



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:19 AM GMT

PDB ID : 2ZZS
Title : Crystal structure of cytochrome c554 from *Vibrio parahaemolyticus* strain RIMD2210633
Authors : Akazaki, H.; Kawai, F.; Kumaki, Y.; Sekine, K.; Hakamata, W.; Nishio, T.; Park, S.-Y.; Oku, T.
Deposited on : 2009-02-24
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

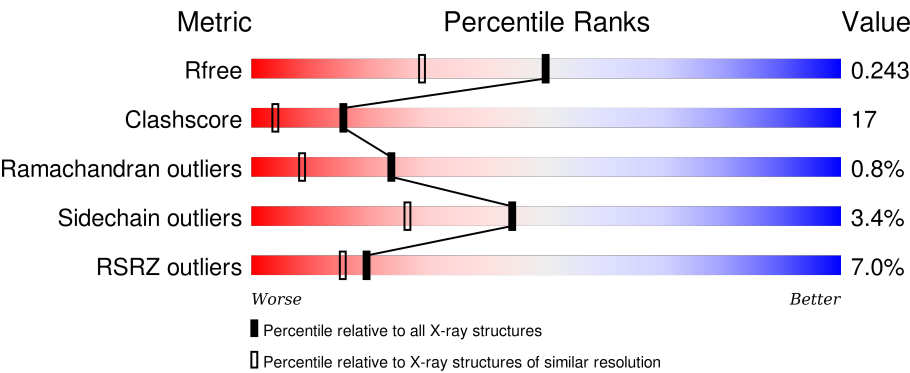
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 91344 | 4533 (1.80-1.80) |
| Clashscore | 102246 | 5383 (1.80-1.80) |
| Ramachandran outliers | 100387 | 5320 (1.80-1.80) |
| Sidechain outliers | 100360 | 5319 (1.80-1.80) |
| RSRZ outliers | 91569 | 4547 (1.80-1.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 1 | 103 | <div><div>8%</div><div><div></div><div>63%</div><div>15%</div><div>•</div><div>21%</div></div></div> |
| 1 | 2 | 103 | <div><div>16%</div><div><div></div><div>58%</div><div>16%</div><div>• •</div><div>21%</div></div></div> |
| 1 | 3 | 103 | <div><div>11%</div><div><div></div><div>59%</div><div>16%</div><div>• •</div><div>21%</div></div></div> |
| 1 | 4 | 103 | <div><div>9%</div><div><div></div><div>54%</div><div>23%</div><div>•</div><div>21%</div></div></div> |
| 1 | 5 | 103 | <div><div>30%</div><div><div></div><div>41%</div><div>29%</div><div>7%</div><div>•</div><div>21%</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 6 | 103 | |
| 1 | A | 103 | |
| 1 | B | 103 | |
| 1 | C | 103 | |
| 1 | D | 103 | |
| 1 | E | 103 | |
| 1 | F | 103 | |
| 1 | G | 103 | |
| 1 | H | 103 | |
| 1 | I | 103 | |
| 1 | J | 103 | |
| 1 | K | 103 | |
| 1 | L | 103 | |
| 1 | M | 103 | |
| 1 | N | 103 | |
| 1 | O | 103 | |
| 1 | P | 103 | |
| 1 | Q | 103 | |
| 1 | R | 103 | |
| 1 | S | 103 | |
| 1 | T | 103 | |
| 1 | U | 103 | |
| 1 | V | 103 | |
| 1 | W | 103 | |
| 1 | X | 103 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | Y | 103 | |
| 1 | Z | 103 | |

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 | HEC | 6 | 220 | - | - | X | - |
| 3 | GOL | P | 104 | - | - | - | X |
| 3 | GOL | R | 104 | - | - | X | - |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21402 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c554.

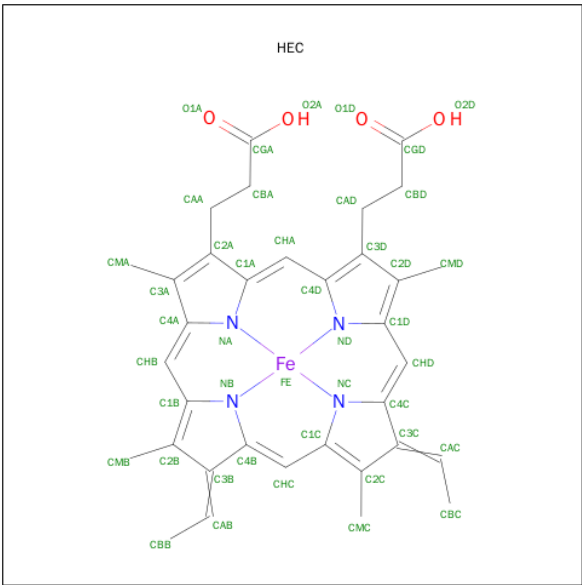
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | B | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | C | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | D | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | E | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | F | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | G | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | H | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | I | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | J | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | K | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | L | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | M | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 567 | 347 | 100 | 117 | 3 | | | |
| 1 | N | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | O | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | P | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | Q | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | R | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | S | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | T | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | U | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | V | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | W | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | X | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | Y | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | Z | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | 1 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | 2 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | 3 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | 4 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | 5 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 353 | 101 | 118 | 3 | | | |
| 1 | 6 | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 561 | 344 | 99 | 115 | 3 | | | |

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 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 |
| 2 | U | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | V | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | W | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | X | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | Y | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | Z | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | 1 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | 2 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | 3 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | 4 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | 5 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 2 | 6 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 3 | E | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 3 | P | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 3 | R | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 91 | Total | O | 0 | 0 |
| | | | 91 | 91 | | |
| 4 | B | 101 | Total | O | 0 | 0 |
| | | | 101 | 101 | | |
| 4 | C | 73 | Total | O | 0 | 0 |
| | | | 73 | 73 | | |
| 4 | D | 62 | Total | O | 0 | 0 |
| | | | 62 | 62 | | |
| 4 | E | 76 | Total | O | 0 | 0 |
| | | | 76 | 76 | | |
| 4 | F | 64 | Total | O | 0 | 0 |
| | | | 64 | 64 | | |
| 4 | G | 62 | Total | O | 0 | 0 |
| | | | 62 | 62 | | |
| 4 | H | 70 | Total | O | 0 | 0 |
| | | | 70 | 70 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4 | I | 62 | Total O 62 62 | 0 | 0 |
| 4 | J | 24 | Total O 24 24 | 0 | 0 |
| 4 | K | 35 | Total O 35 35 | 0 | 0 |
| 4 | L | 53 | Total O 53 53 | 0 | 0 |
| 4 | M | 51 | Total O 51 51 | 0 | 0 |
| 4 | N | 37 | Total O 37 37 | 0 | 0 |
| 4 | O | 71 | Total O 71 71 | 0 | 0 |
| 4 | P | 35 | Total O 35 35 | 0 | 0 |
| 4 | Q | 63 | Total O 63 63 | 0 | 0 |
| 4 | R | 46 | Total O 46 46 | 0 | 0 |
| 4 | S | 42 | Total O 42 42 | 0 | 0 |
| 4 | T | 69 | Total O 69 69 | 0 | 0 |
| 4 | U | 67 | Total O 67 67 | 0 | 0 |
| 4 | V | 59 | Total O 59 59 | 0 | 0 |
| 4 | W | 53 | Total O 53 53 | 0 | 0 |
| 4 | X | 21 | Total O 21 21 | 0 | 0 |
| 4 | Y | 55 | Total O 55 55 | 0 | 0 |
| 4 | Z | 48 | Total O 48 48 | 0 | 0 |
| 4 | 1 | 34 | Total O 34 34 | 0 | 0 |
| 4 | 2 | 15 | Total O 15 15 | 0 | 0 |
| 4 | 3 | 21 | Total O 21 21 | 0 | 0 |

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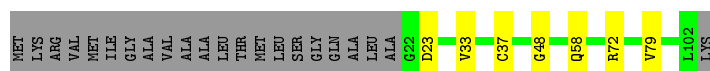
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4 | 4 | 28 | Total 28 | O 28 | 0 | 0 |
| 4 | 5 | 27 | Total 27 | O 27 | 0 | 0 |
| 4 | 6 | 9 | Total 9 | O 9 | 0 | 0 |

3 Residue-property plots [i](#)

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.

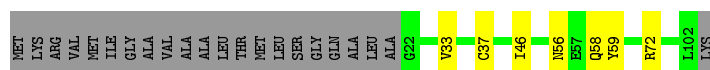
• Molecule 1: Cytochrome c554

Chain A: 



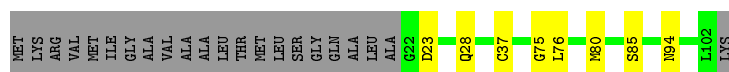
• Molecule 1: Cytochrome c554

Chain B: 



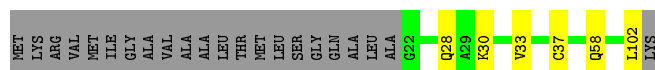
• Molecule 1: Cytochrome c554

Chain C: 



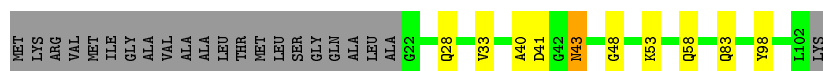
• Molecule 1: Cytochrome c554

Chain D: 



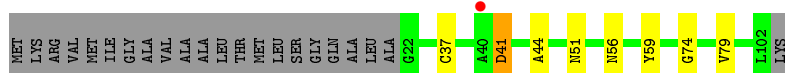
• Molecule 1: Cytochrome c554

Chain E: 

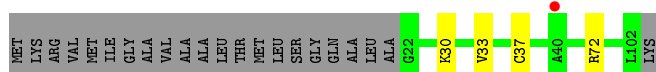
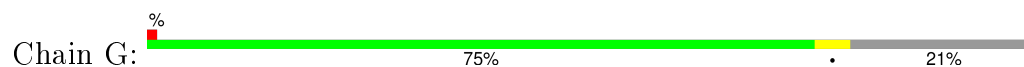


• Molecule 1: Cytochrome c554

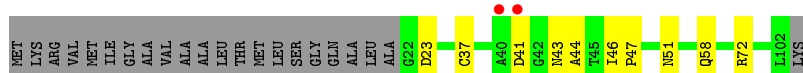
Chain F: 



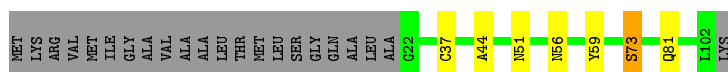
- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



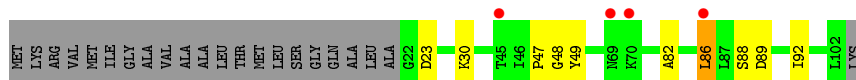
- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



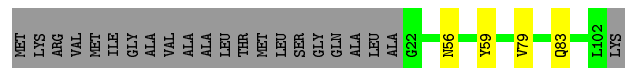
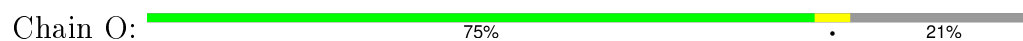
LEU
LYS

- Molecule 1: Cytochrome c554



L102
LYS

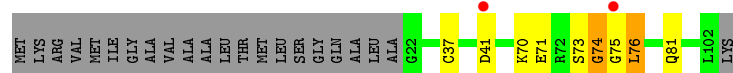
- Molecule 1: Cytochrome c554



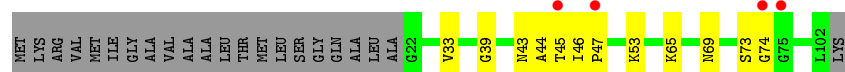
- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554

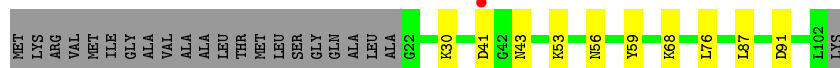


- Molecule 1: Cytochrome c554

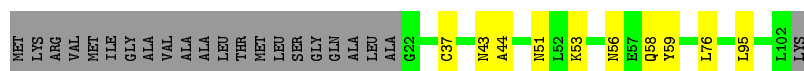




- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554



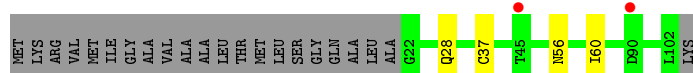
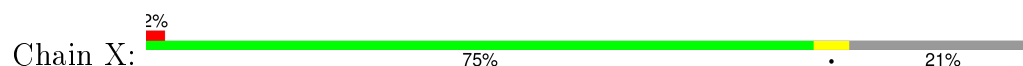
- Molecule 1: Cytochrome c554



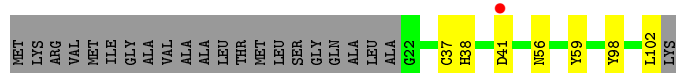
- Molecule 1: Cytochrome c554



- Molecule 1: Cytochrome c554

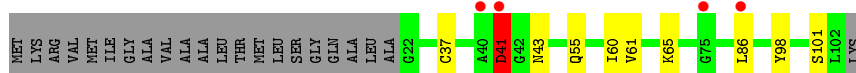


- Molecule 1: Cytochrome c554

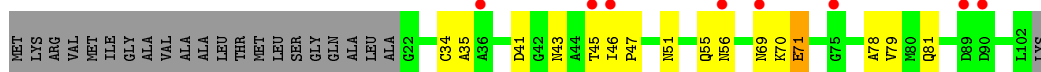


- Molecule 1: Cytochrome c554

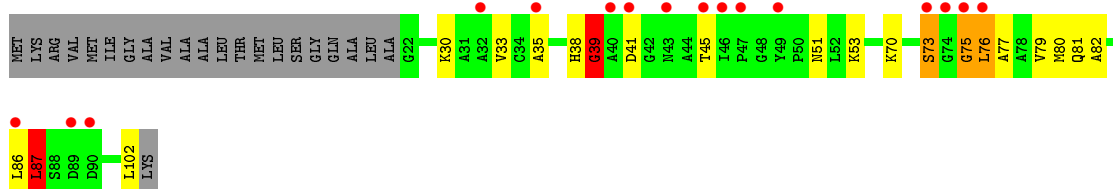




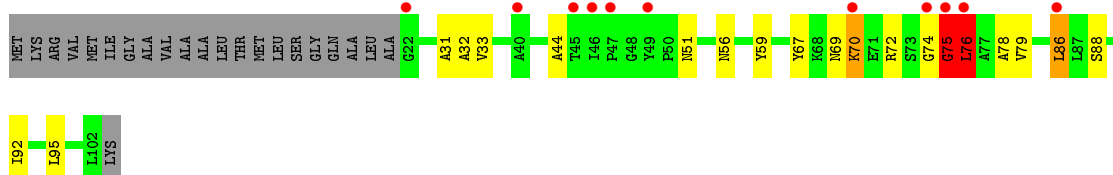
• Molecule 1: Cytochrome c554



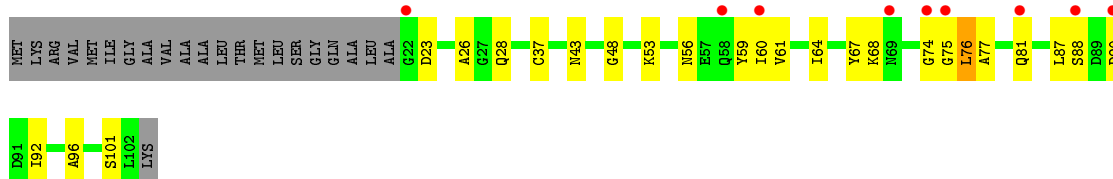
• Molecule 1: Cytochrome c554



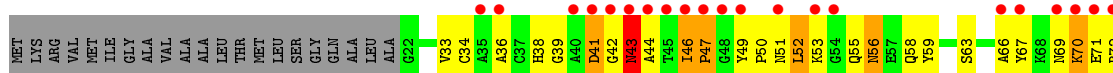
• Molecule 1: Cytochrome c554

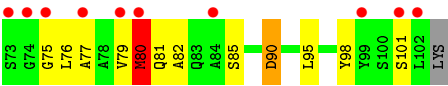


• Molecule 1: Cytochrome c554

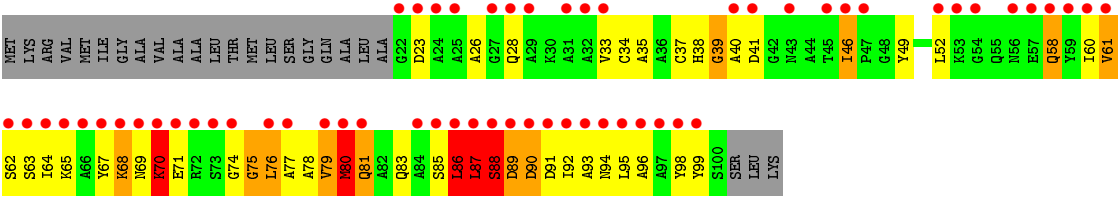
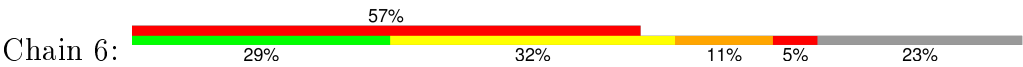


• Molecule 1: Cytochrome c554





● Molecule 1: Cytochrome c554



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 84.95Å 87.61Å 103.85Å 71.50° 72.98° 83.68° | Depositor |
| Resolution (Å) | 20.00 – 1.80 20.03 – 1.80 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (20.00-1.80) 86.3 (20.03-1.80) | Depositor EDS |
| R_{merge} | 0.06 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.60 (at 1.80Å) | Xtriage |
| Refinement program | REFMAC 5.4.0067 | Depositor |
| R, R_{free} | 0.193 , 0.242 0.194 , 0.243 | Depositor DCC |
| R_{free} test set | 11820 reflections (5.28%) | DCC |
| Wilson B-factor (Å ²) | 18.2 | Xtriage |
| Anisotropy | 0.301 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.39 , 55.3 | EDS |
| Estimated twinning fraction | 0.026 for -k,-h,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Outliers | 0 of 235784 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 21402 | wwPDB-VP |
| Average B, all atoms (Å ²) | 26.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% 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: GOL, HEC

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 | 1 | 0.78 | 1/582 (0.2%) | 0.79 | 0/787 |
| 1 | 2 | 0.62 | 0/582 | 0.75 | 1/787 (0.1%) |
| 1 | 3 | 0.65 | 0/582 | 0.77 | 2/787 (0.3%) |
| 1 | 4 | 0.62 | 0/582 | 0.65 | 0/787 |
| 1 | 5 | 0.71 | 0/582 | 0.89 | 1/787 (0.1%) |
| 1 | 6 | 0.64 | 0/568 | 1.06 | 4/768 (0.5%) |
| 1 | A | 1.04 | 1/582 (0.2%) | 0.89 | 1/787 (0.1%) |
| 1 | B | 0.97 | 0/582 | 0.86 | 0/787 |
| 1 | C | 0.86 | 0/582 | 0.78 | 0/787 |
| 1 | D | 0.79 | 0/582 | 0.75 | 0/787 |
| 1 | E | 0.88 | 0/582 | 0.75 | 0/787 |
| 1 | F | 0.89 | 0/582 | 0.86 | 0/787 |
| 1 | G | 0.81 | 0/582 | 0.71 | 0/787 |
| 1 | H | 0.80 | 0/582 | 0.80 | 1/787 (0.1%) |
| 1 | I | 0.74 | 0/582 | 0.76 | 0/787 |
| 1 | J | 0.65 | 0/582 | 0.71 | 0/787 |
| 1 | K | 0.74 | 0/582 | 0.73 | 0/787 |
| 1 | L | 0.80 | 0/582 | 0.82 | 3/787 (0.4%) |
| 1 | M | 0.92 | 0/574 | 0.97 | 1/776 (0.1%) |
| 1 | N | 0.81 | 1/582 (0.2%) | 0.75 | 0/787 |
| 1 | O | 0.85 | 0/582 | 0.81 | 0/787 |
| 1 | P | 0.80 | 1/582 (0.2%) | 0.78 | 0/787 |
| 1 | Q | 0.73 | 0/582 | 0.93 | 2/787 (0.3%) |
| 1 | R | 0.80 | 0/582 | 0.72 | 0/787 |
| 1 | S | 0.80 | 0/582 | 0.80 | 0/787 |
| 1 | T | 0.91 | 0/582 | 0.84 | 0/787 |
| 1 | U | 0.85 | 0/582 | 0.75 | 0/787 |
| 1 | V | 0.88 | 1/582 (0.2%) | 0.79 | 0/787 |
| 1 | W | 0.75 | 0/582 | 0.69 | 0/787 |
| 1 | X | 0.68 | 0/582 | 0.70 | 0/787 |
| 1 | Y | 0.79 | 0/582 | 0.73 | 0/787 |
| 1 | Z | 0.83 | 0/582 | 0.79 | 0/787 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.80 | 5/18602 (0.0%) | 0.80 | 16/25154 (0.1%) |

