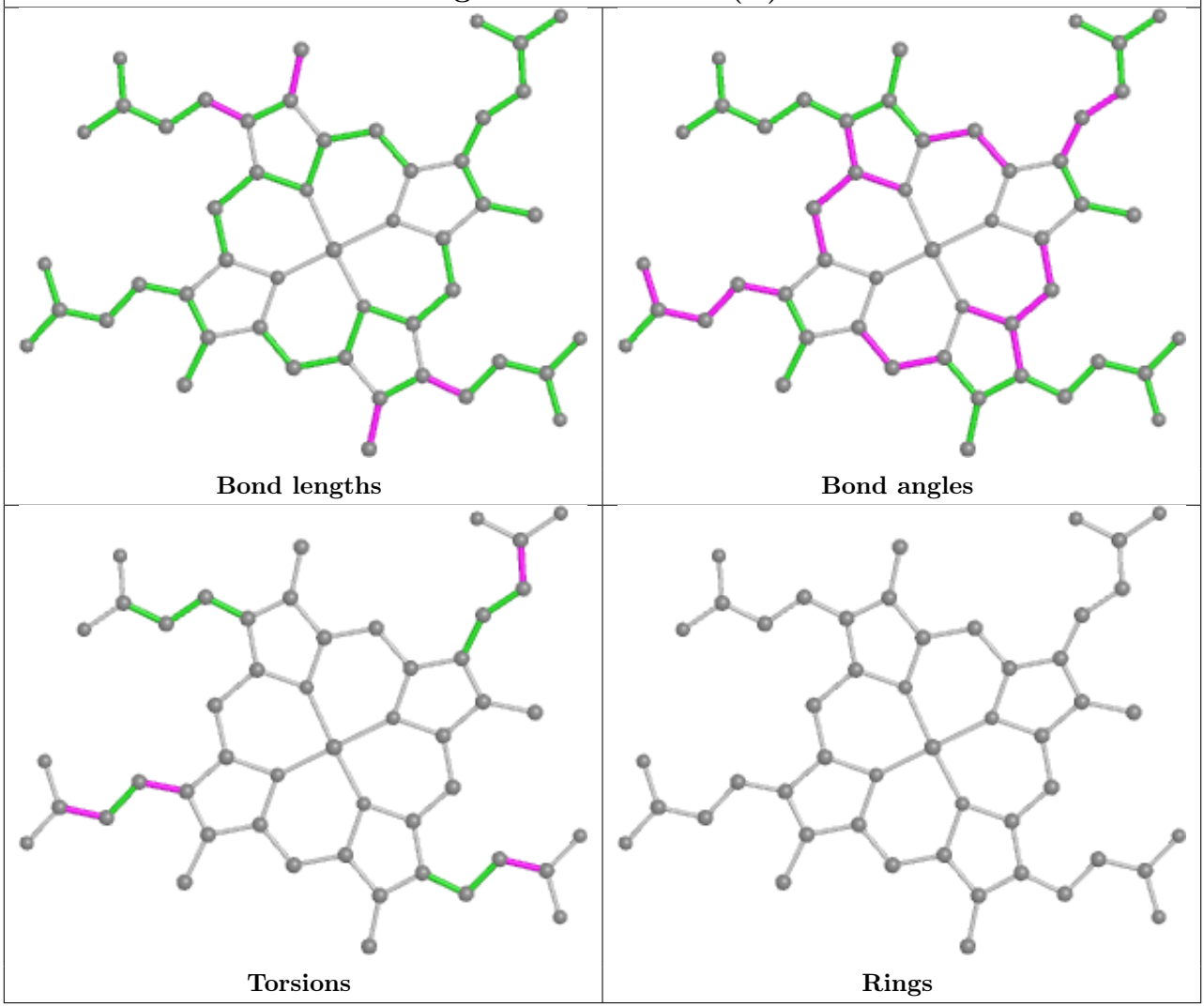


**Torsions**



**Rings**

**Ligand FEC D 1311 (B)**




## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 169/179 (94%) | 0.11 | 10 (5%) | 22 | 30 | 16, 24, 43, 65 | 0 |
| 1 | B | 170/179 (94%) | -0.03 | 9 (5%) | 26 | 35 | 15, 24, 45, 65 | 0 |
| 1 | C | 170/179 (94%) | -0.05 | 8 (4%) | 31 | 41 | 16, 25, 45, 65 | 0 |
| 1 | D | 170/179 (94%) | 0.02 | 9 (5%) | 26 | 35 | 16, 25, 44, 65 | 1 (0%) |
| 1 | E | 170/179 (94%) | 0.05 | 9 (5%) | 26 | 35 | 17, 25, 47, 65 | 1 (0%) |
| 1 | F | 170/179 (94%) | -0.03 | 7 (4%) | 37 | 46 | 16, 25, 46, 68 | 1 (0%) |
| 1 | G | 169/179 (94%) | -0.08 | 4 (2%) | 59 | 68 | 15, 24, 43, 65 | 0 |
| 1 | H | 170/179 (94%) | 0.01 | 12 (7%) | 16 | 24 | 16, 25, 44, 65 | 0 |
| 1 | I | 170/179 (94%) | -0.00 | 6 (3%) | 44 | 53 | 16, 24, 43, 65 | 0 |
| 1 | J | 170/179 (94%) | -0.02 | 9 (5%) | 26 | 35 | 17, 25, 47, 65 | 0 |
| 1 | K | 170/179 (94%) | -0.06 | 4 (2%) | 59 | 68 | 16, 24, 46, 68 | 0 |
| 1 | L | 170/179 (94%) | -0.01 | 4 (2%) | 59 | 68 | 16, 24, 43, 65 | 1 (0%) |
| 1 | M | 170/179 (94%) | -0.04 | 7 (4%) | 37 | 46 | 15, 24, 47, 65 | 0 |
| 1 | N | 170/179 (94%) | -0.03 | 6 (3%) | 44 | 53 | 16, 24, 43, 65 | 0 |
| 1 | O | 169/179 (94%) | 0.10 | 6 (3%) | 42 | 52 | 16, 25, 44, 68 | 1 (0%) |
| 1 | P | 170/179 (94%) | -0.09 | 7 (4%) | 37 | 46 | 17, 25, 48, 65 | 0 |
| All | All | 2717/2864 (94%) | -0.01 | 117 (4%) | 35 | 45 | 15, 25, 46, 68 | 5 (0%) |

