



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:50 AM GMT

PDB ID : 3Q09
Title : Crystal Structure of Chlorite Dismutase from *D. Aromatica* at pH 9.0
Authors : Goblirsch, B.R.; Wilmot, C.M.
Deposited on : 2010-12-15
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

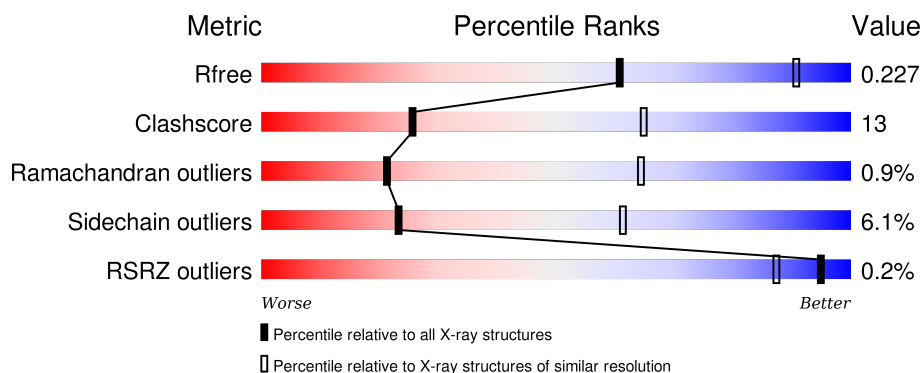
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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} | 91344 | 1578 (3.00-3.00) |
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 248 | <div> <div>70%</div> <div>25%</div> <div>..</div> </div> |
| 1 | B | 248 | <div> <div>72%</div> <div>22%</div> <div>..</div> </div> |
| 1 | C | 248 | <div> <div>%</div> <div>73%</div> <div>20%</div> <div>..</div> </div> |
| 1 | D | 248 | <div> <div>73%</div> <div>22%</div> <div>..</div> </div> |
| 1 | E | 248 | <div> <div>71%</div> <div>23%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | F | 248 |  71% 25% . . |
| 1 | G | 248 |  70% 24% . . |
| 1 | H | 248 |  76% 19% . . |
| 1 | I | 248 |  75% 19% . . |
| 1 | J | 248 |  73% 20% . . |
| 1 | K | 248 |  75% 21% . . |
| 1 | L | 248 |  74% 20% . . |
| 1 | M | 248 |  74% 21% . . |
| 1 | N | 248 |  70% 24% . . |
| 1 | O | 248 |  76% 19% . . |
| 1 | P | 248 |  70% 24% . . |
| 1 | Q | 248 |  67% 25% 5% . |
| 1 | R | 248 |  70% 24% . . |
| 1 | S | 248 |  2% 67% 28% . . |
| 1 | T | 248 |  62% 31% 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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | HEM | G | 1000 | - | - | - | X |
| 3 | NO2 | A | 2000 | - | - | - | X |
| 3 | NO2 | B | 2000 | - | - | - | X |
| 3 | NO2 | C | 2000 | - | - | - | X |
| 3 | NO2 | I | 2000 | - | - | - | X |
| 3 | NO2 | K | 2000 | - | - | - | X |
| 3 | NO2 | N | 2000 | - | - | - | X |
| 3 | NO2 | R | 2000 | - | - | - | X |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39520 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 Chlorite dismutase.

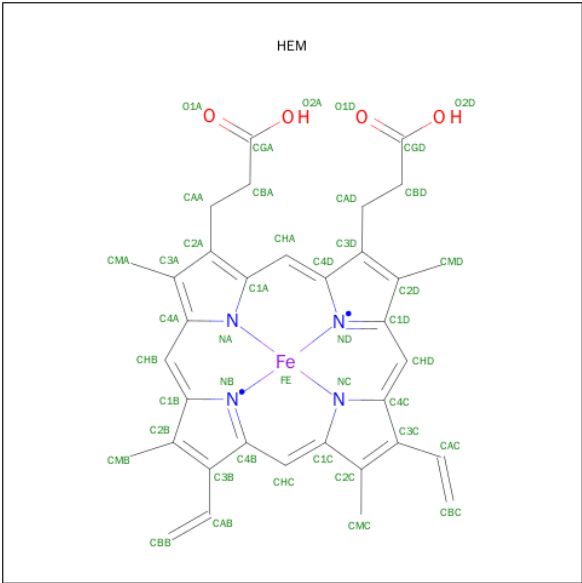
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | B | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | C | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | D | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | E | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | F | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | G | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | H | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | I | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | J | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | K | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | L | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | M | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | N | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | O | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | P | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | Q | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | R | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | S | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |
| 1 | T | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1928 | 1239 | 325 | 359 | 5 | | | |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



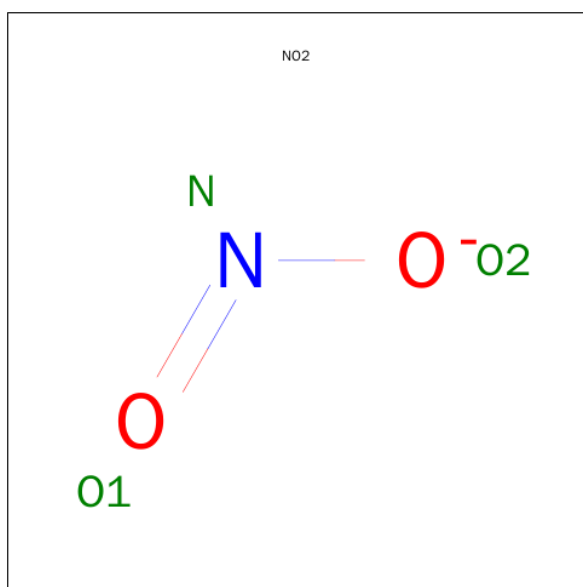
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | B | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | C | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | D | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | E | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | F | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 2 | G | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | H | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | I | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | J | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | K | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | L | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | M | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | N | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | O | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | P | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | Q | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | R | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | S | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | T | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | A | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | B | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | C | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | D | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | E | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | F | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | G | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | H | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | I | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | J | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | K | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | L | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | M | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | N | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | O | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | P | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | Q | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | R | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | S | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |
| 3 | T | 1 | Total | N | O | 0 | 0 |
| | | | 3 | 1 | 2 | | |

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | P | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | G | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | J | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | Q | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | D | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | K | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | E | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | H | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | B | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | I | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | C | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | A | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | T | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | N | 1 | Total 1 | Ca 1 | 0 | 0 |
| 4 | O | 1 | Total 1 | Ca 1 | 0 | 0 |
| 4 | R | 1 | Total 1 | Ca 1 | 0 | 0 |
| 4 | L | 1 | Total 1 | Ca 1 | 0 | 0 |
| 4 | S | 1 | Total 1 | Ca 1 | 0 | 0 |
| 4 | F | 1 | Total 1 | Ca 1 | 0 | 0 |
| 4 | M | 1 | Total 1 | Ca 1 | 0 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 5 | A | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | B | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | C | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | D | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | E | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | F | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | G | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | H | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | I | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | J | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | K | 1 | Total 1 | O 1 | 0 | 0 |
| 5 | L | 1 | Total 1 | O 1 | 0 | 0 |

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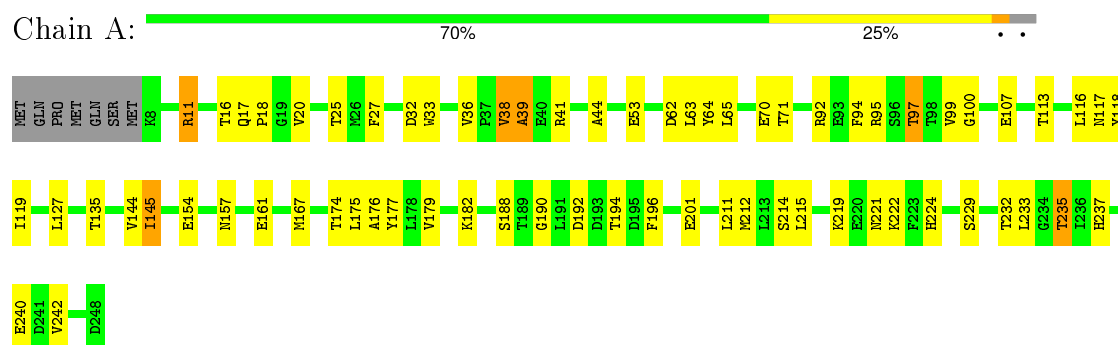
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 5 | M | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | N | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | O | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | P | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | Q | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | R | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | S | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | T | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

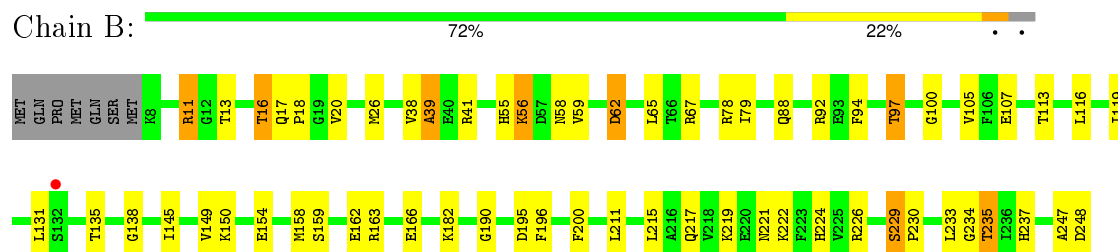
3 Residue-property plots

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

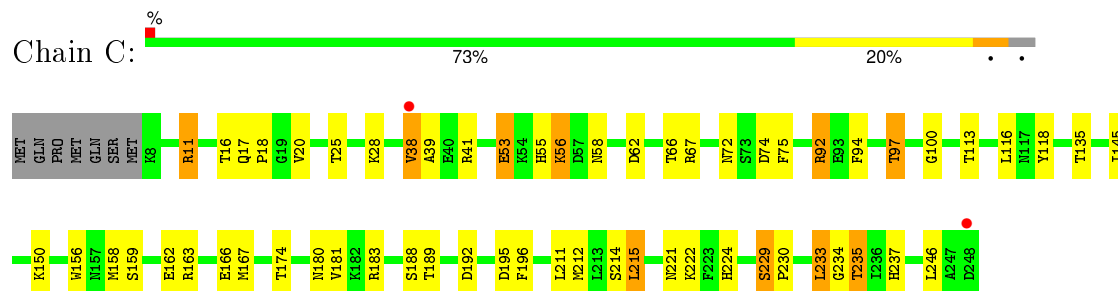
• Molecule 1: Chlorite dismutase



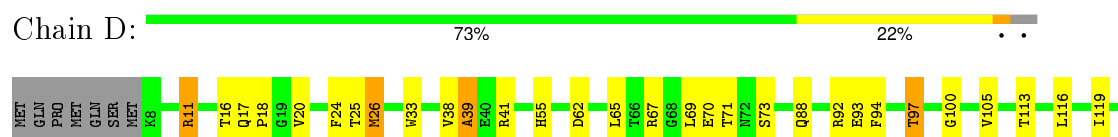
• Molecule 1: Chlorite dismutase



• Molecule 1: Chlorite dismutase



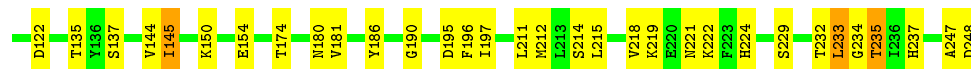
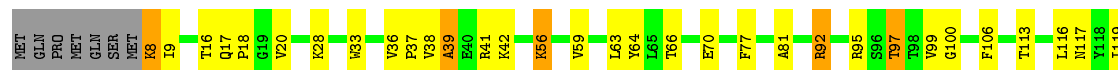
• Molecule 1: Chlorite dismutase





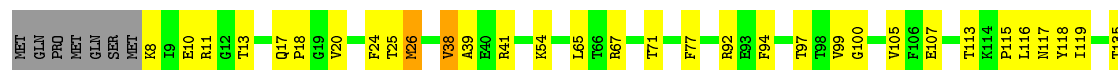
- Molecule 1: Chlorite dismutase

Chain E: 71% 23%



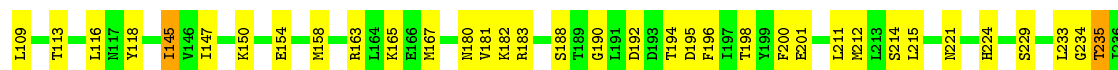
- Molecule 1: Chlorite dismutase

Chain F: 71% 25%



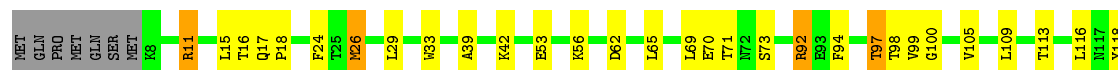
- Molecule 1: Chlorite dismutase

Chain G: 70% 24%



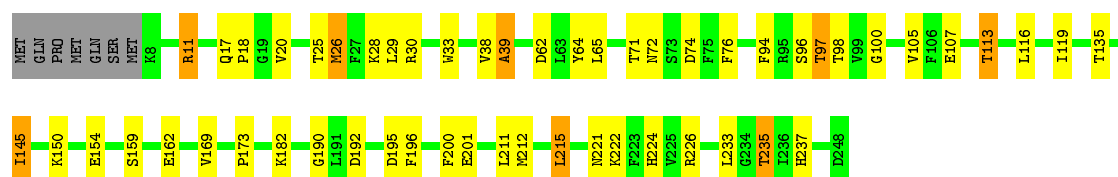
- Molecule 1: Chlorite dismutase

Chain H: 76% 19%



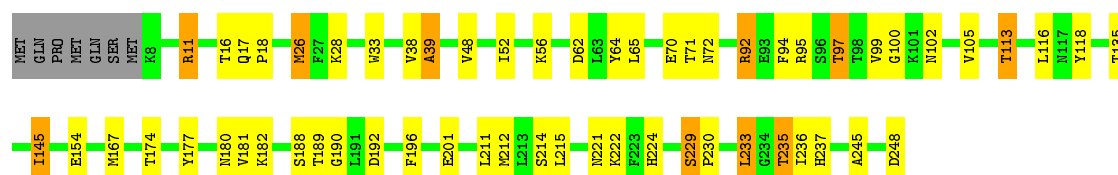
- Molecule 1: Chlorite dismutase

Chain I: 75% 19%



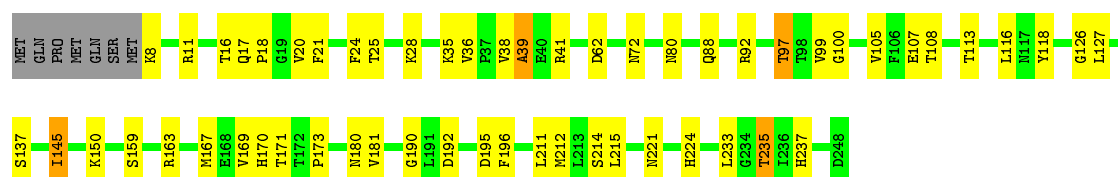
- Molecule 1: Chlorite dismutase

Chain J: 73% 20%



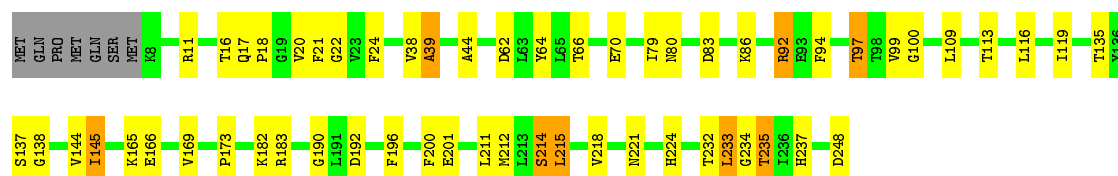
- Molecule 1: Chlorite dismutase

Chain K: 75% 21%



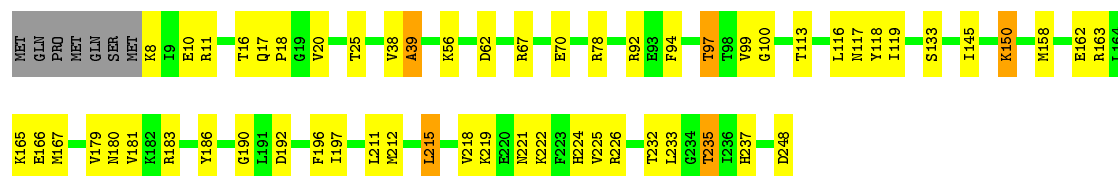
- Molecule 1: Chlorite dismutase

Chain L: 74% 20%



- Molecule 1: Chlorite dismutase

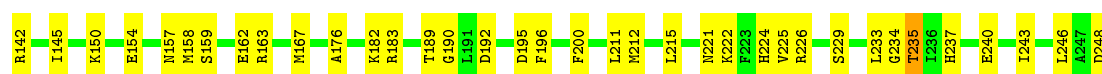
Chain M: 74% 21%



- Molecule 1: Chlorite dismutase

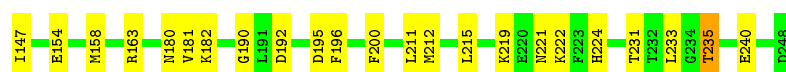
Chain N: 70% 24%





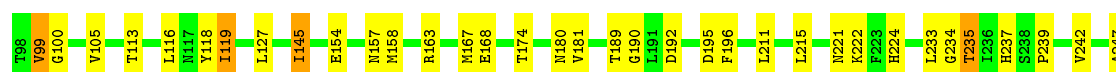
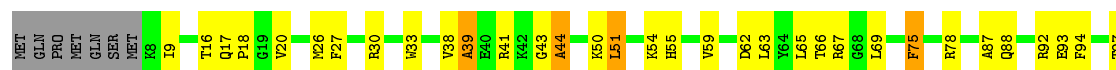
• Molecule 1: Chlorite dismutase

Chain O: 76% 19%



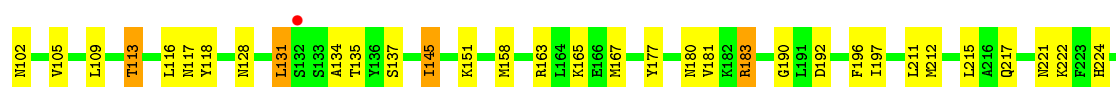
• Molecule 1: Chlorite dismutase

Chain P: 70% 24%



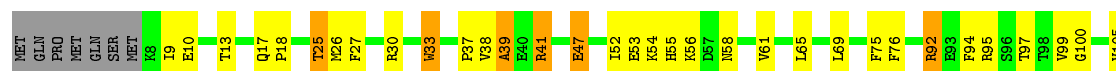
• Molecule 1: Chlorite dismutase

Chain Q: 67% 25% 5%

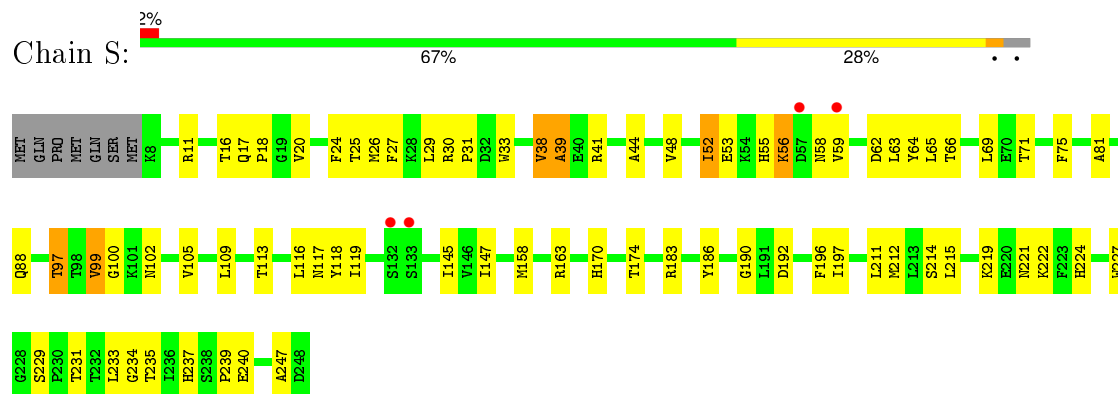


• Molecule 1: Chlorite dismutase

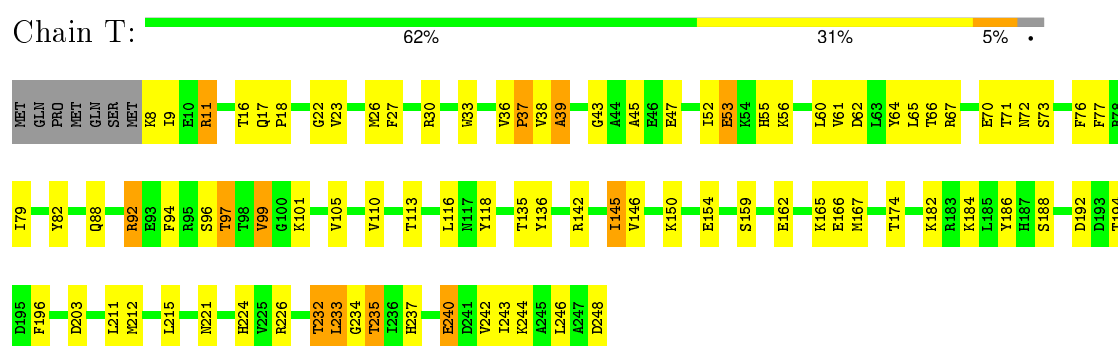
Chain R: 70% 24%



- Molecule 1: Chlorite dismutase



- Molecule 1: Chlorite dismutase



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 122.70Å 202.85Å 247.10Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 48.31 – 3.00 48.31 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (48.31-3.00) 99.7 (48.31-3.00) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 5.59 (at 3.01Å) | Xtriage |
| Refinement program | REFMAC 5.5.0109 | Depositor |
| R, R_{free} | 0.185 , 0.234 0.183 , 0.227 | Depositor DCC |
| R_{free} test set | 6174 reflections (5.28%) | DCC |
| Wilson B-factor (Å ²) | 39.8 | Xtriage |
| Anisotropy | 0.038 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 17.6 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Outliers | 2 of 123079 reflections (0.002%) | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 39520 | wwPDB-VP |
| Average B, all atoms (Å ²) | 40.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CA, NO2