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 | 2 | 0 | 3 |
| 1 | 3 | 0 | 2 |
| 1 | 6 | 0 | 5 |
| 1 | L | 0 | 2 |
| 1 | Q | 0 | 2 |
| 1 | Z | 0 | 1 |
| All | All | 0 | 15 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | N | 37 | CYS | CB-SG | -5.86 | 1.72 | 1.81 |
| 1 | A | 79 | VAL | CB-CG2 | 5.42 | 1.64 | 1.52 |
| 1 | P | 59 | TYR | CD1-CE1 | 5.15 | 1.47 | 1.39 |
| 1 | V | 49 | TYR | CD2-CE2 | 5.12 | 1.47 | 1.39 |
| 1 | 1 | 34 | CYS | CB-SG | -5.10 | 1.73 | 1.81 |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | Q | 74 | GLY | N-CA-C | 11.32 | 141.40 | 113.10 |
| 1 | 6 | 87 | LEU | N-CA-C | 6.35 | 128.15 | 111.00 |
| 1 | 5 | 80 | MET | CB-CG-SD | -6.07 | 94.18 | 112.40 |
| 1 | L | 76 | LEU | N-CA-C | -5.98 | 94.86 | 111.00 |
| 1 | 2 | 39 | GLY | N-CA-C | 5.98 | 128.04 | 113.10 |
| 1 | L | 75 | GLY | N-CA-C | -5.95 | 98.23 | 113.10 |
| 1 | 3 | 76 | LEU | CA-CB-CG | -5.90 | 101.73 | 115.30 |
| 1 | 6 | 80 | MET | CG-SD-CE | -5.78 | 90.95 | 100.20 |
| 1 | 6 | 90 | ASP | N-CA-C | -5.62 | 95.84 | 111.00 |
| 1 | Q | 76 | LEU | N-CA-C | -5.58 | 95.93 | 111.00 |
| 1 | 6 | 89 | ASP | N-CA-C | 5.55 | 126.00 | 111.00 |
| 1 | 3 | 76 | LEU | N-CA-C | 5.53 | 125.93 | 111.00 |
| 1 | L | 23 | ASP | CB-CG-OD1 | 5.42 | 123.17 | 118.30 |
| 1 | H | 23 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | M | 23 | ASP | CB-CG-OD2 | 5.13 | 122.92 | 118.30 |
| 1 | A | 23 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | 2 | 38 | HIS | Peptide |
| 1 | 2 | 73 | SER | Peptide |
| 1 | 2 | 75 | GLY | Peptide |
| 1 | 3 | 74 | GLY | Peptide |
| 1 | 3 | 75 | GLY | Peptide |
| 1 | 6 | 38 | HIS | Peptide |
| 1 | 6 | 70 | LYS | Peptide |
| 1 | 6 | 75 | GLY | Peptide |
| 1 | 6 | 86 | LEU | Peptide |
| 1 | 6 | 88 | SER | Peptide |
| 1 | L | 75 | GLY | Mainchain,Peptide |
| 1 | Q | 73 | SER | Peptide |
| 1 | Q | 75 | GLY | Peptide |
| 1 | Z | 41 | ASP | 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 | 1 | 575 | 0 | 555 | 16 | 0 |
| 1 | 2 | 575 | 0 | 555 | 36 | 0 |
| 1 | 3 | 575 | 0 | 555 | 26 | 0 |
| 1 | 4 | 575 | 0 | 556 | 21 | 0 |
| 1 | 5 | 575 | 0 | 555 | 72 | 0 |
| 1 | 6 | 561 | 0 | 539 | 128 | 0 |
| 1 | A | 575 | 0 | 556 | 10 | 0 |
| 1 | B | 575 | 0 | 555 | 10 | 0 |
| 1 | C | 575 | 0 | 556 | 9 | 0 |
| 1 | D | 575 | 0 | 556 | 9 | 0 |
| 1 | E | 575 | 0 | 555 | 13 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | F | 575 | 0 | 556 | 12 | 0 |
| 1 | G | 575 | 0 | 556 | 6 | 0 |
| 1 | H | 575 | 0 | 556 | 15 | 0 |
| 1 | I | 575 | 0 | 556 | 9 | 0 |
| 1 | J | 575 | 0 | 556 | 31 | 0 |
| 1 | K | 575 | 0 | 555 | 12 | 0 |
| 1 | L | 575 | 0 | 555 | 17 | 0 |
| 1 | M | 567 | 0 | 545 | 31 | 0 |
| 1 | N | 575 | 0 | 555 | 24 | 0 |
| 1 | O | 575 | 0 | 555 | 9 | 0 |
| 1 | P | 575 | 0 | 555 | 9 | 0 |
| 1 | Q | 575 | 0 | 556 | 6 | 0 |
| 1 | R | 575 | 0 | 555 | 15 | 0 |
| 1 | S | 575 | 0 | 556 | 13 | 0 |
| 1 | T | 575 | 0 | 555 | 6 | 0 |
| 1 | U | 575 | 0 | 555 | 17 | 0 |
| 1 | V | 575 | 0 | 556 | 12 | 0 |
| 1 | W | 575 | 0 | 555 | 10 | 0 |
| 1 | X | 575 | 0 | 556 | 4 | 0 |
| 1 | Y | 575 | 0 | 556 | 9 | 0 |
| 1 | Z | 575 | 0 | 555 | 13 | 0 |
| 2 | 1 | 43 | 0 | 30 | 2 | 0 |
| 2 | 2 | 43 | 0 | 30 | 8 | 0 |
| 2 | 3 | 43 | 0 | 30 | 6 | 0 |
| 2 | 4 | 43 | 0 | 31 | 7 | 0 |
| 2 | 5 | 43 | 0 | 30 | 10 | 0 |
| 2 | 6 | 43 | 0 | 30 | 28 | 0 |
| 2 | A | 43 | 0 | 31 | 8 | 0 |
| 2 | B | 43 | 0 | 30 | 3 | 0 |
| 2 | C | 43 | 0 | 31 | 7 | 0 |
| 2 | D | 43 | 0 | 31 | 8 | 0 |
| 2 | E | 43 | 0 | 30 | 2 | 0 |
| 2 | F | 43 | 0 | 31 | 6 | 0 |
| 2 | G | 43 | 0 | 31 | 9 | 0 |
| 2 | H | 43 | 0 | 31 | 7 | 0 |
| 2 | I | 43 | 0 | 31 | 6 | 0 |
| 2 | J | 43 | 0 | 31 | 7 | 0 |
| 2 | K | 43 | 0 | 30 | 2 | 0 |
| 2 | L | 43 | 0 | 30 | 6 | 0 |
| 2 | M | 43 | 0 | 31 | 8 | 0 |
| 2 | N | 43 | 0 | 30 | 5 | 0 |
| 2 | O | 43 | 0 | 30 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | P | 43 | 0 | 30 | 2 | 0 |
| 2 | Q | 43 | 0 | 31 | 6 | 0 |
| 2 | R | 43 | 0 | 30 | 1 | 0 |
| 2 | S | 43 | 0 | 31 | 10 | 0 |
| 2 | T | 43 | 0 | 30 | 2 | 0 |
| 2 | U | 43 | 0 | 31 | 6 | 0 |
| 2 | V | 43 | 0 | 31 | 5 | 0 |
| 2 | W | 43 | 0 | 30 | 2 | 0 |
| 2 | X | 43 | 0 | 31 | 7 | 0 |
| 2 | Y | 43 | 0 | 31 | 8 | 0 |
| 2 | Z | 43 | 0 | 30 | 4 | 0 |
| 3 | C | 6 | 0 | 8 | 0 | 0 |
| 3 | E | 6 | 0 | 8 | 0 | 0 |
| 3 | P | 6 | 0 | 8 | 0 | 0 |
| 3 | R | 6 | 0 | 8 | 7 | 0 |
| 4 | 1 | 34 | 0 | 0 | 2 | 0 |
| 4 | 2 | 15 | 0 | 0 | 0 | 0 |
| 4 | 3 | 21 | 0 | 0 | 0 | 0 |
| 4 | 4 | 28 | 0 | 0 | 1 | 0 |
| 4 | 5 | 27 | 0 | 0 | 3 | 0 |
| 4 | 6 | 9 | 0 | 0 | 0 | 0 |
| 4 | A | 91 | 0 | 0 | 1 | 0 |
| 4 | B | 101 | 0 | 0 | 1 | 0 |
| 4 | C | 73 | 0 | 0 | 1 | 0 |
| 4 | D | 62 | 0 | 0 | 2 | 0 |
| 4 | E | 76 | 0 | 0 | 2 | 0 |
| 4 | F | 64 | 0 | 0 | 2 | 0 |
| 4 | G | 62 | 0 | 0 | 0 | 0 |
| 4 | H | 70 | 0 | 0 | 2 | 0 |
| 4 | I | 62 | 0 | 0 | 1 | 0 |
| 4 | J | 24 | 0 | 0 | 0 | 0 |
| 4 | K | 35 | 0 | 0 | 0 | 0 |
| 4 | L | 53 | 0 | 0 | 0 | 0 |
| 4 | M | 51 | 0 | 0 | 3 | 0 |
| 4 | N | 37 | 0 | 0 | 0 | 0 |
| 4 | O | 71 | 0 | 0 | 0 | 0 |
| 4 | P | 35 | 0 | 0 | 3 | 0 |
| 4 | Q | 63 | 0 | 0 | 0 | 0 |
| 4 | R | 46 | 0 | 0 | 1 | 0 |
| 4 | S | 42 | 0 | 0 | 1 | 0 |
| 4 | T | 69 | 0 | 0 | 0 | 0 |
| 4 | U | 67 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | V | 59 | 0 | 0 | 0 | 0 |
| 4 | W | 53 | 0 | 0 | 0 | 0 |
| 4 | X | 21 | 0 | 0 | 0 | 0 |
| 4 | Y | 55 | 0 | 0 | 0 | 0 |
| 4 | Z | 48 | 0 | 0 | 0 | 0 |
| All | All | 21402 | 0 | 18756 | 643 | 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 17.