All (117) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 166 | THR | 7.2 |
| 1 | A | 166 | THR | 7.1 |
| 1 | E | 168[A] | SER | 6.8 |
| 1 | N | 166 | THR | 6.6 |
| 1 | I | 166 | THR | 6.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | G | 168[A] | SER | 6.3 |
| 1 | O | 166 | THR | 6.2 |
| 1 | B | 166 | THR | 6.0 |
| 1 | I | 168[A] | SER | 5.8 |
| 1 | L | 166 | THR | 5.8 |
| 1 | P | 168[A] | SER | 5.4 |
| 1 | N | 168[A] | SER | 5.3 |
| 1 | F | 166 | THR | 5.2 |
| 1 | E | 166 | THR | 5.2 |
| 1 | M | 166 | THR | 4.9 |
| 1 | A | 168[A] | SER | 4.9 |
| 1 | D | 168[A] | SER | 4.8 |
| 1 | K | 168[A] | SER | 4.7 |
| 1 | L | 168[A] | SER | 4.7 |
| 1 | M | 168[A] | SER | 4.6 |
| 1 | F | 168[A] | SER | 4.6 |
| 1 | J | 168[A] | SER | 4.5 |
| 1 | H | 166 | THR | 4.3 |
| 1 | F | 165 | GLY | 4.3 |
| 1 | A | 167 | ALA | 4.2 |
| 1 | B | 168[A] | SER | 4.2 |
| 1 | C | 3 | GLY | 4.1 |
| 1 | O | 4 | ASN | 4.1 |
| 1 | M | 167 | ALA | 4.1 |
| 1 | H | 168[A] | SER | 4.0 |
| 1 | O | 168[A] | SER | 4.0 |
| 1 | G | 167 | ALA | 4.0 |
| 1 | J | 4 | ASN | 3.9 |
| 1 | N | 167 | ALA | 3.9 |
| 1 | P | 166 | THR | 3.8 |
| 1 | C | 168[A] | SER | 3.7 |
| 1 | F | 3 | GLY | 3.6 |
| 1 | J | 166 | THR | 3.6 |
| 1 | K | 166 | THR | 3.6 |
| 1 | C | 165 | GLY | 3.4 |
| 1 | A | 27 | ILE | 3.4 |
| 1 | D | 166 | THR | 3.4 |
| 1 | J | 3 | GLY | 3.3 |
| 1 | A | 165 | GLY | 3.3 |
| 1 | P | 3 | GLY | 3.3 |
| 1 | G | 166 | THR | 3.3 |
| 1 | I | 169[A] | LYS | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 7 | ASP | 3.3 |
| 1 | C | 4 | ASN | 3.2 |
| 1 | D | 3 | GLY | 3.2 |
| 1 | F | 7 | ASP | 3.2 |
| 1 | H | 4 | ASN | 3.1 |
| 1 | O | 167 | ALA | 3.1 |
| 1 | M | 6 | GLU | 3.0 |
| 1 | B | 4 | ASN | 3.0 |
| 1 | D | 4 | ASN | 3.0 |
| 1 | E | 167 | ALA | 2.9 |
| 1 | M | 3 | GLY | 2.9 |
| 1 | C | 7 | ASP | 2.9 |
| 1 | L | 60 | ALA | 2.9 |
| 1 | D | 165 | GLY | 2.8 |
| 1 | M | 169[A] | LYS | 2.8 |
| 1 | J | 169[A] | LYS | 2.7 |
| 1 | D | 7 | ASP | 2.7 |
| 1 | C | 27 | ILE | 2.7 |
| 1 | E | 165 | GLY | 2.7 |
| 1 | L | 167 | ALA | 2.7 |
| 1 | G | 169[A] | LYS | 2.6 |
| 1 | D | 5 | ARG | 2.6 |
| 1 | M | 4 | ASN | 2.6 |
| 1 | H | 27 | ILE | 2.6 |
| 1 | E | 6 | GLU | 2.6 |
| 1 | O | 165 | GLY | 2.6 |
| 1 | F | 167 | ALA | 2.5 |
| 1 | J | 7 | ASP | 2.5 |
| 1 | I | 3 | GLY | 2.5 |
| 1 | H | 3 | GLY | 2.5 |
| 1 | E | 7 | ASP | 2.5 |
| 1 | C | 167 | ALA | 2.5 |
| 1 | A | 127[A] | ARG | 2.5 |
| 1 | N | 165 | GLY | 2.5 |
| 1 | E | 77 | GLN | 2.5 |
| 1 | B | 169[A] | LYS | 2.5 |
| 1 | N | 3 | GLY | 2.4 |
| 1 | H | 169[A] | LYS | 2.4 |
| 1 | A | 169[A] | LYS | 2.4 |
| 1 | H | 167 | ALA | 2.4 |
| 1 | H | 165 | GLY | 2.4 |
| 1 | B | 7 | ASP | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 81 | LYS | 2.3 |
| 1 | I | 167 | ALA | 2.3 |
| 1 | E | 27 | ILE | 2.3 |
| 1 | K | 169[A] | LYS | 2.3 |
| 1 | P | 6 | GLU | 2.3 |
| 1 | H | 108 | GLN | 2.3 |
| 1 | O | 90 | VAL | 2.3 |
| 1 | D | 169[A] | LYS | 2.3 |
| 1 | P | 79 | GLU | 2.2 |
| 1 | H | 24 | LEU | 2.2 |
| 1 | B | 167 | ALA | 2.2 |
| 1 | E | 4 | ASN | 2.2 |
| 1 | J | 81 | LYS | 2.2 |
| 1 | B | 165 | GLY | 2.2 |
| 1 | J | 5 | ARG | 2.2 |
| 1 | K | 27 | ILE | 2.2 |
| 1 | P | 167 | ALA | 2.2 |
| 1 | A | 4 | ASN | 2.1 |
| 1 | I | 27 | ILE | 2.1 |
| 1 | J | 165 | GLY | 2.1 |
| 1 | F | 4 | ASN | 2.1 |
| 1 | B | 27 | ILE | 2.1 |
| 1 | H | 7 | ASP | 2.1 |
| 1 | B | 3 | GLY | 2.1 |
| 1 | A | 24 | LEU | 2.0 |
| 1 | A | 31 | MET | 2.0 |
| 1 | D | 77[A] | GLN | 2.0 |
| 1 | N | 6 | GLU | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | SO4 | A | 1004 | 5/5 | 0.45 | 0.48 | 66,66,67,67 | 5 |
| 3 | SO4 | G | 1607 | 5/5 | 0.61 | 0.38 | 67,67,70,70 | 0 |
| 3 | SO4 | J | 1901 | 5/5 | 0.73 | 0.29 | 66,67,67,69 | 0 |
| 3 | SO4 | K | 1504 | 5/5 | 0.73 | 0.23 | 78,78,78,79 | 0 |
| 3 | SO4 | E | 1304 | 5/5 | 0.75 | 0.39 | 65,65,67,67 | 0 |
| 3 | SO4 | O | 2409 | 5/5 | 0.76 | 0.40 | 57,63,66,67 | 0 |
| 4 | GOL | E | 1411 | 6/6 | 0.77 | 0.19 | 34,56,92,108 | 0 |
| 2 | FE | B | 201 | 1/1 | 0.78 | 0.09 | 44,44,44,44 | 0 |
| 3 | SO4 | D | 1303 | 5/5 | 0.78 | 0.23 | 39,44,45,50 | 5 |
| 4 | GOL | J | 1910 | 6/6 | 0.78 | 0.30 | 46,52,80,104 | 0 |
| 3 | SO4 | G | 1603 | 5/5 | 0.79 | 0.41 | 73,73,74,75 | 0 |
| 3 | SO4 | P | 2503 | 5/5 | 0.79 | 0.28 | 42,43,47,49 | 5 |
| 2 | FE | L | 201 | 1/1 | 0.79 | 0.11 | 42,42,42,42 | 0 |