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 | 0.83 | 2/1973 (0.1%) | 0.86 | 2/2676 (0.1%) |
| 1 | B | 0.87 | 0/1973 | 0.89 | 2/2676 (0.1%) |
| 1 | C | 0.85 | 1/1973 (0.1%) | 0.85 | 1/2676 (0.0%) |
| 1 | D | 0.80 | 0/1973 | 0.83 | 0/2676 |
| 1 | E | 0.84 | 0/1973 | 0.86 | 2/2676 (0.1%) |
| 1 | F | 0.75 | 1/1973 (0.1%) | 0.81 | 0/2676 |
| 1 | G | 0.77 | 0/1973 | 0.81 | 0/2676 |
| 1 | H | 0.76 | 0/1973 | 0.83 | 0/2676 |
| 1 | I | 0.80 | 0/1973 | 0.84 | 0/2676 |
| 1 | J | 0.75 | 0/1973 | 0.81 | 0/2676 |
| 1 | K | 0.76 | 0/1973 | 0.83 | 0/2676 |
| 1 | L | 0.76 | 0/1973 | 0.79 | 0/2676 |
| 1 | M | 0.80 | 1/1973 (0.1%) | 0.85 | 1/2676 (0.0%) |
| 1 | N | 0.75 | 1/1973 (0.1%) | 0.79 | 0/2676 |
| 1 | O | 0.71 | 0/1973 | 0.77 | 1/2676 (0.0%) |
| 1 | P | 0.82 | 6/1973 (0.3%) | 0.83 | 5/2676 (0.2%) |
| 1 | Q | 0.99 | 6/1973 (0.3%) | 0.88 | 6/2676 (0.2%) |
| 1 | R | 0.78 | 4/1973 (0.2%) | 0.77 | 1/2676 (0.0%) |
| 1 | S | 0.76 | 1/1973 (0.1%) | 0.73 | 0/2676 |
| 1 | T | 0.88 | 7/1973 (0.4%) | 0.83 | 1/2676 (0.0%) |
| All | All | 0.80 | 30/39460 (0.1%) | 0.82 | 22/53520 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | H | 0 | 1 |
| 1 | L | 0 | 1 |
| 1 | M | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | O | 0 | 1 |
| All | All | 0 | 5 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | Q | 93 | GLU | CD-OE1 | 16.32 | 1.43 | 1.25 |
| 1 | Q | 33 | TRP | CG-CD1 | 11.41 | 1.52 | 1.36 |
| 1 | Q | 33 | TRP | CB-CG | 10.37 | 1.69 | 1.50 |
| 1 | R | 33 | TRP | CB-CG | 8.30 | 1.65 | 1.50 |
| 1 | Q | 96 | SER | CB-OG | 7.63 | 1.52 | 1.42 |
| 1 | T | 53 | GLU | CD-OE2 | 7.52 | 1.33 | 1.25 |
| 1 | A | 53 | GLU | CG-CD | 7.42 | 1.63 | 1.51 |
| 1 | R | 41 | ARG | CZ-NH2 | 7.24 | 1.42 | 1.33 |
| 1 | M | 162 | GLU | CG-CD | 6.37 | 1.61 | 1.51 |
| 1 | C | 53 | GLU | CG-CD | 6.37 | 1.61 | 1.51 |
| 1 | N | 142 | ARG | CZ-NH2 | 6.27 | 1.41 | 1.33 |
| 1 | P | 43 | GLY | C-O | 6.22 | 1.33 | 1.23 |
| 1 | Q | 33 | TRP | CD1-NE1 | -5.95 | 1.27 | 1.38 |
| 1 | S | 52 | ILE | CB-CG1 | 5.87 | 1.70 | 1.54 |
| 1 | Q | 97 | THR | C-O | -5.86 | 1.12 | 1.23 |
| 1 | R | 47 | GLU | CB-CG | 5.84 | 1.63 | 1.52 |
| 1 | P | 44 | ALA | C-N | 5.73 | 1.47 | 1.34 |
| 1 | F | 54 | LYS | CD-CE | 5.61 | 1.65 | 1.51 |
| 1 | T | 47 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | P | 75 | PHE | CD2-CE2 | 5.46 | 1.50 | 1.39 |
| 1 | T | 82 | TYR | CE1-CZ | -5.45 | 1.31 | 1.38 |
| 1 | A | 161 | GLU | CG-CD | 5.43 | 1.60 | 1.51 |
| 1 | P | 51 | LEU | C-O | 5.33 | 1.33 | 1.23 |
| 1 | T | 82 | TYR | CG-CD2 | -5.33 | 1.32 | 1.39 |
| 1 | T | 43 | GLY | C-O | 5.31 | 1.32 | 1.23 |
| 1 | R | 54 | LYS | CA-CB | 5.31 | 1.65 | 1.53 |
| 1 | P | 54 | LYS | N-CA | 5.26 | 1.56 | 1.46 |
| 1 | P | 55 | HIS | CD2-NE2 | 5.10 | 1.52 | 1.42 |
| 1 | T | 53 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 1 | T | 43 | GLY | C-N | 5.03 | 1.45 | 1.34 |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | Q | 33 | TRP | CD1-CG-CD2 | -8.99 | 99.11 | 106.30 |
| 1 | P | 75 | PHE | CB-CG-CD1 | 8.80 | 126.96 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | Q | 33 | TRP | CG-CD2-CE3 | -8.24 | 126.48 | 133.90 |
| 1 | Q | 33 | TRP | CB-CG-CD2 | 8.17 | 137.22 | 126.60 |
| 1 | Q | 131 | LEU | CA-CB-CG | 7.86 | 133.39 | 115.30 |
| 1 | R | 41 | ARG | NE-CZ-NH2 | 6.58 | 123.59 | 120.30 |
| 1 | P | 65 | LEU | CB-CG-CD1 | 6.57 | 122.17 | 111.00 |
| 1 | Q | 33 | TRP | CE2-CD2-CE3 | 6.31 | 126.27 | 118.70 |
| 1 | C | 215 | LEU | CB-CG-CD1 | 6.06 | 121.31 | 111.00 |
| 1 | E | 92 | ARG | NE-CZ-NH2 | -6.05 | 117.27 | 120.30 |
| 1 | P | 55 | HIS | CA-CB-CG | -5.98 | 103.44 | 113.60 |
| 1 | A | 92 | ARG | NE-CZ-NH1 | 5.89 | 123.25 | 120.30 |
| 1 | P | 55 | HIS | CG-ND1-CE1 | 5.82 | 116.34 | 108.20 |
| 1 | P | 54 | LYS | CA-CB-CG | 5.59 | 125.70 | 113.40 |
| 1 | M | 215 | LEU | CA-CB-CG | 5.58 | 128.14 | 115.30 |
| 1 | E | 122 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | B | 78 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 1 | T | 55 | HIS | CA-C-N | -5.33 | 105.48 | 117.20 |
| 1 | Q | 33 | TRP | CG-CD1-NE1 | 5.25 | 115.34 | 110.10 |
| 1 | O | 104 | ASP | CB-CG-OD2 | -5.22 | 113.60 | 118.30 |
| 1 | A | 92 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 |
| 1 | B | 62 | ASP | CB-CG-OD1 | -5.09 | 113.72 | 118.30 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | H | 138 | GLY | Peptide |
| 1 | L | 138 | GLY | Peptide |
| 1 | M | 133 | SER | Peptide |
| 1 | M | 179 | VAL | Peptide |
| 1 | O | 138 | GLY | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1928 | 0 | 1938 | 57 | 0 |
| 1 | B | 1928 | 0 | 1938 | 51 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 1928 | 0 | 1938 | 50 | 0 |
| 1 | D | 1928 | 0 | 1938 | 57 | 0 |
| 1 | E | 1928 | 0 | 1938 | 54 | 0 |
| 1 | F | 1928 | 0 | 1938 | 54 | 0 |
| 1 | G | 1928 | 0 | 1938 | 65 | 0 |
| 1 | H | 1928 | 0 | 1938 | 43 | 0 |
| 1 | I | 1928 | 0 | 1938 | 49 | 0 |
| 1 | J | 1928 | 0 | 1938 | 56 | 0 |
| 1 | K | 1928 | 0 | 1938 | 41 | 0 |
| 1 | L | 1928 | 0 | 1938 | 47 | 0 |
| 1 | M | 1928 | 0 | 1938 | 41 | 0 |
| 1 | N | 1928 | 0 | 1938 | 59 | 0 |
| 1 | O | 1928 | 0 | 1938 | 41 | 0 |
| 1 | P | 1928 | 0 | 1938 | 58 | 0 |
| 1 | Q | 1928 | 0 | 1938 | 60 | 0 |
| 1 | R | 1928 | 0 | 1938 | 60 | 0 |
| 1 | S | 1928 | 0 | 1938 | 62 | 0 |
| 1 | T | 1928 | 0 | 1938 | 61 | 0 |
| 2 | A | 43 | 0 | 30 | 8 | 0 |
| 2 | B | 43 | 0 | 30 | 6 | 0 |
| 2 | C | 43 | 0 | 30 | 7 | 0 |
| 2 | D | 43 | 0 | 30 | 9 | 0 |
| 2 | E | 43 | 0 | 30 | 8 | 0 |
| 2 | F | 43 | 0 | 30 | 11 | 0 |
| 2 | G | 43 | 0 | 30 | 15 | 0 |
| 2 | H | 43 | 0 | 30 | 9 | 0 |
| 2 | I | 43 | 0 | 30 | 7 | 0 |
| 2 | J | 43 | 0 | 30 | 10 | 0 |
| 2 | K | 43 | 0 | 30 | 5 | 0 |
| 2 | L | 43 | 0 | 30 | 7 | 0 |
| 2 | M | 43 | 0 | 30 | 6 | 0 |
| 2 | N | 43 | 0 | 30 | 10 | 0 |
| 2 | O | 43 | 0 | 30 | 5 | 0 |
| 2 | P | 43 | 0 | 30 | 3 | 0 |
| 2 | Q | 43 | 0 | 30 | 10 | 0 |
| 2 | R | 43 | 0 | 30 | 14 | 0 |
| 2 | S | 43 | 0 | 30 | 9 | 0 |
| 2 | T | 43 | 0 | 30 | 6 | 0 |
| 3 | A | 3 | 0 | 0 | 0 | 0 |
| 3 | B | 3 | 0 | 0 | 0 | 0 |
| 3 | C | 3 | 0 | 0 | 1 | 0 |
| 3 | D | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | E | 3 | 0 | 0 | 0 | 0 |
| 3 | F | 3 | 0 | 0 | 0 | 0 |
| 3 | G | 3 | 0 | 0 | 1 | 0 |
| 3 | H | 3 | 0 | 0 | 0 | 0 |
| 3 | I | 3 | 0 | 0 | 0 | 0 |
| 3 | J | 3 | 0 | 0 | 0 | 0 |
| 3 | K | 3 | 0 | 0 | 0 | 0 |
| 3 | L | 3 | 0 | 0 | 1 | 0 |
| 3 | M | 3 | 0 | 0 | 0 | 0 |
| 3 | N | 3 | 0 | 0 | 0 | 0 |
| 3 | O | 3 | 0 | 0 | 0 | 0 |
| 3 | P | 3 | 0 | 0 | 0 | 0 |
| 3 | Q | 3 | 0 | 0 | 0 | 0 |
| 3 | R | 3 | 0 | 0 | 0 | 0 |
| 3 | S | 3 | 0 | 0 | 0 | 0 |
| 3 | T | 3 | 0 | 0 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | I | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 4 | K | 1 | 0 | 0 | 0 | 0 |
| 4 | L | 1 | 0 | 0 | 0 | 0 |
| 4 | M | 1 | 0 | 0 | 0 | 0 |
| 4 | N | 1 | 0 | 0 | 0 | 0 |
| 4 | O | 1 | 0 | 0 | 0 | 0 |
| 4 | P | 1 | 0 | 0 | 0 | 0 |
| 4 | Q | 1 | 0 | 0 | 0 | 0 |
| 4 | R | 1 | 0 | 0 | 0 | 0 |
| 4 | S | 1 | 0 | 0 | 0 | 0 |
| 4 | T | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 1 | 0 | 0 | 2 | 0 |
| 5 | C | 1 | 0 | 0 | 1 | 0 |
| 5 | D | 1 | 0 | 0 | 0 | 0 |
| 5 | E | 1 | 0 | 0 | 0 | 0 |
| 5 | F | 1 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | G | 1 | 0 | 0 | 0 | 0 |
| 5 | H | 1 | 0 | 0 | 2 | 0 |
| 5 | I | 1 | 0 | 0 | 0 | 0 |
| 5 | J | 1 | 0 | 0 | 0 | 0 |
| 5 | K | 1 | 0 | 0 | 0 | 0 |
| 5 | L | 1 | 0 | 0 | 2 | 0 |
| 5 | M | 1 | 0 | 0 | 0 | 0 |
| 5 | N | 1 | 0 | 0 | 0 | 0 |
| 5 | O | 1 | 0 | 0 | 0 | 0 |
| 5 | P | 1 | 0 | 0 | 0 | 0 |
| 5 | Q | 1 | 0 | 0 | 0 | 0 |
| 5 | R | 1 | 0 | 0 | 0 | 0 |
| 5 | S | 1 | 0 | 0 | 0 | 0 |
| 5 | T | 1 | 0 | 0 | 0 | 0 |
| All | All | 39520 | 0 | 39360 | 988 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (988) 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:O:97:THR:HG22 | 1:O:100:GLY:H | 1.10 | 1.15 |
| 1:C:18:PRO:HA | 1:C:113:THR:HG22 | 1.23 | 1.15 |
| 1:J:18:PRO:HA | 1:J:113:THR:HG22 | 1.26 | 1.12 |
| 1:K:18:PRO:HA | 1:K:113:THR:HG22 | 1.33 | 1.10 |
| 1:N:18:PRO:HA | 1:N:113:THR:HG22 | 1.28 | 1.10 |
| 1:L:18:PRO:HA | 1:L:113:THR:HG22 | 1.33 | 1.10 |
| 1:M:97:THR:HG22 | 1:M:100:GLY:H | 1.16 | 1.10 |
| 1:L:17:GLN:O | 1:L:113:THR:HG21 | 1.51 | 1.09 |
| 1:G:18:PRO:HA | 1:G:113:THR:HG22 | 1.35 | 1.08 |
| 1:B:138:GLY:HA2 | 1:F:115:PRO:HG2 | 1.35 | 1.08 |
| 1:E:18:PRO:HA | 1:E:113:THR:HG22 | 1.28 | 1.07 |
| 1:L:196:PHE:CZ | 2:L:1000:HEM:O2D | 2.07 | 1.06 |
| 1:D:18:PRO:HA | 1:D:113:THR:HG22 | 1.38 | 1.06 |
| 1:A:18:PRO:HA | 1:A:113:THR:HG22 | 1.32 | 1.05 |
| 1:C:18:PRO:HA | 1:C:113:THR:CG2 | 1.86 | 1.05 |
| 1:M:18:PRO:HA | 1:M:113:THR:HG22 | 1.35 | 1.05 |
| 1:C:97:THR:HG22 | 1:C:100:GLY:H | 1.14 | 1.05 |
| 1:G:221:ASN:HD22 | 1:G:224:HIS:CD2 | 1.75 | 1.05 |
| 1:H:97:THR:HG22 | 1:H:100:GLY:H | 1.17 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:196:PHE:CZ | 2:D:1000:HEM:O2D | 2.12 | 1.03 |
| 1:I:18:PRO:HA | 1:I:113:THR:HG22 | 1.39 | 1.03 |
| 1:K:17:GLN:O | 1:K:113:THR:HG21 | 1.59 | 1.02 |
| 1:K:196:PHE:CZ | 2:K:1000:HEM:O2D | 2.13 | 1.01 |
| 1:G:97:THR:HG22 | 1:G:100:GLY:H | 1.24 | 1.01 |
| 1:N:221:ASN:HD22 | 1:N:224:HIS:CD2 | 1.77 | 1.01 |
| 1:C:221:ASN:HD22 | 1:C:224:HIS:CD2 | 1.76 | 1.01 |
| 1:E:221:ASN:HD22 | 1:E:224:HIS:CD2 | 1.79 | 1.01 |
| 1:I:97:THR:HG22 | 1:I:100:GLY:H | 1.25 | 1.00 |
| 1:A:174:THR:HB | 2:A:1000:HEM:HBB2 | 1.44 | 0.99 |
| 1:O:17:GLN:O | 1:O:113:THR:HG21 | 1.62 | 0.99 |
| 1:M:17:GLN:O | 1:M:113:THR:HG21 | 1.64 | 0.98 |
| 1:G:221:ASN:ND2 | 1:G:224:HIS:HD2 | 1.60 | 0.98 |
| 1:D:97:THR:HG22 | 1:D:100:GLY:H | 1.28 | 0.97 |
| 1:A:221:ASN:HD22 | 1:A:224:HIS:HD2 | 0.99 | 0.97 |
| 1:E:221:ASN:ND2 | 1:E:224:HIS:HD2 | 1.63 | 0.97 |
| 1:R:18:PRO:HA | 1:R:113:THR:HG22 | 1.45 | 0.97 |
| 1:Q:97:THR:HG22 | 1:Q:100:GLY:H | 1.29 | 0.97 |
| 1:B:97:THR:HG22 | 1:B:100:GLY:H | 1.28 | 0.96 |
| 1:H:221:ASN:HD22 | 1:H:224:HIS:HD2 | 1.13 | 0.96 |
| 1:N:221:ASN:ND2 | 1:N:224:HIS:HD2 | 1.64 | 0.96 |
| 1:P:18:PRO:HA | 1:P:113:THR:HG22 | 1.43 | 0.96 |
| 1:S:221:ASN:HD22 | 1:S:224:HIS:CD2 | 1.83 | 0.96 |
| 1:J:18:PRO:HA | 1:J:113:THR:CG2 | 1.95 | 0.95 |
| 2:L:1000:HEM:HBB2 | 2:L:1000:HEM:HHC | 1.48 | 0.95 |
| 1:C:221:ASN:ND2 | 1:C:224:HIS:HD2 | 1.62 | 0.95 |
| 1:F:18:PRO:HA | 1:F:113:THR:HG22 | 1.49 | 0.95 |
| 1:H:18:PRO:HA | 1:H:113:THR:HG22 | 1.45 | 0.95 |
| 1:B:221:ASN:HD22 | 1:B:224:HIS:HD2 | 0.98 | 0.95 |
| 1:P:221:ASN:HD22 | 1:P:224:HIS:HD2 | 1.12 | 0.95 |
| 1:T:18:PRO:HA | 1:T:113:THR:HG22 | 1.50 | 0.94 |
| 1:F:221:ASN:HD22 | 1:F:224:HIS:HD2 | 1.04 | 0.94 |
| 1:L:221:ASN:HD22 | 1:L:224:HIS:HD2 | 1.00 | 0.94 |
| 1:N:18:PRO:HA | 1:N:113:THR:CG2 | 1.97 | 0.94 |
| 1:B:221:ASN:HD22 | 1:B:224:HIS:CD2 | 1.86 | 0.94 |
| 1:O:221:ASN:HD22 | 1:O:224:HIS:HD2 | 0.97 | 0.94 |
| 1:C:196:PHE:CZ | 2:C:1000:HEM:O2D | 2.21 | 0.94 |
| 1:Q:17:GLN:O | 1:Q:113:THR:HG21 | 1.68 | 0.93 |
| 1:D:221:ASN:HD22 | 1:D:224:HIS:HD2 | 1.03 | 0.93 |
| 2:H:1000:HEM:HHC | 2:H:1000:HEM:HBB2 | 1.48 | 0.93 |
| 1:A:221:ASN:HD22 | 1:A:224:HIS:CD2 | 1.87 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:221:ASN:HD22 | 1:J:224:HIS:CD2 | 1.86 | 0.93 |
| 1:J:221:ASN:HD22 | 1:J:224:HIS:HD2 | 1.03 | 0.93 |
| 1:I:221:ASN:HD22 | 1:I:224:HIS:CD2 | 1.87 | 0.93 |
| 1:F:196:PHE:CZ | 2:F:1000:HEM:O2D | 2.22 | 0.93 |
| 1:R:221:ASN:HD22 | 1:R:224:HIS:HD2 | 1.05 | 0.93 |
| 1:N:17:GLN:O | 1:N:113:THR:HG21 | 1.69 | 0.93 |
| 1:A:196:PHE:CZ | 2:A:1000:HEM:O2D | 2.21 | 0.93 |
| 1:G:211:LEU:HD11 | 2:G:1000:HEM:HBB2 | 1.49 | 0.93 |
| 1:O:221:ASN:HD22 | 1:O:224:HIS:CD2 | 1.87 | 0.92 |
| 1:E:97:THR:HG22 | 1:E:100:GLY:H | 1.34 | 0.92 |
| 1:Q:145:ILE:HD13 | 1:Q:233:LEU:HD13 | 1.52 | 0.92 |
| 1:A:97:THR:HG22 | 1:A:100:GLY:H | 1.33 | 0.92 |
| 1:N:221:ASN:HD22 | 1:N:224:HIS:HD2 | 0.94 | 0.92 |
| 1:C:17:GLN:O | 1:C:113:THR:HG21 | 1.70 | 0.92 |
| 1:N:159:SER:OG | 1:N:162:GLU:HG3 | 1.70 | 0.92 |
| 1:C:221:ASN:HD22 | 1:C:224:HIS:HD2 | 0.95 | 0.92 |
| 1:A:235:THR:HG23 | 1:A:237:HIS:NE2 | 1.85 | 0.91 |
| 1:K:221:ASN:HD22 | 1:K:224:HIS:CD2 | 1.88 | 0.91 |
| 1:T:221:ASN:HD22 | 1:T:224:HIS:HD2 | 1.16 | 0.91 |
| 1:I:17:GLN:O | 1:I:113:THR:HG21 | 1.71 | 0.91 |
| 1:T:196:PHE:CZ | 2:T:1000:HEM:O2D | 2.22 | 0.91 |
| 1:A:18:PRO:HA | 1:A:113:THR:CG2 | 2.00 | 0.91 |
| 1:L:221:ASN:HD22 | 1:L:224:HIS:CD2 | 1.89 | 0.90 |
| 1:D:221:ASN:HD22 | 1:D:224:HIS:CD2 | 1.88 | 0.90 |
| 1:H:196:PHE:CZ | 2:H:1000:HEM:O2D | 2.24 | 0.90 |
| 1:S:18:PRO:HA | 1:S:113:THR:HG22 | 1.50 | 0.90 |
| 1:K:221:ASN:HD22 | 1:K:224:HIS:HD2 | 0.96 | 0.90 |
| 1:G:18:PRO:HA | 1:G:113:THR:CG2 | 2.00 | 0.90 |
| 1:K:18:PRO:HA | 1:K:113:THR:CG2 | 2.01 | 0.90 |
| 1:I:18:PRO:HA | 1:I:113:THR:CG2 | 2.01 | 0.89 |
| 1:S:33:TRP:CH2 | 1:S:99:VAL:HG13 | 2.08 | 0.89 |
| 1:H:221:ASN:HD22 | 1:H:224:HIS:CD2 | 1.89 | 0.89 |
| 1:S:48:VAL:O | 1:S:52:ILE:HG13 | 1.72 | 0.89 |
| 1:B:18:PRO:HA | 1:B:113:THR:HG22 | 1.54 | 0.88 |
| 1:I:221:ASN:HD22 | 1:I:224:HIS:HD2 | 0.95 | 0.88 |
| 1:L:18:PRO:HA | 1:L:113:THR:CG2 | 2.02 | 0.88 |
| 1:J:17:GLN:O | 1:J:113:THR:HG21 | 1.73 | 0.88 |
| 1:S:221:ASN:HD22 | 1:S:224:HIS:HD2 | 0.91 | 0.87 |
| 1:S:97:THR:HG22 | 1:S:100:GLY:H | 1.39 | 0.87 |
| 1:A:17:GLN:O | 1:A:113:THR:HG21 | 1.75 | 0.87 |
| 1:T:211:LEU:HD11 | 2:T:1000:HEM:HBB2 | 1.54 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:94:PHE:O | 1:D:97:THR:HB | 1.73 | 0.87 |
| 1:G:221:ASN:HD22 | 1:G:224:HIS:HD2 | 0.89 | 0.86 |
| 1:E:221:ASN:HD22 | 1:E:224:HIS:HD2 | 0.91 | 0.86 |
| 1:E:196:PHE:CZ | 2:E:1000:HEM:O2D | 2.28 | 0.86 |
| 1:B:221:ASN:ND2 | 1:B:224:HIS:HD2 | 1.73 | 0.86 |
| 1:B:94:PHE:O | 1:B:97:THR:HB | 1.76 | 0.86 |
| 1:B:196:PHE:CZ | 2:B:1000:HEM:O2D | 2.29 | 0.85 |
| 1:R:196:PHE:CZ | 2:R:1000:HEM:O2D | 2.30 | 0.85 |
| 1:P:69:LEU:HG | 1:T:88:GLN:HG3 | 1.56 | 0.85 |
| 1:L:97:THR:HG22 | 1:L:100:GLY:H | 1.41 | 0.85 |
| 1:R:17:GLN:O | 1:R:113:THR:HG21 | 1.76 | 0.85 |
| 1:B:17:GLN:O | 1:B:113:THR:HG21 | 1.75 | 0.85 |
| 1:D:18:PRO:HA | 1:D:113:THR:CG2 | 2.06 | 0.84 |
| 1:J:196:PHE:CZ | 2:J:1000:HEM:O2D | 2.29 | 0.84 |
| 1:O:97:THR:HG22 | 1:O:100:GLY:N | 1.91 | 0.84 |
| 1:P:94:PHE:O | 1:P:97:THR:HG22 | 1.77 | 0.84 |
| 1:A:221:ASN:ND2 | 1:A:224:HIS:HD2 | 1.75 | 0.84 |
| 1:O:18:PRO:HA | 1:O:113:THR:HG22 | 1.58 | 0.84 |
| 1:B:235:THR:HG23 | 1:B:237:HIS:NE2 | 1.93 | 0.84 |
| 1:O:221:ASN:ND2 | 1:O:224:HIS:HD2 | 1.74 | 0.84 |
| 1:O:97:THR:CG2 | 1:O:100:GLY:H | 1.89 | 0.83 |
| 1:E:97:THR:CG2 | 1:E:100:GLY:H | 1.91 | 0.83 |
| 1:Q:196:PHE:CZ | 2:Q:1000:HEM:O2D | 2.32 | 0.82 |
| 1:N:97:THR:HG22 | 1:N:100:GLY:H | 1.44 | 0.82 |
| 1:E:17:GLN:O | 1:E:113:THR:HG21 | 1.78 | 0.82 |
| 1:I:212:MET:HG3 | 1:J:190:GLY:CA | 2.10 | 0.82 |
| 1:E:18:PRO:HA | 1:E:113:THR:CG2 | 2.09 | 0.82 |
| 1:H:221:ASN:ND2 | 1:H:224:HIS:HD2 | 1.77 | 0.82 |
| 1:J:221:ASN:ND2 | 1:J:224:HIS:HD2 | 1.76 | 0.82 |
| 1:O:196:PHE:CZ | 2:O:1000:HEM:O2D | 2.34 | 0.81 |
| 1:C:94:PHE:O | 1:C:97:THR:HB | 1.80 | 0.81 |
| 1:L:221:ASN:ND2 | 1:L:224:HIS:HD2 | 1.77 | 0.81 |
| 1:S:221:ASN:ND2 | 1:S:224:HIS:HD2 | 1.75 | 0.81 |
| 1:D:221:ASN:ND2 | 1:D:224:HIS:HD2 | 1.77 | 0.81 |
| 1:A:97:THR:CG2 | 1:A:100:GLY:H | 1.94 | 0.81 |
| 1:L:196:PHE:HZ | 2:L:1000:HEM:O2D | 1.64 | 0.80 |
| 1:P:27:PHE:HB2 | 1:P:75:PHE:CZ | 2.17 | 0.80 |
| 1:M:97:THR:CG2 | 1:M:100:GLY:H | 1.93 | 0.79 |
| 1:A:174:THR:CB | 2:A:1000:HEM:HBB2 | 2.12 | 0.79 |
| 1:K:97:THR:HG22 | 1:K:100:GLY:H | 1.46 | 0.79 |
| 1:C:97:THR:HG22 | 1:C:100:GLY:N | 1.95 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:R:221:ASN:HD22 | 1:R:224:HIS:CD2 | 1.97 | 0.78 |
| 1:P:221:ASN:HD22 | 1:P:224:HIS:CD2 | 1.99 | 0.78 |
| 1:M:97:THR:HG22 | 1:M:100:GLY:N | 1.97 | 0.78 |
| 1:J:97:THR:HG22 | 1:J:100:GLY:H | 1.49 | 0.77 |
| 1:Q:212:MET:HG3 | 1:R:190:GLY:HA3 | 1.65 | 0.77 |
| 1:F:17:GLN:O | 1:F:113:THR:HG21 | 1.84 | 0.77 |
| 1:O:94:PHE:O | 1:O:97:THR:HB | 1.85 | 0.77 |
| 1:I:196:PHE:CZ | 2:I:1000:HEM:O2D | 2.39 | 0.76 |
| 1:R:211:LEU:HD11 | 2:R:1000:HEM:HBB2 | 1.67 | 0.76 |
| 1:K:221:ASN:ND2 | 1:K:224:HIS:HD2 | 1.80 | 0.76 |
| 1:S:221:ASN:HA | 1:S:224:HIS:CD2 | 2.20 | 0.75 |
| 1:E:235:THR:HG23 | 1:E:237:HIS:NE2 | 2.01 | 0.75 |
| 1:J:97:THR:CG2 | 1:J:100:GLY:H | 1.99 | 0.75 |
| 1:S:66:THR:HG22 | 1:S:234:GLY:HA3 | 1.69 | 0.75 |
| 1:M:18:PRO:HA | 1:M:113:THR:CG2 | 2.13 | 0.74 |
| 1:G:196:PHE:CZ | 2:G:1000:HEM:O2D | 2.40 | 0.74 |
| 1:M:221:ASN:HD22 | 1:M:224:HIS:CD2 | 2.05 | 0.74 |
| 1:N:212:MET:HG3 | 1:O:190:GLY:CA | 2.16 | 0.74 |
| 1:H:212:MET:HG3 | 1:I:190:GLY:CA | 2.17 | 0.74 |
| 1:T:53:GLU:O | 1:T:56:LYS:HG3 | 1.87 | 0.74 |
| 1:G:65:LEU:HB3 | 1:G:235:THR:HG22 | 1.69 | 0.74 |
| 1:K:212:MET:HG3 | 1:L:190:GLY:CA | 2.18 | 0.74 |
| 1:F:145:ILE:HD13 | 1:F:233:LEU:HD13 | 1.70 | 0.74 |
| 1:I:94:PHE:O | 1:I:97:THR:HB | 1.86 | 0.74 |
| 1:T:221:ASN:HD22 | 1:T:224:HIS:CD2 | 2.04 | 0.74 |
| 1:D:17:GLN:O | 1:D:113:THR:HG21 | 1.87 | 0.73 |
| 1:H:97:THR:HG22 | 1:H:100:GLY:N | 2.00 | 0.73 |
| 1:L:235:THR:HG23 | 1:L:237:HIS:NE2 | 2.02 | 0.73 |
| 1:G:212:MET:HG3 | 1:H:190:GLY:HA3 | 1.68 | 0.73 |
| 1:N:59:VAL:HG12 | 1:N:81:ALA:HB2 | 1.70 | 0.73 |
| 1:H:145:ILE:HD13 | 1:H:233:LEU:HD13 | 1.70 | 0.73 |
| 1:J:235:THR:HG23 | 1:J:237:HIS:NE2 | 2.02 | 0.73 |
| 1:B:190:GLY:CA | 1:D:212:MET:HG3 | 2.19 | 0.73 |
| 1:J:65:LEU:HB3 | 1:J:235:THR:HG22 | 1.70 | 0.72 |
| 1:L:97:THR:CG2 | 1:L:100:GLY:H | 2.02 | 0.72 |
| 1:P:196:PHE:CZ | 2:P:1000:HEM:O2D | 2.43 | 0.72 |
| 1:F:221:ASN:HD22 | 1:F:224:HIS:CD2 | 1.97 | 0.72 |
| 1:P:105:VAL:HG12 | 1:S:71:THR:HG23 | 1.71 | 0.72 |
| 1:I:211:LEU:HD11 | 2:I:1000:HEM:HBB2 | 1.71 | 0.72 |
| 1:G:94:PHE:O | 1:G:97:THR:HB | 1.89 | 0.72 |
| 1:I:221:ASN:ND2 | 1:I:224:HIS:HD2 | 1.79 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:212:MET:HG3 | 1:G:190:GLY:CA | 2.18 | 0.72 |
| 1:F:212:MET:HG3 | 1:G:190:GLY:HA3 | 1.69 | 0.72 |
| 1:H:18:PRO:HA | 1:H:113:THR:CG2 | 2.20 | 0.72 |
| 1:Q:221:ASN:HD22 | 1:Q:224:HIS:CD2 | 2.08 | 0.72 |
| 1:B:105:VAL:HG12 | 1:D:71:THR:HG23 | 1.72 | 0.71 |
| 1:A:154:GLU:OE1 | 1:E:222:LYS:HE2 | 1.90 | 0.71 |
| 1:O:65:LEU:HB3 | 1:O:235:THR:HG22 | 1.70 | 0.71 |
| 1:B:18:PRO:HA | 1:B:113:THR:CG2 | 2.19 | 0.71 |
| 1:M:221:ASN:HD22 | 1:M:224:HIS:HD2 | 1.38 | 0.71 |
| 1:A:71:THR:HG23 | 1:D:105:VAL:HG12 | 1.71 | 0.71 |
| 1:H:212:MET:HG3 | 1:I:190:GLY:HA3 | 1.72 | 0.71 |
| 1:G:17:GLN:O | 1:G:113:THR:HG21 | 1.89 | 0.71 |
| 1:K:180:ASN:HB3 | 1:K:181:VAL:HG23 | 1.71 | 0.71 |
| 1:S:97:THR:CG2 | 1:S:100:GLY:H | 2.03 | 0.70 |
| 1:I:212:MET:HG3 | 1:J:190:GLY:HA2 | 1.74 | 0.70 |
| 1:F:190:GLY:HA3 | 1:J:212:MET:HG3 | 1.73 | 0.70 |
| 1:E:211:LEU:HD11 | 2:E:1000:HEM:HBB2 | 1.74 | 0.70 |
| 1:S:235:THR:HG23 | 1:S:237:HIS:NE2 | 2.06 | 0.70 |
| 1:K:235:THR:HG23 | 1:K:237:HIS:NE2 | 2.07 | 0.70 |
| 1:F:38:VAL:HB | 1:F:41:ARG:NH1 | 2.07 | 0.69 |
| 1:N:196:PHE:CZ | 2:N:1000:HEM:O2D | 2.45 | 0.69 |
| 1:C:211:LEU:HD11 | 2:C:1000:HEM:HBB2 | 1.75 | 0.69 |
| 1:R:118:TYR:HE2 | 2:R:1000:HEM:O1D | 1.76 | 0.69 |
| 1:R:212:MET:HG3 | 1:S:190:GLY:HA3 | 1.73 | 0.69 |
| 1:A:190:GLY:HA3 | 1:E:212:MET:HG3 | 1.73 | 0.69 |
| 1:N:18:PRO:CA | 1:N:113:THR:HG22 | 2.15 | 0.69 |
| 1:P:190:GLY:HA3 | 1:S:212:MET:HG3 | 1.72 | 0.69 |
| 1:P:17:GLN:O | 1:P:113:THR:HG21 | 1.92 | 0.69 |
| 1:A:97:THR:HG22 | 1:A:100:GLY:N | 2.06 | 0.69 |
| 1:K:221:ASN:HA | 1:K:224:HIS:CD2 | 2.28 | 0.69 |
| 1:T:26:MET:HG3 | 1:T:76:PHE:HB3 | 1.75 | 0.69 |
| 1:S:196:PHE:CZ | 2:S:1000:HEM:O2D | 2.45 | 0.69 |
| 1:A:174:THR:HG22 | 1:A:211:LEU:HD11 | 1.75 | 0.69 |
| 1:G:116:LEU:HA | 2:G:1000:HEM:O1A | 1.93 | 0.69 |
| 1:K:212:MET:HG3 | 1:L:190:GLY:HA2 | 1.75 | 0.69 |
| 1:G:235:THR:HG23 | 1:G:237:HIS:NE2 | 2.09 | 0.68 |
| 1:P:66:THR:HG22 | 1:P:234:GLY:HA3 | 1.76 | 0.68 |
| 1:S:17:GLN:O | 1:S:113:THR:HG21 | 1.93 | 0.68 |
| 1:K:145:ILE:HD13 | 1:K:233:LEU:HD13 | 1.74 | 0.68 |
| 1:G:145:ILE:HD13 | 1:G:233:LEU:HD13 | 1.75 | 0.68 |
| 1:Q:11:ARG:NH2 | 1:Q:62:ASP:OD1 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:150:LYS:HA | 1:D:195:ASP:HB2 | 1.76 | 0.67 |
| 1:G:212:MET:HG3 | 1:H:190:GLY:CA | 2.24 | 0.67 |
| 1:K:105:VAL:HG12 | 1:O:71:THR:HG23 | 1.75 | 0.67 |
| 1:F:235:THR:HG23 | 1:F:237:HIS:NE2 | 2.09 | 0.67 |
| 1:Q:94:PHE:O | 1:Q:97:THR:HB | 1.93 | 0.67 |
| 1:P:222:LYS:HE2 | 1:T:154:GLU:OE1 | 1.95 | 0.67 |
| 1:D:235:THR:HG23 | 1:D:237:HIS:NE2 | 2.09 | 0.67 |
| 1:R:235:THR:HG23 | 1:R:237:HIS:NE2 | 2.09 | 0.67 |
| 1:A:70:GLU:OE2 | 1:A:232:THR:HA | 1.94 | 0.67 |
| 1:A:145:ILE:HD13 | 1:A:233:LEU:HD13 | 1.76 | 0.67 |
| 1:A:235:THR:CG2 | 1:A:237:HIS:NE2 | 2.56 | 0.67 |
| 1:Q:55:HIS:CD2 | 1:Q:58:ASN:HD22 | 2.12 | 0.67 |
| 1:R:221:ASN:ND2 | 1:R:224:HIS:HD2 | 1.88 | 0.66 |
| 1:I:71:THR:HG23 | 1:J:105:VAL:HG12 | 1.77 | 0.66 |
| 1:A:174:THR:HG22 | 1:A:211:LEU:CD1 | 2.26 | 0.66 |
| 1:P:27:PHE:HB2 | 1:P:75:PHE:CE2 | 2.31 | 0.66 |
| 1:M:116:LEU:HA | 2:M:1000:HEM:O1A | 1.95 | 0.66 |
| 1:L:97:THR:HG22 | 1:L:100:GLY:N | 2.09 | 0.66 |
| 1:B:235:THR:CG2 | 1:B:237:HIS:NE2 | 2.58 | 0.66 |
| 1:A:38:VAL:O | 1:A:39:ALA:CB | 2.42 | 0.66 |
| 1:A:44:ALA:HB1 | 1:A:99:VAL:HG22 | 1.76 | 0.66 |
| 1:L:116:LEU:HA | 2:L:1000:HEM:O1A | 1.95 | 0.66 |
| 1:K:211:LEU:HD11 | 2:K:1000:HEM:HBB2 | 1.78 | 0.66 |
| 1:D:38:VAL:O | 1:D:39:ALA:CB | 2.44 | 0.66 |
| 1:F:221:ASN:ND2 | 1:F:224:HIS:HD2 | 1.87 | 0.66 |
| 1:Q:116:LEU:HA | 2:Q:1000:HEM:O1A | 1.96 | 0.66 |
| 1:N:212:MET:HG3 | 1:O:190:GLY:HA2 | 1.78 | 0.66 |
| 1:Q:55:HIS:HD2 | 1:Q:58:ASN:HD22 | 1.44 | 0.66 |