All (643) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 1:6:60:ILE:HD11 | 1:6:96:ALA:CB | 1.43 | 1.45 |
| 1:5:44:ALA:CB | 1:5:49:TYR:HB3 | 1.47 | 1.41 |
| 1:5:44:ALA:HB1 | 1:5:49:TYR:CB | 1.53 | 1.36 |
| 1:6:88:SER:OG | 1:6:92:ILE:HG13 | 1.25 | 1.34 |
| 1:5:39:GLY:HA3 | 1:5:43:ASN:ND2 | 1.44 | 1.31 |
| 1:J:37:CYS:SG | 2:J:220:HEC:HAC | 1.69 | 1.28 |
| 1:2:80:MET:HG3 | 2:2:220:HEC:C4D | 1.63 | 1.27 |
| 1:5:46:ILE:HG12 | 1:5:49:TYR:CE1 | 1.69 | 1.27 |
| 1:R:45:THR:N | 3:R:104:GOL:H31 | 1.51 | 1.24 |
| 1:4:37:CYS:SG | 2:4:220:HEC:HBC3 | 1.77 | 1.24 |
| 1:2:75:GLY:HA3 | 1:2:77:ALA:N | 1.53 | 1.22 |
| 1:4:67:TYR:O | 1:4:81:GLN:HG2 | 1.40 | 1.20 |
| 1:4:37:CYS:SG | 2:4:220:HEC:CBC | 2.28 | 1.20 |
| 1:6:77:ALA:HB2 | 2:6:220:HEC:O2D | 1.34 | 1.20 |
| 1:5:39:GLY:CA | 1:5:43:ASN:HD21 | 1.54 | 1.19 |
| 1:2:75:GLY:CA | 1:2:77:ALA:H | 1.54 | 1.19 |
| 1:6:23:ASP:H | 1:6:94:ASN:HB3 | 0.99 | 1.16 |
| 1:6:69:ASN:ND2 | 1:6:70:LYS:H | 1.42 | 1.14 |
| 1:6:86:LEU:O | 1:6:86:LEU:HD12 | 1.47 | 1.13 |
| 1:6:60:ILE:CD1 | 1:6:96:ALA:HB2 | 1.77 | 1.13 |
| 1:X:37:CYS:SG | 2:X:220:HEC:HAC | 1.88 | 1.12 |
| 1:R:45:THR:H | 3:R:104:GOL:C3 | 1.63 | 1.12 |
| 1:6:23:ASP:O | 1:6:94:ASN:HB2 | 1.52 | 1.08 |
| 1:H:41:ASP:OD2 | 1:H:43:ASN:HB2 | 1.53 | 1.08 |
| 1:L:70:LYS:HG2 | 1:L:81:GLN:NE2 | 1.67 | 1.07 |
| 1:6:76:LEU:H | 1:6:76:LEU:HD12 | 1.20 | 1.07 |
| 1:6:60:ILE:HD11 | 1:6:96:ALA:CA | 1.84 | 1.06 |
| 1:H:46:ILE:HD12 | 4:H:927:HOH:O | 1.56 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:V:37:CYS:SG | 2:V:220:HEC:HAC | 1.96 | 1.06 |
| 1:6:23:ASP:N | 1:6:94:ASN:HB3 | 1.71 | 1.05 |
| 1:6:60:ILE:CD1 | 1:6:96:ALA:CB | 2.35 | 1.04 |
| 1:6:60:ILE:HD11 | 1:6:96:ALA:HB2 | 1.15 | 1.04 |
| 1:M:37:CYS:SG | 2:M:220:HEC:HAC | 1.97 | 1.04 |
| 1:S:37:CYS:SG | 2:S:220:HEC:HAC | 1.96 | 1.03 |
| 1:6:69:ASN:CG | 1:6:70:LYS:H | 1.53 | 1.01 |
| 1:6:77:ALA:CB | 2:6:220:HEC:O2D | 2.09 | 1.01 |
| 1:6:75:GLY:CA | 1:6:77:ALA:H | 1.74 | 1.00 |
| 1:J:37:CYS:HG | 2:J:220:HEC:CAC | 1.61 | 1.00 |
| 1:2:80:MET:HG3 | 2:2:220:HEC:ND | 1.74 | 1.00 |
| 1:N:70:LYS:HD2 | 1:N:81:GLN:HE21 | 1.24 | 0.99 |
| 1:6:88:SER:OG | 1:6:89:ASP:HB3 | 1.60 | 0.99 |
| 1:6:88:SER:CB | 1:6:89:ASP:HB3 | 1.93 | 0.98 |
| 1:2:86:LEU:O | 1:2:87:LEU:HD13 | 1.63 | 0.98 |
| 1:6:75:GLY:HA3 | 1:6:78:ALA:H | 1.29 | 0.98 |
| 1:5:46:ILE:HD13 | 4:5:1265:HOH:O | 1.61 | 0.98 |
| 1:6:52:LEU:HD22 | 2:6:220:HEC:HMA3 | 1.44 | 0.97 |
| 1:6:37:CYS:SG | 2:6:220:HEC:C3C | 2.52 | 0.97 |
| 1:6:75:GLY:HA2 | 1:6:77:ALA:H | 1.26 | 0.97 |
| 1:U:37:CYS:SG | 2:U:220:HEC:HAC | 2.04 | 0.97 |
| 1:5:46:ILE:HG13 | 1:5:47:PRO:N | 1.76 | 0.97 |
| 1:E:83:GLN:HE21 | 1:O:83:GLN:HE21 | 0.97 | 0.97 |
| 1:6:35:ALA:O | 1:6:39:GLY:HA2 | 1.63 | 0.97 |
| 1:G:37:CYS:SG | 2:G:220:HEC:HAC | 2.03 | 0.96 |
| 1:6:88:SER:HB3 | 1:6:89:ASP:CB | 1.95 | 0.96 |
| 1:V:23:ASP:H | 1:V:94:ASN:ND2 | 1.64 | 0.95 |
| 1:N:44:ALA:H | 1:N:51:ASN:HD22 | 1.13 | 0.95 |
| 1:6:52:LEU:HD22 | 2:6:220:HEC:CMA | 1.97 | 0.94 |
| 1:N:44:ALA:H | 1:N:51:ASN:ND2 | 1.66 | 0.94 |
| 1:1:55:GLN:HE21 | 1:1:56:ASN:H | 1.17 | 0.93 |
| 1:J:30:LYS:CE | 1:J:91:ASP:HB3 | 1.99 | 0.93 |
| 1:V:23:ASP:H | 1:V:94:ASN:HD22 | 1.05 | 0.93 |
| 1:D:37:CYS:SG | 2:D:220:HEC:HAC | 2.06 | 0.92 |
| 1:3:76:LEU:HD13 | 1:3:79:VAL:HG23 | 1.51 | 0.92 |
| 1:5:47:PRO:HA | 1:6:58:GLN:NE2 | 1.85 | 0.92 |
| 1:J:57:GLU:H | 1:J:57:GLU:CD | 1.74 | 0.91 |
| 1:5:44:ALA:HB3 | 1:5:49:TYR:C | 1.91 | 0.90 |
| 1:Z:41:ASP:HB3 | 1:Z:43:ASN:HB2 | 1.53 | 0.90 |
| 1:F:41:ASP:OD2 | 1:F:41:ASP:N | 2.03 | 0.90 |
| 1:J:37:CYS:HG | 2:J:220:HEC:HAC | 0.76 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:23:ASP:H | 1:W:94:ASN:HD22 | 1.20 | 0.90 |
| 1:P:75:GLY:HA3 | 4:P:1604:HOH:O | 1.69 | 0.90 |
| 1:6:75:GLY:CA | 1:6:77:ALA:N | 2.33 | 0.90 |
| 1:6:69:ASN:CG | 1:6:70:LYS:N | 2.23 | 0.90 |
| 1:6:70:LYS:HB2 | 1:6:71:GLU:CA | 2.03 | 0.89 |
| 1:6:52:LEU:CD2 | 2:6:220:HEC:HMA3 | 2.02 | 0.89 |
| 1:F:37:CYS:SG | 2:F:220:HEC:HAC | 2.09 | 0.89 |
| 1:L:70:LYS:HG2 | 1:L:81:GLN:HE22 | 1.35 | 0.88 |
| 1:6:68:LYS:HG3 | 1:6:68:LYS:O | 1.71 | 0.88 |
| 1:5:43:ASN:HA | 1:5:51:ASN:OD1 | 1.74 | 0.88 |
| 1:6:60:ILE:HG22 | 2:6:220:HEC:CMA | 2.03 | 0.87 |
| 1:2:75:GLY:HA3 | 1:2:77:ALA:H | 0.73 | 0.87 |
| 1:M:41:ASP:OD2 | 1:M:41:ASP:N | 2.05 | 0.87 |
| 1:2:82:ALA:O | 1:2:86:LEU:CD1 | 2.22 | 0.87 |
| 1:5:47:PRO:HA | 1:6:58:GLN:HE22 | 1.36 | 0.87 |
| 1:R:33:VAL:HG12 | 1:R:33:VAL:O | 1.72 | 0.87 |
| 1:F:44:ALA:H | 1:F:51:ASN:HD22 | 1.22 | 0.86 |
| 1:V:44:ALA:H | 1:V:51:ASN:HD22 | 1.23 | 0.86 |
| 1:6:88:SER:OG | 1:6:92:ILE:CG1 | 2.20 | 0.86 |
| 2:3:220:HEC:HMC1 | 2:3:220:HEC:HBC3 | 1.57 | 0.86 |
| 1:I:44:ALA:H | 1:I:51:ASN:HD22 | 1.20 | 0.86 |
| 1:6:76:LEU:N | 1:6:76:LEU:HD12 | 1.89 | 0.86 |
| 1:N:41:ASP:O | 1:N:53:LYS:HG3 | 1.75 | 0.86 |
| 1:5:69:ASN:O | 1:5:70:LYS:HB2 | 1.73 | 0.85 |
| 1:Z:41:ASP:CB | 1:Z:43:ASN:HB2 | 2.06 | 0.85 |
| 1:J:30:LYS:HD3 | 1:J:95:LEU:HD11 | 1.58 | 0.85 |
| 1:6:60:ILE:HD11 | 1:6:96:ALA:HA | 1.59 | 0.85 |
| 1:2:80:MET:HG2 | 2:2:220:HEC:C1D | 2.06 | 0.84 |
| 1:Y:37:CYS:SG | 2:Y:220:HEC:HAC | 2.17 | 0.84 |
| 1:6:46:ILE:HD13 | 1:6:49:TYR:CD1 | 2.11 | 0.84 |
| 1:2:35:ALA:O | 1:2:39:GLY:HA2 | 1.76 | 0.84 |
| 1:M:96:ALA:O | 1:M:100:SER:HB3 | 1.77 | 0.84 |
| 1:C:37:CYS:SG | 2:C:220:HEC:HAC | 2.17 | 0.83 |
| 1:5:79:VAL:HG11 | 2:5:220:HEC:HBC2 | 1.59 | 0.83 |
| 1:N:70:LYS:HD2 | 1:N:81:GLN:NE2 | 1.93 | 0.83 |
| 1:Y:37:CYS:SG | 2:Y:220:HEC:C3C | 2.67 | 0.82 |
| 1:6:88:SER:CB | 1:6:89:ASP:CB | 2.57 | 0.82 |
| 1:H:44:ALA:H | 1:H:51:ASN:HD22 | 1.27 | 0.82 |
| 1:E:83:GLN:NE2 | 1:O:83:GLN:HE21 | 1.78 | 0.82 |
| 1:A:37:CYS:SG | 2:A:220:HEC:CBC | 2.68 | 0.82 |
| 1:6:23:ASP:H | 1:6:94:ASN:CB | 1.88 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:1:35:ALA:HB2 | 4:1:1037:HOH:O | 1.79 | 0.81 |
| 1:M:30:LYS:O | 1:M:33:VAL:HG12 | 1.82 | 0.80 |
| 1:X:37:CYS:SG | 2:X:220:HEC:C3C | 2.69 | 0.80 |
| 1:J:30:LYS:HE2 | 1:J:91:ASP:CG | 2.01 | 0.80 |
| 1:6:78:ALA:HA | 1:6:81:GLN:HB2 | 1.64 | 0.80 |
| 1:M:33:VAL:HG23 | 4:M:511:HOH:O | 1.81 | 0.80 |
| 1:6:46:ILE:HG23 | 1:6:49:TYR:HB2 | 1.63 | 0.79 |
| 1:U:37:CYS:SG | 2:U:220:HEC:C3C | 2.70 | 0.79 |
| 1:6:35:ALA:HA | 1:6:39:GLY:O | 1.83 | 0.79 |
| 1:1:70:LYS:CG | 1:1:81:GLN:HE21 | 1.95 | 0.79 |
| 1:4:56:ASN:HD22 | 1:4:59:TYR:H | 1.31 | 0.79 |
| 1:5:39:GLY:HA3 | 1:5:43:ASN:HD21 | 0.66 | 0.78 |
| 1:T:56:ASN:HD22 | 1:T:59:TYR:H | 1.32 | 0.78 |
| 1:2:80:MET:HG3 | 2:2:220:HEC:CHA | 2.14 | 0.78 |
| 1:B:37:CYS:SG | 2:B:220:HEC:C3C | 2.72 | 0.78 |
| 1:6:68:LYS:HB2 | 1:6:68:LYS:HZ2 | 1.49 | 0.78 |
| 1:M:42:GLY:C | 1:M:53:LYS:HB2 | 2.03 | 0.78 |
| 1:4:37:CYS:SG | 2:4:220:HEC:C3C | 2.71 | 0.77 |
| 1:6:70:LYS:HB2 | 1:6:71:GLU:HA | 1.64 | 0.77 |
| 1:Q:37:CYS:SG | 2:Q:220:HEC:CBC | 2.73 | 0.77 |
| 1:J:30:LYS:HE3 | 1:J:91:ASP:HB3 | 1.65 | 0.77 |
| 1:H:37:CYS:SG | 2:H:220:HEC:CBC | 2.73 | 0.77 |
| 1:R:45:THR:HB | 3:R:104:GOL:H2 | 1.67 | 0.77 |
| 1:V:37:CYS:SG | 2:V:220:HEC:C3C | 2.73 | 0.76 |
| 1:1:70:LYS:HG2 | 1:1:81:GLN:NE2 | 2.00 | 0.76 |
| 1:5:56:ASN:ND2 | 1:5:59:TYR:HB2 | 1.99 | 0.76 |
| 1:6:52:LEU:CD2 | 2:6:220:HEC:CMA | 2.60 | 0.76 |
| 1:S:37:CYS:SG | 2:S:220:HEC:C3C | 2.74 | 0.76 |
| 1:N:70:LYS:CD | 1:N:81:GLN:HE21 | 1.99 | 0.76 |
| 1:L:37:CYS:SG | 2:L:220:HEC:C3C | 2.73 | 0.76 |
| 1:Z:37:CYS:SG | 2:Z:220:HEC:C3C | 2.74 | 0.76 |
| 1:2:80:MET:CG | 2:2:220:HEC:C4D | 2.49 | 0.76 |
| 1:5:39:GLY:CA | 1:5:43:ASN:ND2 | 2.29 | 0.75 |
| 1:J:37:CYS:SG | 2:J:220:HEC:C3C | 2.75 | 0.75 |
| 1:3:56:ASN:HD22 | 1:3:59:TYR:H | 1.34 | 0.75 |
| 1:6:46:ILE:CD1 | 1:6:49:TYR:CD1 | 2.68 | 0.75 |
| 1:6:75:GLY:HA3 | 1:6:78:ALA:N | 2.01 | 0.75 |
| 1:W:23:ASP:H | 1:W:94:ASN:ND2 | 1.85 | 0.75 |
| 1:I:56:ASN:HD22 | 1:I:59:TYR:H | 1.32 | 0.75 |
| 1:E:83:GLN:HE21 | 1:O:83:GLN:NE2 | 1.81 | 0.74 |
| 1:Q:37:CYS:SG | 2:Q:220:HEC:C3C | 2.75 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:56:ASN:HD22 | 1:Y:59:TYR:H | 1.34 | 0.74 |
| 1:6:69:ASN:ND2 | 1:6:70:LYS:N | 2.27 | 0.74 |
| 1:6:77:ALA:CA | 2:6:220:HEC:O2D | 2.35 | 0.74 |
| 1:D:37:CYS:SG | 2:D:220:HEC:C3C | 2.75 | 0.74 |
| 1:6:88:SER:HB3 | 1:6:89:ASP:HB3 | 1.59 | 0.73 |
| 1:F:37:CYS:SG | 2:F:220:HEC:C3C | 2.76 | 0.73 |
| 1:5:56:ASN:ND2 | 1:5:59:TYR:CB | 2.51 | 0.73 |
| 1:6:60:ILE:CD1 | 1:6:96:ALA:CA | 2.66 | 0.73 |
| 1:U:37:CYS:SG | 2:U:220:HEC:CBC | 2.76 | 0.73 |
| 1:2:82:ALA:O | 1:2:86:LEU:HD12 | 1.87 | 0.73 |
| 1:I:44:ALA:H | 1:I:51:ASN:ND2 | 1.86 | 0.73 |
| 1:G:37:CYS:SG | 2:G:220:HEC:C3C | 2.76 | 0.73 |
| 1:3:69:ASN:O | 1:3:70:LYS:HG3 | 1.89 | 0.73 |
| 1:5:70:LYS:HE2 | 1:5:81:GLN:NE2 | 2.04 | 0.72 |
| 1:6:88:SER:CB | 1:6:89:ASP:CA | 2.67 | 0.72 |
| 1:5:56:ASN:HD21 | 1:5:59:TYR:HB2 | 1.54 | 0.72 |
| 1:6:60:ILE:CD1 | 1:6:96:ALA:HA | 2.18 | 0.72 |
| 1:J:23:ASP:H | 1:J:94:ASN:HD22 | 1.38 | 0.72 |
| 1:3:44:ALA:H | 1:3:51:ASN:HD22 | 1.37 | 0.72 |
| 1:T:68:LYS:NZ | 1:T:87:LEU:O | 2.22 | 0.72 |
| 1:3:75:GLY:N | 1:3:76:LEU:HD23 | 2.05 | 0.72 |
| 1:Q:71:GLU:OE1 | 1:R:74:GLY:HA3 | 1.90 | 0.71 |
| 1:U:44:ALA:H | 1:U:51:ASN:HD22 | 1.36 | 0.71 |
| 2:S:220:HEC:HBB3 | 2:S:220:HEC:HMB1 | 1.72 | 0.71 |
| 1:U:43:ASN:HD21 | 1:U:53:LYS:NZ | 1.88 | 0.71 |
| 1:6:28:GLN:HE21 | 1:6:98:TYR:HE2 | 1.38 | 0.71 |
| 1:6:68:LYS:HD3 | 1:6:87:LEU:HD11 | 1.73 | 0.71 |
| 1:3:56:ASN:HD21 | 1:4:48:GLY:H | 1.38 | 0.71 |
| 1:6:79:VAL:HG23 | 2:6:220:HEC:HBC2 | 1.73 | 0.71 |
| 1:A:37:CYS:SG | 2:A:220:HEC:HAC | 2.29 | 0.71 |
| 1:S:44:ALA:H | 1:S:51:ASN:HD22 | 1.38 | 0.71 |
| 1:5:79:VAL:HG11 | 2:5:220:HEC:CBC | 2.20 | 0.71 |
| 1:6:75:GLY:HA3 | 1:6:77:ALA:N | 2.03 | 0.71 |
| 1:1:55:GLN:HE22 | 1:2:51:ASN:H | 1.36 | 0.70 |
| 1:R:33:VAL:CG1 | 1:R:33:VAL:O | 2.38 | 0.70 |
| 1:5:41:ASP:C | 1:5:41:ASP:OD2 | 2.29 | 0.70 |
| 1:6:68:LYS:CD | 1:6:87:LEU:HD11 | 2.22 | 0.70 |
| 1:1:70:LYS:HG2 | 1:1:81:GLN:HE21 | 1.56 | 0.70 |
| 1:R:45:THR:H | 3:R:104:GOL:H31 | 0.68 | 0.70 |
| 1:2:80:MET:HG2 | 2:2:220:HEC:ND | 1.91 | 0.70 |
| 1:6:83:GLN:HG3 | 2:6:220:HEC:C2C | 2.21 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:23:ASP:H | 1:J:94:ASN:ND2 | 1.90 | 0.69 |
| 1:6:60:ILE:HD11 | 1:6:96:ALA:HB1 | 1.64 | 0.69 |
| 1:A:37:CYS:SG | 2:A:220:HEC:C3C | 2.80 | 0.69 |
| 1:3:76:LEU:CD2 | 1:3:78:ALA:HB3 | 2.23 | 0.69 |
| 2:G:220:HEC:HBC3 | 2:G:220:HEC:HMC1 | 1.74 | 0.69 |
| 1:I:37:CYS:SG | 2:I:220:HEC:CBC | 2.80 | 0.69 |
| 1:6:60:ILE:HG22 | 2:6:220:HEC:HMA2 | 1.75 | 0.68 |
| 1:H:37:CYS:SG | 2:H:220:HEC:C3C | 2.81 | 0.68 |
| 1:5:38:HIS:O | 1:5:43:ASN:ND2 | 2.25 | 0.68 |
| 1:O:56:ASN:HD22 | 1:O:59:TYR:H | 1.42 | 0.68 |
| 1:6:71:GLU:CD | 1:6:71:GLU:O | 2.32 | 0.68 |
| 1:5:33:VAL:O | 2:5:220:HEC:HMC3 | 1.94 | 0.68 |
| 1:4:75:GLY:O | 1:4:76:LEU:HB2 | 1.92 | 0.68 |
| 1:M:98:TYR:C | 1:M:100:SER:H | 1.93 | 0.68 |
| 1:Y:98:TYR:O | 1:Y:102:LEU:HD13 | 1.93 | 0.68 |
| 2:Z:220:HEC:HBC3 | 2:Z:220:HEC:HMC1 | 1.76 | 0.68 |
| 1:6:46:ILE:HD13 | 1:6:49:TYR:CG | 2.29 | 0.67 |
| 1:5:38:HIS:O | 1:5:43:ASN:N | 2.27 | 0.67 |
| 1:3:76:LEU:HD22 | 1:3:78:ALA:HB3 | 1.76 | 0.67 |
| 1:6:85:SER:O | 1:6:86:LEU:HB3 | 1.94 | 0.67 |
| 1:5:53:LYS:O | 1:5:53:LYS:HD3 | 1.95 | 0.67 |
| 1:H:41:ASP:OD1 | 1:H:41:ASP:N | 2.27 | 0.67 |
| 1:C:37:CYS:SG | 2:C:220:HEC:C3C | 2.83 | 0.67 |
| 1:L:79:VAL:CG1 | 2:L:220:HEC:HBC2 | 2.25 | 0.67 |
| 1:J:30:LYS:CE | 1:J:91:ASP:CB | 2.72 | 0.67 |
| 1:U:56:ASN:HD22 | 1:U:59:TYR:H | 1.43 | 0.67 |
| 1:5:44:ALA:CB | 1:5:49:TYR:C | 2.63 | 0.66 |
| 1:2:35:ALA:O | 1:2:39:GLY:CA | 2.43 | 0.66 |
| 1:M:43:ASN:HB2 | 1:M:53:LYS:HG3 | 1.76 | 0.66 |
| 1:F:44:ALA:H | 1:F:51:ASN:ND2 | 1.93 | 0.66 |
| 1:6:76:LEU:HD13 | 2:6:220:HEC:CGD | 2.25 | 0.66 |
| 1:Z:41:ASP:HB3 | 1:Z:43:ASN:CB | 2.25 | 0.66 |
| 1:6:86:LEU:O | 1:6:86:LEU:CD1 | 2.35 | 0.66 |
| 1:6:68:LYS:HB2 | 1:6:68:LYS:NZ | 2.10 | 0.66 |
| 1:I:37:CYS:SG | 2:I:220:HEC:C3C | 2.83 | 0.66 |
| 1:6:76:LEU:N | 1:6:76:LEU:CD1 | 2.59 | 0.66 |
| 1:2:86:LEU:O | 1:2:87:LEU:CD1 | 2.43 | 0.66 |
| 1:N:40:ALA:C | 1:N:42:GLY:H | 1.99 | 0.66 |
| 1:K:47:PRO:HB3 | 1:L:58:GLN:NE2 | 2.11 | 0.66 |
| 1:6:65:LYS:HB2 | 1:6:65:LYS:NZ | 2.11 | 0.65 |
| 1:6:52:LEU:HD21 | 2:6:220:HEC:C3A | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:44:ALA:H | 1:W:51:ASN:HD22 | 1.45 | 0.65 |
| 1:5:59:TYR:OH | 1:5:72:ARG:NH2 | 2.27 | 0.65 |
| 1:5:46:ILE:CG1 | 1:5:47:PRO:N | 2.56 | 0.65 |
| 1:I:37:CYS:SG | 2:I:220:HEC:HAC | 2.33 | 0.65 |
| 2:X:220:HEC:HBB3 | 2:X:220:HEC:HMB1 | 1.78 | 0.65 |
| 1:5:71:GLU:CD | 1:6:74:GLY:HA3 | 2.18 | 0.64 |
| 1:6:99:TYR:HE2 | 2:6:220:HEC:HMB3 | 1.61 | 0.64 |
| 1:C:23:ASP:H | 1:C:94:ASN:HD22 | 1.43 | 0.64 |
| 1:6:64:ILE:HD12 | 1:6:92:ILE:HG23 | 1.80 | 0.64 |
| 1:A:58:GLN:HG2 | 4:F:1412:HOH:O | 1.97 | 0.64 |
| 1:M:42:GLY:O | 1:M:53:LYS:HB2 | 1.98 | 0.63 |
| 1:6:78:ALA:HA | 1:6:81:GLN:CB | 2.27 | 0.63 |
| 1:6:46:ILE:CD1 | 1:6:49:TYR:CE1 | 2.81 | 0.63 |
| 1:2:82:ALA:O | 1:2:86:LEU:HD13 | 1.96 | 0.63 |
| 1:1:55:GLN:NE2 | 1:1:56:ASN:H | 1.94 | 0.63 |
| 1:J:30:LYS:HE3 | 1:J:87:LEU:HD22 | 1.81 | 0.63 |
| 1:5:75:GLY:C | 1:5:77:ALA:H | 2.01 | 0.63 |
| 2:C:220:HEC:HMC1 | 2:C:220:HEC:HBC3 | 1.81 | 0.63 |
| 1:2:79:VAL:HG12 | 2:2:220:HEC:HBC2 | 1.81 | 0.63 |
| 1:J:30:LYS:HE2 | 1:J:91:ASP:CB | 2.29 | 0.62 |
| 1:I:73:SER:HB3 | 1:4:28:GLN:HE21 | 1.65 | 0.62 |
| 1:L:75:GLY:HA2 | 1:L:78:ALA:H | 1.65 | 0.62 |
| 2:D:220:HEC:HMB1 | 2:D:220:HEC:HBB3 | 1.82 | 0.62 |
| 1:G:37:CYS:SG | 2:G:220:HEC:CBC | 2.88 | 0.62 |
| 2:K:220:HEC:HMC1 | 2:K:220:HEC:HBC3 | 1.81 | 0.62 |
| 1:C:37:CYS:SG | 2:C:220:HEC:CBC | 2.88 | 0.62 |
| 1:5:38:HIS:C | 1:5:43:ASN:HD22 | 2.03 | 0.61 |
| 1:M:98:TYR:C | 1:M:100:SER:N | 2.52 | 0.61 |
| 1:3:88:SER:O | 1:3:92:ILE:HG13 | 2.00 | 0.61 |
| 1:M:98:TYR:O | 1:M:100:SER:N | 2.33 | 0.61 |
| 1:1:56:ASN:HB3 | 4:1:466:HOH:O | 1.99 | 0.61 |