| 4 | GOL | I | 1713 | 6/6 | 0.79 | 0.21 | 52,57,84,157 | 0 |
| 3 | SO4 | L | 2103 | 5/5 | 0.79 | 0.36 | 78,78,78,79 | 0 |
| 3 | SO4 | H | 1703 | 5/5 | 0.80 | 0.48 | 40,43,48,48 | 0 |
| 4 | GOL | A | 1010 | 6/6 | 0.81 | 0.29 | 42,68,89,111 | 0 |
| 4 | GOL | I | 1810 | 6/6 | 0.81 | 0.30 | 27,42,66,76 | 0 |
| 3 | SO4 | F | 1502 | 5/5 | 0.81 | 0.44 | 69,69,69,71 | 0 |
| 3 | SO4 | K | 2001 | 5/5 | 0.82 | 0.26 | 51,53,53,54 | 0 |
| 4 | GOL | B | 1110 | 6/6 | 0.82 | 0.20 | 40,46,69,84 | 0 |
| 4 | GOL | H | 1710 | 6/6 | 0.83 | 0.26 | 50,52,61,94 | 0 |
| 4 | GOL | H | 1814 | 6/6 | 0.83 | 0.16 | 38,49,55,61 | 0 |
| 3 | SO4 | E | 1401 | 5/5 | 0.83 | 0.28 | 67,68,68,68 | 0 |
| 3 | SO4 | L | 2101 | 5/5 | 0.83 | 0.20 | 64,64,65,65 | 0 |
| 4 | GOL | G | 1611 | 6/6 | 0.83 | 0.19 | 31,53,70,78 | 0 |
| 3 | SO4 | C | 1201 | 5/5 | 0.84 | 0.19 | 65,65,67,67 | 0 |
| 3 | SO4 | P | 2501 | 5/5 | 0.84 | 0.18 | 62,62,63,63 | 0 |
| 3 | SO4 | J | 1906 | 5/5 | 0.85 | 0.35 | 50,51,59,59 | 0 |
| 3 | SO4 | M | 2206 | 5/5 | 0.85 | 0.31 | 58,60,67,70 | 0 |
| 3 | SO4 | G | 1606 | 5/5 | 0.86 | 0.26 | 58,65,67,73 | 0 |
| 4 | GOL | G | 1610 | 6/6 | 0.86 | 0.20 | 44,46,56,106 | 0 |
| 4 | GOL | M | 2211 | 6/6 | 0.86 | 0.16 | 40,61,98,143 | 0 |
| 4 | GOL | P | 2510 | 6/6 | 0.86 | 0.28 | 32,51,74,105 | 0 |
| 2 | FE | M | 201 | 1/1 | 0.87 | 0.10 | 40,40,40,40 | 0 |
| 4 | GOL | C | 1210 | 6/6 | 0.87 | 0.29 | 32,43,67,71 | 0 |
| 3 | SO4 | C | 1206 | 5/5 | 0.87 | 0.36 | 46,46,47,49 | 0 |
| 3 | SO4 | D | 1301 | 5/5 | 0.87 | 0.24 | 58,59,60,60 | 0 |
| 3 | SO4 | I | 1803 | 5/5 | 0.87 | 0.36 | 67,67,70,70 | 0 |
| 4 | GOL | N | 2310 | 6/6 | 0.87 | 0.18 | 38,48,69,155 | 0 |
| 4 | GOL | O | 2410 | 6/6 | 0.87 | 0.21 | 47,53,59,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | FE | A | 201 | 1/1 | 0.87 | 0.12 | 44,44,44,44 | 0 |
| 6 | 3PY | D | 1310 | 6/7 | 0.87 | 0.19 | 50,63,70,78 | 0 |
| 3 | SO4 | A | 1001 | 5/5 | 0.88 | 0.22 | 53,54,54,55 | 0 |
| 2 | FE | D | 201 | 1/1 | 0.88 | 0.09 | 46,46,46,46 | 0 |
| 4 | GOL | J | 1811 | 6/6 | 0.88 | 0.23 | 40,57,107,154 | 0 |
| 3 | SO4 | O | 2406 | 5/5 | 0.88 | 0.20 | 41,44,46,47 | 5 |
| 4 | GOL | F | 1510 | 6/6 | 0.88 | 0.21 | 52,62,92,104 | 0 |
| 3 | SO4 | B | 1101 | 5/5 | 0.88 | 0.17 | 66,66,67,67 | 0 |
| 3 | SO4 | B | 1106 | 5/5 | 0.88 | 0.34 | 64,66,74,75 | 0 |
| 2 | FE | F | 201 | 1/1 | 0.88 | 0.06 | 46,46,46,46 | 0 |
| 3 | SO4 | H | 1706 | 5/5 | 0.88 | 0.34 | 47,55,58,60 | 0 |
| 3 | SO4 | A | 1105 | 5/5 | 0.89 | 0.47 | 51,53,55,61 | 0 |
| 3 | SO4 | N | 2306 | 5/5 | 0.89 | 0.23 | 60,65,69,71 | 0 |
| 3 | SO4 | A | 1006 | 5/5 | 0.89 | 0.36 | 56,67,69,74 | 0 |
| 3 | SO4 | C | 1203 | 5/5 | 0.89 | 0.34 | 56,58,62,64 | 0 |
| 3 | SO4 | B | 1104 | 5/5 | 0.90 | 0.15 | 73,73,74,75 | 0 |
| 3 | SO4 | H | 1701 | 5/5 | 0.90 | 0.21 | 54,54,55,56 | 0 |
| 3 | SO4 | N | 2303 | 5/5 | 0.90 | 0.50 | 64,68,70,72 | 0 |
| 4 | GOL | B | 1011 | 6/6 | 0.90 | 0.17 | 24,48,57,79 | 0 |
| 4 | GOL | M | 2210 | 6/6 | 0.90 | 0.25 | 34,50,95,99 | 0 |
| 3 | SO4 | A | 1008 | 5/5 | 0.91 | 0.42 | 51,53,55,61 | 0 |
| 4 | GOL | D | 1211 | 6/6 | 0.91 | 0.12 | 45,49,55,68 | 0 |
| 3 | SO4 | I | 1806 | 5/5 | 0.91 | 0.30 | 62,65,67,69 | 0 |
| 3 | SO4 | F | 1506 | 5/5 | 0.91 | 0.25 | 65,67,68,69 | 0 |
| 3 | SO4 | L | 2107 | 5/5 | 0.91 | 0.19 | 78,78,78,79 | 0 |
| 3 | SO4 | M | 2201 | 5/5 | 0.91 | 0.18 | 51,51,52,53 | 0 |
| 2 | FE | K | 201 | 1/1 | 0.91 | 0.09 | 43,43,43,43 | 0 |
| 3 | SO4 | N | 2301 | 5/5 | 0.91 | 0.21 | 62,63,63,63 | 0 |
| 3 | SO4 | F | 1501 | 5/5 | 0.91 | 0.15 | 66,66,67,67 | 0 |
| 2 | FE | G | 201 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 4 | GOL | K | 2011 | 6/6 | 0.92 | 0.14 | 46,57,59,146 | 0 |
| 4 | GOL | O | 2411 | 6/6 | 0.92 | 0.10 | 26,52,74,76 | 0 |
| 2 | FE | H | 201 | 1/1 | 0.92 | 0.09 | 43,43,43,43 | 0 |
| 4 | GOL | E | 1410 | 6/6 | 0.92 | 0.24 | 39,50,75,155 | 0 |
| 2 | FE | J | 201 | 1/1 | 0.93 | 0.07 | 46,46,46,46 | 0 |
| 3 | SO4 | J | 1904 | 5/5 | 0.93 | 0.21 | 61,61,62,63 | 5 |
| 2 | FE | N | 201 | 1/1 | 0.93 | 0.09 | 43,43,43,43 | 0 |
| 2 | FE | C | 201 | 1/1 | 0.93 | 0.08 | 46,46,46,46 | 0 |
| 3 | SO4 | B | 1005 | 5/5 | 0.93 | 0.28 | 51,53,55,61 | 0 |
| 3 | SO4 | K | 2003 | 5/5 | 0.93 | 0.29 | 69,69,69,71 | 0 |
| 2 | FE | I | 201 | 1/1 | 0.93 | 0.09 | 43,43,43,43 | 0 |
| 3 | SO4 | E | 1406 | 5/5 | 0.94 | 0.22 | 62,67,67,70 | 0 |