| 1:K:116:LEU:HA | 2:K:1000:HEM:O1A | 1.94 | 0.65 |
| 1:I:235:THR:HG23 | 1:I:237:HIS:NE2 | 2.11 | 0.65 |
| 1:Q:190:GLY:HA3 | 1:T:212:MET:HG3 | 1.79 | 0.65 |
| 1:F:118:TYR:HE2 | 2:F:1000:HEM:O1D | 1.80 | 0.65 |
| 1:G:44:ALA:HB1 | 1:G:99:VAL:HG23 | 1.78 | 0.65 |
| 1:M:196:PHE:CZ | 2:M:1000:HEM:O2D | 2.50 | 0.65 |
| 1:O:18:PRO:HA | 1:O:113:THR:CG2 | 2.25 | 0.65 |
| 1:P:44:ALA:HB1 | 1:P:99:VAL:HG22 | 1.78 | 0.65 |
| 1:N:235:THR:HG23 | 1:N:237:HIS:NE2 | 2.11 | 0.65 |
| 1:R:94:PHE:O | 1:R:97:THR:HG22 | 1.95 | 0.65 |
| 1:P:221:ASN:ND2 | 1:P:224:HIS:HD2 | 1.91 | 0.65 |
| 1:T:221:ASN:ND2 | 1:T:224:HIS:HD2 | 1.90 | 0.65 |
| 1:F:180:ASN:HB3 | 1:F:181:VAL:HG23 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:1000:HEM:HHC | 2:H:1000:HEM:CBB | 2.25 | 0.64 |
| 1:P:127:LEU:HD12 | 1:P:168:GLU:HG2 | 1.78 | 0.64 |
| 1:H:116:LEU:HA | 2:H:1000:HEM:O1A | 1.97 | 0.64 |
| 1:F:190:GLY:CA | 1:J:212:MET:HG3 | 2.27 | 0.64 |
| 1:A:38:VAL:O | 1:A:39:ALA:HB2 | 1.98 | 0.64 |
| 1:D:70:GLU:OE2 | 1:D:232:THR:HA | 1.96 | 0.64 |
| 1:B:116:LEU:HA | 2:B:1000:HEM:O1A | 1.98 | 0.64 |
| 1:N:212:MET:HG3 | 1:O:190:GLY:HA3 | 1.79 | 0.64 |
| 1:C:212:MET:HG3 | 1:E:190:GLY:HA3 | 1.79 | 0.64 |
| 1:F:222:LYS:HE2 | 1:G:154:GLU:OE1 | 1.98 | 0.64 |
| 1:C:212:MET:HG3 | 1:E:190:GLY:CA | 2.28 | 0.64 |
| 1:M:212:MET:HG3 | 1:N:190:GLY:HA3 | 1.80 | 0.64 |
| 1:I:212:MET:HG3 | 1:J:190:GLY:HA3 | 1.79 | 0.64 |
| 1:N:222:LYS:HE2 | 1:O:154:GLU:OE1 | 1.98 | 0.64 |
| 1:O:211:LEU:HD11 | 2:O:1000:HEM:HBB2 | 1.79 | 0.64 |
| 1:Q:222:LYS:HE2 | 1:R:154:GLU:OE1 | 1.98 | 0.63 |
| 1:F:18:PRO:HA | 1:F:113:THR:CG2 | 2.26 | 0.63 |
| 1:R:30:ARG:O | 1:R:33:TRP:HB3 | 1.97 | 0.63 |
| 1:B:41:ARG:NH2 | 1:B:247:ALA:O | 2.31 | 0.63 |
| 1:S:59:VAL:HG12 | 1:S:81:ALA:HB2 | 1.80 | 0.63 |
| 1:B:190:GLY:HA2 | 1:D:212:MET:HG3 | 1.79 | 0.63 |
| 1:F:150:LYS:HA | 1:F:195:ASP:HB2 | 1.79 | 0.63 |
| 1:F:221:ASN:HA | 1:F:224:HIS:CD2 | 2.34 | 0.63 |
| 1:N:117:ASN:N | 2:N:1000:HEM:O1A | 2.31 | 0.63 |
| 1:Q:59:VAL:HG12 | 1:Q:81:ALA:HB2 | 1.81 | 0.63 |
| 1:P:9:ILE:HG22 | 1:P:9:ILE:O | 1.98 | 0.63 |
| 1:H:17:GLN:O | 1:H:113:THR:HG21 | 1.98 | 0.62 |
| 1:A:190:GLY:CA | 1:E:212:MET:HG3 | 2.29 | 0.62 |
| 1:L:11:ARG:NH2 | 1:L:62:ASP:OD1 | 2.31 | 0.62 |
| 1:R:97:THR:CG2 | 1:R:100:GLY:H | 2.12 | 0.62 |
| 1:Q:17:GLN:O | 1:Q:113:THR:CG2 | 2.43 | 0.62 |
| 1:O:33:TRP:CH2 | 1:O:41:ARG:HG2 | 2.35 | 0.62 |
| 1:I:119:ILE:HG13 | 2:I:1000:HEM:HMA2 | 1.80 | 0.62 |
| 1:D:116:LEU:HD13 | 1:D:119:ILE:O | 2.00 | 0.62 |
| 1:A:177:TYR:HB2 | 2:A:1000:HEM:HBB1 | 1.82 | 0.62 |
| 1:N:97:THR:CG2 | 1:N:100:GLY:H | 2.12 | 0.62 |
| 1:N:38:VAL:O | 1:N:39:ALA:HB2 | 1.99 | 0.62 |
| 1:T:116:LEU:HA | 2:T:1000:HEM:O1A | 2.00 | 0.62 |
| 1:J:116:LEU:HA | 2:J:1000:HEM:O1A | 1.99 | 0.62 |
| 1:C:235:THR:HG23 | 1:C:237:HIS:NE2 | 2.15 | 0.62 |
| 1:A:174:THR:HB | 2:A:1000:HEM:CBB | 2.26 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:211:LEU:HD11 | 2:F:1000:HEM:HBB2 | 1.82 | 0.61 |
| 1:O:116:LEU:HA | 2:O:1000:HEM:O1A | 2.00 | 0.61 |
| 1:J:201:GLU:HG2 | 1:J:236:ILE:HD11 | 1.81 | 0.61 |
| 1:N:150:LYS:HA | 1:N:195:ASP:HB2 | 1.82 | 0.61 |
| 1:B:190:GLY:HA3 | 1:D:212:MET:HG3 | 1.81 | 0.61 |
| 1:K:150:LYS:HA | 1:K:195:ASP:HB2 | 1.82 | 0.61 |
| 1:B:145:ILE:HD13 | 1:B:233:LEU:HD13 | 1.82 | 0.61 |
| 1:L:20:VAL:H | 1:L:113:THR:HB | 1.65 | 0.61 |
| 1:P:20:VAL:H | 1:P:113:THR:HB | 1.66 | 0.61 |
| 1:F:38:VAL:HB | 1:F:41:ARG:HH12 | 1.64 | 0.61 |
| 1:N:67:ARG:HB2 | 1:N:74:ASP:HB3 | 1.83 | 0.61 |
| 1:G:211:LEU:HD11 | 2:G:1000:HEM:CBB | 2.28 | 0.61 |
| 1:E:97:THR:HG22 | 1:E:100:GLY:N | 2.09 | 0.61 |
| 1:J:174:THR:HB | 2:J:1000:HEM:HBB2 | 1.83 | 0.61 |
| 1:P:116:LEU:HA | 2:P:1000:HEM:O1A | 2.00 | 0.61 |
| 1:L:224:HIS:HE1 | 5:L:3000:HOH:O | 1.82 | 0.60 |
| 1:Q:18:PRO:HA | 1:Q:113:THR:HG22 | 1.82 | 0.60 |
| 1:A:116:LEU:HA | 2:A:1000:HEM:O1A | 2.01 | 0.60 |
| 1:B:97:THR:HG22 | 1:B:100:GLY:N | 2.09 | 0.60 |
| 1:T:9:ILE:O | 1:T:9:ILE:HG22 | 2.01 | 0.60 |
| 1:G:97:THR:HG22 | 1:G:100:GLY:N | 2.07 | 0.60 |
| 1:R:18:PRO:HA | 1:R:113:THR:CG2 | 2.28 | 0.60 |
| 1:N:11:ARG:NH2 | 1:N:62:ASP:OD1 | 2.35 | 0.60 |
| 1:M:158:MET:O | 1:M:163:ARG:NH1 | 2.34 | 0.60 |
| 1:P:97:THR:HG23 | 1:P:100:GLY:H | 1.67 | 0.60 |
| 1:T:235:THR:HG23 | 1:T:237:HIS:NE2 | 2.16 | 0.60 |
| 1:M:221:ASN:ND2 | 1:M:224:HIS:HD2 | 2.00 | 0.60 |
| 1:D:174:THR:HB | 2:D:1000:HEM:HBB2 | 1.84 | 0.60 |
| 1:P:18:PRO:HA | 1:P:113:THR:CG2 | 2.27 | 0.60 |
| 1:P:190:GLY:CA | 1:S:212:MET:HG3 | 2.31 | 0.60 |
| 1:J:48:VAL:O | 1:J:52:ILE:HG13 | 2.01 | 0.60 |
| 1:L:211:LEU:O | 1:L:214:SER:HB2 | 2.02 | 0.60 |
| 1:L:224:HIS:CE1 | 5:L:3000:HOH:O | 2.53 | 0.59 |
| 1:S:97:THR:HG22 | 1:S:100:GLY:N | 2.14 | 0.59 |
| 1:B:65:LEU:HB3 | 1:B:235:THR:HG22 | 1.82 | 0.59 |
| 1:F:71:THR:HG23 | 1:G:105:VAL:HG12 | 1.84 | 0.59 |
| 1:C:97:THR:CG2 | 1:C:100:GLY:H | 2.03 | 0.59 |
| 1:P:221:ASN:HA | 1:P:224:HIS:CD2 | 2.38 | 0.59 |
| 1:B:159:SER:OG | 1:B:162:GLU:HG3 | 2.01 | 0.59 |
| 1:N:71:THR:HG23 | 1:O:105:VAL:HG12 | 1.83 | 0.59 |
| 1:F:20:VAL:H | 1:F:113:THR:HB | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:158:MET:O | 1:N:163:ARG:NH1 | 2.36 | 0.59 |
| 1:B:11:ARG:NH2 | 1:B:62:ASP:OD1 | 2.35 | 0.59 |
| 1:M:180:ASN:HB3 | 1:M:181:VAL:HG23 | 1.84 | 0.59 |
| 1:K:18:PRO:CA | 1:K:113:THR:HG22 | 2.22 | 0.59 |
| 1:R:116:LEU:HA | 2:R:1000:HEM:O1A | 2.03 | 0.59 |
| 1:N:97:THR:HG22 | 1:N:100:GLY:N | 2.17 | 0.59 |
| 1:L:70:GLU:OE2 | 1:L:232:THR:HA | 2.03 | 0.59 |
| 1:A:222:LYS:HE2 | 1:D:154:GLU:OE1 | 2.03 | 0.59 |
| 1:D:20:VAL:H | 1:D:113:THR:HB | 1.68 | 0.58 |
| 1:B:97:THR:CG2 | 1:B:100:GLY:H | 2.09 | 0.58 |
| 1:C:66:THR:HG22 | 1:C:234:GLY:HA3 | 1.84 | 0.58 |
| 1:H:94:PHE:O | 1:H:97:THR:HB | 2.03 | 0.58 |
| 1:T:174:THR:HG22 | 1:T:211:LEU:CD1 | 2.33 | 0.58 |
| 1:S:41:ARG:O | 1:S:44:ALA:HB3 | 2.03 | 0.58 |
| 1:J:174:THR:HB | 2:J:1000:HEM:CBB | 2.33 | 0.58 |
| 1:A:145:ILE:CD1 | 1:A:233:LEU:HD13 | 2.33 | 0.58 |
| 1:D:116:LEU:HA | 2:D:1000:HEM:O1A | 2.03 | 0.58 |
| 1:H:212:MET:HG3 | 1:I:190:GLY:HA2 | 1.84 | 0.58 |
| 1:C:183:ARG:NH2 | 3:C:2000:NO2:O2 | 2.36 | 0.58 |
| 1:K:11:ARG:NH2 | 1:K:62:ASP:OD1 | 2.35 | 0.58 |
| 1:C:116:LEU:HA | 2:C:1000:HEM:O1A | 2.04 | 0.58 |
| 1:N:55:HIS:CD2 | 1:N:58:ASN:HD22 | 2.22 | 0.58 |
| 1:P:235:THR:HG23 | 1:P:237:HIS:NE2 | 2.18 | 0.57 |
| 1:D:174:THR:HG22 | 1:D:211:LEU:CD1 | 2.34 | 0.57 |
| 1:P:66:THR:HG22 | 1:P:234:GLY:CA | 2.34 | 0.57 |
| 1:L:212:MET:HG3 | 1:M:190:GLY:HA3 | 1.86 | 0.57 |
| 1:T:211:LEU:CD1 | 2:T:1000:HEM:HBB2 | 2.32 | 0.57 |
| 1:Q:118:TYR:HE2 | 2:Q:1000:HEM:O1D | 1.87 | 0.57 |
| 1:O:221:ASN:HA | 1:O:224:HIS:CD2 | 2.39 | 0.57 |
| 1:A:65:LEU:HB3 | 1:A:235:THR:HG22 | 1.87 | 0.57 |
| 1:E:145:ILE:HD13 | 1:E:233:LEU:HD13 | 1.86 | 0.57 |
| 1:F:118:TYR:CD2 | 1:F:167:MET:HG3 | 2.39 | 0.57 |
| 1:G:235:THR:CG2 | 1:G:237:HIS:NE2 | 2.67 | 0.57 |
| 1:A:219:LYS:O | 1:A:222:LYS:HB2 | 2.04 | 0.57 |
| 1:B:166:GLU:OE1 | 1:B:166:GLU:HA | 2.05 | 0.57 |
| 1:T:159:SER:OG | 1:T:162:GLU:HG3 | 2.05 | 0.57 |
| 1:R:221:ASN:HA | 1:R:224:HIS:CD2 | 2.40 | 0.57 |
| 1:H:11:ARG:NH2 | 1:H:62:ASP:OD1 | 2.36 | 0.57 |
| 1:M:235:THR:HG23 | 1:M:237:HIS:NE2 | 2.19 | 0.57 |
| 1:M:20:VAL:H | 1:M:113:THR:HB | 1.69 | 0.57 |
| 1:P:27:PHE:CD2 | 1:P:75:PHE:CE2 | 2.93 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:R:97:THR:HG22 | 1:R:100:GLY:H | 1.70 | 0.57 |
| 1:K:118:TYR:CD2 | 1:K:167:MET:HG3 | 2.40 | 0.57 |
| 1:G:221:ASN:HA | 1:G:224:HIS:CD2 | 2.40 | 0.57 |
| 2:K:1000:HEM:HHC | 2:K:1000:HEM:HBB2 | 1.86 | 0.56 |
| 1:Q:109:LEU:HB3 | 1:Q:197:ILE:CD1 | 2.34 | 0.56 |
| 1:D:97:THR:HG22 | 1:D:100:GLY:N | 2.10 | 0.56 |
| 1:J:167:MET:CE | 2:J:1000:HEM:HBD1 | 2.35 | 0.56 |
| 1:E:174:THR:HB | 2:E:1000:HEM:CBB | 2.35 | 0.56 |
| 1:K:235:THR:CG2 | 1:K:237:HIS:NE2 | 2.68 | 0.56 |
| 1:M:212:MET:HG3 | 1:N:190:GLY:CA | 2.35 | 0.56 |
| 1:F:94:PHE:O | 1:F:97:THR:HG22 | 2.03 | 0.56 |
| 1:T:23:VAL:HG22 | 1:T:110:VAL:HG22 | 1.87 | 0.56 |
| 1:E:20:VAL:H | 1:E:113:THR:HB | 1.71 | 0.56 |
| 1:N:38:VAL:O | 1:N:39:ALA:CB | 2.52 | 0.56 |
| 1:R:117:ASN:N | 2:R:1000:HEM:O1A | 2.39 | 0.56 |
| 1:R:65:LEU:HB3 | 1:R:235:THR:HG22 | 1.87 | 0.56 |
| 1:T:150:LYS:HB3 | 1:T:226:ARG:HB3 | 1.87 | 0.56 |
| 1:P:195:ASP:HB3 | 1:P:196:PHE:CE2 | 2.40 | 0.56 |
| 1:R:26:MET:HG3 | 1:R:76:PHE:HB3 | 1.88 | 0.56 |
| 1:I:11:ARG:NH2 | 1:I:62:ASP:OD1 | 2.39 | 0.56 |
| 1:O:20:VAL:H | 1:O:113:THR:HB | 1.71 | 0.56 |
| 1:K:190:GLY:HA3 | 1:O:212:MET:HG3 | 1.88 | 0.56 |
| 1:M:145:ILE:CD1 | 1:M:233:LEU:HD13 | 2.35 | 0.56 |
| 1:O:145:ILE:HD13 | 1:O:233:LEU:HD13 | 1.88 | 0.56 |
| 1:E:235:THR:CG2 | 1:E:237:HIS:NE2 | 2.68 | 0.55 |
| 1:T:118:TYR:CD2 | 1:T:167:MET:HG3 | 2.41 | 0.55 |
| 1:H:65:LEU:HB3 | 1:H:235:THR:HG22 | 1.87 | 0.55 |
| 1:G:66:THR:HG22 | 1:G:234:GLY:HA3 | 1.88 | 0.55 |
| 1:J:180:ASN:HB3 | 1:J:181:VAL:HG23 | 1.88 | 0.55 |
| 1:H:224:HIS:CE1 | 5:H:3000:HOH:O | 2.59 | 0.55 |
| 1:C:38:VAL:HB | 1:C:41:ARG:HH12 | 1.71 | 0.55 |
| 1:D:174:THR:HG22 | 1:D:211:LEU:HD11 | 1.88 | 0.55 |
| 1:S:30:ARG:O | 1:S:33:TRP:HB3 | 2.06 | 0.55 |
| 1:E:116:LEU:HA | 2:E:1000:HEM:O1A | 2.07 | 0.55 |
| 1:K:212:MET:HG3 | 1:L:190:GLY:HA3 | 1.87 | 0.55 |
| 1:L:182:LYS:O | 1:L:200:PHE:HA | 2.07 | 0.55 |
| 1:E:59:VAL:HG12 | 1:E:81:ALA:HB2 | 1.88 | 0.55 |
| 1:P:41:ARG:NH2 | 1:P:247:ALA:O | 2.37 | 0.55 |
| 1:C:222:LYS:HE3 | 1:E:154:GLU:OE1 | 2.05 | 0.55 |
| 2:H:1000:HEM:CHC | 2:H:1000:HEM:HBB2 | 2.19 | 0.55 |
| 1:I:38:VAL:O | 1:I:39:ALA:CB | 2.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:97:THR:CG2 | 1:G:100:GLY:H | 2.10 | 0.55 |
| 1:G:196:PHE:HZ | 2:G:1000:HEM:O2D | 1.85 | 0.55 |
| 1:C:211:LEU:CD1 | 2:C:1000:HEM:HBB2 | 2.36 | 0.55 |
| 1:L:221:ASN:HA | 1:L:224:HIS:CD2 | 2.42 | 0.54 |
| 1:Q:18:PRO:HA | 1:Q:113:THR:CG2 | 2.36 | 0.54 |
| 1:P:174:THR:HG22 | 1:P:211:LEU:HD11 | 1.88 | 0.54 |
| 1:J:26:MET:N | 1:J:26:MET:SD | 2.80 | 0.54 |
| 1:C:221:ASN:ND2 | 1:C:224:HIS:CD2 | 2.52 | 0.54 |
| 1:P:27:PHE:CB | 1:P:75:PHE:CZ | 2.88 | 0.54 |
| 1:Q:158:MET:O | 1:Q:163:ARG:NH1 | 2.41 | 0.54 |
| 1:P:154:GLU:OE1 | 1:S:222:LYS:HE2 | 2.07 | 0.54 |
| 1:B:182:LYS:O | 1:B:200:PHE:HA | 2.08 | 0.54 |
| 1:C:20:VAL:H | 1:C:113:THR:HB | 1.72 | 0.54 |
| 1:H:145:ILE:CD1 | 1:H:233:LEU:HD13 | 2.36 | 0.54 |
| 2:L:1000:HEM:CBB | 2:L:1000:HEM:HHC | 2.31 | 0.54 |
| 1:L:196:PHE:CE1 | 2:L:1000:HEM:O2D | 2.60 | 0.54 |
| 1:B:88:GLN:HG3 | 1:D:69:LEU:HG | 1.90 | 0.54 |
| 1:K:97:THR:HG22 | 1:K:100:GLY:N | 2.21 | 0.54 |
| 1:F:116:LEU:HA | 2:F:1000:HEM:O1A | 2.07 | 0.54 |
| 1:B:154:GLU:OE1 | 1:D:222:LYS:HE3 | 2.08 | 0.54 |
| 1:F:92:ARG:NH1 | 1:J:245:ALA:HB1 | 2.23 | 0.54 |
| 1:M:94:PHE:O | 1:M:97:THR:HB | 2.07 | 0.54 |
| 1:I:235:THR:CG2 | 1:I:237:HIS:NE2 | 2.71 | 0.54 |
| 1:A:33:TRP:CZ2 | 1:A:41:ARG:HG2 | 2.43 | 0.53 |
| 1:A:11:ARG:NH2 | 1:A:62:ASP:OD1 | 2.40 | 0.53 |
| 1:F:97:THR:CG2 | 1:F:100:GLY:H | 2.21 | 0.53 |
| 1:D:221:ASN:HA | 1:D:224:HIS:CD2 | 2.43 | 0.53 |
| 1:S:41:ARG:NH2 | 1:S:247:ALA:O | 2.36 | 0.53 |
| 1:C:158:MET:O | 1:C:163:ARG:NH1 | 2.41 | 0.53 |
| 1:Q:221:ASN:HD22 | 1:Q:224:HIS:HD2 | 1.54 | 0.53 |
| 1:S:235:THR:HG23 | 1:S:237:HIS:CD2 | 2.43 | 0.53 |
| 1:H:118:TYR:HE2 | 2:H:1000:HEM:O1D | 1.91 | 0.53 |
| 1:L:21:PHE:O | 1:L:80:ASN:HA | 2.09 | 0.53 |
| 1:T:17:GLN:O | 1:T:113:THR:HG21 | 2.08 | 0.53 |
| 1:F:177:TYR:HB2 | 2:F:1000:HEM:HBB1 | 1.88 | 0.53 |
| 1:F:119:ILE:HG13 | 2:F:1000:HEM:HMA2 | 1.91 | 0.53 |
| 1:K:97:THR:CG2 | 1:K:100:GLY:H | 2.17 | 0.53 |
| 1:T:174:THR:HG22 | 1:T:211:LEU:HD11 | 1.89 | 0.53 |
| 1:E:211:LEU:O | 1:E:214:SER:HB2 | 2.07 | 0.53 |
| 1:I:65:LEU:HB3 | 1:I:235:THR:HG22 | 1.91 | 0.53 |
| 1:H:118:TYR:CD2 | 1:H:167:MET:HG3 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:38:VAL:O | 1:K:39:ALA:CB | 2.56 | 0.53 |
| 1:G:182:LYS:O | 1:G:200:PHE:HA | 2.09 | 0.53 |
| 1:I:116:LEU:HA | 2:I:1000:HEM:O1A | 2.08 | 0.53 |
| 1:G:158:MET:O | 1:G:163:ARG:NH1 | 2.41 | 0.53 |
| 1:F:26:MET:HB2 | 1:F:107:GLU:HB2 | 1.91 | 0.53 |
| 1:A:127:LEU:HD23 | 1:A:175:LEU:HD11 | 1.91 | 0.53 |
| 1:R:99:VAL:HG21 | 1:R:243:ILE:HD12 | 1.90 | 0.53 |
| 1:D:235:THR:CG2 | 1:D:237:HIS:NE2 | 2.72 | 0.52 |
| 1:D:182:LYS:O | 1:D:200:PHE:HA | 2.09 | 0.52 |
| 1:P:88:GLN:OE1 | 1:S:235:THR:HG21 | 2.08 | 0.52 |
| 1:N:167:MET:CE | 2:N:1000:HEM:HBD1 | 2.39 | 0.52 |
| 1:C:75:PHE:CD1 | 1:C:246:LEU:HD11 | 2.44 | 0.52 |
| 1:N:150:LYS:HB3 | 1:N:226:ARG:HB3 | 1.91 | 0.52 |
| 1:M:235:THR:CG2 | 1:M:237:HIS:NE2 | 2.72 | 0.52 |
| 1:B:67:ARG:HG2 | 1:C:92:ARG:HG3 | 1.91 | 0.52 |
| 1:M:211:LEU:HD11 | 2:M:1000:HEM:HBB2 | 1.90 | 0.52 |
| 1:S:63:LEU:HB3 | 1:S:239:PRO:HA | 1.92 | 0.52 |
| 1:G:221:ASN:ND2 | 1:G:224:HIS:CD2 | 2.51 | 0.52 |
| 1:E:221:ASN:ND2 | 1:E:224:HIS:CD2 | 2.55 | 0.52 |
| 1:A:94:PHE:O | 1:A:97:THR:HB | 2.10 | 0.52 |
| 1:Q:118:TYR:CD2 | 1:Q:167:MET:HG3 | 2.44 | 0.52 |
| 1:J:70:GLU:HA | 1:J:70:GLU:OE1 | 2.10 | 0.52 |
| 1:T:22:GLY:HA2 | 1:T:79:ILE:O | 2.09 | 0.52 |
| 1:T:66:THR:HG22 | 1:T:234:GLY:HA3 | 1.91 | 0.52 |
| 1:H:224:HIS:HE1 | 5:H:3000:HOH:O | 1.92 | 0.52 |
| 1:R:119:ILE:HG13 | 2:R:1000:HEM:HMA2 | 1.92 | 0.52 |
| 1:D:11:ARG:NH2 | 1:D:62:ASP:OD1 | 2.43 | 0.52 |
| 1:M:38:VAL:O | 1:M:39:ALA:HB2 | 2.09 | 0.52 |
| 1:G:118:TYR:HE2 | 2:G:1000:HEM:O1D | 1.91 | 0.52 |
| 1:J:118:TYR:HE2 | 2:J:1000:HEM:O1D | 1.93 | 0.52 |
| 1:G:235:THR:HG23 | 1:G:237:HIS:CD2 | 2.45 | 0.52 |
| 1:N:150:LYS:HG2 | 1:N:225:VAL:CG2 | 2.40 | 0.52 |
| 1:E:150:LYS:HA | 1:E:195:ASP:HB2 | 1.92 | 0.52 |
| 1:O:196:PHE:CE2 | 2:O:1000:HEM:O2D | 2.63 | 0.52 |
| 1:T:66:THR:HG22 | 1:T:234:GLY:CA | 2.40 | 0.52 |
| 1:A:27:PHE:CE1 | 1:A:95:ARG:HD2 | 2.45 | 0.52 |
| 1:G:180:ASN:HB3 | 1:G:181:VAL:HG23 | 1.92 | 0.52 |
| 1:F:105:VAL:HG12 | 1:J:71:THR:HG23 | 1.92 | 0.51 |
| 1:O:11:ARG:NH2 | 1:O:62:ASP:OD1 | 2.43 | 0.51 |
| 1:J:221:ASN:HA | 1:J:224:HIS:CD2 | 2.45 | 0.51 |
| 1:I:119:ILE:CG1 | 2:I:1000:HEM:HMA2 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:159:SER:OG | 1:H:162:GLU:HG3 | 2.10 | 0.51 |
| 1:S:44:ALA:HB1 | 1:S:99:VAL:HG22 | 1.92 | 0.51 |
| 1:F:212:MET:HG3 | 1:G:190:GLY:HA2 | 1.91 | 0.51 |
| 1:Q:235:THR:HG23 | 1:Q:237:HIS:NE2 | 2.25 | 0.51 |
| 1:C:18:PRO:HA | 1:C:113:THR:HG21 | 1.89 | 0.51 |
| 2:B:1000:HEM:HHC | 2:B:1000:HEM:CBB | 2.41 | 0.51 |
| 1:I:222:LYS:HE2 | 1:J:154:GLU:OE1 | 2.10 | 0.51 |
| 1:Q:117:ASN:N | 2:Q:1000:HEM:O1A | 2.41 | 0.51 |
| 1:A:212:MET:HG3 | 1:D:190:GLY:HA3 | 1.93 | 0.51 |
| 1:F:67:ARG:HG2 | 1:G:92:ARG:HG3 | 1.93 | 0.51 |
| 1:S:33:TRP:HB2 | 1:S:102:ASN:HB3 | 1.91 | 0.51 |
| 2:B:1000:HEM:HHC | 2:B:1000:HEM:HBB2 | 1.93 | 0.51 |
| 1:R:41:ARG:NH2 | 1:R:247:ALA:O | 2.43 | 0.51 |
| 1:D:65:LEU:HB3 | 1:D:235:THR:HG22 | 1.93 | 0.51 |
| 1:M:145:ILE:HD13 | 1:M:233:LEU:HD13 | 1.93 | 0.51 |
| 1:M:118:TYR:CD2 | 1:M:167:MET:HG3 | 2.46 | 0.51 |
| 1:E:9:ILE:O | 1:E:9:ILE:HG22 | 2.11 | 0.51 |
| 1:Q:221:ASN:ND2 | 1:Q:224:HIS:HD2 | 2.09 | 0.51 |
| 1:L:145:ILE:HD13 | 1:L:233:LEU:HD13 | 1.93 | 0.51 |
| 1:R:92:ARG:HH11 | 1:R:92:ARG:HG2 | 1.75 | 0.51 |
| 1:S:29:LEU:HD21 | 1:S:99:VAL:HG12 | 1.93 | 0.51 |
| 1:O:38:VAL:O | 1:O:39:ALA:HB2 | 2.10 | 0.51 |
| 1:E:195:ASP:HB3 | 1:E:196:PHE:CE2 | 2.47 | 0.50 |
| 1:B:154:GLU:OE1 | 1:D:222:LYS:CE | 2.59 | 0.50 |
| 1:L:66:THR:HG22 | 1:L:234:GLY:HA3 | 1.93 | 0.50 |
| 1:E:70:GLU:OE2 | 1:E:232:THR:HA | 2.11 | 0.50 |
| 1:L:235:THR:CG2 | 1:L:237:HIS:NE2 | 2.71 | 0.50 |
| 1:G:11:ARG:NH2 | 1:G:62:ASP:OD1 | 2.44 | 0.50 |
| 1:R:145:ILE:HD13 | 1:R:233:LEU:HD13 | 1.93 | 0.50 |
| 1:C:174:THR:HG22 | 1:C:211:LEU:CD1 | 2.41 | 0.50 |
| 1:G:118:TYR:CD2 | 1:G:167:MET:HG3 | 2.46 | 0.50 |
| 1:S:66:THR:HG22 | 1:S:234:GLY:CA | 2.40 | 0.50 |
| 1:E:36:VAL:O | 1:E:41:ARG:HD3 | 2.12 | 0.50 |
| 1:T:142:ARG:NE | 1:T:203:ASP:OD1 | 2.40 | 0.50 |
| 1:P:67:ARG:HG2 | 1:T:92:ARG:HG3 | 1.93 | 0.50 |
| 1:C:11:ARG:NH2 | 1:C:62:ASP:OD1 | 2.45 | 0.50 |
| 1:F:196:PHE:HZ | 2:F:1000:HEM:O2D | 1.87 | 0.50 |
| 1:S:116:LEU:HA | 2:S:1000:HEM:O1A | 2.12 | 0.50 |
| 1:O:180:ASN:HB3 | 1:O:181:VAL:HG23 | 1.93 | 0.50 |
| 1:J:235:THR:CG2 | 1:J:237:HIS:NE2 | 2.74 | 0.50 |
| 1:Q:224:HIS:CD2 | 1:Q:227:TRP:CD1 | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:116:LEU:HD22 | 2:N:1000:HEM:HBA2 | 1.94 | 0.50 |
| 1:I:28:LYS:NZ | 1:I:72:ASN:HD22 | 2.09 | 0.50 |
| 1:G:71:THR:HG23 | 1:H:105:VAL:HG12 | 1.94 | 0.50 |
| 1:D:175:LEU:HD12 | 1:K:126:GLY:HA2 | 1.94 | 0.50 |
| 1:B:235:THR:HG23 | 1:B:237:HIS:CD2 | 2.46 | 0.50 |
| 1:N:75:PHE:CD1 | 1:N:246:LEU:HD11 | 2.46 | 0.50 |
| 1:J:18:PRO:CA | 1:J:113:THR:HG22 | 2.19 | 0.49 |
| 1:Q:212:MET:HG3 | 1:R:190:GLY:CA | 2.37 | 0.49 |
| 1:Q:31:PRO:HB3 | 1:R:30:ARG:NH2 | 2.27 | 0.49 |
| 1:L:183:ARG:NH2 | 3:L:2000:NO2:O2 | 2.41 | 0.49 |
| 1:M:119:ILE:O | 1:M:119:ILE:HG22 | 2.12 | 0.49 |
| 1:I:38:VAL:O | 1:I:39:ALA:HB2 | 2.13 | 0.49 |
| 1:J:97:THR:HG22 | 1:J:100:GLY:N | 2.24 | 0.49 |
| 1:C:180:ASN:HB3 | 1:C:181:VAL:HG23 | 1.94 | 0.49 |
| 1:F:148:PRO:HG2 | 1:F:228:GLY:O | 2.12 | 0.49 |
| 1:E:119:ILE:HG13 | 2:E:1000:HEM:HMA3 | 1.95 | 0.49 |
| 1:N:44:ALA:HB1 | 1:N:99:VAL:HG22 | 1.93 | 0.49 |
| 1:C:67:ARG:HG2 | 1:E:92:ARG:HG3 | 1.93 | 0.49 |
| 1:E:63:LEU:HD13 | 1:E:77:PHE:CE1 | 2.46 | 0.49 |
| 1:G:55:HIS:CD2 | 1:G:58:ASN:HD22 | 2.30 | 0.49 |
| 1:S:38:VAL:O | 1:S:39:ALA:HB2 | 2.12 | 0.49 |
| 1:L:44:ALA:HB1 | 1:L:99:VAL:CG2 | 2.42 | 0.49 |
| 1:L:92:ARG:HH11 | 1:L:92:ARG:HG2 | 1.78 | 0.49 |
| 1:S:33:TRP:CH2 | 1:S:41:ARG:HG2 | 2.47 | 0.49 |
| 1:Q:105:VAL:HG12 | 1:T:71:THR:HG23 | 1.94 | 0.49 |
| 1:J:95:ARG:HA | 1:J:100:GLY:HA3 | 1.95 | 0.49 |
| 1:S:119:ILE:HB | 2:S:1000:HEM:HMA2 | 1.95 | 0.49 |
| 1:A:237:HIS:HB2 | 1:A:242:VAL:HG23 | 1.94 | 0.48 |
| 1:B:13:THR:O | 1:B:16:THR:HB | 2.13 | 0.48 |
| 1:I:20:VAL:H | 1:I:113:THR:HB | 1.77 | 0.48 |
| 1:G:211:LEU:HD21 | 2:G:1000:HEM:CBB | 2.43 | 0.48 |
| 1:Q:118:TYR:CE2 | 2:Q:1000:HEM:O1D | 2.66 | 0.48 |
| 1:R:38:VAL:O | 1:R:39:ALA:HB2 | 2.13 | 0.48 |
| 1:E:186:TYR:HB2 | 1:E:197:ILE:HB | 1.94 | 0.48 |
| 1:G:147:ILE:HG21 | 2:G:1000:HEM:HBC1 | 1.95 | 0.48 |
| 1:O:211:LEU:CD1 | 2:O:1000:HEM:HBB2 | 2.44 | 0.48 |
| 1:C:118:TYR:CD2 | 1:C:167:MET:HG3 | 2.48 | 0.48 |
| 1:J:38:VAL:O | 1:J:39:ALA:HB2 | 2.13 | 0.48 |
| 1:G:44:ALA:HB1 | 1:G:99:VAL:CG2 | 2.42 | 0.48 |
| 1:Q:27:PHE:CE1 | 1:Q:105:VAL:HG22 | 2.49 | 0.48 |
| 1:B:158:MET:O | 1:B:163:ARG:NH1 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:116:LEU:HD13 | 1:A:119:ILE:O | 2.14 | 0.48 |
| 1:E:211:LEU:HD11 | 2:E:1000:HEM:CBB | 2.43 | 0.48 |
| 1:P:27:PHE:CD2 | 1:P:75:PHE:HE2 | 2.31 | 0.48 |
| 1:D:196:PHE:CE1 | 2:D:1000:HEM:O2D | 2.64 | 0.48 |
| 1:Q:196:PHE:HZ | 2:Q:1000:HEM:O2D | 1.93 | 0.48 |
| 1:S:27:PHE:CE1 | 1:S:105:VAL:HG22 | 2.48 | 0.48 |
| 1:G:38:VAL:O | 1:G:39:ALA:HB2 | 2.14 | 0.48 |
| 1:Q:26:MET:SD | 1:Q:26:MET:N | 2.87 | 0.48 |
| 1:T:11:ARG:NH1 | 1:T:60:LEU:HD11 | 2.28 | 0.48 |
| 1:R:10:GLU:HB2 | 1:R:13:THR:HB | 1.96 | 0.48 |
| 1:D:195:ASP:HB3 | 1:D:196:PHE:CE2 | 2.48 | 0.48 |
| 1:Q:183:ARG:HD2 | 2:Q:1000:HEM:HMB2 | 1.95 | 0.48 |
| 1:P:62:ASP:HB2 | 1:P:78:ARG:HB3 | 1.96 | 0.48 |
| 1:I:159:SER:OG | 1:I:162:GLU:HG3 | 2.14 | 0.48 |
| 1:S:147:ILE:HG12 | 1:S:231:THR:HG23 | 1.96 | 0.48 |
| 1:Q:180:ASN:HB3 | 1:Q:181:VAL:HG23 | 1.95 | 0.48 |
| 1:B:145:ILE:CD1 | 1:B:233:LEU:HD13 | 2.43 | 0.48 |
| 1:K:88:GLN:O | 1:K:92:ARG:HB2 | 2.14 | 0.48 |
| 1:E:235:THR:HG23 | 1:E:237:HIS:CD2 | 2.48 | 0.48 |
| 1:A:44:ALA:HB1 | 1:A:99:VAL:CG2 | 2.44 | 0.48 |
| 1:F:180:ASN:CB | 1:F:181:VAL:HG23 | 2.43 | 0.48 |
| 1:S:53:GLU:HB3 | 1:S:56:LYS:HZ3 | 1.79 | 0.48 |
| 1:P:30:ARG:NH2 | 1:S:31:PRO:HB3 | 2.28 | 0.48 |
| 1:R:116:LEU:CD2 | 2:R:1000:HEM:HBA2 | 2.44 | 0.47 |
| 1:T:26:MET:HG3 | 1:T:76:PHE:CB | 2.44 | 0.47 |
| 1:L:24:PHE:HB2 | 1:L:109:LEU:HB2 | 1.96 | 0.47 |
| 1:M:38:VAL:O | 1:M:39:ALA:CB | 2.61 | 0.47 |
| 1:C:150:LYS:HA | 1:C:195:ASP:HB2 | 1.96 | 0.47 |
| 1:P:145:ILE:HD13 | 1:P:233:LEU:HD13 | 1.95 | 0.47 |
| 1:N:21:PHE:O | 1:N:80:ASN:HA | 2.14 | 0.47 |
| 1:P:27:PHE:CE1 | 1:P:105:VAL:HG22 | 2.50 | 0.47 |
| 1:L:235:THR:HG23 | 1:L:237:HIS:CD2 | 2.49 | 0.47 |
| 1:E:64:TYR:CD1 | 1:E:144:VAL:HG11 | 2.49 | 0.47 |
| 1:Q:97:THR:CG2 | 1:Q:100:GLY:H | 2.15 | 0.47 |
| 1:B:59:VAL:HB | 1:B:79:ILE:HG23 | 1.95 | 0.47 |
| 1:I:97:THR:HG22 | 1:I:100:GLY:N | 2.09 | 0.47 |
| 1:J:118:TYR:CD2 | 1:J:167:MET:HG3 | 2.50 | 0.47 |
| 1:P:180:ASN:HB3 | 1:P:181:VAL:HG23 | 1.96 | 0.47 |
| 1:A:63:LEU:HG | 1:A:242:VAL:HG11 | 1.95 | 0.47 |
| 1:R:38:VAL:O | 1:R:39:ALA:CB | 2.62 | 0.47 |
| 1:Q:41:ARG:NE | 1:Q:247:ALA:O | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:183:ARG:NH2 | 3:G:2000:NO2:O2 | 2.44 | 0.47 |
| 1:L:119:ILE:HG13 | 2:L:1000:HEM:HMA3 | 1.96 | 0.47 |
| 1:R:211:LEU:HD11 | 2:R:1000:HEM:CBB | 2.42 | 0.47 |
| 1:J:211:LEU:HD11 | 2:J:1000:HEM:HBB2 | 1.96 | 0.47 |
| 1:R:145:ILE:CD1 | 1:R:233:LEU:HD13 | 2.45 | 0.47 |
| 1:K:169:VAL:O | 1:K:173:PRO:HD3 | 2.14 | 0.47 |
| 1:D:26:MET:HB3 | 1:D:73:SER:HB3 | 1.97 | 0.47 |
| 1:G:211:LEU:CD1 | 2:G:1000:HEM:HBB2 | 2.33 | 0.47 |
| 1:L:38:VAL:O | 1:L:39:ALA:CB | 2.62 | 0.47 |
| 1:Q:128:ASN:O | 1:Q:131:LEU:HB3 | 2.15 | 0.47 |
| 1:C:55:HIS:CD2 | 1:C:58:ASN:HD22 | 2.32 | 0.47 |
| 1:F:211:LEU:CD1 | 2:F:1000:HEM:HBB2 | 2.44 | 0.47 |
| 1:S:174:THR:HB | 2:S:1000:HEM:CBB | 2.45 | 0.47 |
| 1:T:45:ALA:CB | 1:T:244:LYS:HG3 | 2.45 | 0.47 |
| 1:C:145:ILE:HD13 | 1:C:233:LEU:HD13 | 1.97 | 0.47 |
| 1:S:186:TYR:HB2 | 1:S:197:ILE:HB | 1.97 | 0.47 |
| 1:S:55:HIS:CD2 | 1:S:58:ASN:HD22 | 2.33 | 0.47 |
| 1:E:28:LYS:HD2 | 1:E:106:PHE:CE1 | 2.50 | 0.47 |
| 1:B:150:LYS:HA | 1:B:195:ASP:HB2 | 1.95 | 0.47 |
| 1:R:53:GLU:O | 1:R:56:LYS:HG3 | 2.15 | 0.47 |