| 1:Z:41:ASP:CB | 1:Z:43:ASN:H | 2.12 | 0.61 |
| 1:5:80:MET:HE3 | 2:5:220:HEC:C4D | 2.30 | 0.61 |
| 1:K:48:GLY:N | 1:L:56:ASN:HD21 | 1.99 | 0.61 |
| 1:6:23:ASP:N | 1:6:94:ASN:CB | 2.56 | 0.60 |
| 1:5:46:ILE:HB | 1:5:47:PRO:HD2 | 1.83 | 0.60 |
| 1:N:44:ALA:N | 1:N:51:ASN:ND2 | 2.44 | 0.60 |
| 1:1:70:LYS:CG | 1:1:81:GLN:NE2 | 2.61 | 0.60 |
| 1:Z:37:CYS:SG | 2:Z:220:HEC:CBC | 2.88 | 0.60 |
| 1:H:58:GLN:HG3 | 4:H:719:HOH:O | 2.01 | 0.60 |
| 1:3:69:ASN:C | 1:3:70:LYS:HG3 | 2.22 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:33:VAL:HG13 | 1:M:34:CYS:SG | 2.42 | 0.60 |
| 1:C:23:ASP:H | 1:C:94:ASN:ND2 | 2.00 | 0.60 |
| 1:M:23:ASP:C | 1:M:23:ASP:OD1 | 2.39 | 0.60 |
| 2:A:220:HEC:HBC3 | 2:A:220:HEC:HMC1 | 1.84 | 0.60 |
| 1:V:37:CYS:SG | 2:V:220:HEC:CBC | 2.88 | 0.59 |
| 1:M:40:ALA:N | 1:M:41:ASP:OD2 | 2.36 | 0.59 |
| 1:6:70:LYS:HB2 | 1:6:71:GLU:CB | 2.32 | 0.59 |
| 2:F:220:HEC:HMC1 | 2:F:220:HEC:HBC3 | 1.85 | 0.59 |
| 1:J:30:LYS:HE2 | 1:J:91:ASP:HB3 | 1.83 | 0.59 |
| 1:H:41:ASP:OD2 | 1:H:43:ASN:CB | 2.40 | 0.59 |
| 2:3:220:HEC:HBB3 | 2:3:220:HEC:HMB1 | 1.84 | 0.59 |
| 2:4:220:HEC:CBC | 2:4:220:HEC:HMC1 | 2.32 | 0.59 |
| 1:5:95:LEU:HD13 | 2:5:220:HEC:HMB1 | 1.85 | 0.59 |
| 1:6:60:ILE:HD12 | 1:6:96:ALA:HB2 | 1.79 | 0.59 |
| 1:6:70:LYS:HG3 | 1:6:71:GLU:HB2 | 1.85 | 0.59 |
| 2:D:220:HEC:HMC1 | 2:D:220:HEC:HBC3 | 1.85 | 0.58 |
| 1:J:57:GLU:N | 1:J:57:GLU:CD | 2.50 | 0.58 |
| 1:D:37:CYS:SG | 2:D:220:HEC:CBC | 2.91 | 0.58 |
| 1:S:37:CYS:HG | 2:S:220:HEC:HAC | 1.67 | 0.58 |
| 1:B:56:ASN:HD22 | 1:B:59:TYR:H | 1.51 | 0.58 |
| 1:A:48:GLY:H | 1:B:56:ASN:HD21 | 1.51 | 0.58 |
| 1:3:70:LYS:O | 1:3:70:LYS:HE3 | 2.04 | 0.58 |
| 2:E:220:HEC:HBB3 | 2:E:220:HEC:HMB1 | 1.86 | 0.58 |
| 1:M:37:CYS:SG | 2:M:220:HEC:C3C | 2.91 | 0.58 |
| 1:5:44:ALA:CB | 1:5:49:TYR:CB | 2.39 | 0.58 |
| 1:U:43:ASN:ND2 | 1:U:53:LYS:HD3 | 2.19 | 0.58 |
| 1:Y:37:CYS:SG | 2:Y:220:HEC:CBC | 2.92 | 0.57 |
| 1:K:48:GLY:H | 1:L:56:ASN:HD21 | 1.52 | 0.57 |
| 1:4:75:GLY:O | 1:4:76:LEU:CB | 2.51 | 0.57 |
| 1:V:44:ALA:H | 1:V:51:ASN:ND2 | 1.96 | 0.57 |
| 1:S:55:GLN:HB3 | 1:S:60:ILE:HD11 | 1.86 | 0.57 |
| 1:6:68:LYS:NZ | 1:6:68:LYS:CB | 2.66 | 0.57 |
| 1:U:43:ASN:HD21 | 1:U:53:LYS:CE | 2.16 | 0.57 |
| 1:5:58:GLN:HG3 | 4:5:1352:HOH:O | 2.04 | 0.57 |
| 1:3:76:LEU:CD1 | 1:3:79:VAL:HG23 | 2.31 | 0.57 |
| 1:N:40:ALA:O | 1:N:42:GLY:N | 2.37 | 0.57 |
| 2:O:220:HEC:HBB3 | 2:O:220:HEC:HMB1 | 1.85 | 0.57 |
| 1:H:37:CYS:SG | 2:H:220:HEC:HBC3 | 2.44 | 0.57 |
| 1:M:57:GLU:CD | 4:M:849:HOH:O | 2.42 | 0.57 |
| 1:5:90:ASP:OD1 | 1:5:90:ASP:N | 2.37 | 0.56 |
| 1:S:36:ALA:HB3 | 4:S:429:HOH:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:34:CYS:HB2 | 1:M:99:TYR:OH | 2.04 | 0.56 |
| 1:Y:41:ASP:O | 1:Y:41:ASP:CG | 2.43 | 0.56 |
| 1:U:56:ASN:ND2 | 1:U:59:TYR:H | 2.02 | 0.56 |
| 1:5:51:ASN:C | 1:5:52:LEU:HD13 | 2.25 | 0.56 |
| 1:5:55:GLN:HE21 | 1:5:59:TYR:HD2 | 1.52 | 0.56 |
| 1:5:44:ALA:HB3 | 1:5:49:TYR:O | 2.05 | 0.56 |
| 1:Q:37:CYS:SG | 2:Q:220:HEC:HBC3 | 2.44 | 0.56 |
| 1:6:70:LYS:HB2 | 1:6:71:GLU:HB2 | 1.87 | 0.56 |
| 1:H:44:ALA:H | 1:H:51:ASN:ND2 | 2.00 | 0.56 |
| 1:6:28:GLN:NE2 | 1:6:98:TYR:CE2 | 2.63 | 0.56 |
| 1:B:56:ASN:ND2 | 1:B:58:GLN:OE1 | 2.39 | 0.56 |
| 1:N:73:SER:O | 1:N:74:GLY:O | 2.24 | 0.56 |
| 1:R:44:ALA:HA | 3:R:104:GOL:H32 | 1.87 | 0.56 |
| 1:5:46:ILE:HG12 | 1:5:49:TYR:HE1 | 1.54 | 0.55 |
| 1:5:42:GLY:O | 1:5:43:ASN:CB | 2.53 | 0.55 |
| 1:P:33:VAL:HG23 | 4:P:842:HOH:O | 2.05 | 0.55 |
| 1:4:37:CYS:HG | 2:4:220:HEC:CAC | 2.14 | 0.55 |
| 1:O:56:ASN:ND2 | 1:O:59:TYR:H | 2.05 | 0.55 |
| 1:B:58:GLN:CD | 1:B:58:GLN:H | 2.09 | 0.55 |
| 1:E:41:ASP:OD2 | 1:E:53:LYS:NZ | 2.34 | 0.55 |
| 2:D:220:HEC:HBC3 | 2:L:220:HEC:HBC3 | 1.88 | 0.55 |
| 1:5:46:ILE:CB | 1:5:47:PRO:HD2 | 2.37 | 0.55 |
| 1:3:76:LEU:HD22 | 1:3:78:ALA:H | 1.71 | 0.55 |
| 1:6:95:LEU:HD13 | 2:6:220:HEC:HMB1 | 1.87 | 0.55 |
| 1:6:60:ILE:HG22 | 2:6:220:HEC:HMA3 | 1.84 | 0.55 |
| 1:1:55:GLN:HE22 | 1:2:51:ASN:N | 2.03 | 0.55 |
| 1:5:44:ALA:HB3 | 1:5:50:PRO:N | 2.23 | 0.54 |
| 1:B:46:ILE:HD12 | 4:B:114:HOH:O | 2.06 | 0.54 |
| 1:A:37:CYS:SG | 2:A:220:HEC:HBC3 | 2.44 | 0.54 |
| 1:2:80:MET:O | 1:2:80:MET:HE3 | 2.07 | 0.54 |
| 1:6:76:LEU:O | 1:6:79:VAL:HG13 | 2.08 | 0.54 |
| 1:J:30:LYS:HD3 | 1:J:95:LEU:CD1 | 2.35 | 0.54 |
| 1:U:44:ALA:H | 1:U:51:ASN:ND2 | 2.04 | 0.54 |
| 1:6:88:SER:OG | 1:6:89:ASP:CB | 2.45 | 0.54 |
| 2:S:220:HEC:HBC3 | 2:S:220:HEC:HMC1 | 1.89 | 0.54 |
| 1:5:38:HIS:C | 1:5:43:ASN:ND2 | 2.61 | 0.54 |
| 1:D:58:GLN:HG2 | 4:D:138:HOH:O | 2.07 | 0.54 |
| 1:3:67:TYR:CZ | 1:3:72:ARG:HD2 | 2.43 | 0.54 |
| 2:X:220:HEC:HMC1 | 2:X:220:HEC:HBC3 | 1.91 | 0.53 |
| 1:Q:37:CYS:SG | 2:Q:220:HEC:HAC | 2.38 | 0.53 |
| 1:5:80:MET:CE | 2:5:220:HEC:C4D | 2.86 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:70:LYS:CG | 1:L:81:GLN:NE2 | 2.57 | 0.53 |
| 1:N:74:GLY:O | 1:N:77:ALA:HB3 | 2.08 | 0.53 |
| 1:6:65:LYS:HB2 | 1:6:65:LYS:HZ2 | 1.74 | 0.53 |
| 1:H:37:CYS:SG | 2:H:220:HEC:HAC | 2.40 | 0.52 |
| 1:V:23:ASP:N | 1:V:94:ASN:HD22 | 1.89 | 0.52 |
| 1:6:46:ILE:HG23 | 1:6:49:TYR:CB | 2.36 | 0.52 |
| 1:6:46:ILE:HG21 | 1:6:49:TYR:CD2 | 2.44 | 0.52 |
| 1:5:72:ARG:HB3 | 4:5:1138:HOH:O | 2.07 | 0.52 |
| 1:E:40:ALA:HB3 | 4:E:622:HOH:O | 2.10 | 0.52 |
| 1:C:76:LEU:HG | 2:C:220:HEC:HMD1 | 1.91 | 0.52 |
| 1:F:37:CYS:SG | 2:F:220:HEC:CBC | 2.94 | 0.52 |
| 1:6:41:ASP:OD2 | 1:6:41:ASP:N | 2.41 | 0.52 |
| 1:5:46:ILE:CG1 | 1:5:49:TYR:CE1 | 2.65 | 0.52 |
| 1:6:52:LEU:CD2 | 2:6:220:HEC:C3A | 2.87 | 0.52 |
| 1:J:30:LYS:HE3 | 1:J:91:ASP:CB | 2.35 | 0.52 |
| 1:J:95:LEU:HD13 | 2:J:220:HEC:HMB1 | 1.91 | 0.52 |
| 1:6:85:SER:O | 1:6:86:LEU:CB | 2.58 | 0.52 |
| 1:F:56:ASN:HD22 | 1:F:59:TYR:H | 1.58 | 0.52 |
| 1:N:38:HIS:HE1 | 2:N:220:HEC:C4D | 2.22 | 0.52 |
| 1:M:41:ASP:O | 1:M:53:LYS:HG2 | 2.09 | 0.52 |
| 1:3:44:ALA:H | 1:3:51:ASN:ND2 | 2.05 | 0.52 |
| 1:E:48:GLY:H | 1:F:56:ASN:HD21 | 1.58 | 0.52 |
| 1:E:58:GLN:NE2 | 4:E:629:HOH:O | 2.42 | 0.52 |
| 1:S:30:LYS:HG3 | 1:S:95:LEU:HD21 | 1.91 | 0.52 |
| 2:Y:220:HEC:HMB1 | 2:Y:220:HEC:HBB3 | 1.91 | 0.51 |
| 2:M:220:HEC:HBB3 | 2:M:220:HEC:HMB1 | 1.92 | 0.51 |
| 1:M:79:VAL:CG1 | 2:M:220:HEC:HBC2 | 2.40 | 0.51 |
| 1:U:43:ASN:HD21 | 1:U:53:LYS:HD3 | 1.75 | 0.51 |
| 2:Y:220:HEC:O1A | 2:Z:220:HEC:O1A | 2.29 | 0.51 |
| 1:5:55:GLN:CD | 1:5:56:ASN:H | 2.13 | 0.51 |
| 1:M:27:GLY:HA3 | 1:M:94:ASN:O | 2.10 | 0.51 |
| 1:D:28:GLN:O | 1:D:28:GLN:HG2 | 2.07 | 0.51 |
| 1:A:48:GLY:H | 1:B:56:ASN:ND2 | 2.08 | 0.51 |
| 1:C:76:LEU:HB2 | 4:C:1107:HOH:O | 2.10 | 0.51 |
| 1:K:86:LEU:N | 1:K:86:LEU:CD1 | 2.74 | 0.51 |
| 1:3:56:ASN:ND2 | 1:4:48:GLY:H | 2.06 | 0.51 |
| 1:U:95:LEU:HD13 | 2:U:220:HEC:HMB1 | 1.92 | 0.51 |
| 1:5:56:ASN:ND2 | 1:5:59:TYR:HB3 | 2.26 | 0.51 |
| 1:N:40:ALA:C | 1:N:42:GLY:N | 2.64 | 0.51 |
| 4:I:1571:HOH:O | 1:J:47:PRO:HA | 2.10 | 0.51 |
| 1:6:46:ILE:CD1 | 1:6:49:TYR:CG | 2.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:5:46:ILE:HG12 | 1:5:49:TYR:CD1 | 2.38 | 0.51 |
| 1:W:69:ASN:C | 1:W:70:LYS:HG3 | 2.30 | 0.51 |
| 1:X:56:ASN:O | 1:X:60:ILE:HG13 | 2.10 | 0.51 |
| 1:O:56:ASN:ND2 | 1:P:48:GLY:H | 2.09 | 0.50 |
| 1:K:86:LEU:N | 1:K:86:LEU:HD13 | 2.26 | 0.50 |
| 1:J:46:ILE:HG13 | 1:J:47:PRO:HD2 | 1.93 | 0.50 |
| 1:3:76:LEU:HD22 | 1:3:78:ALA:CB | 2.41 | 0.50 |
| 1:6:37:CYS:CB | 2:6:220:HEC:C3C | 2.89 | 0.50 |
| 1:3:86:LEU:H | 1:3:86:LEU:HD12 | 1.76 | 0.50 |
| 1:N:82:ALA:O | 1:N:85:SER:OG | 2.25 | 0.50 |
| 1:6:80:MET:HG3 | 1:6:83:GLN:HB2 | 1.93 | 0.50 |
| 1:B:37:CYS:SG | 2:B:220:HEC:CBC | 2.95 | 0.50 |
| 2:G:220:HEC:HBC3 | 2:Y:220:HEC:HBC3 | 1.91 | 0.50 |
| 1:6:88:SER:HA | 1:6:91:ASP:OD1 | 2.12 | 0.50 |
| 1:A:33:VAL:HG23 | 4:A:1503:HOH:O | 2.10 | 0.50 |
| 2:G:220:HEC:HBC3 | 2:Y:220:HEC:CBC | 2.42 | 0.50 |
| 1:J:57:GLU:HG3 | 1:J:100:SER:CB | 2.42 | 0.50 |
| 1:Z:55:GLN:HB3 | 1:Z:60:ILE:HD11 | 1.94 | 0.50 |
| 1:T:56:ASN:ND2 | 1:T:59:TYR:H | 2.04 | 0.50 |
| 1:C:85:SER:HB3 | 1:6:26:ALA:HB2 | 1.93 | 0.50 |
| 1:5:51:ASN:O | 1:5:52:LEU:HD13 | 2.12 | 0.50 |
| 1:Z:41:ASP:HB3 | 1:Z:43:ASN:H | 1.77 | 0.49 |
| 1:M:33:VAL:CG2 | 4:M:511:HOH:O | 2.51 | 0.49 |
| 2:H:220:HEC:HBC3 | 2:H:220:HEC:HMC1 | 1.95 | 0.49 |
| 1:S:30:LYS:O | 1:S:33:VAL:HG22 | 2.12 | 0.49 |
| 1:6:60:ILE:CG2 | 2:6:220:HEC:CMA | 2.83 | 0.49 |
| 1:J:30:LYS:CE | 1:J:91:ASP:CG | 2.75 | 0.49 |
| 1:5:55:GLN:NE2 | 1:5:59:TYR:HD2 | 2.10 | 0.49 |
| 1:5:80:MET:CE | 2:5:220:HEC:ND | 2.74 | 0.49 |
| 2:T:220:HEC:HBC3 | 2:T:220:HEC:HMC1 | 1.93 | 0.49 |
| 1:5:80:MET:HE3 | 2:5:220:HEC:CHA | 2.43 | 0.49 |
| 1:6:86:LEU:N | 1:6:87:LEU:HB2 | 2.27 | 0.49 |
| 1:O:56:ASN:HD21 | 1:P:48:GLY:H | 1.61 | 0.49 |
| 1:6:71:GLU:OE2 | 1:6:71:GLU:O | 2.31 | 0.49 |
| 2:3:220:HEC:CMC | 2:3:220:HEC:HBC3 | 2.36 | 0.48 |
| 1:P:76:LEU:N | 4:P:1604:HOH:O | 2.35 | 0.48 |
| 1:W:44:ALA:H | 1:W:51:ASN:ND2 | 2.11 | 0.48 |
| 1:B:33:VAL:HG11 | 1:M:78:ALA:HB3 | 1.95 | 0.48 |
| 1:Z:61:VAL:CG1 | 1:Z:65:LYS:HE3 | 2.43 | 0.48 |
| 2:Q:220:HEC:HBC3 | 2:Q:220:HEC:HMC1 | 1.94 | 0.48 |
| 1:4:68:LYS:HE3 | 1:4:87:LEU:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:72:ARG:HG2 | 1:H:72:ARG:HG2 | 1.94 | 0.48 |
| 1:6:99:TYR:CE2 | 2:6:220:HEC:HMB3 | 2.46 | 0.48 |
| 1:N:38:HIS:HE1 | 2:N:220:HEC:ND | 1.98 | 0.48 |
| 1:M:42:GLY:O | 1:M:53:LYS:N | 2.33 | 0.48 |
| 1:2:33:VAL:HG22 | 1:2:33:VAL:O | 2.14 | 0.48 |
| 2:1:220:HEC:HMC1 | 2:1:220:HEC:HBC3 | 1.95 | 0.48 |
| 1:1:46:ILE:HG22 | 1:1:47:PRO:O | 2.12 | 0.48 |
| 1:6:87:LEU:HD23 | 1:6:88:SER:C | 2.34 | 0.48 |
| 1:5:34:CYS:C | 1:5:36:ALA:N | 2.65 | 0.48 |
| 1:4:76:LEU:N | 4:4:610:HOH:O | 2.37 | 0.48 |
| 1:J:37:CYS:CB | 2:J:220:HEC:C3C | 2.92 | 0.48 |
| 1:D:58:GLN:CG | 4:D:138:HOH:O | 2.61 | 0.48 |
| 1:U:76:LEU:HA | 1:U:76:LEU:HD23 | 1.60 | 0.48 |
| 1:6:85:SER:HA | 1:6:87:LEU:HD12 | 1.96 | 0.48 |
| 1:6:23:ASP:O | 1:6:94:ASN:CB | 2.44 | 0.48 |
| 1:6:75:GLY:HA2 | 1:6:77:ALA:N | 2.05 | 0.47 |
| 1:Z:41:ASP:C | 1:Z:43:ASN:H | 2.16 | 0.47 |
| 1:E:48:GLY:H | 1:F:56:ASN:ND2 | 2.12 | 0.47 |
| 1:N:58:GLN:H | 1:N:58:GLN:NE2 | 2.12 | 0.47 |
| 2:G:220:HEC:HMB1 | 2:G:220:HEC:HBB3 | 1.96 | 0.47 |
| 2:I:220:HEC:HBC3 | 2:I:220:HEC:HMC1 | 1.97 | 0.47 |
| 1:2:86:LEU:O | 1:2:87:LEU:CB | 2.63 | 0.47 |
| 1:5:70:LYS:HE2 | 1:5:81:GLN:HE22 | 1.78 | 0.47 |
| 1:6:70:LYS:CG | 1:6:71:GLU:HB2 | 2.45 | 0.47 |
| 1:6:93:ALA:O | 1:6:96:ALA:HB3 | 2.15 | 0.47 |
| 2:W:220:HEC:O1A | 2:X:220:HEC:O1A | 2.33 | 0.47 |
| 1:6:86:LEU:CA | 1:6:87:LEU:HB2 | 2.45 | 0.47 |
| 1:5:42:GLY:O | 1:5:43:ASN:HB3 | 2.15 | 0.47 |
| 1:R:44:ALA:HA | 3:R:104:GOL:C3 | 2.44 | 0.47 |
| 1:2:75:GLY:C | 1:2:77:ALA:H | 2.15 | 0.47 |
| 1:3:76:LEU:HA | 1:3:76:LEU:HD23 | 1.21 | 0.47 |
| 1:J:57:GLU:HG3 | 1:J:100:SER:OG | 2.15 | 0.47 |
| 1:6:77:ALA:O | 1:6:81:GLN:N | 2.48 | 0.46 |
| 2:S:220:HEC:CMB | 2:S:220:HEC:HBB3 | 2.42 | 0.46 |
| 1:D:58:GLN:HE22 | 1:F:79:VAL:HA | 1.81 | 0.46 |
| 2:4:220:HEC:HBC2 | 2:4:220:HEC:HMC1 | 1.97 | 0.46 |
| 1:2:35:ALA:HA | 1:2:39:GLY:HA2 | 1.96 | 0.46 |
| 1:J:46:ILE:HG12 | 1:J:49:TYR:CE1 | 2.50 | 0.46 |
| 1:M:43:ASN:N | 1:M:53:LYS:HB2 | 2.29 | 0.46 |
| 1:6:46:ILE:HG23 | 1:6:49:TYR:CG | 2.51 | 0.46 |
| 1:K:48:GLY:H | 1:L:56:ASN:ND2 | 2.12 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:220:HEC:HMC1 | 2:O:220:HEC:HBC3 | 1.98 | 0.46 |
| 2:A:220:HEC:HMC1 | 2:A:220:HEC:CBC | 2.46 | 0.46 |
| 1:M:79:VAL:HG13 | 2:M:220:HEC:HBC2 | 1.98 | 0.46 |
| 1:D:30:LYS:O | 1:D:33:VAL:HG22 | 2.16 | 0.46 |
| 1:N:28:GLN:NE2 | 1:W:40:ALA:H | 2.13 | 0.46 |
| 1:C:80:MET:CE | 2:C:220:HEC:NB | 2.78 | 0.46 |
| 1:K:49:TYR:N | 1:L:56:ASN:HD21 | 2.14 | 0.46 |
| 2:G:220:HEC:O1A | 2:H:220:HEC:O1A | 2.34 | 0.46 |
| 1:6:88:SER:HB3 | 1:6:89:ASP:CG | 2.35 | 0.46 |
| 1:S:39:GLY:HA3 | 1:S:43:ASN:O | 2.16 | 0.46 |
| 1:6:60:ILE:O | 1:6:61:VAL:C | 2.53 | 0.46 |
| 1:2:75:GLY:HA3 | 1:2:77:ALA:CB | 2.45 | 0.46 |
| 1:S:37:CYS:CB | 2:S:220:HEC:C3C | 2.94 | 0.46 |
| 1:L:56:ASN:ND2 | 1:L:59:TYR:HB2 | 2.31 | 0.46 |
| 1:M:57:GLU:CD | 1:M:97:ALA:HA | 2.35 | 0.46 |
| 1:Z:98:TYR:O | 1:Z:101:SER:HB2 | 2.15 | 0.46 |
| 1:U:37:CYS:CB | 2:U:220:HEC:C3C | 2.94 | 0.46 |
| 1:N:38:HIS:CD2 | 2:N:220:HEC:C4B | 2.99 | 0.46 |
| 1:S:46:ILE:HG23 | 1:S:47:PRO:HD2 | 1.98 | 0.46 |
| 1:V:37:CYS:CB | 2:V:220:HEC:C3C | 2.94 | 0.45 |
| 1:2:35:ALA:C | 1:2:39:GLY:HA2 | 2.37 | 0.45 |
| 1:6:89:ASP:OD2 | 1:6:89:ASP:N | 2.36 | 0.45 |
| 1:2:79:VAL:CG1 | 2:2:220:HEC:HBC2 | 2.46 | 0.45 |
| 1:R:43:ASN:HD21 | 1:R:53:LYS:HD3 | 1.81 | 0.45 |
| 2:M:220:HEC:O1A | 2:N:220:HEC:O1A | 2.34 | 0.45 |
| 1:5:82:ALA:O | 1:5:85:SER:HB3 | 2.17 | 0.45 |
| 1:S:38:HIS:CD2 | 2:S:220:HEC:NB | 2.84 | 0.45 |
| 1:F:74:GLY:C | 4:F:1568:HOH:O | 2.54 | 0.45 |
| 2:U:220:HEC:O1A | 2:V:220:HEC:O1A | 2.34 | 0.45 |
| 1:5:63:SER:O | 1:5:66:ALA:HB3 | 2.17 | 0.45 |
| 1:Y:56:ASN:ND2 | 1:Y:59:TYR:H | 2.08 | 0.45 |
| 1:T:43:ASN:ND2 | 1:T:53:LYS:HD3 | 2.32 | 0.45 |
| 1:G:30:LYS:O | 1:G:33:VAL:HG22 | 2.16 | 0.45 |
| 1:3:76:LEU:HD13 | 1:3:79:VAL:CG2 | 2.35 | 0.45 |
| 2:O:220:HEC:O1A | 2:P:220:HEC:O1A | 2.35 | 0.45 |
| 1:5:43:ASN:CA | 1:5:51:ASN:OD1 | 2.57 | 0.45 |
| 1:N:58:GLN:N | 1:N:58:GLN:CD | 2.70 | 0.45 |
| 1:6:67:TYR:CZ | 2:6:220:HEC:HHA | 2.52 | 0.45 |
| 1:3:95:LEU:HD13 | 2:3:220:HEC:HMB1 | 1.99 | 0.45 |
| 1:E:28:GLN:HB2 | 1:E:98:TYR:CE1 | 2.52 | 0.45 |
| 1:V:30:LYS:O | 1:V:33:VAL:HG22 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:220:HEC:O1A | 2:J:220:HEC:O1A | 2.34 | 0.44 |
| 1:2:76:LEU:O | 1:2:79:VAL:HG23 | 2.17 | 0.44 |
| 1:W:80:MET:HG3 | 1:W:80:MET:O | 2.17 | 0.44 |
| 2:K:220:HEC:O1A | 2:L:220:HEC:O1A | 2.36 | 0.44 |
| 2:M:220:HEC:HBC3 | 2:M:220:HEC:HMC1 | 1.98 | 0.44 |
| 1:3:76:LEU:HD22 | 1:3:78:ALA:N | 2.32 | 0.44 |
| 1:3:76:LEU:HD21 | 1:3:78:ALA:HB3 | 1.95 | 0.44 |
| 1:6:60:ILE:HA | 1:6:63:SER:OG | 2.18 | 0.44 |