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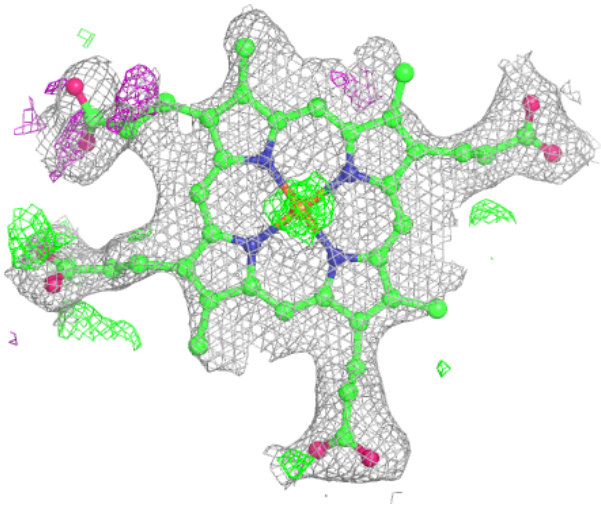
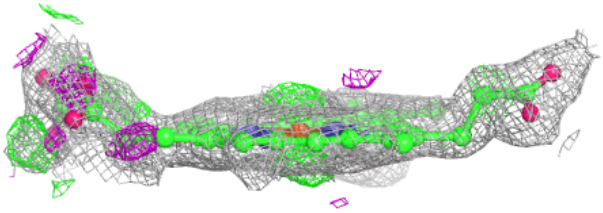
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | SO4 | I | 1801 | 5/5 | 0.94 | 0.17 | 61,61,62,63 | 0 |
| 2 | FE | E | 201 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 4 | GOL | F | 1512 | 6/6 | 0.95 | 0.14 | 22,37,47,49 | 0 |
| 3 | SO4 | K | 2006 | 5/5 | 0.95 | 0.23 | 52,55,60,61 | 0 |
| 3 | SO4 | P | 2506 | 5/5 | 0.95 | 0.24 | 57,63,66,67 | 0 |
| 3 | SO4 | I | 1802 | 5/5 | 0.95 | 0.15 | 36,37,38,38 | 0 |
| 5 | FEC | D | 1311[A] | 49/49 | 0.95 | 0.19 | 15,19,28,37 | 49 |
| 5 | FEC | D | 1311[B] | 49/49 | 0.95 | 0.19 | 10,19,28,46 | 49 |
| 2 | FE | P | 201 | 1/1 | 0.95 | 0.05 | 45,45,45,45 | 0 |
| 5 | FEC | B | 1107[B] | 49/49 | 0.96 | 0.20 | 15,18,27,38 | 49 |
| 2 | FE | O | 201 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 3 | SO4 | L | 2102 | 5/5 | 0.96 | 0.16 | 78,78,78,79 | 5 |
| 5 | FEC | F | 1507[A] | 49/49 | 0.96 | 0.17 | 15,19,29,36 | 49 |
| 5 | FEC | F | 1507[B] | 49/49 | 0.96 | 0.17 | 16,19,31,38 | 49 |
| 5 | FEC | G | 1608[A] | 49/49 | 0.96 | 0.19 | 15,18,28,37 | 49 |
| 5 | FEC | G | 1608[B] | 49/49 | 0.96 | 0.19 | 10,17,29,38 | 49 |
| 5 | FEC | P | 2507[A] | 49/49 | 0.96 | 0.17 | 15,18,28,37 | 49 |
| 5 | FEC | P | 2507[B] | 49/49 | 0.96 | 0.17 | 16,18,28,33 | 49 |
| 5 | FEC | B | 1107[A] | 49/49 | 0.96 | 0.20 | 15,18,28,37 | 49 |
| 5 | FEC | L | 2108[B] | 49/49 | 0.97 | 0.19 | 13,18,28,39 | 49 |
| 5 | FEC | M | 2207[A] | 49/49 | 0.97 | 0.18 | 14,18,28,37 | 49 |
| 5 | FEC | M | 2207[B] | 49/49 | 0.97 | 0.18 | 13,18,27,39 | 49 |
| 5 | FEC | I | 1807[A] | 49/49 | 0.97 | 0.18 | 15,19,28,37 | 49 |
| 5 | FEC | I | 1807[B] | 49/49 | 0.97 | 0.18 | 14,19,27,38 | 49 |
| 5 | FEC | L | 2108[A] | 49/49 | 0.97 | 0.19 | 15,18,28,37 | 49 |
| 2 | FE | A | 200 | 1/1 | 0.98 | 0.07 | 27,27,27,27 | 0 |
| 2 | FE | K | 200 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 2 | FE | C | 200 | 1/1 | 0.99 | 0.04 | 28,28,28,28 | 0 |
| 2 | FE | L | 200 | 1/1 | 0.99 | 0.07 | 26,26,26,26 | 0 |
| 2 | FE | H | 200 | 1/1 | 0.99 | 0.04 | 26,26,26,26 | 0 |
| 2 | FE | M | 200 | 1/1 | 0.99 | 0.07 | 26,26,26,26 | 0 |
| 2 | FE | F | 200 | 1/1 | 0.99 | 0.06 | 29,29,29,29 | 0 |
| 2 | FE | N | 200 | 1/1 | 0.99 | 0.05 | 25,25,25,25 | 0 |
| 2 | FE | I | 200 | 1/1 | 0.99 | 0.06 | 27,27,27,27 | 0 |
| 2 | FE | O | 200 | 1/1 | 0.99 | 0.07 | 29,29,29,29 | 0 |
| 2 | FE | E | 200 | 1/1 | 0.99 | 0.08 | 29,29,29,29 | 0 |
| 2 | FE | P | 200 | 1/1 | 0.99 | 0.05 | 28,28,28,28 | 0 |
| 2 | FE | J | 200 | 1/1 | 0.99 | 0.05 | 30,30,30,30 | 0 |
| 2 | FE | G | 200 | 1/1 | 0.99 | 0.06 | 26,26,26,26 | 0 |
| 2 | FE | D | 200 | 1/1 | 1.00 | 0.06 | 29,29,29,29 | 0 |
| 2 | FE | B | 200 | 1/1 | 1.00 | 0.07 | 25,25,25,25 | 0 |