| 1:Q:217:GLN:HA | 1:R:156:TRP:O | 2.15 | 0.47 |
| 1:H:24:PHE:HB2 | 1:H:109:LEU:HB2 | 1.97 | 0.47 |
| 1:D:177:TYR:HB2 | 2:D:1000:HEM:HBB1 | 1.98 | 0.46 |
| 1:F:118:TYR:CE2 | 2:F:1000:HEM:O1D | 2.65 | 0.46 |
| 1:N:150:LYS:HG2 | 1:N:225:VAL:HG23 | 1.96 | 0.46 |
| 1:A:157:ASN:HD21 | 1:E:218:VAL:C | 2.18 | 0.46 |
| 1:I:97:THR:HG23 | 1:I:98:THR:N | 2.30 | 0.46 |
| 1:K:35:LYS:HE3 | 1:K:35:LYS:HB2 | 1.73 | 0.46 |
| 1:O:182:LYS:O | 1:O:200:PHE:HA | 2.15 | 0.46 |
| 1:Q:151:LYS:NZ | 2:Q:1000:HEM:HBD2 | 2.31 | 0.46 |
| 1:I:212:MET:CG | 1:J:190:GLY:HA3 | 2.43 | 0.46 |
| 1:N:65:LEU:HB3 | 1:N:235:THR:HG22 | 1.97 | 0.46 |
| 1:L:94:PHE:O | 1:L:97:THR:HB | 2.14 | 0.46 |
| 1:F:65:LEU:HB3 | 1:F:235:THR:HG22 | 1.97 | 0.46 |
| 1:O:147:ILE:HG12 | 1:O:231:THR:HG23 | 1.97 | 0.46 |
| 1:S:211:LEU:O | 1:S:214:SER:HB2 | 2.16 | 0.46 |
| 1:N:221:ASN:ND2 | 1:N:224:HIS:CD2 | 2.55 | 0.46 |
| 1:G:196:PHE:CZ | 2:G:1000:HEM:HAD1 | 2.50 | 0.46 |
| 1:I:29:LEU:N | 1:I:74:ASP:OD2 | 2.45 | 0.46 |
| 1:N:26:MET:HB3 | 1:N:73:SER:HB3 | 1.97 | 0.46 |
| 1:S:118:TYR:CE2 | 2:S:1000:HEM:O1D | 2.69 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:T:33:TRP:CH2 | 1:T:99:VAL:HG13 | 2.51 | 0.46 |
| 1:H:92:ARG:HH11 | 1:H:92:ARG:HG2 | 1.80 | 0.46 |
| 1:F:154:GLU:OE1 | 1:J:222:LYS:HE2 | 2.16 | 0.46 |
| 1:K:36:VAL:O | 1:K:41:ARG:HD3 | 2.16 | 0.46 |
| 1:P:63:LEU:HD23 | 1:P:239:PRO:O | 2.16 | 0.46 |
| 1:L:22:GLY:HA2 | 1:L:79:ILE:O | 2.15 | 0.46 |
| 1:N:195:ASP:HB3 | 1:N:196:PHE:CE2 | 2.51 | 0.46 |
| 1:B:211:LEU:HD11 | 2:B:1000:HEM:HBB2 | 1.97 | 0.46 |
| 1:M:218:VAL:C | 1:N:157:ASN:HD21 | 2.18 | 0.46 |
| 1:Q:177:TYR:CD2 | 1:Q:211:LEU:HD13 | 2.51 | 0.46 |
| 1:Q:44:ALA:HB1 | 1:Q:99:VAL:HG22 | 1.97 | 0.46 |
| 1:I:215:LEU:HD12 | 1:I:215:LEU:HA | 1.81 | 0.46 |
| 1:H:221:ASN:HA | 1:H:224:HIS:CD2 | 2.51 | 0.46 |
| 1:N:116:LEU:CD2 | 2:N:1000:HEM:HBA2 | 2.46 | 0.46 |
| 1:C:159:SER:OG | 1:C:162:GLU:HG3 | 2.15 | 0.46 |
| 1:S:33:TRP:CZ2 | 1:S:99:VAL:HG13 | 2.51 | 0.45 |
| 1:J:11:ARG:NH2 | 1:J:62:ASP:OD1 | 2.49 | 0.45 |
| 1:L:215:LEU:O | 1:L:218:VAL:HG22 | 2.16 | 0.45 |
| 1:K:159:SER:O | 1:K:163:ARG:HG3 | 2.16 | 0.45 |
| 1:M:222:LYS:HE2 | 1:N:154:GLU:OE1 | 2.16 | 0.45 |
| 1:G:38:VAL:O | 1:G:38:VAL:HG13 | 2.16 | 0.45 |
| 1:G:70:GLU:HA | 1:G:70:GLU:OE1 | 2.15 | 0.45 |
| 1:R:159:SER:OG | 1:R:162:GLU:HG3 | 2.16 | 0.45 |
| 1:R:177:TYR:CD2 | 1:R:211:LEU:HD13 | 2.51 | 0.45 |
| 1:T:145:ILE:HD13 | 1:T:233:LEU:HD13 | 1.98 | 0.45 |
| 1:T:146:VAL:HG12 | 1:T:146:VAL:O | 2.16 | 0.45 |
| 1:T:77:PHE:HE2 | 1:T:94:PHE:CE2 | 2.34 | 0.45 |
| 1:A:212:MET:HG3 | 1:D:190:GLY:CA | 2.47 | 0.45 |
| 1:T:70:GLU:OE2 | 1:T:232:THR:HA | 2.17 | 0.45 |
| 1:G:211:LEU:O | 1:G:214:SER:HB2 | 2.16 | 0.45 |
| 1:Q:151:LYS:HZ2 | 2:Q:1000:HEM:HBD2 | 1.81 | 0.45 |
| 1:B:219:LYS:O | 1:B:222:LYS:HB2 | 2.16 | 0.45 |
| 1:N:159:SER:HG | 1:N:162:GLU:HG3 | 1.78 | 0.45 |
| 1:J:177:TYR:HB2 | 2:J:1000:HEM:HBB1 | 1.99 | 0.45 |
| 1:P:196:PHE:CE1 | 2:P:1000:HEM:O2D | 2.69 | 0.45 |
| 1:P:119:ILE:O | 1:P:119:ILE:HG22 | 2.17 | 0.45 |
| 2:B:1000:HEM:HBB2 | 2:B:1000:HEM:CHC | 2.47 | 0.45 |
| 1:R:118:TYR:CE2 | 2:R:1000:HEM:O1D | 2.62 | 0.45 |
| 1:S:117:ASN:N | 2:S:1000:HEM:O1A | 2.40 | 0.45 |
| 1:M:219:LYS:N | 1:N:157:ASN:HD21 | 2.14 | 0.45 |
| 1:Q:52:ILE:HG12 | 1:Q:61:VAL:HG21 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:217:GLN:HG2 | 1:C:156:TRP:O | 2.17 | 0.45 |
| 1:F:8:LYS:HE2 | 1:F:8:LYS:HB3 | 1.76 | 0.45 |
| 1:F:242:VAL:O | 1:F:246:LEU:HG | 2.17 | 0.45 |
| 1:E:145:ILE:CD1 | 1:E:233:LEU:HD13 | 2.46 | 0.45 |
| 1:L:169:VAL:O | 1:L:173:PRO:HD3 | 2.15 | 0.45 |
| 1:T:27:PHE:O | 1:T:73:SER:HA | 2.16 | 0.45 |
| 1:J:182:LYS:HB2 | 1:J:201:GLU:HB2 | 1.99 | 0.45 |
| 1:B:92:ARG:HG3 | 1:D:67:ARG:HG2 | 1.98 | 0.45 |
| 1:K:92:ARG:HG3 | 1:O:67:ARG:HG2 | 1.99 | 0.44 |
| 1:E:37:PRO:O | 1:E:39:ALA:N | 2.50 | 0.44 |
| 1:K:24:PHE:O | 1:K:108:THR:HA | 2.18 | 0.44 |
| 1:S:24:PHE:HB2 | 1:S:109:LEU:HB2 | 1.99 | 0.44 |
| 1:J:188:SER:O | 1:J:189:THR:C | 2.55 | 0.44 |
| 1:H:167:MET:O | 1:H:170:HIS:HB3 | 2.16 | 0.44 |
| 1:I:221:ASN:HA | 1:I:224:HIS:CD2 | 2.52 | 0.44 |
| 1:F:117:ASN:N | 2:F:1000:HEM:O1A | 2.47 | 0.44 |
| 1:J:167:MET:HE2 | 2:J:1000:HEM:HBD1 | 1.99 | 0.44 |
| 1:C:212:MET:HG3 | 1:E:190:GLY:HA2 | 2.00 | 0.44 |
| 1:M:62:ASP:HB2 | 1:M:78:ARG:HB3 | 1.99 | 0.44 |
| 1:D:211:LEU:HD21 | 2:D:1000:HEM:HMC2 | 1.98 | 0.44 |
| 1:Q:95:ARG:HB3 | 1:T:67:ARG:NH2 | 2.32 | 0.44 |
| 1:F:174:THR:HB | 2:F:1000:HEM:CBB | 2.48 | 0.44 |
| 1:T:62:ASP:HB3 | 1:T:64:TYR:CZ | 2.52 | 0.44 |
| 1:R:47:GLU:OE2 | 1:R:97:THR:HA | 2.17 | 0.44 |
| 1:R:215:LEU:O | 1:R:218:VAL:HG22 | 2.17 | 0.44 |
| 1:E:8:LYS:HE2 | 1:E:8:LYS:HB2 | 1.45 | 0.44 |
| 1:C:196:PHE:HZ | 2:C:1000:HEM:O2D | 1.94 | 0.44 |
| 1:E:95:ARG:HA | 1:E:100:GLY:HA3 | 1.98 | 0.44 |
| 1:E:174:THR:HB | 2:E:1000:HEM:HBB2 | 2.00 | 0.44 |
| 1:Q:30:ARG:O | 1:Q:33:TRP:HB3 | 2.17 | 0.44 |
| 1:G:88:GLN:O | 1:G:92:ARG:HB2 | 2.18 | 0.44 |
| 1:T:38:VAL:O | 1:T:39:ALA:CB | 2.66 | 0.44 |
| 1:S:11:ARG:NH2 | 1:S:62:ASP:OD1 | 2.30 | 0.44 |
| 1:E:117:ASN:N | 2:E:1000:HEM:O1A | 2.43 | 0.44 |
| 1:P:97:THR:CG2 | 1:P:100:GLY:H | 2.29 | 0.44 |
| 1:T:27:PHE:CE1 | 1:T:105:VAL:HG22 | 2.53 | 0.44 |
| 1:J:28:LYS:NZ | 1:J:72:ASN:HD22 | 2.16 | 0.44 |
| 1:Q:94:PHE:O | 1:Q:97:THR:CB | 2.64 | 0.44 |
| 1:C:211:LEU:CD1 | 2:C:1000:HEM:CBB | 2.95 | 0.44 |
| 1:B:233:LEU:HD12 | 1:B:234:GLY:N | 2.32 | 0.44 |
| 1:T:65:LEU:HB3 | 1:T:235:THR:HG22 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:235:THR:HG23 | 1:H:237:HIS:CD2 | 2.53 | 0.44 |
| 1:C:75:PHE:CD1 | 1:C:246:LEU:CD1 | 3.01 | 0.44 |
| 1:I:150:LYS:HB3 | 1:I:226:ARG:HB3 | 2.00 | 0.44 |
| 1:L:83:ASP:HB3 | 1:L:86:LYS:HD2 | 1.98 | 0.44 |
| 1:C:211:LEU:HD11 | 2:C:1000:HEM:CBB | 2.47 | 0.44 |
| 1:F:150:LYS:HB3 | 1:F:226:ARG:HB3 | 2.00 | 0.44 |
| 1:T:235:THR:HG23 | 1:T:237:HIS:CD2 | 2.52 | 0.44 |
| 1:I:26:MET:HB2 | 1:I:107:GLU:HB2 | 2.00 | 0.44 |
| 1:H:26:MET:HB3 | 1:H:73:SER:HB3 | 2.00 | 0.44 |
| 1:J:94:PHE:O | 1:J:97:THR:HG22 | 2.18 | 0.44 |
| 1:P:66:THR:CG2 | 1:P:234:GLY:HA3 | 2.44 | 0.44 |
| 1:G:62:ASP:HB3 | 1:G:64:TYR:CZ | 2.53 | 0.44 |
| 1:Q:25:THR:HB | 1:Q:27:PHE:HE2 | 1.83 | 0.44 |
| 1:O:110:VAL:CG1 | 1:O:111:GLY:N | 2.81 | 0.44 |
| 1:R:69:LEU:HG | 1:S:88:GLN:HB2 | 1.99 | 0.44 |
| 1:A:182:LYS:HB2 | 1:A:201:GLU:HB2 | 1.99 | 0.44 |
| 1:F:97:THR:HG22 | 1:F:100:GLY:H | 1.82 | 0.44 |
| 1:H:42:LYS:HD3 | 1:H:247:ALA:HB1 | 2.00 | 0.44 |
| 1:T:184:LYS:HG2 | 1:T:186:TYR:CE2 | 2.53 | 0.44 |
| 1:K:21:PHE:O | 1:K:80:ASN:HA | 2.18 | 0.44 |
| 1:G:61:VAL:HG22 | 1:G:79:ILE:HD12 | 2.00 | 0.44 |
| 1:L:166:GLU:HA | 1:L:166:GLU:OE1 | 2.17 | 0.44 |
| 1:C:166:GLU:OE1 | 1:C:166:GLU:HA | 2.17 | 0.44 |
| 1:O:195:ASP:HB3 | 1:O:196:PHE:CE2 | 2.53 | 0.43 |
| 1:P:27:PHE:HD2 | 1:P:75:PHE:CE2 | 2.34 | 0.43 |
| 1:I:211:LEU:CD1 | 2:I:1000:HEM:HBB2 | 2.42 | 0.43 |
| 1:P:145:ILE:CD1 | 1:P:233:LEU:HD13 | 2.48 | 0.43 |
| 1:T:240:GLU:O | 1:T:244:LYS:HB2 | 2.18 | 0.43 |
| 1:M:150:LYS:HB3 | 1:M:226:ARG:HB3 | 2.00 | 0.43 |
| 1:P:158:MET:O | 1:P:163:ARG:NH1 | 2.51 | 0.43 |
| 1:G:118:TYR:CE2 | 2:G:1000:HEM:O1D | 2.70 | 0.43 |
| 1:F:145:ILE:CD1 | 1:F:233:LEU:HD13 | 2.43 | 0.43 |
| 1:P:237:HIS:HB2 | 1:P:242:VAL:HG23 | 1.99 | 0.43 |
| 1:E:180:ASN:HB3 | 1:E:181:VAL:HG23 | 2.00 | 0.43 |
| 1:D:196:PHE:CE2 | 2:D:1000:HEM:O2D | 2.70 | 0.43 |
| 1:A:235:THR:HG23 | 1:A:237:HIS:CD2 | 2.50 | 0.43 |
| 1:F:237:HIS:HB2 | 1:F:242:VAL:HG23 | 2.00 | 0.43 |
| 1:R:55:HIS:CD2 | 1:R:58:ASN:HD22 | 2.37 | 0.43 |
| 1:G:33:TRP:CZ2 | 1:G:41:ARG:HG2 | 2.53 | 0.43 |
| 1:T:136:TYR:CD2 | 1:T:182:LYS:HE3 | 2.53 | 0.43 |
| 1:F:141:PRO:HA | 1:F:203:ASP:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:211:LEU:HD11 | 2:N:1000:HEM:HBB2 | 2.00 | 0.43 |
| 1:R:52:ILE:HG12 | 1:R:61:VAL:HG11 | 1.99 | 0.43 |
| 1:D:180:ASN:HB3 | 1:D:181:VAL:HG23 | 2.01 | 0.43 |
| 1:G:211:LEU:CD1 | 2:G:1000:HEM:CBB | 2.94 | 0.43 |
| 1:P:44:ALA:HB1 | 1:P:99:VAL:CG2 | 2.46 | 0.43 |
| 1:R:95:ARG:HA | 1:R:100:GLY:HA3 | 2.00 | 0.43 |
| 1:R:38:VAL:HB | 1:R:41:ARG:NH1 | 2.33 | 0.43 |
| 2:H:1000:HEM:CHC | 2:H:1000:HEM:CBB | 2.90 | 0.43 |
| 1:T:221:ASN:HA | 1:T:224:HIS:CD2 | 2.53 | 0.43 |
| 1:T:64:TYR:CD2 | 1:T:76:PHE:CE2 | 3.06 | 0.43 |
| 1:A:36:VAL:O | 1:A:41:ARG:HD3 | 2.19 | 0.43 |
| 1:L:215:LEU:HA | 1:L:215:LEU:HD12 | 1.80 | 0.43 |
| 1:T:188:SER:HB2 | 1:T:194:THR:HG23 | 2.00 | 0.43 |
| 1:B:224:HIS:HE1 | 5:B:3000:HOH:O | 2.01 | 0.43 |
| 1:T:196:PHE:CE1 | 2:T:1000:HEM:O2D | 2.68 | 0.43 |
| 1:G:235:THR:CG2 | 1:G:237:HIS:CD2 | 3.02 | 0.43 |
| 1:L:182:LYS:HB2 | 1:L:201:GLU:HB2 | 2.00 | 0.43 |
| 1:N:66:THR:HG22 | 1:N:234:GLY:HA3 | 2.00 | 0.43 |
| 1:P:38:VAL:O | 1:P:39:ALA:CB | 2.65 | 0.43 |
| 1:T:52:ILE:HG12 | 1:T:61:VAL:HG21 | 2.01 | 0.43 |
| 1:R:163:ARG:O | 1:R:167:MET:HG2 | 2.19 | 0.43 |
| 1:Q:72:ASN:O | 1:Q:73:SER:HB3 | 2.19 | 0.43 |
| 1:H:69:LEU:HD23 | 1:H:69:LEU:HA | 1.84 | 0.43 |
| 1:J:97:THR:HG23 | 1:J:99:VAL:N | 2.34 | 0.43 |
| 1:D:38:VAL:O | 1:D:39:ALA:HB2 | 2.17 | 0.43 |
| 1:P:33:TRP:CH2 | 1:P:99:VAL:HG13 | 2.54 | 0.43 |
| 1:D:145:ILE:HA | 1:D:232:THR:O | 2.19 | 0.43 |
| 1:J:62:ASP:HB3 | 1:J:64:TYR:CZ | 2.54 | 0.43 |
| 1:Q:63:LEU:HB3 | 1:Q:239:PRO:HA | 2.01 | 0.43 |
| 1:C:221:ASN:HA | 1:C:224:HIS:CD2 | 2.53 | 0.42 |
| 1:S:18:PRO:HA | 1:S:113:THR:CG2 | 2.36 | 0.42 |
| 1:B:20:VAL:H | 1:B:113:THR:HB | 1.83 | 0.42 |
| 1:Q:183:ARG:HD2 | 2:Q:1000:HEM:CMB | 2.49 | 0.42 |
| 1:R:235:THR:HG23 | 1:R:237:HIS:CD2 | 2.53 | 0.42 |
| 1:L:64:TYR:CD1 | 1:L:144:VAL:HG11 | 2.54 | 0.42 |
| 1:I:145:ILE:HD13 | 1:I:233:LEU:HD13 | 1.99 | 0.42 |
| 1:F:224:HIS:HE1 | 5:F:3000:HOH:O | 2.02 | 0.42 |
| 1:P:88:GLN:HB2 | 1:S:69:LEU:HD21 | 2.01 | 0.42 |
| 1:T:97:THR:CG2 | 1:T:99:VAL:HG23 | 2.48 | 0.42 |
| 1:B:149:VAL:HA | 1:B:226:ARG:O | 2.19 | 0.42 |
| 1:A:118:TYR:CD2 | 1:A:167:MET:HG3 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:20:VAL:H | 1:K:113:THR:HB | 1.84 | 0.42 |
| 1:I:196:PHE:CE1 | 2:I:1000:HEM:O2D | 2.73 | 0.42 |
| 2:M:1000:HEM:HHC | 2:M:1000:HEM:HBB2 | 2.02 | 0.42 |
| 1:K:167:MET:O | 1:K:170:HIS:HB3 | 2.18 | 0.42 |
| 1:C:67:ARG:HD2 | 1:C:74:ASP:OD1 | 2.20 | 0.42 |
| 1:J:38:VAL:O | 1:J:39:ALA:CB | 2.66 | 0.42 |
| 1:M:11:ARG:HH22 | 1:M:62:ASP:CG | 2.20 | 0.42 |
| 1:I:182:LYS:HB2 | 1:I:201:GLU:HB2 | 2.00 | 0.42 |
| 1:K:127:LEU:HD22 | 1:K:171:THR:HG22 | 2.02 | 0.42 |
| 1:T:36:VAL:O | 1:T:37:PRO:C | 2.56 | 0.42 |
| 1:N:221:ASN:HA | 1:N:224:HIS:CD2 | 2.55 | 0.42 |
| 1:R:118:TYR:CD2 | 1:R:167:MET:HG3 | 2.55 | 0.42 |
| 1:M:117:ASN:N | 2:M:1000:HEM:O1A | 2.51 | 0.42 |
| 1:P:127:LEU:HA | 1:P:127:LEU:HD23 | 1.86 | 0.42 |
| 1:N:182:LYS:O | 1:N:200:PHE:HA | 2.19 | 0.42 |
| 1:Q:31:PRO:C | 1:Q:33:TRP:H | 2.23 | 0.42 |
| 1:G:182:LYS:HB2 | 1:G:201:GLU:HB2 | 2.01 | 0.42 |
| 1:I:169:VAL:O | 1:I:173:PRO:HD2 | 2.19 | 0.42 |
| 1:C:224:HIS:HE1 | 5:C:3000:HOH:O | 2.03 | 0.42 |
| 1:R:196:PHE:HZ | 2:R:1000:HEM:O2D | 1.96 | 0.42 |
| 1:O:110:VAL:HG12 | 1:O:111:GLY:N | 2.35 | 0.42 |
| 1:E:221:ASN:HA | 1:E:224:HIS:CD2 | 2.55 | 0.42 |
| 1:A:221:ASN:HA | 1:A:224:HIS:CD2 | 2.55 | 0.42 |
| 1:N:183:ARG:HD2 | 2:N:1000:HEM:C3B | 2.55 | 0.42 |
| 2:M:1000:HEM:HHC | 2:M:1000:HEM:CBB | 2.49 | 0.42 |
| 1:D:38:VAL:O | 1:D:39:ALA:HB3 | 2.20 | 0.42 |
| 1:O:21:PHE:O | 1:O:80:ASN:HA | 2.20 | 0.42 |
| 1:M:8:LYS:HE3 | 1:M:10:GLU:OE2 | 2.20 | 0.42 |
| 1:I:64:TYR:CD2 | 1:I:76:PHE:CE2 | 3.08 | 0.42 |
| 1:A:117:ASN:N | 2:A:1000:HEM:O1A | 2.52 | 0.42 |
| 1:B:224:HIS:CE1 | 5:B:3000:HOH:O | 2.73 | 0.42 |
| 1:H:196:PHE:HZ | 2:H:1000:HEM:O2D | 1.93 | 0.42 |
| 1:G:198:THR:HG21 | 2:G:1000:HEM:CHD | 2.49 | 0.42 |
| 1:R:119:ILE:CG1 | 2:R:1000:HEM:HMA2 | 2.49 | 0.42 |
| 1:D:219:LYS:O | 1:D:222:LYS:HB2 | 2.19 | 0.42 |
| 1:D:182:LYS:HB2 | 1:D:201:GLU:HB2 | 2.01 | 0.42 |
| 1:E:36:VAL:HG12 | 1:E:41:ARG:HG3 | 2.02 | 0.42 |
| 1:Q:63:LEU:HG | 1:Q:242:VAL:HG11 | 2.02 | 0.42 |
| 1:A:64:TYR:CD1 | 1:A:144:VAL:HG11 | 2.55 | 0.42 |
| 1:C:229:SER:HA | 1:C:230:PRO:HA | 1.76 | 0.42 |
| 1:A:176:ALA:O | 1:A:179:VAL:HG22 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:66:THR:HG22 | 1:E:234:GLY:HA3 | 2.02 | 0.42 |
| 1:M:70:GLU:OE2 | 1:M:232:THR:HA | 2.20 | 0.42 |
| 1:T:166:GLU:OE1 | 1:T:166:GLU:HA | 2.20 | 0.42 |
| 1:H:97:THR:HG23 | 1:H:98:THR:N | 2.33 | 0.42 |
| 1:S:174:THR:HB | 2:S:1000:HEM:HBB2 | 2.02 | 0.42 |
| 1:E:33:TRP:O | 1:E:41:ARG:HD2 | 2.20 | 0.42 |
| 1:M:67:ARG:HG2 | 1:N:92:ARG:HG3 | 2.01 | 0.42 |
| 1:A:188:SER:HB2 | 1:A:194:THR:O | 2.20 | 0.42 |
| 1:M:166:GLU:OE1 | 1:M:166:GLU:HA | 2.20 | 0.42 |
| 1:Q:97:THR:HG22 | 1:Q:100:GLY:N | 2.12 | 0.42 |
| 1:Q:20:VAL:O | 1:Q:113:THR:HB | 2.20 | 0.42 |
| 1:K:196:PHE:HZ | 2:K:1000:HEM:O2D | 1.89 | 0.41 |
| 1:O:18:PRO:CA | 1:O:113:THR:HG22 | 2.41 | 0.41 |
| 1:O:17:GLN:O | 1:O:113:THR:CG2 | 2.50 | 0.41 |
| 1:Q:18:PRO:CA | 1:Q:113:THR:HG22 | 2.50 | 0.41 |
| 1:T:196:PHE:HZ | 2:T:1000:HEM:O2D | 1.93 | 0.41 |
| 1:S:20:VAL:H | 1:S:113:THR:HB | 1.85 | 0.41 |
| 1:J:196:PHE:HZ | 2:J:1000:HEM:O2D | 1.91 | 0.41 |
| 1:N:235:THR:CG2 | 1:N:237:HIS:NE2 | 2.83 | 0.41 |
| 1:Q:235:THR:CG2 | 1:Q:237:HIS:NE2 | 2.83 | 0.41 |
| 1:I:150:LYS:HA | 1:I:195:ASP:HB2 | 2.01 | 0.41 |
| 1:I:182:LYS:O | 1:I:200:PHE:HA | 2.20 | 0.41 |
| 1:G:150:LYS:HA | 1:G:195:ASP:HB2 | 2.01 | 0.41 |
| 1:D:188:SER:O | 1:D:189:THR:C | 2.58 | 0.41 |
| 1:D:174:THR:HB | 2:D:1000:HEM:CBB | 2.49 | 0.41 |
| 1:N:116:LEU:HA | 2:N:1000:HEM:O1A | 2.20 | 0.41 |
| 1:S:38:VAL:O | 1:S:39:ALA:CB | 2.68 | 0.41 |
| 1:J:92:ARG:HG2 | 1:J:92:ARG:HH11 | 1.84 | 0.41 |
| 1:S:196:PHE:CE1 | 2:S:1000:HEM:O2D | 2.72 | 0.41 |
| 1:Q:33:TRP:HB2 | 1:Q:102:ASN:HB3 | 2.02 | 0.41 |
| 1:D:55:HIS:HE1 | 1:D:93:GLU:OE1 | 2.03 | 0.41 |
| 1:S:145:ILE:HD13 | 1:S:233:LEU:HD13 | 2.02 | 0.41 |
| 1:S:170:HIS:HE1 | 2:S:1000:HEM:C4C | 2.38 | 0.41 |
| 1:D:211:LEU:HD11 | 2:D:1000:HEM:HBB2 | 2.02 | 0.41 |
| 1:N:167:MET:HE2 | 2:N:1000:HEM:HBD1 | 2.02 | 0.41 |
| 1:M:11:ARG:NH2 | 1:M:62:ASP:OD1 | 2.38 | 0.41 |
| 1:H:222:LYS:HE2 | 1:I:154:GLU:OE1 | 2.20 | 0.41 |
| 1:R:170:HIS:O | 1:R:173:PRO:HD2 | 2.20 | 0.41 |
| 1:N:63:LEU:HD21 | 1:N:243:ILE:HD11 | 2.03 | 0.41 |
| 1:G:188:SER:HB2 | 1:G:194:THR:HG23 | 2.01 | 0.41 |
| 1:C:188:SER:O | 1:C:189:THR:C | 2.58 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:15:LEU:HD23 | 1:H:15:LEU:HA | 1.83 | 0.41 |
| 1:H:198:THR:HG21 | 2:H:1000:HEM:HBC2 | 2.02 | 0.41 |
| 1:A:157:ASN:HD21 | 1:E:219:LYS:N | 2.19 | 0.41 |
| 1:C:28:LYS:NZ | 1:C:72:ASN:HD22 | 2.19 | 0.41 |
| 1:F:170:HIS:O | 1:F:173:PRO:HD2 | 2.20 | 0.41 |
| 1:H:70:GLU:OE2 | 1:H:232:THR:HA | 2.20 | 0.41 |
| 1:P:118:TYR:CD2 | 1:P:167:MET:HG3 | 2.56 | 0.41 |
| 1:B:88:GLN:O | 1:B:92:ARG:HB2 | 2.21 | 0.41 |
| 1:S:62:ASP:HB3 | 1:S:64:TYR:CZ | 2.55 | 0.41 |
| 1:G:26:MET:HB2 | 1:G:107:GLU:HB2 | 2.03 | 0.41 |
| 1:J:145:ILE:HD13 | 1:J:233:LEU:HD13 | 2.02 | 0.41 |
| 1:I:30:ARG:O | 1:I:33:TRP:HB3 | 2.21 | 0.41 |
| 1:A:33:TRP:CH2 | 1:A:41:ARG:HG2 | 2.55 | 0.41 |
| 1:S:53:GLU:HB3 | 1:S:56:LYS:NZ | 2.36 | 0.41 |
| 1:T:97:THR:HG23 | 1:T:99:VAL:HG23 | 2.02 | 0.41 |
| 1:T:99:VAL:HG11 | 1:T:243:ILE:HG23 | 2.03 | 0.41 |
| 1:T:145:ILE:CD1 | 1:T:233:LEU:HD13 | 2.51 | 0.41 |
| 1:O:219:LYS:O | 1:O:222:LYS:HB2 | 2.21 | 0.41 |
| 1:T:242:VAL:O | 1:T:246:LEU:HG | 2.20 | 0.41 |
| 1:H:29:LEU:HD13 | 1:H:33:TRP:CD1 | 2.56 | 0.41 |
| 1:R:25:THR:HG22 | 1:R:105:VAL:HG13 | 2.02 | 0.41 |
| 1:B:229:SER:HA | 1:B:230:PRO:HA | 1.85 | 0.41 |
| 1:D:88:GLN:O | 1:D:92:ARG:HB2 | 2.21 | 0.41 |
| 1:D:24:PHE:CD2 | 1:D:24:PHE:N | 2.88 | 0.41 |
| 1:N:17:GLN:O | 1:N:113:THR:CG2 | 2.54 | 0.41 |
| 1:G:116:LEU:CA | 2:G:1000:HEM:O1A | 2.67 | 0.41 |
| 1:R:116:LEU:CA | 2:R:1000:HEM:O1A | 2.69 | 0.41 |
| 1:N:196:PHE:HZ | 2:N:1000:HEM:O2D | 2.00 | 0.41 |
| 1:M:150:LYS:HG2 | 1:M:225:VAL:HG23 | 2.01 | 0.41 |
| 1:O:158:MET:O | 1:O:163:ARG:NH1 | 2.53 | 0.41 |
| 1:G:24:PHE:HB2 | 1:G:109:LEU:HB2 | 2.03 | 0.41 |
| 1:C:53:GLU:O | 1:C:56:LYS:HB2 | 2.21 | 0.41 |
| 1:H:71:THR:HG23 | 1:I:105:VAL:HG12 | 2.03 | 0.41 |
| 1:L:119:ILE:O | 1:L:119:ILE:HG22 | 2.21 | 0.40 |
| 1:J:33:TRP:HB2 | 1:J:102:ASN:HB3 | 2.03 | 0.40 |
| 1:P:59:VAL:HG11 | 1:P:87:ALA:HA | 2.03 | 0.40 |
| 1:P:157:ASN:HD21 | 1:S:219:LYS:N | 2.19 | 0.40 |
| 1:R:9:ILE:O | 1:R:9:ILE:HG22 | 2.20 | 0.40 |
| 1:D:33:TRP:CZ2 | 1:D:41:ARG:HG2 | 2.57 | 0.40 |
| 1:K:28:LYS:NZ | 1:K:72:ASN:HD22 | 2.19 | 0.40 |
| 1:B:38:VAL:O | 1:B:39:ALA:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:T:30:ARG:NH2 | 1:T:101:LYS:O | 2.36 | 0.40 |
| 1:Q:95:ARG:HA | 1:Q:100:GLY:HA3 | 2.03 | 0.40 |
| 1:R:119:ILE:HG12 | 2:R:1000:HEM:HAA1 | 2.02 | 0.40 |
| 1:P:127:LEU:CD1 | 1:P:168:GLU:HG2 | 2.47 | 0.40 |
| 1:S:158:MET:O | 1:S:163:ARG:NH1 | 2.54 | 0.40 |
| 1:E:42:LYS:HD3 | 1:E:247:ALA:HB1 | 2.04 | 0.40 |
| 1:J:229:SER:HA | 1:J:230:PRO:HA | 1.84 | 0.40 |
| 1:R:27:PHE:HB2 | 1:R:75:PHE:CZ | 2.57 | 0.40 |
| 1:H:53:GLU:O | 1:H:56:LYS:HG3 | 2.22 | 0.40 |
| 1:A:174:THR:O | 2:A:1000:HEM:CBB | 2.70 | 0.40 |
| 1:G:196:PHE:CE1 | 2:G:1000:HEM:HAD1 | 2.57 | 0.40 |
| 1:B:195:ASP:HB3 | 1:B:196:PHE:CE2 | 2.56 | 0.40 |
| 1:J:97:THR:HG23 | 1:J:99:VAL:H | 1.86 | 0.40 |
| 1:S:65:LEU:HB3 | 1:S:235:THR:HG22 | 2.03 | 0.40 |
| 1:R:97:THR:HG23 | 1:R:100:GLY:H | 1.86 | 0.40 |
| 1:S:38:VAL:HG13 | 1:S:38:VAL:O | 2.22 | 0.40 |
| 1:T:72:ASN:O | 1:T:73:SER:HB3 | 2.21 | 0.40 |
| 1:M:186:TYR:HB2 | 1:M:197:ILE:HB | 2.04 | 0.40 |
| 1:P:51:LEU:HD11 | 1:P:93:GLU:HB3 | 2.04 | 0.40 |
| 1:F:24:PHE:HA | 1:F:77:PHE:O | 2.21 | 0.40 |
| 1:B:55:HIS:CD2 | 1:B:58:ASN:HD22 | 2.40 | 0.40 |
| 1:Q:8:LYS:HB3 | 1:Q:8:LYS:HE2 | 1.78 | 0.40 |
| 1:A:20:VAL:H | 1:A:113:THR:HB | 1.87 | 0.40 |
| 1:B:18:PRO:CA | 1:B:113:THR:HG22 | 2.39 | 0.40 |
| 1:R:183:ARG:HD2 | 2:R:1000:HEM:C2B | 2.56 | 0.40 |
| 1:N:94:PHE:O | 1:N:97:THR:HB | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 239/248 (96%) | 230 (96%) | 8 (3%) | 1 (0%) | 39 | 80 |
| 1 | B | 239/248 (96%) | 228 (95%) | 8 (3%) | 3 (1%) | 15 | 53 |
| 1 | C | 239/248 (96%) | 231 (97%) | 5 (2%) | 3 (1%) | 15 | 53 |
| 1 | D | 239/248 (96%) | 232 (97%) | 6 (2%) | 1 (0%) | 39 | 80 |
| 1 | E | 239/248 (96%) | 228 (95%) | 8 (3%) | 3 (1%) | 15 | 53 |
| 1 | F | 239/248 (96%) | 226 (95%) | 11 (5%) | 2 (1%) | 24 | 66 |
| 1 | G | 239/248 (96%) | 228 (95%) | 9 (4%) | 2 (1%) | 24 | 66 |
| 1 | H | 239/248 (96%) | 227 (95%) | 11 (5%) | 1 (0%) | 39 | 80 |
| 1 | I | 239/248 (96%) | 226 (95%) | 12 (5%) | 1 (0%) | 39 | 80 |
| 1 | J | 239/248 (96%) | 229 (96%) | 9 (4%) | 1 (0%) | 39 | 80 |
| 1 | K | 239/248 (96%) | 228 (95%) | 10 (4%) | 1 (0%) | 39 | 80 |
| 1 | L | 239/248 (96%) | 231 (97%) | 7 (3%) | 1 (0%) | 39 | 80 |
| 1 | M | 239/248 (96%) | 228 (95%) | 9 (4%) | 2 (1%) | 24 | 66 |
| 1 | N | 239/248 (96%) | 225 (94%) | 11 (5%) | 3 (1%) | 15 | 53 |
| 1 | O | 239/248 (96%) | 227 (95%) | 11 (5%) | 1 (0%) | 39 | 80 |
| 1 | P | 239/248 (96%) | 223 (93%) | 13 (5%) | 3 (1%) | 15 | 53 |
| 1 | Q | 239/248 (96%) | 223 (93%) | 12 (5%) | 4 (2%) | 11 | 46 |
| 1 | R | 239/248 (96%) | 225 (94%) | 11 (5%) | 3 (1%) | 15 | 53 |
| 1 | S | 239/248 (96%) | 226 (95%) | 9 (4%) | 4 (2%) | 11 | 46 |
| 1 | T | 239/248 (96%) | 225 (94%) | 12 (5%) | 2 (1%) | 24 | 66 |
| All | All | 4780/4960 (96%) | 4546 (95%) | 192 (4%) | 42 (1%) | 21 | 64 |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 39 | ALA |
| 1 | C | 39 | ALA |
| 1 | E | 39 | ALA |
| 1 | F | 38 | VAL |
| 1 | F | 39 | ALA |
| 1 | G | 39 | ALA |
| 1 | H | 39 | ALA |
| 1 | J | 39 | ALA |
| 1 | K | 39 | ALA |
| 1 | M | 39 | ALA |
| 1 | M | 56 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 39 | ALA |
| 1 | P | 39 | ALA |
| 1 | Q | 39 | ALA |
| 1 | S | 39 | ALA |
| 1 | A | 39 | ALA |
| 1 | B | 56 | LYS |
| 1 | C | 56 | LYS |
| 1 | D | 39 | ALA |
| 1 | E | 38 | VAL |
| 1 | I | 39 | ALA |
| 1 | L | 39 | ALA |
| 1 | N | 39 | ALA |
| 1 | Q | 38 | VAL |
| 1 | R | 39 | ALA |
| 1 | S | 38 | VAL |
| 1 | S | 56 | LYS |
| 1 | T | 39 | ALA |
| 1 | C | 38 | VAL |
| 1 | E | 56 | LYS |
| 1 | Q | 134 | ALA |
| 1 | P | 189 | THR |
| 1 | Q | 32 | ASP |
| 1 | R | 134 | ALA |
| 1 | N | 176 | ALA |
| 1 | R | 37 | PRO |
| 1 | S | 75 | PHE |
| 1 | G | 38 | VAL |
| 1 | T | 37 | PRO |
| 1 | B | 119 | ILE |
| 1 | N | 119 | ILE |
| 1 | P | 119 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 212/219 (97%) | 197 (93%) | 15 (7%) | 18 | 54 |
| 1 | B | 212/219 (97%) | 200 (94%) | 12 (6%) | 25 | 64 |
| 1 | C | 212/219 (97%) | 200 (94%) | 12 (6%) | 25 | 64 |
| 1 | D | 212/219 (97%) | 199 (94%) | 13 (6%) | 23 | 61 |
| 1 | E | 212/219 (97%) | 199 (94%) | 13 (6%) | 23 | 61 |
| 1 | F | 212/219 (97%) | 197 (93%) | 15 (7%) | 18 | 54 |
| 1 | G | 212/219 (97%) | 200 (94%) | 12 (6%) | 25 | 64 |
| 1 | H | 212/219 (97%) | 199 (94%) | 13 (6%) | 23 | 61 |
| 1 | I | 212/219 (97%) | 201 (95%) | 11 (5%) | 29 | 68 |
| 1 | J | 212/219 (97%) | 196 (92%) | 16 (8%) | 17 | 51 |
| 1 | K | 212/219 (97%) | 200 (94%) | 12 (6%) | 25 | 64 |
| 1 | L | 212/219 (97%) | 199 (94%) | 13 (6%) | 23 | 61 |
| 1 | M | 212/219 (97%) | 200 (94%) | 12 (6%) | 25 | 64 |
| 1 | N | 212/219 (97%) | 198 (93%) | 14 (7%) | 21 | 57 |
| 1 | O | 212/219 (97%) | 201 (95%) | 11 (5%) | 29 | 68 |
| 1 | P | 212/219 (97%) | 203 (96%) | 9 (4%) | 36 | 76 |
| 1 | Q | 212/219 (97%) | 193 (91%) | 19 (9%) | 12 | 41 |
| 1 | R | 212/219 (97%) | 202 (95%) | 10 (5%) | 32 | 72 |
| 1 | S | 212/219 (97%) | 201 (95%) | 11 (5%) | 29 | 68 |
| 1 | T | 212/219 (97%) | 195 (92%) | 17 (8%) | 15 | 47 |
| All | All | 4240/4380 (97%) | 3980 (94%) | 260 (6%) | 23 | 61 |