| 1:6:46:ILE:HD12 | 1:6:49:TYR:CE2 | 2.52 | 0.44 |
| 1:4:60:ILE:HG21 | 1:4:96:ALA:HA | 1.99 | 0.44 |
| 1:U:58:GLN:NE2 | 1:V:47:PRO:HB3 | 2.33 | 0.44 |
| 1:4:61:VAL:HG23 | 1:4:96:ALA:CB | 2.48 | 0.44 |
| 1:6:52:LEU:HD22 | 2:6:220:HEC:HMA1 | 1.92 | 0.44 |
| 1:U:43:ASN:HD21 | 1:U:53:LYS:CD | 2.30 | 0.44 |
| 1:E:28:GLN:HB2 | 1:E:98:TYR:CD1 | 2.52 | 0.44 |
| 1:T:76:LEU:HA | 1:T:76:LEU:HD23 | 1.56 | 0.44 |
| 1:R:39:GLY:HA2 | 3:R:104:GOL:H12 | 1.99 | 0.44 |
| 1:6:89:ASP:HB3 | 1:6:92:ILE:HG13 | 1.99 | 0.44 |
| 1:M:55:GLN:O | 1:M:100:SER:HB2 | 2.17 | 0.44 |
| 1:I:37:CYS:SG | 2:I:220:HEC:HBC3 | 2.56 | 0.44 |
| 1:4:74:GLY:O | 1:4:77:ALA:HB3 | 2.18 | 0.44 |
| 1:6:76:LEU:C | 1:6:76:LEU:HD13 | 2.38 | 0.43 |
| 1:G:37:CYS:CB | 2:G:220:HEC:C3C | 2.95 | 0.43 |
| 1:P:23:ASP:C | 1:P:23:ASP:OD1 | 2.56 | 0.43 |
| 1:6:46:ILE:HD12 | 1:6:49:TYR:CZ | 2.53 | 0.43 |
| 1:P:95:LEU:HD13 | 2:P:220:HEC:HMB1 | 2.00 | 0.43 |
| 1:2:75:GLY:HA3 | 1:2:77:ALA:CA | 2.40 | 0.43 |
| 1:2:70:LYS:HE2 | 1:2:70:LYS:HB3 | 1.76 | 0.43 |
| 1:H:46:ILE:HG22 | 1:H:47:PRO:O | 2.18 | 0.43 |
| 1:K:82:ALA:O | 1:K:86:LEU:HD13 | 2.18 | 0.43 |
| 1:2:76:LEU:HD23 | 1:2:79:VAL:HG21 | 2.01 | 0.43 |
| 1:2:73:SER:C | 1:2:75:GLY:N | 2.69 | 0.43 |
| 1:N:38:HIS:HD2 | 2:N:220:HEC:C4B | 2.32 | 0.43 |
| 1:A:72:ARG:HG2 | 1:B:72:ARG:HG2 | 2.01 | 0.43 |
| 1:K:88:SER:O | 1:K:92:ILE:HG13 | 2.18 | 0.43 |
| 2:5:220:HEC:HHA | 2:5:220:HEC:HBD1 | 2.01 | 0.43 |
| 1:T:30:LYS:HE2 | 1:T:91:ASP:CG | 2.38 | 0.43 |
| 1:N:25:ALA:HA | 1:W:45:THR:OG1 | 2.19 | 0.43 |
| 2:3:220:HEC:CMB | 2:3:220:HEC:HBB3 | 2.48 | 0.43 |
| 2:F:220:HEC:HBB3 | 2:F:220:HEC:HMB1 | 2.01 | 0.42 |
| 1:6:28:GLN:NE2 | 1:6:98:TYR:HE2 | 2.09 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:5:75:GLY:C | 1:5:77:ALA:N | 2.68 | 0.42 |
| 1:R:43:ASN:ND2 | 1:R:53:LYS:HD3 | 2.34 | 0.42 |
| 1:N:76:LEU:HA | 1:N:76:LEU:HD23 | 1.84 | 0.42 |
| 1:E:33:VAL:HB | 1:O:79:VAL:HG21 | 2.00 | 0.42 |
| 1:V:41:ASP:N | 1:V:41:ASP:OD2 | 2.50 | 0.42 |
| 1:M:45:THR:HG22 | 1:M:46:ILE:N | 2.35 | 0.42 |
| 1:R:65:LYS:O | 1:R:69:ASN:ND2 | 2.46 | 0.42 |
| 2:A:220:HEC:O1A | 2:B:220:HEC:O1A | 2.38 | 0.42 |
| 1:5:38:HIS:ND1 | 1:5:52:LEU:HD22 | 2.35 | 0.42 |
| 1:6:78:ALA:O | 1:6:81:GLN:HB3 | 2.19 | 0.42 |
| 1:J:39:GLY:O | 1:J:40:ALA:C | 2.57 | 0.42 |
| 2:X:220:HEC:HBB3 | 2:X:220:HEC:CMB | 2.48 | 0.42 |
| 1:6:80:MET:SD | 2:6:220:HEC:C1D | 2.86 | 0.42 |
| 1:5:52:LEU:HD12 | 1:5:52:LEU:HA | 1.47 | 0.42 |
| 2:Q:220:HEC:O1A | 2:R:220:HEC:O1A | 2.37 | 0.42 |
| 1:K:48:GLY:C | 1:L:56:ASN:HD21 | 2.22 | 0.42 |
| 1:J:39:GLY:HA3 | 1:J:43:ASN:O | 2.20 | 0.42 |
| 1:2:41:ASP:O | 1:2:102:LEU:HD13 | 2.20 | 0.42 |
| 1:6:33:VAL:O | 2:6:220:HEC:HMC3 | 2.19 | 0.42 |
| 1:S:83:GLN:HG3 | 2:S:220:HEC:C2C | 2.50 | 0.42 |
| 1:5:39:GLY:N | 1:5:43:ASN:ND2 | 2.68 | 0.42 |
| 1:2:86:LEU:H | 1:2:86:LEU:HD12 | 1.84 | 0.42 |
| 1:Z:41:ASP:HB3 | 1:Z:43:ASN:N | 2.35 | 0.42 |
| 1:5:66:ALA:HB1 | 1:5:72:ARG:HG3 | 2.01 | 0.42 |
| 1:J:33:VAL:HG13 | 1:J:34:CYS:H | 1.84 | 0.42 |
| 1:N:30:LYS:O | 1:N:30:LYS:HG3 | 2.20 | 0.42 |
| 1:Q:70:LYS:HD3 | 1:Q:81:GLN:NE2 | 2.34 | 0.42 |
| 1:D:37:CYS:CB | 2:D:220:HEC:C3C | 2.98 | 0.41 |
| 1:X:37:CYS:CB | 2:X:220:HEC:C3C | 2.97 | 0.41 |
| 1:Y:56:ASN:HD22 | 1:Y:59:TYR:N | 2.09 | 0.41 |
| 1:E:33:VAL:HB | 1:O:79:VAL:CG2 | 2.50 | 0.41 |
| 1:W:30:LYS:HE3 | 1:W:30:LYS:HB3 | 1.84 | 0.41 |
| 1:R:46:ILE:HA | 1:R:47:PRO:HD2 | 1.66 | 0.41 |
| 2:S:220:HEC:O1A | 2:T:220:HEC:O1A | 2.37 | 0.41 |
| 1:6:80:MET:CE | 2:6:220:HEC:C4B | 2.88 | 0.41 |
| 1:5:79:VAL:CG1 | 2:5:220:HEC:CBC | 2.93 | 0.41 |
| 1:I:81:GLN:HE22 | 1:4:28:GLN:NE2 | 2.18 | 0.41 |
| 1:L:38:HIS:CD2 | 2:L:220:HEC:NB | 2.89 | 0.41 |
| 1:Y:38:HIS:CD2 | 2:Y:220:HEC:NB | 2.86 | 0.41 |
| 1:Z:41:ASP:C | 1:Z:43:ASN:N | 2.74 | 0.41 |
| 1:4:56:ASN:ND2 | 1:4:59:TYR:H | 2.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:5:53:LYS:O | 1:5:53:LYS:CD | 2.67 | 0.41 |
| 1:E:43:ASN:HA | 1:E:43:ASN:HD22 | 1.63 | 0.41 |
| 1:5:98:TYR:O | 1:5:101:SER:OG | 2.24 | 0.41 |
| 1:J:71:GLU:OE2 | 1:4:23:ASP:OD2 | 2.39 | 0.41 |
| 1:M:79:VAL:HG11 | 2:M:220:HEC:HBC2 | 2.03 | 0.41 |
| 1:K:48:GLY:CA | 1:L:56:ASN:HD21 | 2.32 | 0.41 |
| 1:P:61:VAL:O | 1:P:65:LYS:HG3 | 2.20 | 0.41 |
| 1:J:61:VAL:HG12 | 1:J:65:LYS:HE2 | 2.01 | 0.41 |
| 2:3:220:HEC:O1A | 2:4:220:HEC:O1A | 2.38 | 0.41 |
| 1:2:86:LEU:O | 1:2:87:LEU:HB2 | 2.21 | 0.41 |
| 1:3:31:ALA:O | 1:3:32:ALA:C | 2.58 | 0.41 |
| 1:6:77:ALA:N | 2:6:220:HEC:O2D | 2.53 | 0.41 |
| 1:F:56:ASN:ND2 | 1:F:59:TYR:H | 2.16 | 0.41 |
| 1:3:56:ASN:HD22 | 1:3:59:TYR:N | 2.10 | 0.41 |
| 1:3:56:ASN:ND2 | 1:3:59:TYR:H | 2.11 | 0.41 |
| 1:6:34:CYS:HA | 2:6:220:HEC:CHC | 2.50 | 0.41 |
| 1:A:37:CYS:CB | 2:A:220:HEC:C3C | 2.99 | 0.41 |
| 1:W:83:GLN:HG3 | 2:W:220:HEC:C2C | 2.51 | 0.41 |
| 1:6:62:SER:O | 1:6:65:LYS:HB3 | 2.20 | 0.41 |
| 1:4:23:ASP:HB3 | 1:4:26:ALA:HB3 | 2.03 | 0.41 |
| 1:1:43:ASN:HD22 | 1:1:51:ASN:HB3 | 1.86 | 0.41 |
| 1:M:41:ASP:OD1 | 1:M:43:ASN:HB3 | 2.20 | 0.41 |
| 1:H:37:CYS:CB | 2:H:220:HEC:C3C | 2.99 | 0.40 |
| 1:5:42:GLY:O | 1:5:43:ASN:CG | 2.58 | 0.40 |
| 1:2:53:LYS:HZ3 | 1:2:102:LEU:C | 2.24 | 0.40 |
| 1:4:64:ILE:HG21 | 1:4:92:ILE:HG12 | 2.02 | 0.40 |
| 1:M:73:SER:O | 1:N:71:GLU:HB3 | 2.21 | 0.40 |
| 1:P:88:SER:O | 1:P:92:ILE:HG13 | 2.21 | 0.40 |
| 1:H:41:ASP:CG | 1:H:43:ASN:H | 2.24 | 0.40 |
| 1:R:74:GLY:N | 4:R:915:HOH:O | 2.41 | 0.40 |
| 1:1:79:VAL:HG13 | 2:1:220:HEC:HBC2 | 2.03 | 0.40 |
| 2:C:220:HEC:O1A | 2:D:220:HEC:O1A | 2.40 | 0.40 |
| 2:E:220:HEC:O1A | 2:F:220:HEC:O1A | 2.39 | 0.40 |
| 1:U:43:ASN:HD21 | 1:U:53:LYS:HZ2 | 1.66 | 0.40 |
| 1:K:49:TYR:N | 1:L:56:ASN:ND2 | 2.69 | 0.40 |
| 1:1:69:ASN:HB2 | 1:1:71:GLU:OE2 | 2.22 | 0.40 |
| 1:5:46:ILE:CB | 1:5:47:PRO:CD | 2.97 | 0.40 |
| 1:1:78:ALA:HA | 1:1:81:GLN:HB3 | 2.02 | 0.40 |
| 1:1:43:ASN:HD22 | 1:1:43:ASN:HA | 1.67 | 0.40 |
| 1:L:37:CYS:CB | 2:L:220:HEC:C3C | 2.99 | 0.40 |
| 1:5:34:CYS:C | 1:5:36:ALA:H | 2.24 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|--------------|-----------|---------|----------|-------------|-----|
| 1 | 1 | 79/103 (77%) | 77 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | 2 | 79/103 (77%) | 72 (91%) | 4 (5%) | 3 (4%) | 4 | 0 |
| 1 | 3 | 79/103 (77%) | 76 (96%) | 2 (2%) | 1 (1%) | 15 | 4 |
| 1 | 4 | 79/103 (77%) | 75 (95%) | 2 (2%) | 2 (2%) | 7 | 1 |
| 1 | 5 | 79/103 (77%) | 70 (89%) | 5 (6%) | 4 (5%) | 2 | 0 |
| 1 | 6 | 77/103 (75%) | 63 (82%) | 8 (10%) | 6 (8%) | 1 | 0 |
| 1 | A | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | B | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | C | 79/103 (77%) | 76 (96%) | 2 (2%) | 1 (1%) | 15 | 4 |
| 1 | D | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | E | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | F | 79/103 (77%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 1 | G | 79/103 (77%) | 77 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | H | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | I | 79/103 (77%) | 77 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | J | 79/103 (77%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 1 | K | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | L | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | M | 78/103 (76%) | 75 (96%) | 3 (4%) | 0 | 100 | 100 |
| 1 | N | 79/103 (77%) | 76 (96%) | 1 (1%) | 2 (2%) | 7 | 1 |
| 1 | O | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | P | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1 | Q | 79/103 (77%) | 75 (95%) | 2 (2%) | 2 (2%) | 7 | 1 |
| 1 | R | 79/103 (77%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 1 | S | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | T | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | U | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | V | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | W | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | X | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | Y | 79/103 (77%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 1 | Z | 79/103 (77%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| All | All | 2525/3296 (77%) | 2451 (97%) | 53 (2%) | 21 (1%) | 24 | 8 |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 41 | ASP |
| 1 | Q | 74 | GLY |
| 1 | Q | 76 | LEU |
| 1 | 2 | 39 | GLY |
| 1 | 5 | 43 | ASN |
| 1 | 5 | 70 | LYS |
| 1 | 6 | 39 | GLY |
| 1 | 6 | 86 | LEU |
| 1 | 6 | 88 | SER |
| 1 | 6 | 90 | ASP |
| 1 | C | 75 | GLY |
| 1 | N | 74 | GLY |
| 1 | 2 | 87 | LEU |
| 1 | 3 | 75 | GLY |
| 1 | 5 | 76 | LEU |
| 1 | 6 | 40 | ALA |
| 1 | 2 | 76 | LEU |
| 1 | 4 | 76 | LEU |
| 1 | 4 | 88 | SER |
| 1 | 5 | 47 | PRO |
| 1 | 6 | 61 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1 | 1 | 55/70 (79%) | 52 (94%) | 3 (6%) | 27 | 10 |
| 1 | 2 | 55/70 (79%) | 51 (93%) | 4 (7%) | 17 | 5 |
| 1 | 3 | 55/70 (79%) | 51 (93%) | 4 (7%) | 17 | 5 |
| 1 | 4 | 55/70 (79%) | 51 (93%) | 4 (7%) | 17 | 5 |
| 1 | 5 | 55/70 (79%) | 47 (86%) | 8 (14%) | 4 | 0 |
| 1 | 6 | 53/70 (76%) | 43 (81%) | 10 (19%) | 2 | 0 |
| 1 | A | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | B | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | C | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | D | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | E | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | F | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | G | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | H | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | I | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | J | 55/70 (79%) | 53 (96%) | 2 (4%) | 42 | 24 |
| 1 | K | 55/70 (79%) | 51 (93%) | 4 (7%) | 17 | 5 |
| 1 | L | 55/70 (79%) | 53 (96%) | 2 (4%) | 42 | 24 |
| 1 | M | 54/70 (77%) | 50 (93%) | 4 (7%) | 17 | 5 |
| 1 | N | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | O | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | P | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | Q | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | R | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | S | 55/70 (79%) | 53 (96%) | 2 (4%) | 42 | 24 |
| 1 | T | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | U | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | V | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | W | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | X | 55/70 (79%) | 54 (98%) | 1 (2%) | 66 | 54 |
| 1 | Y | 55/70 (79%) | 55 (100%) | 0 | 100 | 100 |
| 1 | Z | 55/70 (79%) | 53 (96%) | 2 (4%) | 42 | 24 |
| All | All | 1757/2240 (78%) | 1697 (97%) | 60 (3%) | 44 | 26 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 28 | GLN |
| 1 | D | 102 | LEU |
| 1 | E | 43 | ASN |
| 1 | F | 41 | ASP |
| 1 | I | 73 | SER |
| 1 | J | 33 | VAL |
| 1 | J | 46 | ILE |
| 1 | K | 23 | ASP |
| 1 | K | 30 | LYS |
| 1 | K | 86 | LEU |
| 1 | K | 89 | ASP |
| 1 | L | 56 | ASN |
| 1 | L | 90 | ASP |
| 1 | M | 41 | ASP |
| 1 | M | 45 | THR |
| 1 | M | 53 | LYS |
| 1 | M | 100 | SER |
| 1 | P | 90 | ASP |
| 1 | Q | 41 | ASP |
| 1 | R | 73 | SER |
| 1 | S | 28 | GLN |
| 1 | S | 41 | ASP |
| 1 | T | 41 | ASP |
| 1 | W | 85 | SER |
| 1 | X | 28 | GLN |
| 1 | Z | 41 | ASP |
| 1 | Z | 86 | LEU |
| 1 | 1 | 41 | ASP |
| 1 | 1 | 45 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 71 | GLU |
| 1 | 2 | 30 | LYS |
| 1 | 2 | 45 | THR |
| 1 | 2 | 81 | GLN |
| 1 | 2 | 87 | LEU |
| 1 | 3 | 33 | VAL |
| 1 | 3 | 70 | LYS |
| 1 | 3 | 76 | LEU |
| 1 | 3 | 86 | LEU |
| 1 | 4 | 43 | ASN |
| 1 | 4 | 53 | LYS |
| 1 | 4 | 90 | ASP |
| 1 | 4 | 101 | SER |
| 1 | 5 | 41 | ASP |
| 1 | 5 | 43 | ASN |
| 1 | 5 | 46 | ILE |
| 1 | 5 | 52 | LEU |
| 1 | 5 | 56 | ASN |
| 1 | 5 | 67 | TYR |
| 1 | 5 | 80 | MET |
| 1 | 5 | 90 | ASP |
| 1 | 6 | 46 | ILE |
| 1 | 6 | 58 | GLN |
| 1 | 6 | 68 | LYS |
| 1 | 6 | 70 | LYS |
| 1 | 6 | 76 | LEU |
| 1 | 6 | 79 | VAL |
| 1 | 6 | 80 | MET |
| 1 | 6 | 81 | GLN |
| 1 | 6 | 87 | LEU |
| 1 | 6 | 88 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 56 | ASN |
| 1 | B | 83 | GLN |
| 1 | C | 28 | GLN |
| 1 | C | 69 | ASN |
| 1 | C | 94 | ASN |
| 1 | D | 43 | ASN |
| 1 | D | 58 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 43 | ASN |
| 1 | E | 58 | GLN |
| 1 | E | 69 | ASN |
| 1 | F | 51 | ASN |
| 1 | F | 56 | ASN |
| 1 | G | 58 | GLN |
| 1 | H | 43 | ASN |
| 1 | H | 51 | ASN |
| 1 | I | 51 | ASN |
| 1 | I | 56 | ASN |
| 1 | J | 43 | ASN |
| 1 | J | 94 | ASN |
| 1 | K | 43 | ASN |
| 1 | L | 56 | ASN |
| 1 | L | 58 | GLN |
| 1 | L | 81 | GLN |
| 1 | M | 56 | ASN |
| 1 | M | 83 | GLN |
| 1 | N | 28 | GLN |
| 1 | N | 51 | ASN |
| 1 | N | 58 | GLN |
| 1 | N | 81 | GLN |
| 1 | O | 43 | ASN |
| 1 | O | 56 | ASN |
| 1 | O | 58 | GLN |
| 1 | O | 83 | GLN |
| 1 | Q | 81 | GLN |
| 1 | R | 43 | ASN |
| 1 | S | 28 | GLN |
| 1 | S | 51 | ASN |
| 1 | T | 43 | ASN |
| 1 | T | 56 | ASN |
| 1 | U | 28 | GLN |
| 1 | U | 43 | ASN |
| 1 | U | 51 | ASN |
| 1 | U | 56 | ASN |
| 1 | V | 51 | ASN |
| 1 | V | 69 | ASN |
| 1 | V | 94 | ASN |
| 1 | W | 51 | ASN |
| 1 | W | 81 | GLN |
| 1 | W | 94 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 28 | GLN |
| 1 | X | 43 | ASN |
| 1 | X | 69 | ASN |
| 1 | Y | 56 | ASN |
| 1 | Y | 69 | ASN |
| 1 | 1 | 43 | ASN |
| 1 | 1 | 55 | GLN |
| 1 | 1 | 58 | GLN |
| 1 | 1 | 81 | GLN |
| 1 | 1 | 83 | GLN |
| 1 | 2 | 81 | GLN |
| 1 | 3 | 43 | ASN |
| 1 | 3 | 51 | ASN |
| 1 | 3 | 56 | ASN |
| 1 | 4 | 28 | GLN |
| 1 | 4 | 56 | ASN |
| 1 | 4 | 58 | GLN |
| 1 | 4 | 81 | GLN |
| 1 | 5 | 43 | ASN |
| 1 | 5 | 56 | ASN |
| 1 | 5 | 58 | GLN |
| 1 | 5 | 69 | ASN |
| 1 | 5 | 81 | GLN |
| 1 | 6 | 58 | GLN |
| 1 | 6 | 81 | GLN |