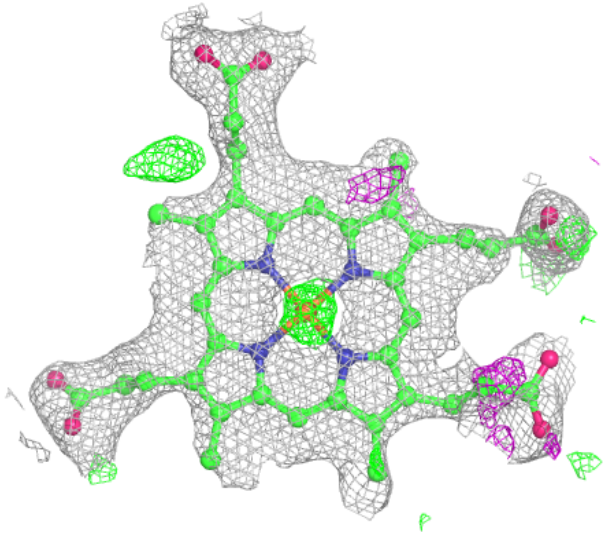
The following is a graphical depiction of the model fit to experimental electron density of all

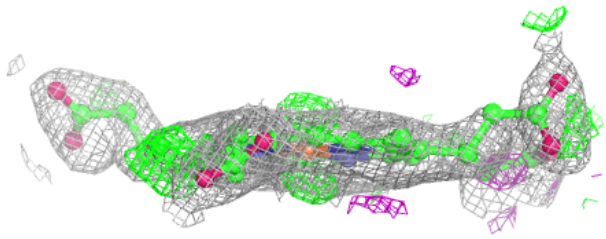
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

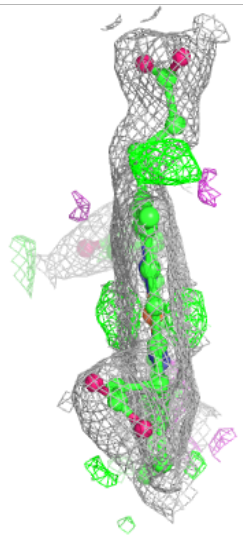
| | |
|---|---|
| **Electron density around FEC D 1311 (A):**<br><br>$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray<br>$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)<br>and green (positive) |  |
|  | |