All (260) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | ARG |
| 1 | A | 16 | THR |
| 1 | A | 25 | THR |
| 1 | A | 32 | ASP |
| 1 | A | 38 | VAL |
| 1 | A | 97 | THR |
| 1 | A | 107 | GLU |
| 1 | A | 135 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 145 | ILE |
| 1 | A | 192 | ASP |
| 1 | A | 214 | SER |
| 1 | A | 215 | LEU |
| 1 | A | 229 | SER |
| 1 | A | 235 | THR |
| 1 | A | 240 | GLU |
| 1 | B | 11 | ARG |
| 1 | B | 16 | THR |
| 1 | B | 26 | MET |
| 1 | B | 56 | LYS |
| 1 | B | 97 | THR |
| 1 | B | 107 | GLU |
| 1 | B | 131 | LEU |
| 1 | B | 135 | THR |
| 1 | B | 215 | LEU |
| 1 | B | 229 | SER |
| 1 | B | 235 | THR |
| 1 | B | 248 | ASP |
| 1 | C | 11 | ARG |
| 1 | C | 16 | THR |
| 1 | C | 25 | THR |
| 1 | C | 92 | ARG |
| 1 | C | 97 | THR |
| 1 | C | 135 | THR |
| 1 | C | 192 | ASP |
| 1 | C | 214 | SER |
| 1 | C | 215 | LEU |
| 1 | C | 229 | SER |
| 1 | C | 233 | LEU |
| 1 | C | 235 | THR |
| 1 | D | 11 | ARG |
| 1 | D | 16 | THR |
| 1 | D | 25 | THR |
| 1 | D | 26 | MET |
| 1 | D | 97 | THR |
| 1 | D | 124 | SER |
| 1 | D | 135 | THR |
| 1 | D | 139 | PRO |
| 1 | D | 145 | ILE |
| 1 | D | 192 | ASP |
| 1 | D | 233 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 235 | THR |
| 1 | D | 248 | ASP |
| 1 | E | 8 | LYS |
| 1 | E | 16 | THR |
| 1 | E | 56 | LYS |
| 1 | E | 97 | THR |
| 1 | E | 99 | VAL |
| 1 | E | 135 | THR |
| 1 | E | 137 | SER |
| 1 | E | 145 | ILE |
| 1 | E | 215 | LEU |
| 1 | E | 229 | SER |
| 1 | E | 233 | LEU |
| 1 | E | 235 | THR |
| 1 | E | 248 | ASP |
| 1 | F | 10 | GLU |
| 1 | F | 11 | ARG |
| 1 | F | 13 | THR |
| 1 | F | 25 | THR |
| 1 | F | 26 | MET |
| 1 | F | 99 | VAL |
| 1 | F | 135 | THR |
| 1 | F | 137 | SER |
| 1 | F | 145 | ILE |
| 1 | F | 192 | ASP |
| 1 | F | 214 | SER |
| 1 | F | 215 | LEU |
| 1 | F | 229 | SER |
| 1 | F | 235 | THR |
| 1 | F | 248 | ASP |
| 1 | G | 11 | ARG |
| 1 | G | 26 | MET |
| 1 | G | 42 | LYS |
| 1 | G | 96 | SER |
| 1 | G | 97 | THR |
| 1 | G | 98 | THR |
| 1 | G | 145 | ILE |
| 1 | G | 165 | LYS |
| 1 | G | 192 | ASP |
| 1 | G | 215 | LEU |
| 1 | G | 229 | SER |
| 1 | G | 235 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 11 | ARG |
| 1 | H | 16 | THR |
| 1 | H | 26 | MET |
| 1 | H | 92 | ARG |
| 1 | H | 97 | THR |
| 1 | H | 99 | VAL |
| 1 | H | 145 | ILE |
| 1 | H | 192 | ASP |
| 1 | H | 214 | SER |
| 1 | H | 215 | LEU |
| 1 | H | 229 | SER |
| 1 | H | 235 | THR |
| 1 | H | 248 | ASP |
| 1 | I | 11 | ARG |
| 1 | I | 25 | THR |
| 1 | I | 26 | MET |
| 1 | I | 96 | SER |
| 1 | I | 97 | THR |
| 1 | I | 113 | THR |
| 1 | I | 135 | THR |
| 1 | I | 145 | ILE |
| 1 | I | 192 | ASP |
| 1 | I | 215 | LEU |
| 1 | I | 235 | THR |
| 1 | J | 11 | ARG |
| 1 | J | 16 | THR |
| 1 | J | 26 | MET |
| 1 | J | 56 | LYS |
| 1 | J | 92 | ARG |
| 1 | J | 97 | THR |
| 1 | J | 113 | THR |
| 1 | J | 135 | THR |
| 1 | J | 145 | ILE |
| 1 | J | 192 | ASP |
| 1 | J | 214 | SER |
| 1 | J | 215 | LEU |
| 1 | J | 229 | SER |
| 1 | J | 233 | LEU |
| 1 | J | 235 | THR |
| 1 | J | 248 | ASP |
| 1 | K | 8 | LYS |
| 1 | K | 16 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 25 | THR |
| 1 | K | 97 | THR |
| 1 | K | 99 | VAL |
| 1 | K | 107 | GLU |
| 1 | K | 137 | SER |
| 1 | K | 145 | ILE |
| 1 | K | 192 | ASP |
| 1 | K | 214 | SER |
| 1 | K | 215 | LEU |
| 1 | K | 235 | THR |
| 1 | L | 16 | THR |
| 1 | L | 92 | ARG |
| 1 | L | 97 | THR |
| 1 | L | 135 | THR |
| 1 | L | 137 | SER |
| 1 | L | 145 | ILE |
| 1 | L | 165 | LYS |
| 1 | L | 192 | ASP |
| 1 | L | 214 | SER |
| 1 | L | 215 | LEU |
| 1 | L | 233 | LEU |
| 1 | L | 235 | THR |
| 1 | L | 248 | ASP |
| 1 | M | 16 | THR |
| 1 | M | 25 | THR |
| 1 | M | 92 | ARG |
| 1 | M | 97 | THR |
| 1 | M | 99 | VAL |
| 1 | M | 150 | LYS |
| 1 | M | 165 | LYS |
| 1 | M | 183 | ARG |
| 1 | M | 192 | ASP |
| 1 | M | 215 | LEU |
| 1 | M | 235 | THR |
| 1 | M | 248 | ASP |
| 1 | N | 11 | ARG |
| 1 | N | 26 | MET |
| 1 | N | 97 | THR |
| 1 | N | 99 | VAL |
| 1 | N | 113 | THR |
| 1 | N | 145 | ILE |
| 1 | N | 189 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 192 | ASP |
| 1 | N | 215 | LEU |
| 1 | N | 229 | SER |
| 1 | N | 233 | LEU |
| 1 | N | 235 | THR |
| 1 | N | 240 | GLU |
| 1 | N | 248 | ASP |
| 1 | O | 11 | ARG |
| 1 | O | 16 | THR |
| 1 | O | 26 | MET |
| 1 | O | 56 | LYS |
| 1 | O | 97 | THR |
| 1 | O | 99 | VAL |
| 1 | O | 145 | ILE |
| 1 | O | 192 | ASP |
| 1 | O | 215 | LEU |
| 1 | O | 235 | THR |
| 1 | O | 240 | GLU |
| 1 | P | 16 | THR |
| 1 | P | 26 | MET |
| 1 | P | 50 | LYS |
| 1 | P | 92 | ARG |
| 1 | P | 99 | VAL |
| 1 | P | 145 | ILE |
| 1 | P | 192 | ASP |
| 1 | P | 215 | LEU |
| 1 | P | 235 | THR |
| 1 | Q | 8 | LYS |
| 1 | Q | 11 | ARG |
| 1 | Q | 16 | THR |
| 1 | Q | 25 | THR |
| 1 | Q | 26 | MET |
| 1 | Q | 56 | LYS |
| 1 | Q | 71 | THR |
| 1 | Q | 96 | SER |
| 1 | Q | 97 | THR |
| 1 | Q | 99 | VAL |
| 1 | Q | 113 | THR |
| 1 | Q | 135 | THR |
| 1 | Q | 137 | SER |
| 1 | Q | 145 | ILE |
| 1 | Q | 165 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 183 | ARG |
| 1 | Q | 192 | ASP |
| 1 | Q | 215 | LEU |
| 1 | Q | 235 | THR |
| 1 | R | 25 | THR |
| 1 | R | 92 | ARG |
| 1 | R | 121 | LYS |
| 1 | R | 135 | THR |
| 1 | R | 145 | ILE |
| 1 | R | 189 | THR |
| 1 | R | 192 | ASP |
| 1 | R | 215 | LEU |
| 1 | R | 235 | THR |
| 1 | R | 248 | ASP |
| 1 | S | 16 | THR |
| 1 | S | 25 | THR |
| 1 | S | 26 | MET |
| 1 | S | 97 | THR |
| 1 | S | 99 | VAL |
| 1 | S | 183 | ARG |
| 1 | S | 192 | ASP |
| 1 | S | 215 | LEU |
| 1 | S | 227 | TRP |
| 1 | S | 229 | SER |
| 1 | S | 240 | GLU |
| 1 | T | 8 | LYS |
| 1 | T | 11 | ARG |
| 1 | T | 16 | THR |
| 1 | T | 92 | ARG |
| 1 | T | 96 | SER |
| 1 | T | 97 | THR |
| 1 | T | 99 | VAL |
| 1 | T | 135 | THR |
| 1 | T | 145 | ILE |
| 1 | T | 165 | LYS |
| 1 | T | 192 | ASP |
| 1 | T | 215 | LEU |
| 1 | T | 232 | THR |
| 1 | T | 233 | LEU |
| 1 | T | 235 | THR |
| 1 | T | 240 | GLU |
| 1 | T | 248 | ASP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 55 | HIS |
| 1 | A | 72 | ASN |
| 1 | A | 157 | ASN |
| 1 | A | 180 | ASN |
| 1 | A | 221 | ASN |
| 1 | A | 224 | HIS |
| 1 | B | 55 | HIS |
| 1 | B | 72 | ASN |
| 1 | B | 157 | ASN |
| 1 | B | 221 | ASN |
| 1 | B | 224 | HIS |
| 1 | C | 55 | HIS |
| 1 | C | 72 | ASN |
| 1 | C | 102 | ASN |
| 1 | C | 157 | ASN |
| 1 | C | 217 | GLN |
| 1 | C | 221 | ASN |
| 1 | C | 224 | HIS |
| 1 | D | 55 | HIS |
| 1 | D | 72 | ASN |
| 1 | D | 80 | ASN |
| 1 | D | 157 | ASN |
| 1 | D | 217 | GLN |
| 1 | D | 221 | ASN |
| 1 | D | 224 | HIS |
| 1 | E | 55 | HIS |
| 1 | E | 72 | ASN |
| 1 | E | 80 | ASN |
| 1 | E | 157 | ASN |
| 1 | E | 221 | ASN |
| 1 | E | 224 | HIS |
| 1 | F | 55 | HIS |
| 1 | F | 72 | ASN |
| 1 | F | 157 | ASN |
| 1 | F | 224 | HIS |
| 1 | G | 55 | HIS |
| 1 | G | 72 | ASN |
| 1 | G | 157 | ASN |
| 1 | G | 217 | GLN |
| 1 | G | 221 | ASN |
| 1 | G | 224 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 72 | ASN |
| 1 | H | 102 | ASN |
| 1 | H | 157 | ASN |
| 1 | H | 221 | ASN |
| 1 | H | 224 | HIS |
| 1 | I | 58 | ASN |
| 1 | I | 72 | ASN |
| 1 | I | 157 | ASN |
| 1 | I | 221 | ASN |
| 1 | I | 224 | HIS |
| 1 | J | 72 | ASN |
| 1 | J | 157 | ASN |
| 1 | J | 217 | GLN |
| 1 | J | 221 | ASN |
| 1 | J | 224 | HIS |
| 1 | K | 58 | ASN |
| 1 | K | 72 | ASN |
| 1 | K | 157 | ASN |
| 1 | K | 221 | ASN |
| 1 | K | 224 | HIS |
| 1 | L | 55 | HIS |
| 1 | L | 72 | ASN |
| 1 | L | 157 | ASN |
| 1 | L | 221 | ASN |
| 1 | L | 224 | HIS |
| 1 | M | 55 | HIS |
| 1 | M | 72 | ASN |
| 1 | M | 157 | ASN |
| 1 | M | 217 | GLN |
| 1 | M | 221 | ASN |
| 1 | M | 224 | HIS |
| 1 | N | 55 | HIS |
| 1 | N | 72 | ASN |
| 1 | N | 157 | ASN |
| 1 | N | 217 | GLN |
| 1 | N | 221 | ASN |
| 1 | N | 224 | HIS |
| 1 | O | 157 | ASN |
| 1 | O | 221 | ASN |
| 1 | O | 224 | HIS |
| 1 | P | 157 | ASN |
| 1 | P | 224 | HIS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 55 | HIS |
| 1 | Q | 157 | ASN |
| 1 | Q | 217 | GLN |
| 1 | Q | 221 | ASN |
| 1 | Q | 224 | HIS |
| 1 | R | 55 | HIS |
| 1 | R | 157 | ASN |
| 1 | R | 224 | HIS |
| 1 | S | 55 | HIS |
| 1 | S | 157 | ASN |
| 1 | S | 217 | GLN |
| 1 | S | 221 | ASN |
| 1 | S | 224 | HIS |
| 1 | T | 72 | ASN |
| 1 | T | 157 | ASN |
| 1 | T | 221 | ASN |
| 1 | T | 224 | HIS |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 20 are monoatomic - leaving 40 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 |
| 2 | HEM | A | 1000 | 1,3 | 30,50,50 | 2.46 | 7 (23%) | 24,82,82 | 2.35 | 10 (41%) |
| 3 | NO2 | A | 2000 | 2 | 2,2,2 | 1.41 | 0 | 1,1,1 | 0.81 | 0 |
| 2 | HEM | B | 1000 | 1,3 | 30,50,50 | 2.42 | 5 (16%) | 24,82,82 | 3.22 | 14 (58%) |
| 3 | NO2 | B | 2000 | 2 | 2,2,2 | 1.59 | 0 | 1,1,1 | 0.97 | 0 |
| 2 | HEM | C | 1000 | 1,3 | 30,50,50 | 2.28 | 5 (16%) | 24,82,82 | 2.59 | 12 (50%) |
| 3 | NO2 | C | 2000 | 2 | 2,2,2 | 1.60 | 0 | 1,1,1 | 0.50 | 0 |
| 2 | HEM | D | 1000 | 1,3 | 30,50,50 | 2.48 | 9 (30%) | 24,82,82 | 2.34 | 12 (50%) |
| 3 | NO2 | D | 2000 | 2 | 2,2,2 | 1.53 | 0 | 1,1,1 | 0.49 | 0 |
| 2 | HEM | E | 1000 | 1,3 | 30,50,50 | 1.90 | 4 (13%) | 24,82,82 | 2.89 | 13 (54%) |
| 3 | NO2 | E | 2000 | 2 | 2,2,2 | 1.44 | 0 | 1,1,1 | 0.86 | 0 |
| 2 | HEM | F | 1000 | 1,3 | 30,50,50 | 2.18 | 7 (23%) | 24,82,82 | 2.44 | 12 (50%) |
| 3 | NO2 | F | 2000 | 2 | 2,2,2 | 1.57 | 0 | 1,1,1 | 0.30 | 0 |
| 2 | HEM | G | 1000 | 1,3 | 30,50,50 | 2.19 | 9 (30%) | 24,82,82 | 3.07 | 13 (54%) |
| 3 | NO2 | G | 2000 | 2 | 2,2,2 | 1.60 | 0 | 1,1,1 | 0.57 | 0 |
| 2 | HEM | H | 1000 | 1,3 | 30,50,50 | 2.09 | 6 (20%) | 24,82,82 | 2.93 | 11 (45%) |
| 3 | NO2 | H | 2000 | 2 | 2,2,2 | 1.53 | 0 | 1,1,1 | 0.76 | 0 |
| 2 | HEM | I | 1000 | 1,3 | 30,50,50 | 2.30 | 9 (30%) | 24,82,82 | 2.61 | 8 (33%) |
| 3 | NO2 | I | 2000 | 2 | 2,2,2 | 1.37 | 0 | 1,1,1 | 0.94 | 0 |
| 2 | HEM | J | 1000 | 1,3 | 30,50,50 | 2.47 | 7 (23%) | 24,82,82 | 2.70 | 11 (45%) |
| 3 | NO2 | J | 2000 | 2 | 2,2,2 | 1.51 | 0 | 1,1,1 | 0.58 | 0 |
| 2 | HEM | K | 1000 | 1,3 | 30,50,50 | 1.95 | 4 (13%) | 24,82,82 | 2.72 | 9 (37%) |
| 3 | NO2 | K | 2000 | 2 | 2,2,2 | 1.61 | 0 | 1,1,1 | 0.85 | 0 |
| 2 | HEM | L | 1000 | 1,3 | 30,50,50 | 2.10 | 7 (23%) | 24,82,82 | 2.73 | 11 (45%) |
| 3 | NO2 | L | 2000 | 2 | 2,2,2 | 1.57 | 0 | 1,1,1 | 0.50 | 0 |
| 2 | HEM | M | 1000 | 1,3 | 30,50,50 | 1.91 | 6 (20%) | 24,82,82 | 3.20 | 16 (66%) |
| 3 | NO2 | M | 2000 | 2 | 2,2,2 | 1.82 | 1 (50%) | 1,1,1 | 0.87 | 0 |
| 2 | HEM | N | 1000 | 1,3 | 30,50,50 | 1.76 | 4 (13%) | 24,82,82 | 2.55 | 12 (50%) |
| 3 | NO2 | N | 2000 | 2 | 2,2,2 | 1.56 | 0 | 1,1,1 | 0.57 | 0 |
| 2 | HEM | O | 1000 | 1,3 | 30,50,50 | 1.98 | 8 (26%) | 24,82,82 | 2.55 | 8 (33%) |
| 3 | NO2 | O | 2000 | 2 | 2,2,2 | 1.47 | 0 | 1,1,1 | 0.55 | 0 |
| 2 | HEM | P | 1000 | 1,3 | 30,50,50 | 1.80 | 5 (16%) | 24,82,82 | 2.80 | 11 (45%) |
| 3 | NO2 | P | 2000 | 2 | 2,2,2 | 1.61 | 0 | 1,1,1 | 0.24 | 0 |
| 2 | HEM | Q | 1000 | 1,3 | 30,50,50 | 2.08 | 8 (26%) | 24,82,82 | 3.04 | 9 (37%) |
| 3 | NO2 | Q | 2000 | 2 | 2,2,2 | 1.51 | 0 | 1,1,1 | 1.02 | 0 |
| 2 | HEM | R | 1000 | 1,3 | 30,50,50 | 2.07 | 9 (30%) | 24,82,82 | 2.50 | 12 (50%) |
| 3 | NO2 | R | 2000 | 2 | 2,2,2 | 1.66 | 0 | 1,1,1 | 0.31 | 0 |
| 2 | HEM | S | 1000 | 1,3 | 30,50,50 | 2.12 | 9 (30%) | 24,82,82 | 2.58 | 11 (45%) |
| 3 | NO2 | S | 2000 | 2 | 2,2,2 | 1.57 | 0 | 1,1,1 | 0.37 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | HEM | T | 1000 | 1,3 | 30,50,50 | 2.15 | 6 (20%) | 24,82,82 | 2.56 | 10 (41%) |
| 3 | NO2 | T | 2000 | 2 | 2,2,2 | 1.49 | 0 | 1,1,1 | 0.66 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | HEM | A | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | A | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | B | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | B | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | C | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | C | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | D | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | D | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | E | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | E | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | F | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | F | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | G | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | G | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | H | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | H | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | I | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | I | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | J | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | J | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | K | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | K | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | L | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | L | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | M | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | M | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | N | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | N | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | O | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | O | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | P | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | P | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | Q | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 3 | NO2 | Q | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | R | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | R | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | S | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | S | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 2 | HEM | T | 1000 | 1,3 | - | 0/10/54/54 | 0/0/8/8 |
| 3 | NO2 | T | 2000 | 2 | - | 0/0/0/0 | 0/0/0/0 |