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 ⓘ

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | HEC | 1 | 220 | 1 | 24,50,50 | 2.50 | 6 (25%) | 19,82,82 | 3.22 | 8 (42%) |
| 2 | HEC | 2 | 220 | 1 | 24,50,50 | 2.19 | 7 (29%) | 19,82,82 | 3.29 | 5 (26%) |
| 2 | HEC | 3 | 220 | 1 | 24,50,50 | 2.27 | 6 (25%) | 19,82,82 | 3.29 | 6 (31%) |
| 2 | HEC | 4 | 220 | 1 | 24,50,50 | 2.40 | 5 (20%) | 19,82,82 | 2.59 | 6 (31%) |
| 2 | HEC | 5 | 220 | 1 | 24,50,50 | 2.19 | 8 (33%) | 19,82,82 | 3.67 | 8 (42%) |
| 2 | HEC | 6 | 220 | 1 | 24,50,50 | 2.18 | 7 (29%) | 19,82,82 | 3.30 | 8 (42%) |
| 2 | HEC | A | 220 | 1 | 24,50,50 | 2.48 | 9 (37%) | 19,82,82 | 3.06 | 7 (36%) |
| 2 | HEC | B | 220 | 1 | 24,50,50 | 2.62 | 8 (33%) | 19,82,82 | 2.96 | 7 (36%) |
| 3 | GOL | C | 104 | - | 5,5,5 | 0.26 | 0 | 5,5,5 | 0.89 | 0 |
| 2 | HEC | C | 220 | 1 | 24,50,50 | 2.58 | 7 (29%) | 19,82,82 | 2.63 | 7 (36%) |
| 2 | HEC | D | 220 | 1 | 24,50,50 | 1.99 | 4 (16%) | 19,82,82 | 2.98 | 8 (42%) |
| 3 | GOL | E | 104 | - | 5,5,5 | 0.20 | 0 | 5,5,5 | 0.83 | 0 |
| 2 | HEC | E | 220 | 1 | 24,50,50 | 2.11 | 4 (16%) | 19,82,82 | 2.67 | 7 (36%) |
| 2 | HEC | F | 220 | 1 | 24,50,50 | 2.32 | 4 (16%) | 19,82,82 | 2.69 | 8 (42%) |
| 2 | HEC | G | 220 | 1 | 24,50,50 | 2.03 | 8 (33%) | 19,82,82 | 3.25 | 10 (52%) |
| 2 | HEC | H | 220 | 1 | 24,50,50 | 2.26 | 9 (37%) | 19,82,82 | 2.83 | 6 (31%) |
| 2 | HEC | I | 220 | 1 | 24,50,50 | 2.80 | 9 (37%) | 19,82,82 | 2.30 | 5 (26%) |
| 2 | HEC | J | 220 | 1 | 24,50,50 | 2.49 | 9 (37%) | 19,82,82 | 2.88 | 6 (31%) |
| 2 | HEC | K | 220 | 1 | 24,50,50 | 2.05 | 5 (20%) | 19,82,82 | 3.17 | 7 (36%) |
| 2 | HEC | L | 220 | 1 | 24,50,50 | 1.89 | 4 (16%) | 19,82,82 | 2.87 | 7 (36%) |
| 2 | HEC | M | 220 | 1 | 24,50,50 | 2.37 | 4 (16%) | 19,82,82 | 2.87 | 6 (31%) |
| 2 | HEC | N | 220 | 1 | 24,50,50 | 1.96 | 6 (25%) | 19,82,82 | 3.63 | 10 (52%) |
| 2 | HEC | O | 220 | 1 | 24,50,50 | 2.20 | 6 (25%) | 19,82,82 | 2.49 | 8 (42%) |
| 3 | GOL | P | 104 | - | 5,5,5 | 0.23 | 0 | 5,5,5 | 0.43 | 0 |
| 2 | HEC | P | 220 | 1 | 24,50,50 | 2.09 | 6 (25%) | 19,82,82 | 3.27 | 9 (47%) |
| 2 | HEC | Q | 220 | 1 | 24,50,50 | 2.05 | 7 (29%) | 19,82,82 | 3.01 | 7 (36%) |
| 3 | GOL | R | 104 | - | 5,5,5 | 0.67 | 0 | 5,5,5 | 0.86 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | HEC | R | 220 | 1 | 24,50,50 | 2.04 | 4 (16%) | 19,82,82 | 3.20 | 9 (47%) |
| 2 | HEC | S | 220 | 1 | 24,50,50 | 2.61 | 6 (25%) | 19,82,82 | 3.29 | 7 (36%) |
| 2 | HEC | T | 220 | 1 | 24,50,50 | 2.34 | 6 (25%) | 19,82,82 | 3.15 | 8 (42%) |
| 2 | HEC | U | 220 | 1 | 24,50,50 | 2.24 | 8 (33%) | 19,82,82 | 2.65 | 7 (36%) |
| 2 | HEC | V | 220 | 1 | 24,50,50 | 2.48 | 5 (20%) | 19,82,82 | 2.65 | 7 (36%) |
| 2 | HEC | W | 220 | 1 | 24,50,50 | 2.09 | 6 (25%) | 19,82,82 | 2.97 | 9 (47%) |
| 2 | HEC | X | 220 | 1 | 24,50,50 | 2.35 | 6 (25%) | 19,82,82 | 3.26 | 8 (42%) |
| 2 | HEC | Y | 220 | 1 | 24,50,50 | 2.16 | 4 (16%) | 19,82,82 | 2.62 | 8 (42%) |
| 2 | HEC | Z | 220 | 1 | 24,50,50 | 2.26 | 6 (25%) | 19,82,82 | 2.92 | 7 (36%) |

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 | HEC | 1 | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | 2 | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | 3 | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | 4 | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | 5 | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | 6 | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | A | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | B | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 3 | GOL | C | 104 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | HEC | C | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | D | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 3 | GOL | E | 104 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | HEC | E | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | F | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | G | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | H | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | I | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | J | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | K | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | L | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | M | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | N | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | O | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 3 | GOL | P | 104 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | HEC | P | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | HEC | Q | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 3 | GOL | R | 104 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | HEC | R | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | S | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | T | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | U | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | V | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | W | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | X | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | Y | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |
| 2 | HEC | Z | 220 | 1 | - | 0/6/54/54 | 0/0/8/8 |

All (199) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 220 | HEC | C3B-C2B | -8.20 | 1.32 | 1.40 |
| 2 | I | 220 | HEC | C3B-C2B | -7.90 | 1.32 | 1.40 |
| 2 | C | 220 | HEC | C3C-C2C | -7.44 | 1.33 | 1.40 |
| 2 | S | 220 | HEC | C3B-C2B | -7.43 | 1.33 | 1.40 |
| 2 | V | 220 | HEC | C3B-C2B | -7.25 | 1.33 | 1.40 |
| 2 | 1 | 220 | HEC | C3C-C2C | -7.18 | 1.33 | 1.40 |
| 2 | E | 220 | HEC | C3B-C2B | -7.16 | 1.33 | 1.40 |
| 2 | M | 220 | HEC | C3C-C2C | -6.86 | 1.33 | 1.40 |
| 2 | M | 220 | HEC | C3B-C2B | -6.71 | 1.33 | 1.40 |
| 2 | S | 220 | HEC | C3C-C2C | -6.67 | 1.33 | 1.40 |
| 2 | R | 220 | HEC | C3B-C2B | -6.65 | 1.33 | 1.40 |
| 2 | Z | 220 | HEC | C3C-C2C | -6.59 | 1.33 | 1.40 |
| 2 | Y | 220 | HEC | C3B-C2B | -6.47 | 1.34 | 1.40 |
| 2 | C | 220 | HEC | C3B-C2B | -6.39 | 1.34 | 1.40 |
| 2 | F | 220 | HEC | C3B-C2B | -6.25 | 1.34 | 1.40 |
| 2 | I | 220 | HEC | C3C-C2C | -6.24 | 1.34 | 1.40 |
| 2 | F | 220 | HEC | C3C-C2C | -6.24 | 1.34 | 1.40 |
| 2 | T | 220 | HEC | C3B-C2B | -6.19 | 1.34 | 1.40 |
| 2 | U | 220 | HEC | C3C-C2C | -6.10 | 1.34 | 1.40 |
| 2 | V | 220 | HEC | C3C-C2C | -6.04 | 1.34 | 1.40 |
| 2 | O | 220 | HEC | C3B-C2B | -6.00 | 1.34 | 1.40 |
| 2 | 4 | 220 | HEC | C3B-C2B | -5.99 | 1.34 | 1.40 |
| 2 | J | 220 | HEC | C3B-C2B | -5.97 | 1.34 | 1.40 |
| 2 | 3 | 220 | HEC | C3B-C2B | -5.93 | 1.34 | 1.40 |
| 2 | X | 220 | HEC | C3B-C2B | -5.85 | 1.34 | 1.40 |
| 2 | D | 220 | HEC | C3C-C2C | -5.71 | 1.34 | 1.40 |
| 2 | X | 220 | HEC | C3C-C2C | -5.62 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | O | 220 | HEC | C3C-C2C | -5.62 | 1.34 | 1.40 |
| 2 | T | 220 | HEC | C3C-C2C | -5.50 | 1.35 | 1.40 |
| 2 | K | 220 | HEC | C3C-C2C | -5.42 | 1.35 | 1.40 |
| 2 | P | 220 | HEC | C3B-C2B | -5.39 | 1.35 | 1.40 |
| 2 | 1 | 220 | HEC | C3B-C2B | -5.33 | 1.35 | 1.40 |
| 2 | J | 220 | HEC | C3C-C2C | -5.23 | 1.35 | 1.40 |
| 2 | 4 | 220 | HEC | C3C-C2C | -5.22 | 1.35 | 1.40 |
| 2 | H | 220 | HEC | C3C-C2C | -5.18 | 1.35 | 1.40 |
| 2 | H | 220 | HEC | C3B-C2B | -5.17 | 1.35 | 1.40 |
| 2 | L | 220 | HEC | C3C-C2C | -5.09 | 1.35 | 1.40 |
| 2 | A | 220 | HEC | C3B-C2B | -5.06 | 1.35 | 1.40 |
| 2 | A | 220 | HEC | C3C-C2C | -5.04 | 1.35 | 1.40 |
| 2 | W | 220 | HEC | C3C-C2C | -4.93 | 1.35 | 1.40 |
| 2 | 6 | 220 | HEC | C3B-C2B | -4.81 | 1.35 | 1.40 |
| 2 | 5 | 220 | HEC | C3C-C2C | -4.77 | 1.35 | 1.40 |
| 2 | U | 220 | HEC | C3B-C2B | -4.68 | 1.35 | 1.40 |
| 2 | G | 220 | HEC | C3B-C2B | -4.66 | 1.35 | 1.40 |
| 2 | 2 | 220 | HEC | C3B-C2B | -4.62 | 1.35 | 1.40 |
| 2 | 2 | 220 | HEC | C3C-C2C | -4.57 | 1.36 | 1.40 |
| 2 | Q | 220 | HEC | C3C-C2C | -4.51 | 1.36 | 1.40 |
| 2 | Z | 220 | HEC | C3B-C2B | -4.50 | 1.36 | 1.40 |
| 2 | 3 | 220 | HEC | C3C-C2C | -4.45 | 1.36 | 1.40 |
| 2 | P | 220 | HEC | C3C-C2C | -4.40 | 1.36 | 1.40 |
| 2 | 6 | 220 | HEC | C3C-C2C | -4.18 | 1.36 | 1.40 |
| 2 | K | 220 | HEC | C3B-C2B | -4.15 | 1.36 | 1.40 |
| 2 | N | 220 | HEC | C3C-C2C | -4.03 | 1.36 | 1.40 |
| 2 | L | 220 | HEC | C3B-C2B | -4.02 | 1.36 | 1.40 |
| 2 | Q | 220 | HEC | C3B-C2B | -3.97 | 1.36 | 1.40 |
| 2 | G | 220 | HEC | C3C-C2C | -3.86 | 1.36 | 1.40 |
| 2 | 5 | 220 | HEC | C3B-C2B | -3.74 | 1.36 | 1.40 |
| 2 | R | 220 | HEC | C3C-C2C | -3.71 | 1.36 | 1.40 |
| 2 | W | 220 | HEC | C3B-C2B | -3.55 | 1.37 | 1.40 |
| 2 | N | 220 | HEC | C3B-C2B | -3.41 | 1.37 | 1.40 |
| 2 | B | 220 | HEC | C3C-C2C | -3.35 | 1.37 | 1.40 |
| 2 | D | 220 | HEC | C3B-C2B | -2.58 | 1.38 | 1.40 |
| 2 | E | 220 | HEC | C3C-C2C | -2.48 | 1.38 | 1.40 |
| 2 | B | 220 | HEC | C1A-NA | -2.20 | 1.33 | 1.36 |
| 2 | 5 | 220 | HEC | CMA-C3A | 2.00 | 1.56 | 1.51 |
| 2 | H | 220 | HEC | CMD-C2D | 2.00 | 1.55 | 1.51 |
| 2 | 6 | 220 | HEC | C1A-NA | 2.00 | 1.39 | 1.36 |
| 2 | I | 220 | HEC | CBB-CAB | 2.01 | 1.57 | 1.49 |
| 2 | C | 220 | HEC | C4B-NB | 2.01 | 1.39 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | D | 220 | HEC | CAA-C2A | 2.02 | 1.56 | 1.52 |
| 2 | 6 | 220 | HEC | CAA-C2A | 2.03 | 1.56 | 1.52 |
| 2 | S | 220 | HEC | CAD-C3D | 2.03 | 1.55 | 1.52 |
| 2 | H | 220 | HEC | CBB-CAB | 2.03 | 1.57 | 1.49 |
| 2 | T | 220 | HEC | CMD-C2D | 2.03 | 1.55 | 1.51 |
| 2 | J | 220 | HEC | CMD-C2D | 2.03 | 1.55 | 1.51 |
| 2 | U | 220 | HEC | CMC-C2C | 2.05 | 1.56 | 1.51 |
| 2 | 1 | 220 | HEC | CMC-C2C | 2.05 | 1.56 | 1.51 |
| 2 | O | 220 | HEC | C3C-C4C | 2.06 | 1.47 | 1.42 |
| 2 | 2 | 220 | HEC | C4A-NA | 2.07 | 1.39 | 1.36 |
| 2 | W | 220 | HEC | CMD-C2D | 2.08 | 1.55 | 1.51 |
| 2 | O | 220 | HEC | C4B-NB | 2.09 | 1.39 | 1.36 |
| 2 | 2 | 220 | HEC | C3C-C4C | 2.11 | 1.47 | 1.42 |
| 2 | U | 220 | HEC | CAA-C2A | 2.11 | 1.56 | 1.52 |
| 2 | 3 | 220 | HEC | C3B-C4B | 2.11 | 1.47 | 1.42 |
| 2 | K | 220 | HEC | CAA-C2A | 2.11 | 1.56 | 1.52 |
| 2 | Q | 220 | HEC | CMB-C2B | 2.12 | 1.56 | 1.51 |
| 2 | Y | 220 | HEC | CMB-C2B | 2.12 | 1.56 | 1.51 |
| 2 | 5 | 220 | HEC | CAA-C2A | 2.12 | 1.56 | 1.52 |
| 2 | J | 220 | HEC | CMA-C3A | 2.13 | 1.56 | 1.51 |
| 2 | C | 220 | HEC | C3C-C4C | 2.14 | 1.47 | 1.42 |
| 2 | G | 220 | HEC | CAD-C3D | 2.16 | 1.55 | 1.52 |
| 2 | U | 220 | HEC | CBB-CAB | 2.16 | 1.58 | 1.49 |
| 2 | 2 | 220 | HEC | CAA-C2A | 2.17 | 1.56 | 1.52 |
| 2 | K | 220 | HEC | C4B-NB | 2.18 | 1.39 | 1.36 |
| 2 | N | 220 | HEC | C3B-C4B | 2.19 | 1.47 | 1.42 |
| 2 | T | 220 | HEC | C4B-NB | 2.19 | 1.39 | 1.36 |
| 2 | H | 220 | HEC | C4A-NA | 2.20 | 1.39 | 1.36 |
| 2 | H | 220 | HEC | CMC-C2C | 2.20 | 1.56 | 1.51 |
| 2 | J | 220 | HEC | CAA-C2A | 2.20 | 1.56 | 1.52 |
| 2 | U | 220 | HEC | C3C-C4C | 2.21 | 1.47 | 1.42 |
| 2 | A | 220 | HEC | CAA-C2A | 2.22 | 1.56 | 1.52 |
| 2 | S | 220 | HEC | CAA-C2A | 2.23 | 1.56 | 1.52 |
| 2 | G | 220 | HEC | CMA-C3A | 2.24 | 1.56 | 1.51 |
| 2 | J | 220 | HEC | CAD-C3D | 2.25 | 1.55 | 1.52 |
| 2 | I | 220 | HEC | C1A-NA | 2.25 | 1.39 | 1.36 |
| 2 | 3 | 220 | HEC | C1A-NA | 2.26 | 1.39 | 1.36 |
| 2 | H | 220 | HEC | CMA-C3A | 2.26 | 1.56 | 1.51 |
| 2 | Z | 220 | HEC | CMA-C3A | 2.27 | 1.56 | 1.51 |
| 2 | I | 220 | HEC | C4A-NA | 2.29 | 1.39 | 1.36 |
| 2 | M | 220 | HEC | CMA-C3A | 2.31 | 1.56 | 1.51 |
| 2 | G | 220 | HEC | C4A-NA | 2.32 | 1.39 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | I | 220 | HEC | CAA-C2A | 2.32 | 1.56 | 1.52 |
| 2 | P | 220 | HEC | CMC-C2C | 2.34 | 1.56 | 1.51 |
| 2 | 5 | 220 | HEC | C4A-NA | 2.34 | 1.39 | 1.36 |
| 2 | 5 | 220 | HEC | C4B-NB | 2.37 | 1.39 | 1.36 |
| 2 | P | 220 | HEC | C1A-NA | 2.39 | 1.39 | 1.36 |
| 2 | 5 | 220 | HEC | C4C-NC | 2.40 | 1.39 | 1.36 |
| 2 | H | 220 | HEC | C4C-NC | 2.40 | 1.39 | 1.36 |
| 2 | Q | 220 | HEC | CMD-C2D | 2.41 | 1.56 | 1.51 |
| 2 | Q | 220 | HEC | CMA-C3A | 2.42 | 1.56 | 1.51 |
| 2 | A | 220 | HEC | CMB-C2B | 2.43 | 1.56 | 1.51 |
| 2 | C | 220 | HEC | CMC-C2C | 2.44 | 1.56 | 1.51 |
| 2 | Z | 220 | HEC | CAA-C2A | 2.45 | 1.56 | 1.52 |
| 2 | X | 220 | HEC | CMC-C2C | 2.47 | 1.57 | 1.51 |
| 2 | I | 220 | HEC | CMD-C2D | 2.47 | 1.56 | 1.51 |
| 2 | G | 220 | HEC | C4B-NB | 2.47 | 1.40 | 1.36 |
| 2 | E | 220 | HEC | CAA-C2A | 2.52 | 1.57 | 1.52 |
| 2 | X | 220 | HEC | CAA-C2A | 2.52 | 1.57 | 1.52 |
| 2 | B | 220 | HEC | CAA-C2A | 2.52 | 1.57 | 1.52 |
| 2 | N | 220 | HEC | C3C-C4C | 2.53 | 1.48 | 1.42 |
| 2 | Z | 220 | HEC | C4B-NB | 2.57 | 1.40 | 1.36 |
| 2 | 6 | 220 | HEC | C3B-C4B | 2.57 | 1.48 | 1.42 |
| 2 | O | 220 | HEC | CAA-C2A | 2.57 | 1.57 | 1.52 |
| 2 | R | 220 | HEC | C3C-C4C | 2.59 | 1.48 | 1.42 |
| 2 | L | 220 | HEC | C4B-NB | 2.60 | 1.40 | 1.36 |
| 2 | J | 220 | HEC | C4B-NB | 2.61 | 1.40 | 1.36 |
| 2 | C | 220 | HEC | CMA-C3A | 2.65 | 1.57 | 1.51 |
| 2 | A | 220 | HEC | C3C-C4C | 2.65 | 1.48 | 1.42 |
| 2 | W | 220 | HEC | C4C-NC | 2.67 | 1.40 | 1.36 |
| 2 | V | 220 | HEC | CAA-C2A | 2.67 | 1.57 | 1.52 |
| 2 | 1 | 220 | HEC | CAA-C2A | 2.68 | 1.57 | 1.52 |
| 2 | F | 220 | HEC | C4B-NB | 2.72 | 1.40 | 1.36 |
| 2 | P | 220 | HEC | CAA-C2A | 2.74 | 1.57 | 1.52 |
| 2 | 6 | 220 | HEC | C4B-NB | 2.74 | 1.40 | 1.36 |
| 2 | X | 220 | HEC | C4B-NB | 2.85 | 1.40 | 1.36 |
| 2 | B | 220 | HEC | C3C-C4C | 2.93 | 1.49 | 1.42 |
| 2 | G | 220 | HEC | CMC-C2C | 2.95 | 1.58 | 1.51 |
| 2 | A | 220 | HEC | C4A-NA | 2.96 | 1.40 | 1.36 |
| 2 | W | 220 | HEC | CMB-C2B | 3.01 | 1.58 | 1.51 |
| 2 | U | 220 | HEC | C4B-NB | 3.07 | 1.40 | 1.36 |
| 2 | 4 | 220 | HEC | CAA-C2A | 3.11 | 1.58 | 1.52 |
| 2 | 3 | 220 | HEC | CAA-C2A | 3.16 | 1.58 | 1.52 |
| 2 | S | 220 | HEC | C4B-NB | 3.22 | 1.41 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | A | 220 | HEC | CMA-C3A | 3.22 | 1.58 | 1.51 |
| 2 | V | 220 | HEC | C4B-NB | 3.22 | 1.41 | 1.36 |
| 2 | Q | 220 | HEC | C4B-NB | 3.28 | 1.41 | 1.36 |
| 2 | N | 220 | HEC | C4B-NB | 3.28 | 1.41 | 1.36 |
| 2 | B | 220 | HEC | CMC-C2C | 3.30 | 1.58 | 1.51 |
| 2 | 1 | 220 | HEC | C4B-NB | 3.32 | 1.41 | 1.36 |
| 2 | 2 | 220 | HEC | C4C-NC | 3.35 | 1.41 | 1.36 |
| 2 | T | 220 | HEC | CMA-C3A | 3.52 | 1.59 | 1.51 |
| 2 | G | 220 | HEC | C3D-C2D | 3.52 | 1.48 | 1.37 |
| 2 | M | 220 | HEC | C3D-C2D | 3.71 | 1.48 | 1.37 |
| 2 | L | 220 | HEC | C3D-C2D | 3.78 | 1.48 | 1.37 |
| 2 | R | 220 | HEC | C3D-C2D | 3.86 | 1.49 | 1.37 |
| 2 | P | 220 | HEC | C3D-C2D | 3.89 | 1.49 | 1.37 |
| 2 | 4 | 220 | HEC | C4B-NB | 4.00 | 1.42 | 1.36 |
| 2 | J | 220 | HEC | C3D-C2D | 4.12 | 1.49 | 1.37 |
| 2 | O | 220 | HEC | C3D-C2D | 4.16 | 1.50 | 1.37 |
| 2 | T | 220 | HEC | C3D-C2D | 4.29 | 1.50 | 1.37 |
| 2 | Y | 220 | HEC | C3D-C2D | 4.32 | 1.50 | 1.37 |
| 2 | A | 220 | HEC | C4B-NB | 4.34 | 1.42 | 1.36 |
| 2 | C | 220 | HEC | C3D-C2D | 4.35 | 1.50 | 1.37 |
| 2 | K | 220 | HEC | C3D-C2D | 4.44 | 1.50 | 1.37 |
| 2 | Q | 220 | HEC | C3D-C2D | 4.45 | 1.50 | 1.37 |
| 2 | B | 220 | HEC | C4B-NB | 4.47 | 1.42 | 1.36 |
| 2 | Z | 220 | HEC | C3D-C2D | 4.50 | 1.51 | 1.37 |
| 2 | I | 220 | HEC | C3D-C2D | 4.51 | 1.51 | 1.37 |
| 2 | F | 220 | HEC | C3D-C2D | 4.60 | 1.51 | 1.37 |
| 2 | B | 220 | HEC | C3D-C2D | 4.61 | 1.51 | 1.37 |
| 2 | E | 220 | HEC | C3D-C2D | 4.62 | 1.51 | 1.37 |
| 2 | V | 220 | HEC | C3D-C2D | 4.67 | 1.51 | 1.37 |
| 2 | H | 220 | HEC | C3D-C2D | 4.73 | 1.51 | 1.37 |
| 2 | U | 220 | HEC | C3D-C2D | 4.81 | 1.51 | 1.37 |
| 2 | D | 220 | HEC | C3D-C2D | 4.84 | 1.52 | 1.37 |
| 2 | N | 220 | HEC | C3D-C2D | 4.87 | 1.52 | 1.37 |
| 2 | Y | 220 | HEC | C4B-NB | 4.89 | 1.43 | 1.36 |
| 2 | X | 220 | HEC | C3D-C2D | 4.93 | 1.52 | 1.37 |
| 2 | 2 | 220 | HEC | C3D-C2D | 4.94 | 1.52 | 1.37 |
| 2 | S | 220 | HEC | C3D-C2D | 4.99 | 1.52 | 1.37 |
| 2 | A | 220 | HEC | C3D-C2D | 5.00 | 1.52 | 1.37 |
| 2 | 4 | 220 | HEC | C3D-C2D | 5.03 | 1.52 | 1.37 |
| 2 | 1 | 220 | HEC | C3D-C2D | 5.12 | 1.52 | 1.37 |
| 2 | J | 220 | HEC | C1A-NA | 5.23 | 1.43 | 1.36 |
| 2 | W | 220 | HEC | C3D-C2D | 5.30 | 1.53 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | I | 220 | HEC | C4C-NC | 5.33 | 1.43 | 1.36 |
| 2 | 6 | 220 | HEC | C3D-C2D | 5.41 | 1.53 | 1.37 |
| 2 | 5 | 220 | HEC | C3D-C2D | 5.43 | 1.53 | 1.37 |
| 2 | 3 | 220 | HEC | C3D-C2D | 5.52 | 1.54 | 1.37 |