**Electron density around FEC D 1311 (B):**

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

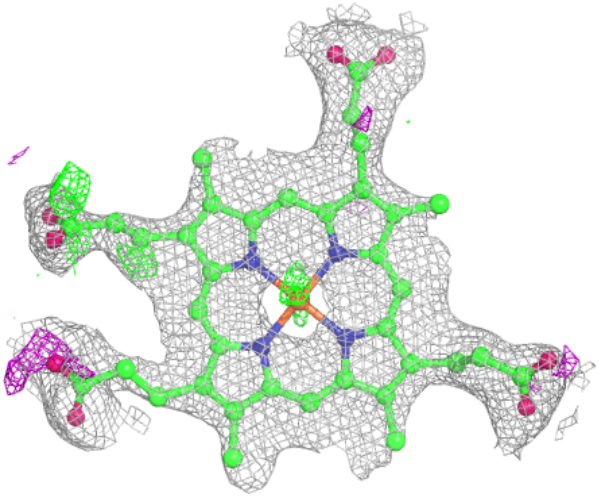


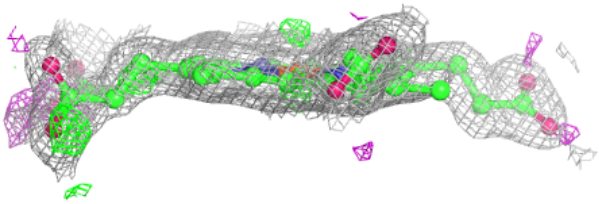


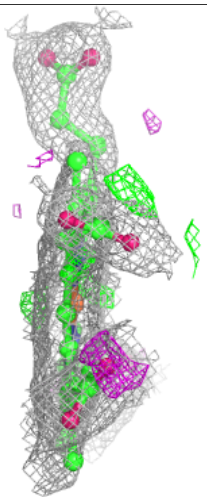


**Electron density around FEC B 1107 (B):**

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

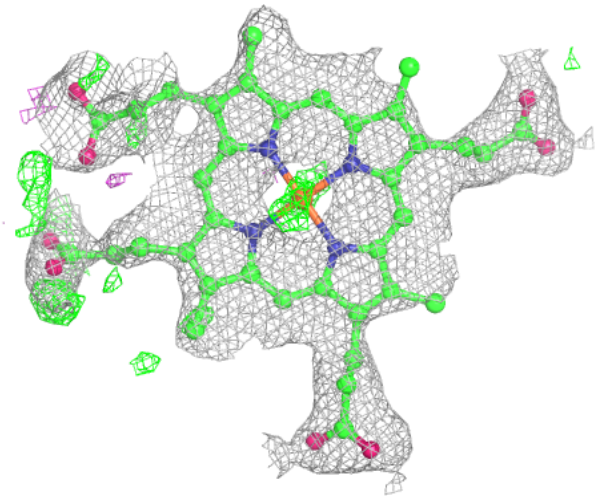


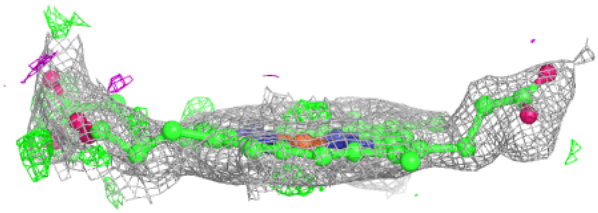


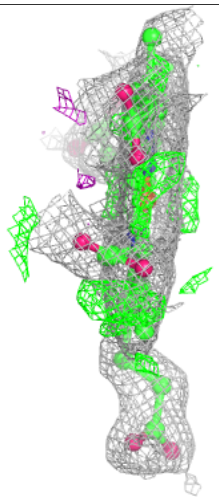


**Electron density around FEC F 1507 (A):**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

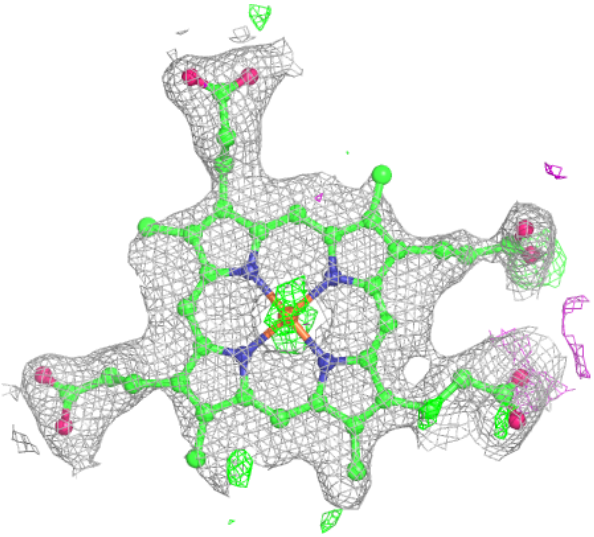


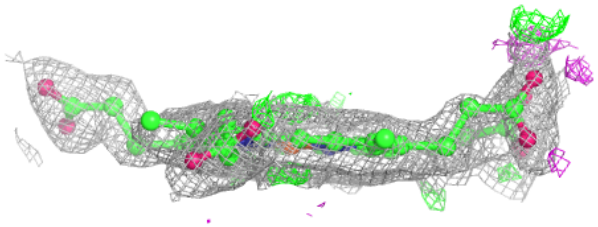


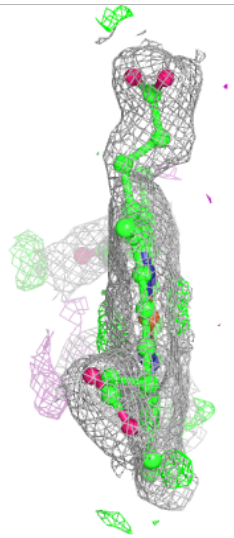


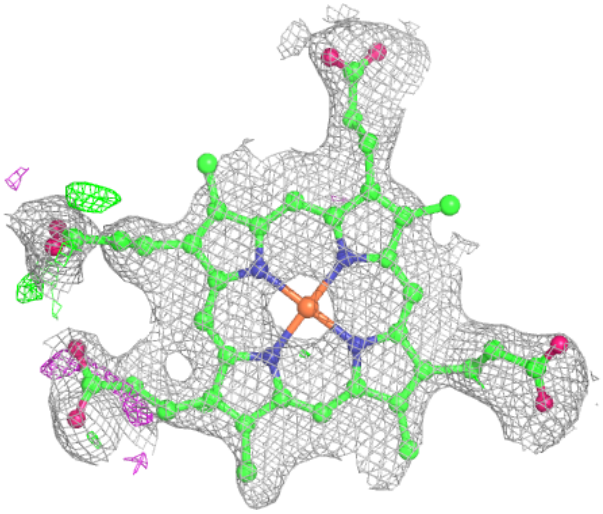
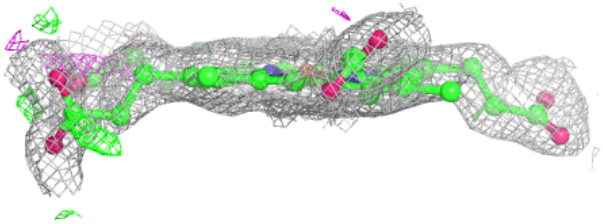
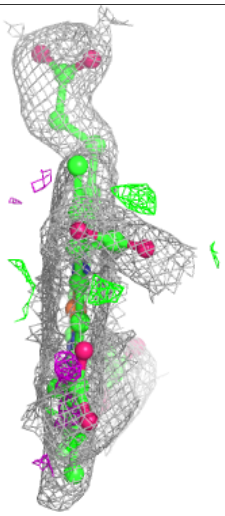
**Electron density around FEC F 1507 (B):**

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



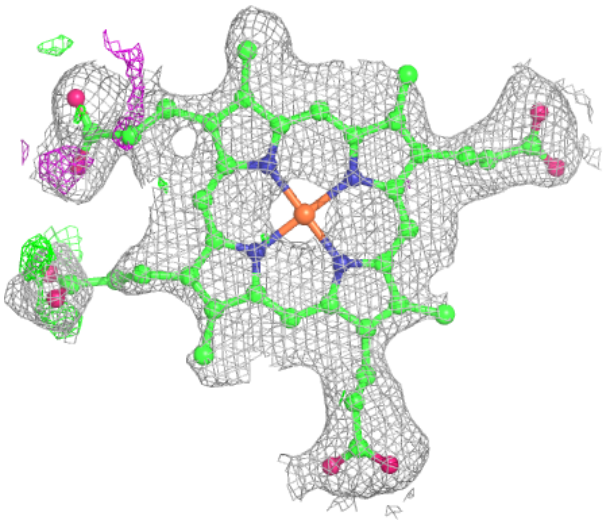


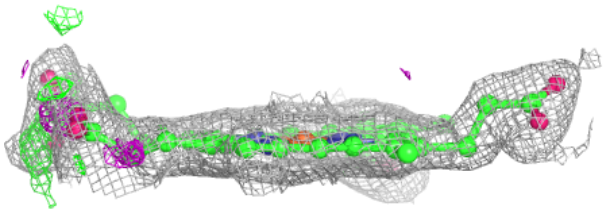


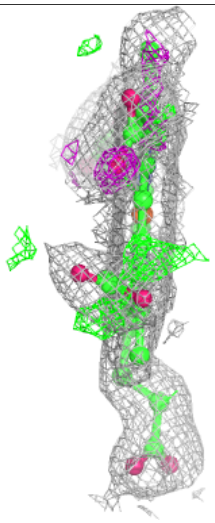
| | |
|---|---|
| **Electron density around FEC G 1608 (A):**<br><br>2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray<br>mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)<br>and green (positive) |  |
|  |  |