All (135) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | D | 1000 | HEM | C3B-C4B | -9.26 | 1.43 | 1.51 |
| 2 | B | 1000 | HEM | C3B-C4B | -8.15 | 1.44 | 1.51 |
| 2 | A | 1000 | HEM | C3B-C4B | -7.78 | 1.44 | 1.51 |
| 2 | J | 1000 | HEM | C3D-C4D | -7.15 | 1.42 | 1.51 |
| 2 | T | 1000 | HEM | C3B-C4B | -6.98 | 1.45 | 1.51 |
| 2 | I | 1000 | HEM | C3B-C4B | -6.98 | 1.45 | 1.51 |
| 2 | J | 1000 | HEM | C3B-C4B | -6.63 | 1.45 | 1.51 |
| 2 | E | 1000 | HEM | C3B-C4B | -6.57 | 1.46 | 1.51 |
| 2 | C | 1000 | HEM | C3D-C4D | -6.53 | 1.43 | 1.51 |
| 2 | A | 1000 | HEM | C3D-C4D | -6.51 | 1.43 | 1.51 |
| 2 | T | 1000 | HEM | C3D-C4D | -6.31 | 1.43 | 1.51 |
| 2 | R | 1000 | HEM | C3B-C4B | -6.28 | 1.46 | 1.51 |
| 2 | B | 1000 | HEM | C3D-C4D | -6.24 | 1.43 | 1.51 |
| 2 | F | 1000 | HEM | C3D-C4D | -6.17 | 1.43 | 1.51 |
| 2 | L | 1000 | HEM | C3D-C4D | -6.14 | 1.43 | 1.51 |
| 2 | G | 1000 | HEM | C3D-C4D | -6.06 | 1.43 | 1.51 |
| 2 | H | 1000 | HEM | C3B-C4B | -6.04 | 1.46 | 1.51 |
| 2 | F | 1000 | HEM | C3B-C4B | -6.00 | 1.46 | 1.51 |
| 2 | D | 1000 | HEM | C3D-C4D | -5.99 | 1.43 | 1.51 |
| 2 | M | 1000 | HEM | C3D-C4D | -5.91 | 1.44 | 1.51 |
| 2 | C | 1000 | HEM | C3B-C4B | -5.66 | 1.46 | 1.51 |
| 2 | I | 1000 | HEM | C3D-C4D | -5.60 | 1.44 | 1.51 |
| 2 | G | 1000 | HEM | C2C-C1C | -5.52 | 1.42 | 1.52 |
| 2 | C | 1000 | HEM | C2C-C1C | -5.46 | 1.42 | 1.52 |
| 2 | S | 1000 | HEM | C3B-C4B | -5.40 | 1.47 | 1.51 |
| 2 | K | 1000 | HEM | C3B-C4B | -5.37 | 1.47 | 1.51 |
| 2 | P | 1000 | HEM | C3D-C4D | -5.23 | 1.44 | 1.51 |
| 2 | O | 1000 | HEM | C3B-C4B | -5.19 | 1.47 | 1.51 |
| 2 | L | 1000 | HEM | C3B-C4B | -5.01 | 1.47 | 1.51 |
| 2 | Q | 1000 | HEM | C3B-C4B | -4.99 | 1.47 | 1.51 |
| 2 | K | 1000 | HEM | C2C-C1C | -4.92 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | O | 1000 | HEM | C3D-C4D | -4.84 | 1.45 | 1.51 |
| 2 | K | 1000 | HEM | C3D-C4D | -4.83 | 1.45 | 1.51 |
| 2 | N | 1000 | HEM | C3B-C4B | -4.78 | 1.47 | 1.51 |
| 2 | J | 1000 | HEM | C2C-C1C | -4.67 | 1.43 | 1.52 |
| 2 | H | 1000 | HEM | C3D-C4D | -4.61 | 1.45 | 1.51 |
| 2 | B | 1000 | HEM | C2C-C1C | -4.46 | 1.44 | 1.52 |
| 2 | M | 1000 | HEM | C3B-C4B | -4.36 | 1.48 | 1.51 |
| 2 | R | 1000 | HEM | C3D-C4D | -4.34 | 1.46 | 1.51 |
| 2 | F | 1000 | HEM | C2C-C1C | -4.29 | 1.44 | 1.52 |
| 2 | E | 1000 | HEM | C3D-C4D | -4.23 | 1.46 | 1.51 |
| 2 | L | 1000 | HEM | C2C-C1C | -4.13 | 1.44 | 1.52 |
| 2 | H | 1000 | HEM | FE-NC | -4.00 | 1.80 | 1.95 |
| 2 | P | 1000 | HEM | C2C-C1C | -3.99 | 1.45 | 1.52 |
| 2 | A | 1000 | HEM | C2C-C1C | -3.88 | 1.45 | 1.52 |
| 2 | S | 1000 | HEM | C3D-C4D | -3.85 | 1.46 | 1.51 |
| 2 | M | 1000 | HEM | C2C-C1C | -3.70 | 1.45 | 1.52 |
| 2 | O | 1000 | HEM | C2C-C1C | -3.65 | 1.45 | 1.52 |
| 2 | R | 1000 | HEM | C2C-C1C | -3.63 | 1.45 | 1.52 |
| 2 | N | 1000 | HEM | C3D-C4D | -3.60 | 1.47 | 1.51 |
| 2 | E | 1000 | HEM | C2C-C1C | -3.60 | 1.45 | 1.52 |
| 2 | G | 1000 | HEM | C3B-C4B | -3.57 | 1.48 | 1.51 |
| 2 | N | 1000 | HEM | C2C-C1C | -3.48 | 1.46 | 1.52 |
| 2 | D | 1000 | HEM | C2C-C1C | -3.42 | 1.46 | 1.52 |
| 2 | Q | 1000 | HEM | C3D-C4D | -3.39 | 1.47 | 1.51 |
| 2 | H | 1000 | HEM | C2C-C1C | -3.26 | 1.46 | 1.52 |
| 2 | S | 1000 | HEM | C2C-C1C | -3.20 | 1.46 | 1.52 |
| 2 | Q | 1000 | HEM | C2C-C1C | -3.06 | 1.46 | 1.52 |
| 2 | T | 1000 | HEM | C2C-C1C | -2.88 | 1.47 | 1.52 |
| 2 | I | 1000 | HEM | C2C-C1C | -2.78 | 1.47 | 1.52 |
| 2 | G | 1000 | HEM | C2D-C1D | -2.62 | 1.43 | 1.51 |
| 2 | A | 1000 | HEM | C2D-C1D | -2.44 | 1.43 | 1.51 |
| 2 | R | 1000 | HEM | C2D-C1D | -2.38 | 1.44 | 1.51 |
| 2 | J | 1000 | HEM | C2D-C1D | -2.37 | 1.44 | 1.51 |
| 2 | G | 1000 | HEM | C2B-C1B | -2.35 | 1.44 | 1.51 |
| 2 | I | 1000 | HEM | C2B-C1B | -2.31 | 1.44 | 1.51 |
| 2 | I | 1000 | HEM | C2D-C1D | -2.24 | 1.44 | 1.51 |
| 2 | D | 1000 | HEM | C2D-C1D | -2.23 | 1.44 | 1.51 |
| 2 | T | 1000 | HEM | C2B-C1B | -2.20 | 1.44 | 1.51 |
| 2 | H | 1000 | HEM | C4A-CHB | -2.20 | 1.33 | 1.39 |
| 2 | B | 1000 | HEM | C2D-C1D | -2.13 | 1.44 | 1.51 |
| 2 | P | 1000 | HEM | C3B-C4B | -2.10 | 1.50 | 1.51 |
| 2 | D | 1000 | HEM | C2B-C1B | -2.04 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2 | L | 1000 | HEM | C4C-NC | 2.02 | 1.38 | 1.36 |
| 2 | F | 1000 | HEM | C4C-NC | 2.03 | 1.38 | 1.36 |
| 2 | G | 1000 | HEM | C3C-CAC | 2.03 | 1.55 | 1.51 |
| 2 | R | 1000 | HEM | FE-ND | 2.05 | 2.08 | 1.97 |
| 2 | T | 1000 | HEM | FE-ND | 2.10 | 2.08 | 1.97 |
| 2 | J | 1000 | HEM | C3C-CAC | 2.11 | 1.55 | 1.51 |
| 2 | O | 1000 | HEM | C3B-CAB | 2.12 | 1.55 | 1.51 |
| 2 | S | 1000 | HEM | CAA-C2A | 2.13 | 1.55 | 1.52 |
| 2 | A | 1000 | HEM | CAA-C2A | 2.15 | 1.55 | 1.52 |
| 2 | M | 1000 | HEM | C3B-CAB | 2.15 | 1.55 | 1.51 |
| 2 | D | 1000 | HEM | C3C-CAC | 2.15 | 1.55 | 1.51 |
| 2 | R | 1000 | HEM | FE-NC | 2.19 | 2.04 | 1.95 |
| 2 | Q | 1000 | HEM | CAD-C3D | 2.19 | 1.58 | 1.54 |
| 2 | O | 1000 | HEM | CAA-C2A | 2.22 | 1.55 | 1.52 |
| 3 | M | 2000 | NO2 | O1-N | 2.26 | 1.53 | 1.23 |
| 2 | D | 1000 | HEM | CAA-C2A | 2.28 | 1.55 | 1.52 |
| 2 | D | 1000 | HEM | CMA-C3A | 2.31 | 1.56 | 1.51 |
| 2 | F | 1000 | HEM | C3C-CAC | 2.35 | 1.55 | 1.51 |
| 2 | I | 1000 | HEM | CMA-C3A | 2.35 | 1.56 | 1.51 |
| 2 | D | 1000 | HEM | FE-ND | 2.40 | 2.10 | 1.97 |
| 2 | R | 1000 | HEM | C3C-CAC | 2.41 | 1.55 | 1.51 |
| 2 | M | 1000 | HEM | FE-ND | 2.47 | 2.10 | 1.97 |
| 2 | S | 1000 | HEM | C3B-CAB | 2.49 | 1.56 | 1.51 |
| 2 | I | 1000 | HEM | C3C-CAC | 2.49 | 1.56 | 1.51 |
| 2 | R | 1000 | HEM | C1C-NC | 2.50 | 1.39 | 1.36 |
| 2 | S | 1000 | HEM | C3C-CAC | 2.51 | 1.56 | 1.51 |
| 2 | A | 1000 | HEM | C3C-CAC | 2.55 | 1.56 | 1.51 |
| 2 | I | 1000 | HEM | C4C-NC | 2.56 | 1.39 | 1.36 |
| 2 | L | 1000 | HEM | C1C-NC | 2.59 | 1.39 | 1.36 |
| 2 | E | 1000 | HEM | C1C-NC | 2.60 | 1.39 | 1.36 |
| 2 | G | 1000 | HEM | C1C-NC | 2.61 | 1.39 | 1.36 |
| 2 | K | 1000 | HEM | C3B-CAB | 2.62 | 1.56 | 1.51 |
| 2 | T | 1000 | HEM | C1C-NC | 2.64 | 1.39 | 1.36 |
| 2 | O | 1000 | HEM | C4C-NC | 2.69 | 1.39 | 1.36 |
| 2 | O | 1000 | HEM | C3C-CAC | 2.71 | 1.56 | 1.51 |
| 2 | O | 1000 | HEM | FE-ND | 2.71 | 2.11 | 1.97 |
| 2 | P | 1000 | HEM | FE-NC | 2.74 | 2.06 | 1.95 |
| 2 | L | 1000 | HEM | FE-ND | 2.78 | 2.12 | 1.97 |
| 2 | M | 1000 | HEM | C1C-NC | 2.81 | 1.39 | 1.36 |
| 2 | S | 1000 | HEM | C4C-NC | 2.88 | 1.39 | 1.36 |
| 2 | F | 1000 | HEM | C1C-NC | 2.92 | 1.39 | 1.36 |
| 2 | P | 1000 | HEM | C3B-CAB | 3.00 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2 | J | 1000 | HEM | C4C-NC | 3.05 | 1.39 | 1.36 |
| 2 | Q | 1000 | HEM | C1C-NC | 3.10 | 1.39 | 1.36 |
| 2 | R | 1000 | HEM | FE-NB | 3.19 | 2.14 | 1.97 |
| 2 | G | 1000 | HEM | C3B-CAB | 3.25 | 1.57 | 1.51 |
| 2 | F | 1000 | HEM | FE-ND | 3.25 | 2.14 | 1.97 |
| 2 | C | 1000 | HEM | C3C-CAC | 3.26 | 1.57 | 1.51 |
| 2 | S | 1000 | HEM | FE-ND | 3.58 | 2.16 | 1.97 |
| 2 | H | 1000 | HEM | C1C-NC | 3.59 | 1.40 | 1.36 |
| 2 | N | 1000 | HEM | FE-ND | 3.62 | 2.16 | 1.97 |
| 2 | L | 1000 | HEM | C3B-CAB | 3.63 | 1.58 | 1.51 |
| 2 | Q | 1000 | HEM | CAA-C2A | 3.65 | 1.58 | 1.52 |
| 2 | C | 1000 | HEM | FE-ND | 3.72 | 2.17 | 1.97 |
| 2 | G | 1000 | HEM | FE-ND | 3.83 | 2.17 | 1.97 |
| 2 | Q | 1000 | HEM | FE-ND | 4.00 | 2.18 | 1.97 |
| 2 | Q | 1000 | HEM | C3B-CAB | 4.05 | 1.58 | 1.51 |
| 2 | S | 1000 | HEM | C1C-NC | 4.19 | 1.41 | 1.36 |
| 2 | J | 1000 | HEM | FE-ND | 4.60 | 2.21 | 1.97 |
| 2 | I | 1000 | HEM | FE-ND | 4.67 | 2.22 | 1.97 |
| 2 | B | 1000 | HEM | FE-ND | 4.77 | 2.22 | 1.97 |
| 2 | A | 1000 | HEM | FE-ND | 4.86 | 2.23 | 1.97 |