All (236) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | N | 220 | HEC | CBB-CAB-C3B | -10.33 | 104.40 | 127.35 |
| 2 | 6 | 220 | HEC | CBB-CAB-C3B | -10.01 | 105.11 | 127.35 |
| 2 | X | 220 | HEC | CBB-CAB-C3B | -10.00 | 105.14 | 127.35 |
| 2 | J | 220 | HEC | CBB-CAB-C3B | -9.33 | 106.63 | 127.35 |
| 2 | 3 | 220 | HEC | CBB-CAB-C3B | -9.24 | 106.83 | 127.35 |
| 2 | S | 220 | HEC | CBB-CAB-C3B | -9.21 | 106.89 | 127.35 |
| 2 | 2 | 220 | HEC | CBC-CAC-C3C | -8.66 | 108.11 | 127.35 |
| 2 | 5 | 220 | HEC | CBC-CAC-C3C | -8.62 | 108.19 | 127.35 |
| 2 | R | 220 | HEC | CBB-CAB-C3B | -8.62 | 108.20 | 127.35 |
| 2 | D | 220 | HEC | CBB-CAB-C3B | -8.57 | 108.30 | 127.35 |
| 2 | 3 | 220 | HEC | CBC-CAC-C3C | -8.49 | 108.48 | 127.35 |
| 2 | P | 220 | HEC | CBB-CAB-C3B | -8.47 | 108.53 | 127.35 |
| 2 | 2 | 220 | HEC | CBB-CAB-C3B | -8.37 | 108.76 | 127.35 |
| 2 | B | 220 | HEC | CBB-CAB-C3B | -8.33 | 108.83 | 127.35 |
| 2 | K | 220 | HEC | CBB-CAB-C3B | -8.26 | 109.00 | 127.35 |
| 2 | 1 | 220 | HEC | CBB-CAB-C3B | -8.24 | 109.04 | 127.35 |
| 2 | T | 220 | HEC | CBB-CAB-C3B | -8.12 | 109.30 | 127.35 |
| 2 | Q | 220 | HEC | CBB-CAB-C3B | -8.06 | 109.45 | 127.35 |
| 2 | V | 220 | HEC | CBB-CAB-C3B | -7.98 | 109.61 | 127.35 |
| 2 | M | 220 | HEC | CBB-CAB-C3B | -7.88 | 109.84 | 127.35 |
| 2 | A | 220 | HEC | CBB-CAB-C3B | -7.86 | 109.88 | 127.35 |
| 2 | G | 220 | HEC | CBB-CAB-C3B | -7.79 | 110.04 | 127.35 |
| 2 | 5 | 220 | HEC | CBD-CAD-C3D | -7.68 | 98.76 | 112.53 |
| 2 | 5 | 220 | HEC | CBB-CAB-C3B | -7.67 | 110.31 | 127.35 |
| 2 | L | 220 | HEC | CBB-CAB-C3B | -7.65 | 110.34 | 127.35 |
| 2 | H | 220 | HEC | CBB-CAB-C3B | -7.63 | 110.39 | 127.35 |
| 2 | E | 220 | HEC | CBB-CAB-C3B | -7.45 | 110.79 | 127.35 |
| 2 | F | 220 | HEC | CBB-CAB-C3B | -7.43 | 110.85 | 127.35 |
| 2 | 4 | 220 | HEC | CBB-CAB-C3B | -7.33 | 111.07 | 127.35 |
| 2 | W | 220 | HEC | CBB-CAB-C3B | -7.24 | 111.26 | 127.35 |
| 2 | C | 220 | HEC | CBB-CAB-C3B | -7.14 | 111.49 | 127.35 |
| 2 | U | 220 | HEC | CBB-CAB-C3B | -7.08 | 111.61 | 127.35 |
| 2 | K | 220 | HEC | CBC-CAC-C3C | -7.06 | 111.65 | 127.35 |
| 2 | I | 220 | HEC | CBB-CAB-C3B | -7.01 | 111.77 | 127.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | O | 220 | HEC | CBB-CAB-C3B | -6.98 | 111.83 | 127.35 |
| 2 | 1 | 220 | HEC | CBC-CAC-C3C | -6.69 | 112.49 | 127.35 |
| 2 | G | 220 | HEC | CBC-CAC-C3C | -6.67 | 112.52 | 127.35 |
| 2 | Z | 220 | HEC | CBB-CAB-C3B | -6.54 | 112.82 | 127.35 |
| 2 | X | 220 | HEC | CBC-CAC-C3C | -6.39 | 113.16 | 127.35 |
| 2 | Z | 220 | HEC | CBC-CAC-C3C | -5.84 | 114.36 | 127.35 |
| 2 | P | 220 | HEC | CBC-CAC-C3C | -5.81 | 114.44 | 127.35 |
| 2 | L | 220 | HEC | CBC-CAC-C3C | -5.79 | 114.49 | 127.35 |
| 2 | S | 220 | HEC | CBC-CAC-C3C | -5.70 | 114.69 | 127.35 |
| 2 | Y | 220 | HEC | CBB-CAB-C3B | -5.68 | 114.74 | 127.35 |
| 2 | R | 220 | HEC | CMC-C2C-C1C | -5.62 | 119.06 | 128.36 |
| 2 | Q | 220 | HEC | CBC-CAC-C3C | -5.51 | 115.10 | 127.35 |
| 2 | A | 220 | HEC | CMC-C2C-C1C | -5.42 | 119.40 | 128.36 |
| 2 | A | 220 | HEC | CBD-CAD-C3D | -5.31 | 103.01 | 112.53 |
| 2 | Z | 220 | HEC | CMB-C2B-C1B | -5.23 | 119.70 | 128.36 |
| 2 | T | 220 | HEC | CAA-C2A-C1A | -5.23 | 121.33 | 127.01 |
| 2 | N | 220 | HEC | CAA-C2A-C1A | -5.16 | 121.41 | 127.01 |
| 2 | H | 220 | HEC | CBD-CAD-C3D | -5.14 | 103.31 | 112.53 |
| 2 | P | 220 | HEC | CMC-C2C-C1C | -5.10 | 119.92 | 128.36 |
| 2 | D | 220 | HEC | CBC-CAC-C3C | -5.04 | 116.16 | 127.35 |
| 2 | C | 220 | HEC | CBC-CAC-C3C | -4.99 | 116.26 | 127.35 |
| 2 | T | 220 | HEC | CBC-CAC-C3C | -4.95 | 116.34 | 127.35 |
| 2 | Y | 220 | HEC | CMC-C2C-C1C | -4.92 | 120.22 | 128.36 |
| 2 | M | 220 | HEC | CBC-CAC-C3C | -4.91 | 116.44 | 127.35 |
| 2 | B | 220 | HEC | CMC-C2C-C1C | -4.88 | 120.29 | 128.36 |
| 2 | 6 | 220 | HEC | CBC-CAC-C3C | -4.84 | 116.60 | 127.35 |
| 2 | M | 220 | HEC | CBD-CAD-C3D | -4.83 | 103.86 | 112.53 |
| 2 | A | 220 | HEC | CBC-CAC-C3C | -4.82 | 116.65 | 127.35 |
| 2 | 6 | 220 | HEC | CBD-CAD-C3D | -4.81 | 103.90 | 112.53 |
| 2 | U | 220 | HEC | CMB-C2B-C1B | -4.76 | 120.48 | 128.36 |
| 2 | W | 220 | HEC | CBC-CAC-C3C | -4.76 | 116.78 | 127.35 |
| 2 | 4 | 220 | HEC | CBC-CAC-C3C | -4.70 | 116.91 | 127.35 |
| 2 | P | 220 | HEC | CMB-C2B-C1B | -4.63 | 120.70 | 128.36 |
| 2 | G | 220 | HEC | CBD-CAD-C3D | -4.57 | 104.33 | 112.53 |
| 2 | F | 220 | HEC | CBC-CAC-C3C | -4.56 | 117.21 | 127.35 |
| 2 | T | 220 | HEC | CMC-C2C-C1C | -4.53 | 120.86 | 128.36 |
| 2 | H | 220 | HEC | CBC-CAC-C3C | -4.52 | 117.31 | 127.35 |
| 2 | S | 220 | HEC | CBA-CAA-C2A | -4.51 | 104.45 | 112.53 |
| 2 | 1 | 220 | HEC | CBD-CAD-C3D | -4.51 | 104.45 | 112.53 |
| 2 | W | 220 | HEC | CBD-CAD-C3D | -4.50 | 104.46 | 112.53 |
| 2 | B | 220 | HEC | CBC-CAC-C3C | -4.43 | 117.50 | 127.35 |
| 2 | N | 220 | HEC | CMC-C2C-C1C | -4.41 | 121.07 | 128.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | R | 220 | HEC | CBA-CAA-C2A | -4.35 | 104.73 | 112.53 |
| 2 | R | 220 | HEC | CBC-CAC-C3C | -4.35 | 117.68 | 127.35 |
| 2 | 5 | 220 | HEC | CBA-CAA-C2A | -4.33 | 104.76 | 112.53 |
| 2 | N | 220 | HEC | CBD-CAD-C3D | -4.32 | 104.78 | 112.53 |
| 2 | D | 220 | HEC | CMB-C2B-C1B | -4.32 | 121.22 | 128.36 |
| 2 | E | 220 | HEC | CMC-C2C-C1C | -4.30 | 121.25 | 128.36 |
| 2 | 5 | 220 | HEC | CMB-C2B-C1B | -4.28 | 121.28 | 128.36 |
| 2 | W | 220 | HEC | CAA-C2A-C1A | -4.22 | 122.43 | 127.01 |
| 2 | D | 220 | HEC | CBD-CAD-C3D | -4.20 | 105.00 | 112.53 |
| 2 | U | 220 | HEC | CBD-CAD-C3D | -4.13 | 105.13 | 112.53 |
| 2 | Q | 220 | HEC | CMB-C2B-C1B | -4.12 | 121.55 | 128.36 |
| 2 | 1 | 220 | HEC | CBA-CAA-C2A | -4.09 | 105.20 | 112.53 |
| 2 | Z | 220 | HEC | CMC-C2C-C1C | -4.03 | 121.69 | 128.36 |
| 2 | G | 220 | HEC | CMB-C2B-C1B | -4.01 | 121.72 | 128.36 |
| 2 | O | 220 | HEC | CBA-CAA-C2A | -4.00 | 105.37 | 112.53 |
| 2 | 4 | 220 | HEC | CBD-CAD-C3D | -3.98 | 105.39 | 112.53 |
| 2 | 2 | 220 | HEC | CBA-CAA-C2A | -3.98 | 105.39 | 112.53 |
| 2 | Y | 220 | HEC | CBA-CAA-C2A | -3.96 | 105.43 | 112.53 |
| 2 | K | 220 | HEC | CMB-C2B-C1B | -3.96 | 121.82 | 128.36 |
| 2 | N | 220 | HEC | CAD-CBD-CGD | -3.94 | 105.52 | 112.75 |
| 2 | 1 | 220 | HEC | CMC-C2C-C1C | -3.94 | 121.85 | 128.36 |
| 2 | K | 220 | HEC | CMC-C2C-C1C | -3.91 | 121.90 | 128.36 |
| 2 | V | 220 | HEC | CMB-C2B-C1B | -3.83 | 122.03 | 128.36 |
| 2 | M | 220 | HEC | CMC-C2C-C1C | -3.79 | 122.10 | 128.36 |
| 2 | K | 220 | HEC | CBA-CAA-C2A | -3.79 | 105.74 | 112.53 |
| 2 | 2 | 220 | HEC | CAD-CBD-CGD | -3.78 | 105.83 | 112.75 |
| 2 | H | 220 | HEC | CMC-C2C-C1C | -3.77 | 122.12 | 128.36 |
| 2 | R | 220 | HEC | CBD-CAD-C3D | -3.74 | 105.82 | 112.53 |
| 2 | 6 | 220 | HEC | CMB-C2B-C1B | -3.74 | 122.17 | 128.36 |
| 2 | Q | 220 | HEC | CMC-C2C-C1C | -3.72 | 122.21 | 128.36 |
| 2 | J | 220 | HEC | CMB-C2B-C1B | -3.72 | 122.22 | 128.36 |
| 2 | R | 220 | HEC | CMB-C2B-C1B | -3.71 | 122.22 | 128.36 |
| 2 | B | 220 | HEC | CAA-C2A-C1A | -3.68 | 123.02 | 127.01 |
| 2 | I | 220 | HEC | CMC-C2C-C1C | -3.65 | 122.32 | 128.36 |
| 2 | G | 220 | HEC | CMC-C2C-C1C | -3.62 | 122.38 | 128.36 |
| 2 | N | 220 | HEC | CBC-CAC-C3C | -3.62 | 119.31 | 127.35 |
| 2 | Z | 220 | HEC | CAD-CBD-CGD | -3.60 | 106.14 | 112.75 |
| 2 | P | 220 | HEC | CBD-CAD-C3D | -3.55 | 106.17 | 112.53 |
| 2 | P | 220 | HEC | CAA-C2A-C1A | -3.52 | 123.19 | 127.01 |
| 2 | Y | 220 | HEC | CAA-C2A-C1A | -3.49 | 123.22 | 127.01 |
| 2 | W | 220 | HEC | CMC-C2C-C1C | -3.47 | 122.63 | 128.36 |
| 2 | 4 | 220 | HEC | CMB-C2B-C1B | -3.45 | 122.65 | 128.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | V | 220 | HEC | CBA-CAA-C2A | -3.43 | 106.39 | 112.53 |
| 2 | G | 220 | HEC | CAD-CBD-CGD | -3.43 | 106.47 | 112.75 |
| 2 | Y | 220 | HEC | CBC-CAC-C3C | -3.42 | 119.75 | 127.35 |
| 2 | C | 220 | HEC | CMC-C2C-C1C | -3.42 | 122.70 | 128.36 |
| 2 | T | 220 | HEC | CBD-CAD-C3D | -3.41 | 106.42 | 112.53 |
| 2 | X | 220 | HEC | CBA-CAA-C2A | -3.38 | 106.47 | 112.53 |
| 2 | J | 220 | HEC | CMC-C2C-C1C | -3.38 | 122.78 | 128.36 |
| 2 | V | 220 | HEC | CBD-CAD-C3D | -3.37 | 106.48 | 112.53 |
| 2 | 2 | 220 | HEC | CMB-C2B-C1B | -3.36 | 122.81 | 128.36 |
| 2 | S | 220 | HEC | CMC-C2C-C1C | -3.34 | 122.84 | 128.36 |
| 2 | B | 220 | HEC | CBA-CAA-C2A | -3.31 | 106.59 | 112.53 |
| 2 | F | 220 | HEC | CBA-CAA-C2A | -3.31 | 106.59 | 112.53 |
| 2 | 6 | 220 | HEC | CMC-C2C-C1C | -3.31 | 122.89 | 128.36 |
| 2 | D | 220 | HEC | CAD-CBD-CGD | -3.31 | 106.68 | 112.75 |
| 2 | F | 220 | HEC | CBD-CAD-C3D | -3.31 | 106.60 | 112.53 |
| 2 | E | 220 | HEC | CMB-C2B-C1B | -3.29 | 122.91 | 128.36 |
| 2 | E | 220 | HEC | CBA-CAA-C2A | -3.29 | 106.64 | 112.53 |
| 2 | E | 220 | HEC | CBC-CAC-C3C | -3.27 | 120.09 | 127.35 |
| 2 | O | 220 | HEC | CMB-C2B-C1B | -3.20 | 123.07 | 128.36 |
| 2 | A | 220 | HEC | CBA-CAA-C2A | -3.18 | 106.83 | 112.53 |
| 2 | E | 220 | HEC | CBD-CAD-C3D | -3.16 | 106.86 | 112.53 |
| 2 | H | 220 | HEC | CAA-C2A-C1A | -3.14 | 123.60 | 127.01 |
| 2 | Z | 220 | HEC | CBD-CAD-C3D | -3.14 | 106.91 | 112.53 |
| 2 | X | 220 | HEC | CMB-C2B-C1B | -3.12 | 123.20 | 128.36 |
| 2 | T | 220 | HEC | CBA-CAA-C2A | -3.12 | 106.94 | 112.53 |
| 2 | N | 220 | HEC | CBA-CAA-C2A | -3.11 | 106.96 | 112.53 |
| 2 | N | 220 | HEC | CMB-C2B-C1B | -3.10 | 123.24 | 128.36 |
| 2 | U | 220 | HEC | CBA-CAA-C2A | -3.09 | 107.00 | 112.53 |
| 2 | U | 220 | HEC | CBC-CAC-C3C | -3.06 | 120.55 | 127.35 |
| 2 | X | 220 | HEC | CBD-CAD-C3D | -3.04 | 107.08 | 112.53 |
| 2 | A | 220 | HEC | CMB-C2B-C1B | -3.04 | 123.34 | 128.36 |
| 2 | T | 220 | HEC | C3C-C4C-NC | -3.03 | 105.21 | 110.94 |
| 2 | Y | 220 | HEC | CBD-CAD-C3D | -3.03 | 107.11 | 112.53 |
| 2 | S | 220 | HEC | CAA-C2A-C1A | -3.00 | 123.75 | 127.01 |
| 2 | M | 220 | HEC | CMB-C2B-C1B | -2.99 | 123.42 | 128.36 |
| 2 | I | 220 | HEC | CBD-CAD-C3D | -2.98 | 107.18 | 112.53 |
| 2 | A | 220 | HEC | C3C-C4C-NC | -2.98 | 105.32 | 110.94 |
| 2 | F | 220 | HEC | CAD-CBD-CGD | -2.96 | 107.31 | 112.75 |
| 2 | I | 220 | HEC | CMB-C2B-C1B | -2.96 | 123.47 | 128.36 |
| 2 | J | 220 | HEC | CBD-CAD-C3D | -2.94 | 107.25 | 112.53 |
| 2 | K | 220 | HEC | CBD-CAD-C3D | -2.94 | 107.26 | 112.53 |
| 2 | 3 | 220 | HEC | CMC-C2C-C1C | -2.92 | 123.53 | 128.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | C | 220 | HEC | CAD-CBD-CGD | -2.92 | 107.40 | 112.75 |
| 2 | W | 220 | HEC | CMB-C2B-C1B | -2.90 | 123.57 | 128.36 |
| 2 | L | 220 | HEC | CMC-C2C-C1C | -2.88 | 123.61 | 128.36 |
| 2 | H | 220 | HEC | CMB-C2B-C1B | -2.87 | 123.62 | 128.36 |
| 2 | Q | 220 | HEC | CBA-CAA-C2A | -2.85 | 107.42 | 112.53 |
| 2 | 5 | 220 | HEC | CAA-C2A-C1A | -2.83 | 123.93 | 127.01 |
| 2 | X | 220 | HEC | CAA-C2A-C1A | -2.83 | 123.94 | 127.01 |
| 2 | F | 220 | HEC | CMC-C2C-C1C | -2.81 | 123.71 | 128.36 |
| 2 | F | 220 | HEC | CMB-C2B-C1B | -2.80 | 123.73 | 128.36 |
| 2 | P | 220 | HEC | CBA-CAA-C2A | -2.79 | 107.52 | 112.53 |
| 2 | Y | 220 | HEC | CAD-CBD-CGD | -2.79 | 107.64 | 112.75 |
| 2 | C | 220 | HEC | CBA-CAA-C2A | -2.78 | 107.55 | 112.53 |
| 2 | V | 220 | HEC | CMC-C2C-C1C | -2.78 | 123.77 | 128.36 |
| 2 | C | 220 | HEC | CBD-CAD-C3D | -2.73 | 107.63 | 112.53 |
| 2 | B | 220 | HEC | C3C-C4C-NC | -2.72 | 105.80 | 110.94 |
| 2 | 1 | 220 | HEC | CMD-C2D-C1D | -2.69 | 123.91 | 128.36 |
| 2 | 1 | 220 | HEC | CAD-CBD-CGD | -2.69 | 107.82 | 112.75 |
| 2 | W | 220 | HEC | CBA-CAA-C2A | -2.67 | 107.73 | 112.53 |
| 2 | I | 220 | HEC | CAD-CBD-CGD | -2.67 | 107.85 | 112.75 |
| 2 | 6 | 220 | HEC | CAA-CBA-CGA | -2.67 | 107.85 | 112.75 |
| 2 | U | 220 | HEC | CMC-C2C-C1C | -2.66 | 123.96 | 128.36 |
| 2 | B | 220 | HEC | CAD-CBD-CGD | -2.64 | 107.91 | 112.75 |
| 2 | W | 220 | HEC | CAD-CBD-CGD | -2.62 | 107.94 | 112.75 |
| 2 | O | 220 | HEC | CMC-C2C-C1C | -2.62 | 124.04 | 128.36 |
| 2 | 6 | 220 | HEC | C3B-C4B-NB | -2.61 | 106.02 | 110.94 |
| 2 | Z | 220 | HEC | CAA-C2A-C1A | -2.58 | 124.21 | 127.01 |
| 2 | P | 220 | HEC | C3C-C4C-NC | -2.56 | 106.11 | 110.94 |
| 2 | L | 220 | HEC | C3C-C4C-NC | -2.53 | 106.17 | 110.94 |
| 2 | G | 220 | HEC | CAA-C2A-C1A | -2.52 | 124.27 | 127.01 |
| 2 | 5 | 220 | HEC | CMC-C2C-C1C | -2.48 | 124.26 | 128.36 |
| 2 | L | 220 | HEC | CAD-C3D-C2D | -2.45 | 122.00 | 129.00 |
| 2 | X | 220 | HEC | CMC-C2C-C1C | -2.41 | 124.38 | 128.36 |
| 2 | L | 220 | HEC | CBA-CAA-C2A | -2.41 | 108.22 | 112.53 |
| 2 | J | 220 | HEC | CBC-CAC-C3C | -2.40 | 122.02 | 127.35 |
| 2 | O | 220 | HEC | CBC-CAC-C3C | -2.40 | 122.02 | 127.35 |
| 2 | D | 220 | HEC | CAA-C2A-C1A | -2.38 | 124.42 | 127.01 |
| 2 | P | 220 | HEC | CAD-CBD-CGD | -2.38 | 108.39 | 112.75 |
| 2 | M | 220 | HEC | CBA-CAA-C2A | -2.37 | 108.29 | 112.53 |
| 2 | V | 220 | HEC | CBC-CAC-C3C | -2.36 | 122.10 | 127.35 |
| 2 | D | 220 | HEC | CMC-C2C-C1C | -2.36 | 124.45 | 128.36 |
| 2 | 4 | 220 | HEC | CAA-C2A-C1A | -2.34 | 124.47 | 127.01 |
| 2 | 3 | 220 | HEC | CBA-CAA-C2A | -2.34 | 108.33 | 112.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | C | 220 | HEC | CMB-C2B-C1B | -2.29 | 124.57 | 128.36 |
| 2 | R | 220 | HEC | C3C-C4C-NC | -2.29 | 106.63 | 110.94 |
| 2 | G | 220 | HEC | CMD-C2D-C1D | -2.26 | 124.63 | 128.36 |
| 2 | S | 220 | HEC | CMB-C2B-C1B | -2.24 | 124.66 | 128.36 |
| 2 | R | 220 | HEC | CAA-C2A-C1A | -2.24 | 124.58 | 127.01 |
| 2 | N | 220 | HEC | CAD-C3D-C2D | -2.22 | 122.66 | 129.00 |
| 2 | K | 220 | HEC | CAA-C2A-C1A | -2.22 | 124.60 | 127.01 |
| 2 | E | 220 | HEC | CAA-C2A-C1A | -2.19 | 124.62 | 127.01 |
| 2 | Q | 220 | HEC | CBD-CAD-C3D | -2.18 | 108.63 | 112.53 |
| 2 | R | 220 | HEC | CAD-CBD-CGD | -2.17 | 108.77 | 112.75 |
| 2 | 3 | 220 | HEC | CAD-CBD-CGD | -2.17 | 108.77 | 112.75 |
| 2 | F | 220 | HEC | C3C-C4C-NC | -2.15 | 106.88 | 110.94 |
| 2 | O | 220 | HEC | C3C-C4C-NC | -2.12 | 106.94 | 110.94 |
| 2 | 3 | 220 | HEC | CBD-CAD-C3D | -2.10 | 108.76 | 112.53 |
| 2 | G | 220 | HEC | CBA-CAA-C2A | -2.10 | 108.77 | 112.53 |
| 2 | O | 220 | HEC | CBD-CAD-C3D | -2.09 | 108.78 | 112.53 |
| 2 | V | 220 | HEC | CAD-CBD-CGD | -2.07 | 108.95 | 112.75 |
| 2 | D | 220 | HEC | CBA-CAA-C2A | -2.06 | 108.84 | 112.53 |
| 2 | U | 220 | HEC | CAA-C2A-C1A | -2.05 | 124.78 | 127.01 |
| 2 | 5 | 220 | HEC | C3B-C4B-NB | -2.01 | 107.15 | 110.94 |
| 2 | X | 220 | HEC | CMA-C3A-C2A | 2.15 | 129.73 | 125.24 |
| 2 | 4 | 220 | HEC | CMA-C3A-C2A | 2.26 | 129.97 | 125.24 |
| 2 | G | 220 | HEC | CMA-C3A-C2A | 2.29 | 130.03 | 125.24 |
| 2 | 6 | 220 | HEC | CAD-C3D-C4D | 2.30 | 129.50 | 127.01 |
| 2 | Y | 220 | HEC | CAD-C3D-C4D | 2.42 | 129.64 | 127.01 |
| 2 | T | 220 | HEC | CAD-C3D-C4D | 2.46 | 129.68 | 127.01 |
| 2 | W | 220 | HEC | CMA-C3A-C2A | 2.74 | 130.97 | 125.24 |
| 2 | 1 | 220 | HEC | CMD-C2D-C3D | 3.03 | 131.57 | 125.24 |
| 2 | O | 220 | HEC | CAD-C3D-C4D | 3.22 | 130.50 | 127.01 |
| 2 | Q | 220 | HEC | CAD-C3D-C4D | 3.91 | 131.25 | 127.01 |
| 2 | J | 220 | HEC | CAD-C3D-C4D | 3.92 | 131.26 | 127.01 |
| 2 | N | 220 | HEC | CAD-C3D-C4D | 4.21 | 131.58 | 127.01 |
| 2 | L | 220 | HEC | CAD-C3D-C4D | 4.43 | 131.82 | 127.01 |
| 2 | S | 220 | HEC | CAD-C3D-C4D | 4.74 | 132.16 | 127.01 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 191 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | 1 | 220 | HEC | 2 | 0 |
| 2 | 2 | 220 | HEC | 8 | 0 |
| 2 | 3 | 220 | HEC | 6 | 0 |
| 2 | 4 | 220 | HEC | 7 | 0 |
| 2 | 5 | 220 | HEC | 10 | 0 |
| 2 | 6 | 220 | HEC | 28 | 0 |
| 2 | A | 220 | HEC | 8 | 0 |
| 2 | B | 220 | HEC | 3 | 0 |
| 2 | C | 220 | HEC | 7 | 0 |
| 2 | D | 220 | HEC | 8 | 0 |
| 2 | E | 220 | HEC | 2 | 0 |
| 2 | F | 220 | HEC | 6 | 0 |
| 2 | G | 220 | HEC | 9 | 0 |
| 2 | H | 220 | HEC | 7 | 0 |
| 2 | I | 220 | HEC | 6 | 0 |
| 2 | J | 220 | HEC | 7 | 0 |
| 2 | K | 220 | HEC | 2 | 0 |
| 2 | L | 220 | HEC | 6 | 0 |
| 2 | M | 220 | HEC | 8 | 0 |
| 2 | N | 220 | HEC | 5 | 0 |
| 2 | O | 220 | HEC | 3 | 0 |
| 2 | P | 220 | HEC | 2 | 0 |
| 2 | Q | 220 | HEC | 6 | 0 |
| 3 | R | 104 | GOL | 7 | 0 |
| 2 | R | 220 | HEC | 1 | 0 |
| 2 | S | 220 | HEC | 10 | 0 |
| 2 | T | 220 | HEC | 2 | 0 |
| 2 | U | 220 | HEC | 6 | 0 |
| 2 | V | 220 | HEC | 5 | 0 |
| 2 | W | 220 | HEC | 2 | 0 |
| 2 | X | 220 | HEC | 7 | 0 |
| 2 | Y | 220 | HEC | 8 | 0 |
| 2 | Z | 220 | HEC | 4 | 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 | 1 | 81/103 (78%) | 0.56 | 8 (9%) 9 7 | 17, 30, 42, 48 | 0 |
| 1 | 2 | 81/103 (78%) | 1.07 | 16 (19%) 1 1 | 21, 38, 54, 57 | 0 |
| 1 | 3 | 81/103 (78%) | 0.81 | 11 (13%) 4 3 | 22, 33, 46, 48 | 0 |
| 1 | 4 | 81/103 (78%) | 0.70 | 9 (11%) 7 5 | 24, 33, 45, 49 | 0 |
| 1 | 5 | 81/103 (78%) | 1.87 | 31 (38%) 0 0 | 25, 37, 58, 63 | 0 |
| 1 | 6 | 79/103 (76%) | 3.17 | 59 (74%) 0 0 | 34, 54, 62, 64 | 0 |
| 1 | A | 81/103 (78%) | -0.36 | 0 100 100 | 10, 17, 24, 30 | 0 |
| 1 | B | 81/103 (78%) | -0.29 | 0 100 100 | 11, 17, 25, 25 | 0 |
| 1 | C | 81/103 (78%) | -0.24 | 0 100 100 | 14, 21, 28, 33 | 0 |
| 1 | D | 81/103 (78%) | -0.20 | 0 100 100 | 14, 22, 31, 34 | 0 |
| 1 | E | 81/103 (78%) | -0.33 | 0 100 100 | 11, 18, 25, 34 | 0 |
| 1 | F | 81/103 (78%) | -0.17 | 1 (1%) 81 78 | 11, 21, 29, 35 | 0 |
| 1 | G | 81/103 (78%) | -0.20 | 1 (1%) 81 78 | 15, 21, 27, 34 | 0 |
| 1 | H | 81/103 (78%) | -0.23 | 2 (2%) 61 56 | 14, 20, 32, 40 | 0 |
| 1 | I | 81/103 (78%) | -0.17 | 0 100 100 | 16, 23, 29, 35 | 0 |
| 1 | J | 81/103 (78%) | 0.55 | 7 (8%) 13 10 | 23, 31, 41, 44 | 0 |
| 1 | K | 81/103 (78%) | 0.40 | 4 (4%) 33 27 | 18, 28, 42, 47 | 0 |
| 1 | L | 81/103 (78%) | 0.01 | 2 (2%) 61 56 | 16, 22, 35, 40 | 0 |
| 1 | M | 80/103 (77%) | 0.61 | 6 (7%) 17 13 | 14, 26, 37, 44 | 0 |
| 1 | N | 81/103 (78%) | 0.40 | 3 (3%) 45 39 | 15, 27, 41, 50 | 0 |
| 1 | O | 81/103 (78%) | -0.20 | 0 100 100 | 12, 18, 29, 33 | 0 |
| 1 | P | 81/103 (78%) | 0.09 | 0 100 100 | 16, 24, 32, 34 | 0 |
| 1 | Q | 81/103 (78%) | -0.14 | 2 (2%) 61 56 | 15, 20, 33, 37 | 0 |
| 1 | R | 81/103 (78%) | 0.16 | 4 (4%) 33 27 | 14, 23, 34, 38 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | S | 81/103 (78%) | 0.28 | 5 (6%) 24 19 | 15, 26, 36, 39 | 0 |
| 1 | T | 81/103 (78%) | -0.09 | 1 (1%) 81 78 | 13, 21, 33, 36 | 0 |
| 1 | U | 81/103 (78%) | -0.14 | 0 100 100 | 14, 22, 30, 33 | 0 |
| 1 | V | 81/103 (78%) | -0.20 | 0 100 100 | 14, 21, 28, 32 | 0 |
| 1 | W | 81/103 (78%) | -0.00 | 1 (1%) 81 78 | 18, 24, 32, 35 | 0 |
| 1 | X | 81/103 (78%) | 0.14 | 2 (2%) 61 56 | 21, 28, 36, 40 | 0 |
| 1 | Y | 81/103 (78%) | 0.01 | 1 (1%) 81 78 | 16, 23, 32, 37 | 0 |
| 1 | Z | 81/103 (78%) | 0.09 | 4 (4%) 33 27 | 17, 23, 33, 38 | 0 |
| All | All | 2589/3296 (78%) | 0.25 | 180 (6%) 19 15 | 10, 24, 45, 64 | 0 |