**Electron density around FEC G 1608 (B):**

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

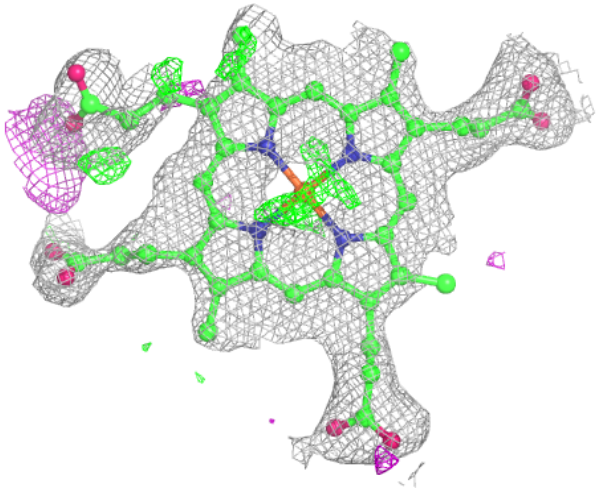


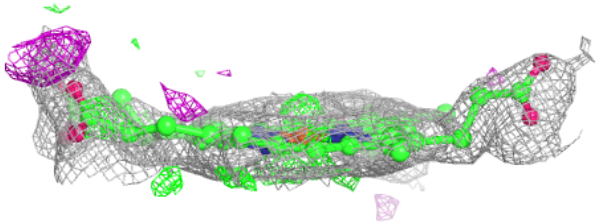


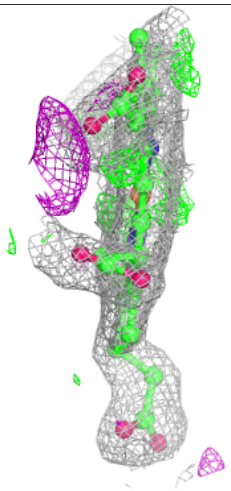


**Electron density around FEC P 2507 (A):**

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

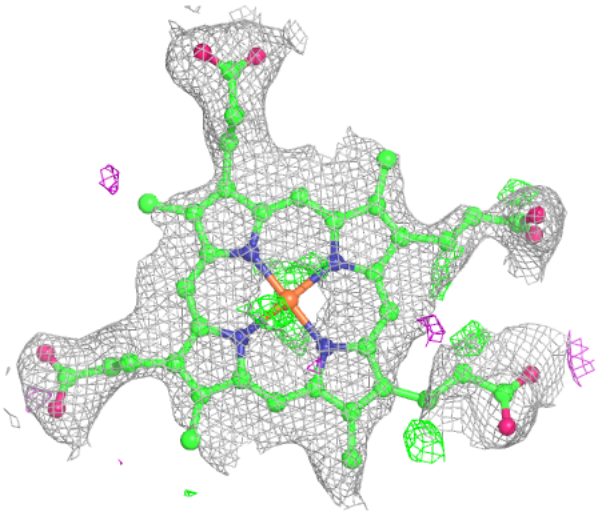


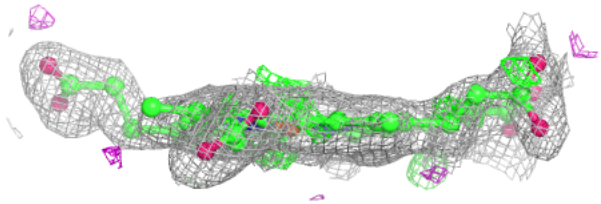


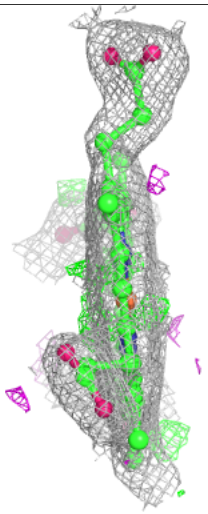


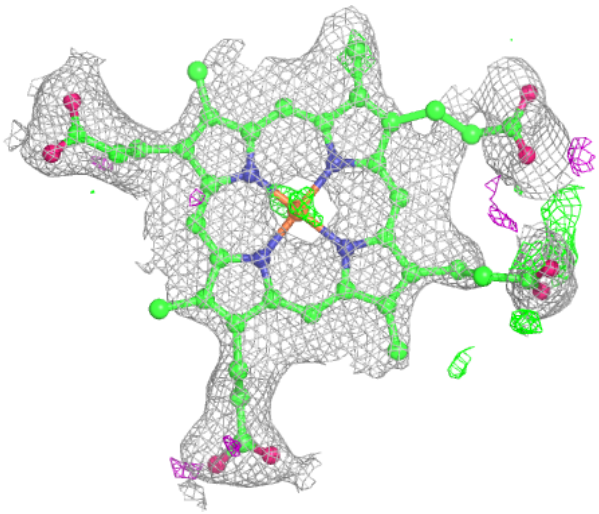
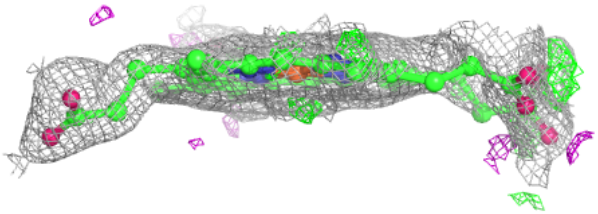
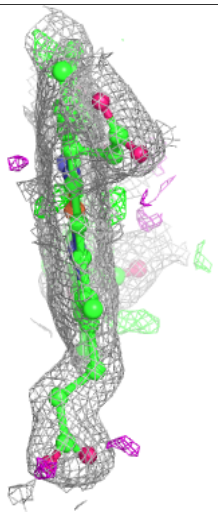
**Electron density around FEC P 2507 (B):**

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



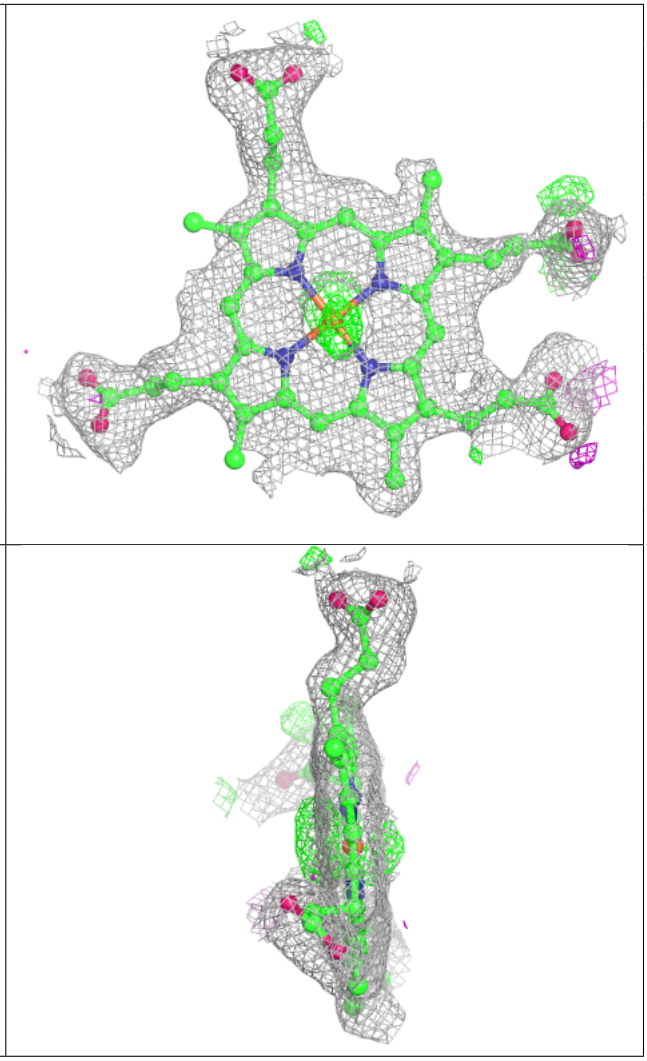




| | |
|---|---|
| **Electron density around FEC B 1107 (A):**<br><br>2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray<br>mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)<br>and green (positive) |  |
|  |  |

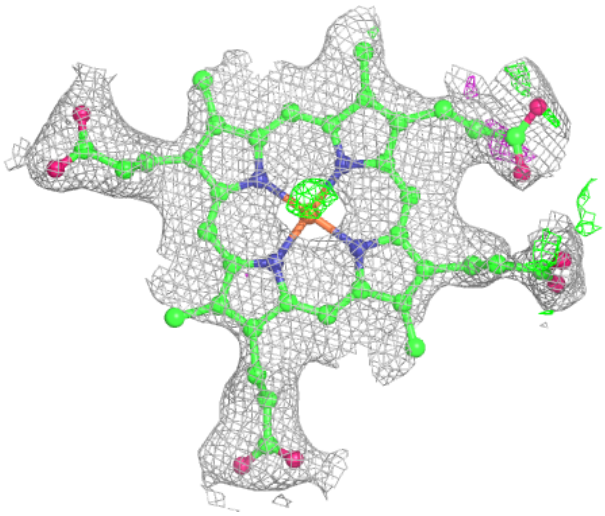
**Electron density around FEC L 2108 (B):**

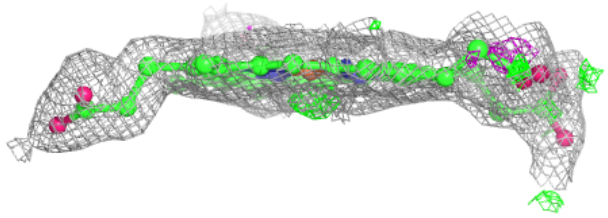
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