All (225) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | M | 1000 | HEM | C3B-CAB-CBB | -9.41 | 110.03 | 124.46 |
| 2 | Q | 1000 | HEM | C3B-CAB-CBB | -9.27 | 110.23 | 124.46 |
| 2 | B | 1000 | HEM | C3B-CAB-CBB | -8.59 | 111.28 | 124.46 |
| 2 | G | 1000 | HEM | C3C-CAC-CBC | -6.98 | 113.75 | 124.46 |
| 2 | E | 1000 | HEM | C3C-CAC-CBC | -6.53 | 114.44 | 124.46 |
| 2 | H | 1000 | HEM | C3B-CAB-CBB | -6.50 | 114.48 | 124.46 |
| 2 | I | 1000 | HEM | C3C-CAC-CBC | -6.26 | 114.86 | 124.46 |
| 2 | O | 1000 | HEM | C3C-CAC-CBC | -5.81 | 115.55 | 124.46 |
| 2 | L | 1000 | HEM | C3B-CAB-CBB | -5.79 | 115.58 | 124.46 |
| 2 | K | 1000 | HEM | C3C-CAC-CBC | -5.74 | 115.65 | 124.46 |
| 2 | Q | 1000 | HEM | C3C-CAC-CBC | -5.48 | 116.04 | 124.46 |
| 2 | P | 1000 | HEM | C3C-CAC-CBC | -5.35 | 116.25 | 124.46 |
| 2 | B | 1000 | HEM | C3C-CAC-CBC | -5.08 | 116.67 | 124.46 |
| 2 | H | 1000 | HEM | CMA-C3A-C4A | -5.04 | 120.02 | 128.36 |
| 2 | J | 1000 | HEM | C3C-CAC-CBC | -4.92 | 116.90 | 124.46 |
| 2 | P | 1000 | HEM | CAA-CBA-CGA | -4.71 | 104.11 | 112.75 |
| 2 | B | 1000 | HEM | CMA-C3A-C4A | -4.55 | 120.84 | 128.36 |
| 2 | G | 1000 | HEM | CMA-C3A-C4A | -4.51 | 120.90 | 128.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | J | 1000 | HEM | C3B-CAB-CBB | -4.48 | 117.58 | 124.46 |
| 2 | N | 1000 | HEM | C3B-CAB-CBB | -4.48 | 117.59 | 124.46 |
| 2 | S | 1000 | HEM | CMA-C3A-C4A | -4.35 | 121.16 | 128.36 |
| 2 | L | 1000 | HEM | C3C-CAC-CBC | -4.32 | 117.84 | 124.46 |
| 2 | H | 1000 | HEM | C3C-CAC-CBC | -4.21 | 118.00 | 124.46 |
| 2 | M | 1000 | HEM | C3C-CAC-CBC | -4.12 | 118.14 | 124.46 |
| 2 | E | 1000 | HEM | C3B-CAB-CBB | -4.12 | 118.14 | 124.46 |
| 2 | E | 1000 | HEM | CMA-C3A-C4A | -4.08 | 121.61 | 128.36 |
| 2 | T | 1000 | HEM | C3C-CAC-CBC | -4.01 | 118.30 | 124.46 |
| 2 | K | 1000 | HEM | C3B-CAB-CBB | -3.99 | 118.33 | 124.46 |
| 2 | S | 1000 | HEM | CAA-CBA-CGA | -3.94 | 105.52 | 112.75 |
| 2 | R | 1000 | HEM | C3B-CAB-CBB | -3.92 | 118.44 | 124.46 |
| 2 | C | 1000 | HEM | C3B-CAB-CBB | -3.87 | 118.52 | 124.46 |
| 2 | C | 1000 | HEM | C3C-CAC-CBC | -3.79 | 118.64 | 124.46 |
| 2 | G | 1000 | HEM | C3B-CAB-CBB | -3.78 | 118.65 | 124.46 |
| 2 | A | 1000 | HEM | C3C-CAC-CBC | -3.66 | 118.84 | 124.46 |
| 2 | C | 1000 | HEM | CMA-C3A-C4A | -3.57 | 122.45 | 128.36 |
| 2 | N | 1000 | HEM | C3C-CAC-CBC | -3.52 | 119.05 | 124.46 |
| 2 | I | 1000 | HEM | CAA-CBA-CGA | -3.46 | 106.40 | 112.75 |
| 2 | N | 1000 | HEM | CAA-CBA-CGA | -3.39 | 106.53 | 112.75 |
| 2 | M | 1000 | HEM | CMA-C3A-C4A | -3.39 | 122.76 | 128.36 |
| 2 | K | 1000 | HEM | CMA-C3A-C4A | -3.36 | 122.80 | 128.36 |
| 2 | R | 1000 | HEM | CAA-CBA-CGA | -3.35 | 106.61 | 112.75 |
| 2 | F | 1000 | HEM | C3C-CAC-CBC | -3.27 | 119.43 | 124.46 |
| 2 | E | 1000 | HEM | CBA-CAA-C2A | -3.23 | 106.73 | 112.53 |
| 2 | D | 1000 | HEM | C3C-CAC-CBC | -3.19 | 119.56 | 124.46 |
| 2 | J | 1000 | HEM | CMA-C3A-C4A | -3.11 | 123.21 | 128.36 |
| 2 | F | 1000 | HEM | CMA-C3A-C4A | -3.05 | 123.31 | 128.36 |
| 2 | S | 1000 | HEM | CBD-CAD-C3D | -3.04 | 104.70 | 113.55 |
| 2 | E | 1000 | HEM | CBD-CAD-C3D | -3.01 | 104.80 | 113.55 |
| 2 | R | 1000 | HEM | CMA-C3A-C4A | -3.00 | 123.40 | 128.36 |
| 2 | L | 1000 | HEM | CMA-C3A-C4A | -2.98 | 123.43 | 128.36 |
| 2 | R | 1000 | HEM | C3C-CAC-CBC | -2.98 | 119.89 | 124.46 |
| 2 | B | 1000 | HEM | CAA-C2A-C1A | -2.92 | 123.83 | 127.01 |
| 2 | S | 1000 | HEM | C3B-CAB-CBB | -2.87 | 120.06 | 124.46 |
| 2 | L | 1000 | HEM | CAA-CBA-CGA | -2.84 | 107.53 | 112.75 |
| 2 | A | 1000 | HEM | CAA-CBA-CGA | -2.83 | 107.56 | 112.75 |
| 2 | E | 1000 | HEM | CAA-C2A-C1A | -2.78 | 123.99 | 127.01 |
| 2 | M | 1000 | HEM | C4B-CHC-C1C | -2.77 | 121.20 | 125.82 |
| 2 | T | 1000 | HEM | CAA-CBA-CGA | -2.71 | 107.78 | 112.75 |
| 2 | A | 1000 | HEM | C3B-CAB-CBB | -2.67 | 120.35 | 124.46 |
| 2 | O | 1000 | HEM | C3B-CAB-CBB | -2.64 | 120.41 | 124.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | M | 1000 | HEM | CBD-CAD-C3D | -2.64 | 105.88 | 113.55 |
| 2 | D | 1000 | HEM | C3B-CAB-CBB | -2.61 | 120.45 | 124.46 |
| 2 | H | 1000 | HEM | C4B-CHC-C1C | -2.58 | 121.52 | 125.82 |
| 2 | L | 1000 | HEM | CAA-C2A-C1A | -2.57 | 124.22 | 127.01 |
| 2 | T | 1000 | HEM | C3B-CAB-CBB | -2.51 | 120.61 | 124.46 |
| 2 | F | 1000 | HEM | C3B-CAB-CBB | -2.51 | 120.61 | 124.46 |
| 2 | O | 1000 | HEM | CMA-C3A-C4A | -2.50 | 124.23 | 128.36 |
| 2 | Q | 1000 | HEM | CMA-C3A-C4A | -2.49 | 124.24 | 128.36 |
| 2 | Q | 1000 | HEM | CBD-CAD-C3D | -2.48 | 106.33 | 113.55 |
| 2 | C | 1000 | HEM | CBD-CAD-C3D | -2.46 | 106.39 | 113.55 |
| 2 | F | 1000 | HEM | CAA-CBA-CGA | -2.39 | 108.36 | 112.75 |
| 2 | D | 1000 | HEM | CAA-CBA-CGA | -2.38 | 108.38 | 112.75 |
| 2 | P | 1000 | HEM | CMA-C3A-C4A | -2.32 | 124.53 | 128.36 |
| 2 | D | 1000 | HEM | CAA-C2A-C1A | -2.31 | 124.50 | 127.01 |
| 2 | D | 1000 | HEM | CMA-C3A-C4A | -2.26 | 124.62 | 128.36 |
| 2 | M | 1000 | HEM | CBA-CAA-C2A | -2.25 | 108.50 | 112.53 |
| 2 | C | 1000 | HEM | C4B-CHC-C1C | -2.24 | 122.07 | 125.82 |
| 2 | R | 1000 | HEM | CBD-CAD-C3D | -2.21 | 107.12 | 113.55 |
| 2 | M | 1000 | HEM | C2C-C1C-NC | -2.20 | 106.50 | 110.21 |
| 2 | G | 1000 | HEM | CAA-C2A-C3A | -2.20 | 122.73 | 129.00 |
| 2 | G | 1000 | HEM | C4B-CHC-C1C | -2.16 | 122.22 | 125.82 |
| 2 | N | 1000 | HEM | CMA-C3A-C4A | -2.13 | 124.84 | 128.36 |
| 2 | M | 1000 | HEM | C3B-C4B-NB | -2.10 | 107.61 | 111.63 |
| 2 | L | 1000 | HEM | CBD-CAD-C3D | -2.05 | 107.58 | 113.55 |
| 2 | B | 1000 | HEM | C4B-CHC-C1C | -2.04 | 122.41 | 125.82 |
| 2 | D | 1000 | HEM | CAD-CBD-CGD | -2.02 | 104.77 | 113.02 |
| 2 | J | 1000 | HEM | C4B-CHC-C1C | -2.02 | 122.45 | 125.82 |
| 2 | A | 1000 | HEM | CMA-C3A-C4A | -2.01 | 125.05 | 128.36 |
| 2 | N | 1000 | HEM | C1D-CHD-C4C | 2.02 | 129.20 | 125.82 |
| 2 | T | 1000 | HEM | C2C-C1C-CHC | 2.03 | 126.77 | 123.68 |
| 2 | M | 1000 | HEM | C3B-C4B-CHC | 2.04 | 126.03 | 123.16 |
| 2 | H | 1000 | HEM | C3B-C4B-CHC | 2.05 | 126.05 | 123.16 |
| 2 | P | 1000 | HEM | C1D-CHD-C4C | 2.07 | 129.28 | 125.82 |
| 2 | B | 1000 | HEM | C2C-C1C-CHC | 2.10 | 126.88 | 123.68 |
| 2 | N | 1000 | HEM | C3B-C4B-CHC | 2.11 | 126.14 | 123.16 |
| 2 | B | 1000 | HEM | C2D-C3D-C4D | 2.12 | 105.09 | 101.50 |
| 2 | F | 1000 | HEM | C3B-C4B-CHC | 2.20 | 126.27 | 123.16 |
| 2 | S | 1000 | HEM | C3B-C4B-CHC | 2.21 | 126.28 | 123.16 |
| 2 | R | 1000 | HEM | C2D-C3D-C4D | 2.21 | 105.25 | 101.50 |
| 2 | F | 1000 | HEM | C2C-C1C-CHC | 2.23 | 127.08 | 123.68 |
| 2 | E | 1000 | HEM | C2C-C1C-CHC | 2.26 | 127.12 | 123.68 |
| 2 | I | 1000 | HEM | C2C-C1C-CHC | 2.26 | 127.12 | 123.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2 | J | 1000 | HEM | C1D-CHD-C4C | 2.27 | 129.62 | 125.82 |
| 2 | P | 1000 | HEM | C2C-C1C-CHC | 2.31 | 127.20 | 123.68 |
| 2 | B | 1000 | HEM | CMB-C2B-C3B | 2.33 | 122.35 | 116.53 |
| 2 | D | 1000 | HEM | C2D-C3D-C4D | 2.34 | 105.46 | 101.50 |
| 2 | G | 1000 | HEM | C1D-CHD-C4C | 2.35 | 129.76 | 125.82 |
| 2 | E | 1000 | HEM | CMA-C3A-C2A | 2.37 | 130.20 | 125.24 |
| 2 | A | 1000 | HEM | CMC-C2C-C3C | 2.39 | 122.49 | 116.53 |
| 2 | R | 1000 | HEM | C3B-C4B-CHC | 2.41 | 126.55 | 123.16 |
| 2 | M | 1000 | HEM | C1D-CHD-C4C | 2.43 | 129.88 | 125.82 |
| 2 | J | 1000 | HEM | C2C-C1C-CHC | 2.43 | 127.37 | 123.68 |
| 2 | G | 1000 | HEM | CMA-C3A-C2A | 2.43 | 130.31 | 125.24 |
| 2 | Q | 1000 | HEM | CMB-C2B-C3B | 2.47 | 122.70 | 116.53 |
| 2 | D | 1000 | HEM | CMD-C2D-C3D | 2.49 | 125.38 | 114.35 |
| 2 | N | 1000 | HEM | C2C-C1C-CHC | 2.50 | 127.48 | 123.68 |
| 2 | A | 1000 | HEM | C2C-C1C-CHC | 2.54 | 127.55 | 123.68 |
| 2 | M | 1000 | HEM | CMB-C2B-C3B | 2.55 | 122.89 | 116.53 |
| 2 | F | 1000 | HEM | CMB-C2B-C3B | 2.55 | 122.91 | 116.53 |
| 2 | K | 1000 | HEM | C1D-CHD-C4C | 2.57 | 130.11 | 125.82 |
| 2 | O | 1000 | HEM | CMD-C2D-C3D | 2.57 | 125.72 | 114.35 |
| 2 | E | 1000 | HEM | CMD-C2D-C3D | 2.63 | 125.97 | 114.35 |
| 2 | F | 1000 | HEM | CMD-C2D-C3D | 2.67 | 126.16 | 114.35 |
| 2 | B | 1000 | HEM | CMA-C3A-C2A | 2.68 | 130.85 | 125.24 |
| 2 | M | 1000 | HEM | CMD-C2D-C3D | 2.70 | 126.28 | 114.35 |
| 2 | C | 1000 | HEM | CMD-C2D-C3D | 2.70 | 126.30 | 114.35 |
| 2 | R | 1000 | HEM | CMD-C2D-C3D | 2.81 | 126.79 | 114.35 |
| 2 | L | 1000 | HEM | CMB-C2B-C3B | 2.83 | 123.61 | 116.53 |
| 2 | N | 1000 | HEM | CMD-C2D-C3D | 2.84 | 126.91 | 114.35 |
| 2 | E | 1000 | HEM | CMC-C2C-C3C | 2.87 | 123.69 | 116.53 |
| 2 | G | 1000 | HEM | CAA-C2A-C1A | 2.89 | 130.15 | 127.01 |
| 2 | S | 1000 | HEM | CMA-C3A-C2A | 2.92 | 131.33 | 125.24 |
| 2 | K | 1000 | HEM | CMD-C2D-C3D | 2.92 | 127.27 | 114.35 |
| 2 | I | 1000 | HEM | CMC-C2C-C3C | 2.93 | 123.85 | 116.53 |
| 2 | F | 1000 | HEM | C1D-CHD-C4C | 2.94 | 130.73 | 125.82 |
| 2 | C | 1000 | HEM | CMA-C3A-C2A | 2.94 | 131.38 | 125.24 |
| 2 | M | 1000 | HEM | CMC-C2C-C3C | 3.00 | 124.01 | 116.53 |
| 2 | C | 1000 | HEM | CMB-C2B-C3B | 3.00 | 124.02 | 116.53 |
| 2 | L | 1000 | HEM | CMD-C2D-C3D | 3.01 | 127.64 | 114.35 |
| 2 | P | 1000 | HEM | CMD-C2D-C3D | 3.02 | 127.70 | 114.35 |
| 2 | Q | 1000 | HEM | CMD-C2D-C3D | 3.02 | 127.72 | 114.35 |
| 2 | J | 1000 | HEM | CMD-C2D-C3D | 3.03 | 127.74 | 114.35 |
| 2 | T | 1000 | HEM | CMD-C2D-C3D | 3.05 | 127.83 | 114.35 |
| 2 | A | 1000 | HEM | CMD-C2D-C3D | 3.06 | 127.87 | 114.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2 | P | 1000 | HEM | C3B-C4B-CHC | 3.06 | 127.48 | 123.16 |
| 2 | I | 1000 | HEM | CMD-C2D-C3D | 3.11 | 128.11 | 114.35 |
| 2 | S | 1000 | HEM | CMD-C2D-C3D | 3.11 | 128.12 | 114.35 |
| 2 | C | 1000 | HEM | C1D-CHD-C4C | 3.13 | 131.05 | 125.82 |
| 2 | H | 1000 | HEM | CMA-C3A-C2A | 3.14 | 131.81 | 125.24 |
| 2 | A | 1000 | HEM | CMB-C2B-C3B | 3.18 | 124.46 | 116.53 |
| 2 | B | 1000 | HEM | CMD-C2D-C3D | 3.18 | 128.40 | 114.35 |
| 2 | H | 1000 | HEM | CMB-C2B-C3B | 3.19 | 124.49 | 116.53 |
| 2 | M | 1000 | HEM | C2C-C1C-CHC | 3.20 | 128.55 | 123.68 |
| 2 | J | 1000 | HEM | CAD-C3D-C4D | 3.20 | 123.77 | 112.47 |
| 2 | K | 1000 | HEM | CMB-C2B-C3B | 3.31 | 124.80 | 116.53 |
| 2 | N | 1000 | HEM | CMC-C2C-C3C | 3.36 | 124.92 | 116.53 |
| 2 | T | 1000 | HEM | CMC-C2C-C3C | 3.37 | 124.95 | 116.53 |
| 2 | R | 1000 | HEM | CMB-C2B-C3B | 3.39 | 124.98 | 116.53 |
| 2 | H | 1000 | HEM | CMD-C2D-C3D | 3.42 | 129.47 | 114.35 |
| 2 | D | 1000 | HEM | CMC-C2C-C3C | 3.43 | 125.10 | 116.53 |
| 2 | C | 1000 | HEM | CMC-C2C-C3C | 3.50 | 125.27 | 116.53 |
| 2 | E | 1000 | HEM | CMB-C2B-C3B | 3.53 | 125.35 | 116.53 |
| 2 | O | 1000 | HEM | CMB-C2B-C3B | 3.57 | 125.43 | 116.53 |
| 2 | N | 1000 | HEM | CMB-C2B-C3B | 3.62 | 125.57 | 116.53 |
| 2 | Q | 1000 | HEM | CMC-C2C-C3C | 3.63 | 125.58 | 116.53 |
| 2 | S | 1000 | HEM | CMC-C2C-C3C | 3.64 | 125.61 | 116.53 |
| 2 | J | 1000 | HEM | CMB-C2B-C3B | 3.67 | 125.69 | 116.53 |
| 2 | S | 1000 | HEM | CMB-C2B-C3B | 3.70 | 125.77 | 116.53 |
| 2 | T | 1000 | HEM | CAD-C3D-C4D | 3.71 | 125.54 | 112.47 |
| 2 | I | 1000 | HEM | CMB-C2B-C3B | 3.72 | 125.81 | 116.53 |
| 2 | R | 1000 | HEM | CMC-C2C-C3C | 3.75 | 125.89 | 116.53 |
| 2 | D | 1000 | HEM | CMB-C2B-C3B | 3.75 | 125.89 | 116.53 |
| 2 | G | 1000 | HEM | CMB-C2B-C3B | 3.75 | 125.90 | 116.53 |
| 2 | P | 1000 | HEM | CAD-C3D-C4D | 3.78 | 125.80 | 112.47 |
| 2 | P | 1000 | HEM | CMC-C2C-C3C | 3.80 | 126.02 | 116.53 |
| 2 | G | 1000 | HEM | CMD-C2D-C3D | 3.83 | 131.29 | 114.35 |
| 2 | B | 1000 | HEM | C1D-CHD-C4C | 3.83 | 132.23 | 125.82 |
| 2 | B | 1000 | HEM | CAD-C3D-C4D | 3.83 | 125.99 | 112.47 |
| 2 | L | 1000 | HEM | CAD-C3D-C4D | 3.88 | 126.16 | 112.47 |
| 2 | T | 1000 | HEM | CMB-C2B-C3B | 3.90 | 126.27 | 116.53 |
| 2 | J | 1000 | HEM | CMC-C2C-C3C | 3.94 | 126.37 | 116.53 |
| 2 | A | 1000 | HEM | CAD-C3D-C4D | 3.95 | 126.39 | 112.47 |
| 2 | B | 1000 | HEM | CMC-C2C-C3C | 3.98 | 126.46 | 116.53 |
| 2 | Q | 1000 | HEM | CAD-C3D-C4D | 4.00 | 126.57 | 112.47 |
| 2 | H | 1000 | HEM | CMC-C2C-C3C | 4.06 | 126.67 | 116.53 |
| 2 | D | 1000 | HEM | CAD-C3D-C4D | 4.06 | 126.79 | 112.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2 | C | 1000 | HEM | CAD-C3D-C4D | 4.09 | 126.88 | 112.47 |
| 2 | G | 1000 | HEM | CAD-C3D-C4D | 4.09 | 126.89 | 112.47 |
| 2 | T | 1000 | HEM | C3B-C4B-CHC | 4.11 | 128.94 | 123.16 |
| 2 | O | 1000 | HEM | CAD-C3D-C4D | 4.12 | 126.98 | 112.47 |
| 2 | F | 1000 | HEM | CMC-C2C-C3C | 4.15 | 126.90 | 116.53 |
| 2 | H | 1000 | HEM | CAD-C3D-C4D | 4.21 | 127.31 | 112.47 |
| 2 | O | 1000 | HEM | CMC-C2C-C3C | 4.22 | 127.06 | 116.53 |
| 2 | S | 1000 | HEM | CAD-C3D-C4D | 4.28 | 127.58 | 112.47 |
| 2 | R | 1000 | HEM | CAD-C3D-C2D | 4.28 | 125.53 | 113.22 |
| 2 | I | 1000 | HEM | CAD-C3D-C4D | 4.29 | 127.60 | 112.47 |
| 2 | M | 1000 | HEM | CAD-C3D-C4D | 4.34 | 127.77 | 112.47 |
| 2 | P | 1000 | HEM | CMB-C2B-C3B | 4.37 | 127.43 | 116.53 |
| 2 | L | 1000 | HEM | CMC-C2C-C3C | 4.40 | 127.53 | 116.53 |
| 2 | F | 1000 | HEM | CAD-C3D-C4D | 4.42 | 128.07 | 112.47 |
| 2 | N | 1000 | HEM | CAD-C3D-C4D | 4.45 | 128.16 | 112.47 |
| 2 | E | 1000 | HEM | CAD-C3D-C2D | 4.45 | 126.02 | 113.22 |
| 2 | K | 1000 | HEM | CAD-C3D-C4D | 4.50 | 128.35 | 112.47 |
| 2 | G | 1000 | HEM | CMC-C2C-C3C | 4.64 | 128.10 | 116.53 |
| 2 | R | 1000 | HEM | CAD-C3D-C4D | 4.75 | 129.22 | 112.47 |
| 2 | E | 1000 | HEM | CAD-C3D-C4D | 4.77 | 129.28 | 112.47 |
| 2 | K | 1000 | HEM | CMC-C2C-C3C | 4.82 | 128.57 | 116.53 |
| 2 | N | 1000 | HEM | CAD-C3D-C2D | 4.86 | 127.19 | 113.22 |
| 2 | D | 1000 | HEM | CAD-C3D-C2D | 5.02 | 127.65 | 113.22 |
| 2 | S | 1000 | HEM | CAD-C3D-C2D | 5.16 | 128.06 | 113.22 |
| 2 | I | 1000 | HEM | CAD-C3D-C2D | 5.17 | 128.09 | 113.22 |
| 2 | M | 1000 | HEM | CAD-C3D-C2D | 5.18 | 128.11 | 113.22 |
| 2 | F | 1000 | HEM | CAD-C3D-C2D | 5.23 | 128.24 | 113.22 |
| 2 | H | 1000 | HEM | CAD-C3D-C2D | 5.26 | 128.34 | 113.22 |
| 2 | K | 1000 | HEM | CAD-C3D-C2D | 5.29 | 128.42 | 113.22 |
| 2 | C | 1000 | HEM | CAD-C3D-C2D | 5.34 | 128.56 | 113.22 |
| 2 | B | 1000 | HEM | CAD-C3D-C2D | 5.45 | 128.89 | 113.22 |
| 2 | G | 1000 | HEM | CAD-C3D-C2D | 5.53 | 129.12 | 113.22 |
| 2 | A | 1000 | HEM | CAD-C3D-C2D | 5.70 | 129.61 | 113.22 |
| 2 | L | 1000 | HEM | CAD-C3D-C2D | 5.75 | 129.75 | 113.22 |
| 2 | Q | 1000 | HEM | CAD-C3D-C2D | 5.83 | 129.98 | 113.22 |
| 2 | O | 1000 | HEM | CAD-C3D-C2D | 5.94 | 130.28 | 113.22 |
| 2 | T | 1000 | HEM | CAD-C3D-C2D | 6.03 | 130.55 | 113.22 |
| 2 | P | 1000 | HEM | CAD-C3D-C2D | 6.46 | 131.79 | 113.22 |
| 2 | J | 1000 | HEM | CAD-C3D-C2D | 6.62 | 132.26 | 113.22 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 168 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 1000 | HEM | 8 | 0 |
| 2 | B | 1000 | HEM | 6 | 0 |
| 2 | C | 1000 | HEM | 7 | 0 |
| 3 | C | 2000 | NO2 | 1 | 0 |
| 2 | D | 1000 | HEM | 9 | 0 |
| 2 | E | 1000 | HEM | 8 | 0 |
| 2 | F | 1000 | HEM | 11 | 0 |
| 2 | G | 1000 | HEM | 15 | 0 |
| 3 | G | 2000 | NO2 | 1 | 0 |
| 2 | H | 1000 | HEM | 9 | 0 |
| 2 | I | 1000 | HEM | 7 | 0 |
| 2 | J | 1000 | HEM | 10 | 0 |
| 2 | K | 1000 | HEM | 5 | 0 |
| 2 | L | 1000 | HEM | 7 | 0 |
| 3 | L | 2000 | NO2 | 1 | 0 |
| 2 | M | 1000 | HEM | 6 | 0 |
| 2 | N | 1000 | HEM | 10 | 0 |
| 2 | O | 1000 | HEM | 5 | 0 |
| 2 | P | 1000 | HEM | 3 | 0 |
| 2 | Q | 1000 | HEM | 10 | 0 |
| 2 | R | 1000 | HEM | 14 | 0 |
| 2 | S | 1000 | HEM | 9 | 0 |
| 2 | T | 1000 | HEM | 6 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1 | A | 241/248 (97%) | -0.78 | 0 100 100 | 11, 24, 52, 62 | 0 |
| 1 | B | 241/248 (97%) | -0.74 | 1 (0%) 93 80 | 13, 24, 48, 70 | 0 |
| 1 | C | 241/248 (97%) | -0.68 | 2 (0%) 87 67 | 11, 23, 50, 68 | 0 |
| 1 | D | 241/248 (97%) | -0.78 | 0 100 100 | 14, 27, 54, 77 | 0 |
| 1 | E | 241/248 (97%) | -0.82 | 0 100 100 | 9, 21, 47, 64 | 0 |
| 1 | F | 241/248 (97%) | -0.51 | 0 100 100 | 17, 40, 75, 96 | 0 |
| 1 | G | 241/248 (97%) | -0.68 | 0 100 100 | 18, 34, 61, 90 | 0 |
| 1 | H | 241/248 (97%) | -0.77 | 0 100 100 | 14, 27, 55, 74 | 0 |
| 1 | I | 241/248 (97%) | -0.70 | 0 100 100 | 13, 28, 62, 80 | 0 |
| 1 | J | 241/248 (97%) | -0.67 | 0 100 100 | 15, 32, 69, 88 | 0 |
| 1 | K | 241/248 (97%) | -0.65 | 0 100 100 | 19, 34, 64, 87 | 0 |
| 1 | L | 241/248 (97%) | -0.62 | 0 100 100 | 17, 31, 60, 81 | 0 |
| 1 | M | 241/248 (97%) | -0.68 | 0 100 100 | 16, 29, 56, 79 | 0 |
| 1 | N | 241/248 (97%) | -0.59 | 0 100 100 | 19, 36, 71, 82 | 0 |
| 1 | O | 241/248 (97%) | -0.52 | 0 100 100 | 22, 41, 71, 96 | 0 |
| 1 | P | 241/248 (97%) | -0.30 | 0 100 100 | 38, 62, 108, 134 | 0 |
| 1 | Q | 241/248 (97%) | -0.49 | 1 (0%) 93 80 | 23, 52, 99, 120 | 0 |
| 1 | R | 241/248 (97%) | -0.30 | 0 100 100 | 27, 56, 101, 124 | 0 |
| 1 | S | 241/248 (97%) | -0.12 | 4 (1%) 73 45 | 39, 68, 110, 129 | 0 |
| 1 | T | 241/248 (97%) | -0.23 | 0 100 100 | 32, 63, 111, 135 | 0 |
| All | All | 4820/4960 (97%) | -0.58 | 8 (0%) 95 87 | 9, 36, 86, 135 | 0 |

All (8) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 132 | SER | 3.7 |
| 1 | S | 132 | SER | 2.6 |
| 1 | Q | 132 | SER | 2.4 |
| 1 | C | 38 | VAL | 2.2 |
| 1 | S | 57 | ASP | 2.2 |
| 1 | S | 59 | VAL | 2.2 |
| 1 | C | 248 | ASP | 2.1 |
| 1 | S | 133 | SER | 2.1 |

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 3 | NO2 | C | 2000 | 3/3 | 0.98 | 0.18 | 3.91 | 25,25,28,31 | 0 |
| 3 | NO2 | A | 2000 | 3/3 | 0.99 | 0.22 | 3.70 | 29,29,31,34 | 0 |
| 3 | NO2 | R | 2000 | 3/3 | 0.97 | 0.33 | 3.30 | 48,48,50,52 | 0 |
| 3 | NO2 | I | 2000 | 3/3 | 0.98 | 0.20 | 3.22 | 27,27,29,32 | 0 |
| 3 | NO2 | B | 2000 | 3/3 | 0.95 | 0.23 | 2.64 | 32,32,36,43 | 0 |
| 2 | HEM | G | 1000 | 43/43 | 0.96 | 0.20 | 2.42 | 21,26,36,39 | 0 |
| 3 | NO2 | N | 2000 | 3/3 | 0.97 | 0.20 | 2.32 | 41,41,45,47 | 0 |
| 3 | NO2 | K | 2000 | 3/3 | 0.98 | 0.17 | 2.03 | 34,34,36,39 | 0 |
| 4 | CA | K | 1001 | 1/1 | 0.94 | 0.18 | 1.70 | 26,26,26,26 | 0 |
| 2 | HEM | D | 1000 | 43/43 | 0.97 | 0.18 | 1.34 | 15,22,31,35 | 0 |
| 4 | CA | M | 1001 | 1/1 | 0.97 | 0.16 | 1.32 | 26,26,26,26 | 0 |
| 3 | NO2 | J | 2000 | 3/3 | 0.99 | 0.16 | 1.26 | 29,29,30,31 | 0 |
| 3 | NO2 | G | 2000 | 3/3 | 0.99 | 0.17 | 1.20 | 36,36,37,39 | 0 |
| 3 | NO2 | D | 2000 | 3/3 | 0.99 | 0.16 | 1.19 | 30,30,32,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3 | NO2 | M | 2000 | 3/3 | 0.96 | 0.18 | 1.07 | 31,31,34,41 | 0 |
| 2 | HEM | Q | 1000 | 43/43 | 0.96 | 0.18 | 1.05 | 29,31,39,45 | 0 |
| 2 | HEM | E | 1000 | 43/43 | 0.97 | 0.16 | 1.04 | 11,16,23,30 | 0 |
| 2 | HEM | I | 1000 | 43/43 | 0.97 | 0.18 | 1.03 | 13,19,27,32 | 0 |
| 2 | HEM | A | 1000 | 43/43 | 0.98 | 0.17 | 0.90 | 13,19,28,36 | 0 |
| 3 | NO2 | H | 2000 | 3/3 | 0.99 | 0.17 | 0.89 | 28,28,30,33 | 0 |
| 2 | HEM | M | 1000 | 43/43 | 0.97 | 0.18 | 0.83 | 17,22,29,34 | 0 |
| 3 | NO2 | O | 2000 | 3/3 | 0.99 | 0.14 | 0.81 | 40,40,42,43 | 0 |
| 2 | HEM | K | 1000 | 43/43 | 0.97 | 0.17 | 0.78 | 21,25,34,37 | 0 |
| 2 | HEM | H | 1000 | 43/43 | 0.97 | 0.17 | 0.77 | 12,19,29,33 | 0 |
| 2 | HEM | B | 1000 | 43/43 | 0.96 | 0.19 | 0.63 | 15,18,27,33 | 0 |
| 2 | HEM | F | 1000 | 43/43 | 0.96 | 0.20 | 0.56 | 24,33,42,47 | 0 |
| 4 | CA | C | 1001 | 1/1 | 0.96 | 0.14 | 0.55 | 20,20,20,20 | 0 |
| 2 | HEM | C | 1000 | 43/43 | 0.97 | 0.16 | 0.51 | 13,17,24,31 | 0 |
| 2 | HEM | L | 1000 | 43/43 | 0.97 | 0.17 | 0.50 | 18,22,30,35 | 0 |
| 3 | NO2 | Q | 2000 | 3/3 | 0.98 | 0.16 | 0.44 | 45,45,45,49 | 0 |
| 2 | HEM | J | 1000 | 43/43 | 0.97 | 0.17 | 0.44 | 15,20,28,35 | 0 |
| 2 | HEM | N | 1000 | 43/43 | 0.97 | 0.17 | 0.41 | 22,31,40,48 | 0 |
| 3 | NO2 | S | 2000 | 3/3 | 0.97 | 0.18 | 0.39 | 63,63,64,65 | 0 |
| 2 | HEM | O | 1000 | 43/43 | 0.97 | 0.17 | 0.32 | 27,34,42,46 | 0 |
| 4 | CA | G | 1001 | 1/1 | 0.92 | 0.14 | 0.29 | 24,24,24,24 | 0 |
| 3 | NO2 | F | 2000 | 3/3 | 0.98 | 0.17 | 0.23 | 40,40,42,44 | 0 |
| 3 | NO2 | L | 2000 | 3/3 | 0.99 | 0.13 | 0.11 | 31,31,32,35 | 0 |
| 2 | HEM | R | 1000 | 43/43 | 0.96 | 0.19 | 0.09 | 30,36,43,53 | 0 |
| 4 | CA | O | 1001 | 1/1 | 0.96 | 0.15 | 0.02 | 29,29,29,29 | 0 |
| 4 | CA | J | 1001 | 1/1 | 0.98 | 0.17 | 0.01 | 29,29,29,29 | 0 |
| 2 | HEM | S | 1000 | 43/43 | 0.94 | 0.20 | -0.05 | 45,55,64,71 | 0 |
| 3 | NO2 | P | 2000 | 3/3 | 0.98 | 0.15 | -0.05 | 55,55,55,55 | 0 |
| 2 | HEM | P | 1000 | 43/43 | 0.97 | 0.17 | -0.13 | 41,45,52,55 | 0 |
| 2 | HEM | T | 1000 | 43/43 | 0.96 | 0.20 | -0.16 | 39,46,52,59 | 0 |
| 4 | CA | L | 1001 | 1/1 | 0.95 | 0.15 | -0.55 | 25,25,25,25 | 0 |
| 4 | CA | A | 1001 | 1/1 | 0.97 | 0.12 | -0.58 | 21,21,21,21 | 0 |
| 4 | CA | H | 1001 | 1/1 | 0.97 | 0.13 | -0.63 | 22,22,22,22 | 0 |
| 4 | CA | T | 1001 | 1/1 | 0.94 | 0.16 | -0.65 | 52,52,52,52 | 0 |
| 4 | CA | N | 1001 | 1/1 | 0.96 | 0.14 | -0.78 | 32,32,32,32 | 0 |
| 4 | CA | R | 1001 | 1/1 | 0.94 | 0.14 | -0.85 | 50,50,50,50 | 0 |
| 4 | CA | D | 1001 | 1/1 | 0.97 | 0.12 | -0.88 | 24,24,24,24 | 0 |
| 3 | NO2 | T | 2000 | 3/3 | 0.99 | 0.17 | -1.13 | 57,57,57,58 | 0 |
| 4 | CA | E | 1001 | 1/1 | 0.98 | 0.12 | -1.14 | 13,13,13,13 | 0 |
| 4 | CA | P | 1001 | 1/1 | 0.97 | 0.12 | -1.19 | 54,54,54,54 | 0 |
| 4 | CA | I | 1001 | 1/1 | 0.94 | 0.11 | -1.34 | 23,23,23,23 | 0 |
| 4 | CA | S | 1001 | 1/1 | 0.84 | 0.14 | -1.61 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 4 | CA | B | 1001 | 1/1 | 0.98 | 0.12 | -1.64 | 17,17,17,17 | 0 |
| 4 | CA | F | 1001 | 1/1 | 0.99 | 0.10 | -1.80 | 30,30,30,30 | 0 |
| 4 | CA | Q | 1001 | 1/1 | 0.96 | 0.12 | -1.99 | 48,48,48,48 | 0 |
| 3 | NO2 | E | 2000 | 3/3 | 1.00 | 0.10 | -2.82 | 22,22,24,28 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.