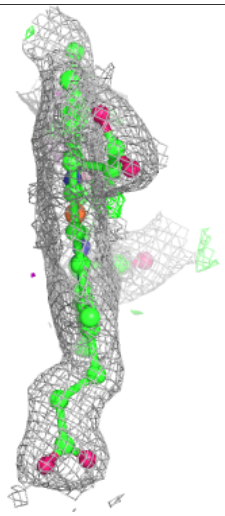


**Electron density around FEC M 2207 (A):**

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

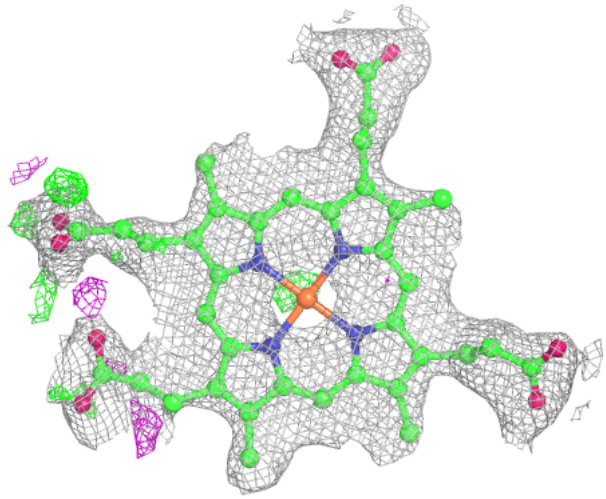


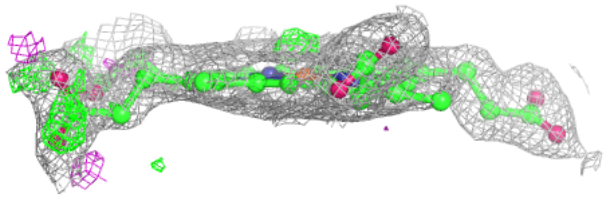


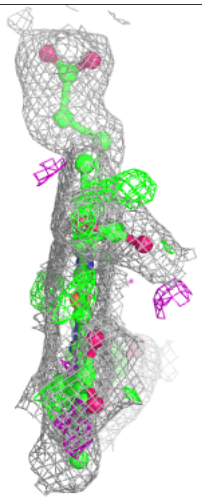


**Electron density around FEC M 2207 (B):**

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

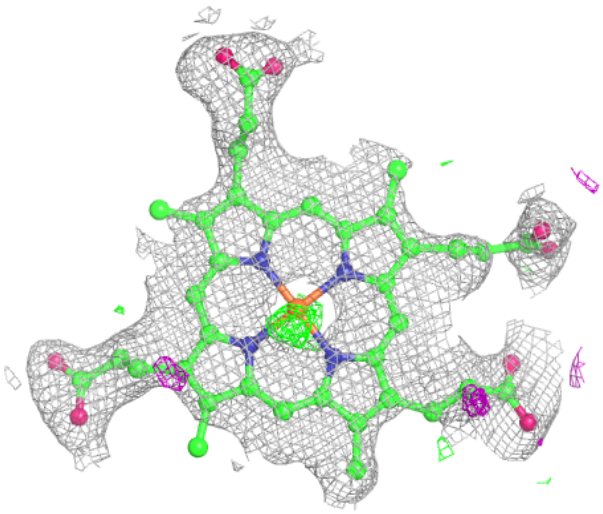


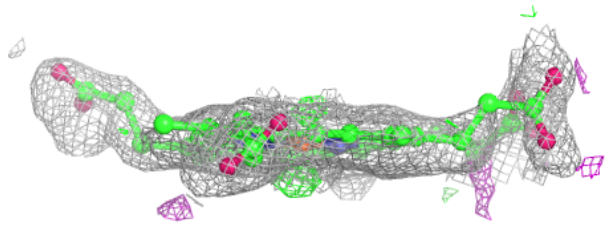


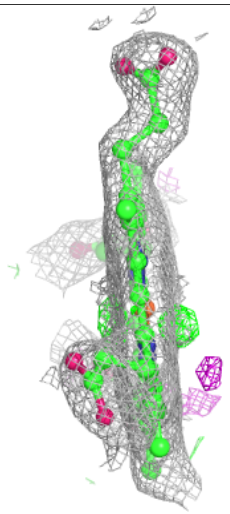


**Electron density around FEC I 1807 (A):**

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

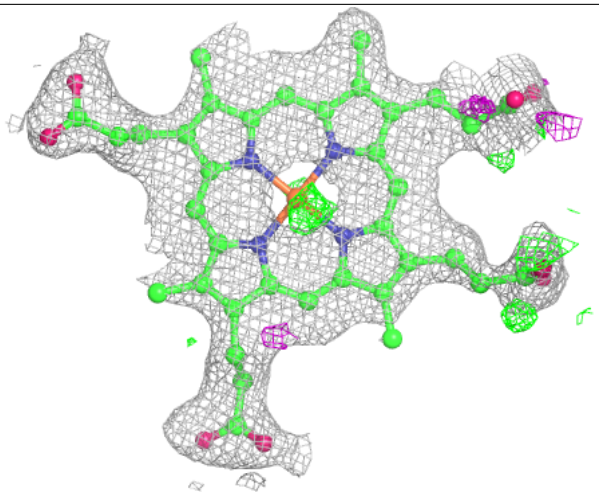


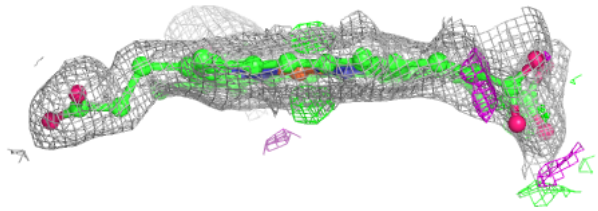


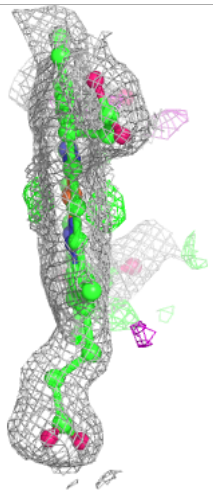


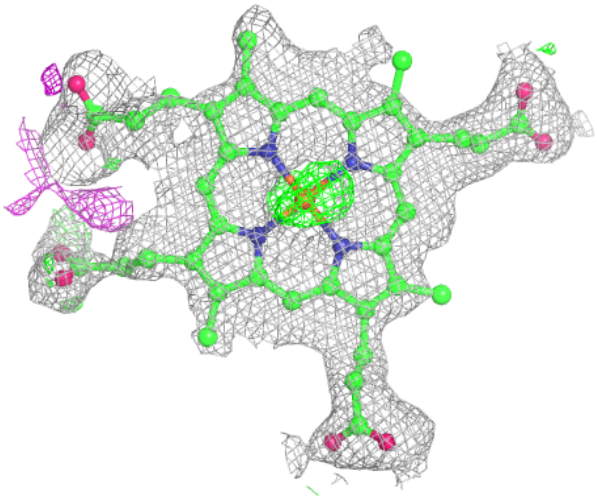
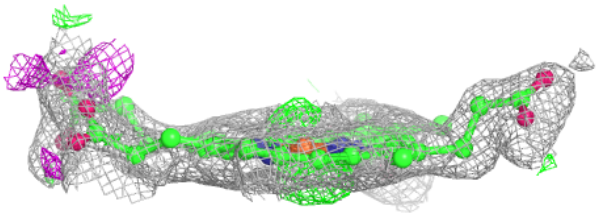
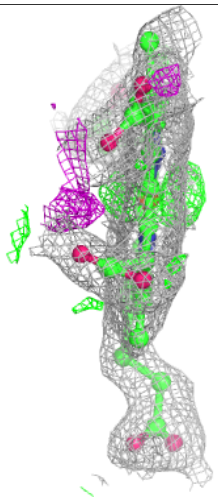
**Electron density around FEC I 1807 (B):**

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







| | |
|---|---|
| **Electron density around FEC L 2108 (A):**<br><br>2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray<br>mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)<br>and green (positive) |  |
|  |  |

## 6.5 Other polymers (i)

There are no such residues in this entry.