All (180) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 6 | 87 | LEU | 9.1 |
| 1 | 6 | 45 | THR | 7.5 |
| 1 | 6 | 77 | ALA | 7.3 |
| 1 | 5 | 47 | PRO | 7.1 |
| 1 | 6 | 74 | GLY | 6.8 |
| 1 | 2 | 86 | LEU | 6.5 |
| 1 | 6 | 29 | ALA | 6.4 |
| 1 | 6 | 86 | LEU | 6.3 |
| 1 | 4 | 75 | GLY | 6.2 |
| 1 | 3 | 75 | GLY | 5.7 |
| 1 | 6 | 95 | LEU | 5.7 |
| 1 | N | 41 | ASP | 5.6 |
| 1 | 5 | 48 | GLY | 5.3 |
| 1 | 5 | 44 | ALA | 5.2 |
| 1 | R | 75 | GLY | 5.2 |
| 1 | 5 | 69 | ASN | 5.1 |
| 1 | 6 | 54 | GLY | 5.1 |
| 1 | 6 | 79 | VAL | 5.1 |
| 1 | 6 | 98 | TYR | 5.1 |
| 1 | 3 | 76 | LEU | 5.1 |
| 1 | 2 | 45 | THR | 5.0 |
| 1 | 6 | 69 | ASN | 5.0 |
| 1 | 3 | 45 | THR | 5.0 |
| 1 | 6 | 31 | ALA | 4.9 |
| 1 | 5 | 71 | GLU | 4.9 |
| 1 | 4 | 74 | GLY | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 6 | 41 | ASP | 4.7 |
| 1 | 6 | 99 | TYR | 4.7 |
| 1 | 2 | 40 | ALA | 4.7 |
| 1 | 6 | 68 | LYS | 4.6 |
| 1 | 6 | 73 | SER | 4.5 |
| 1 | M | 40 | ALA | 4.5 |
| 1 | R | 74 | GLY | 4.4 |
| 1 | 5 | 46 | ILE | 4.4 |
| 1 | 5 | 74 | GLY | 4.4 |
| 1 | 6 | 24 | ALA | 4.4 |
| 1 | 5 | 40 | ALA | 4.3 |
| 1 | M | 41 | ASP | 4.2 |
| 1 | 6 | 67 | TYR | 4.2 |
| 1 | 6 | 27 | GLY | 4.1 |
| 1 | 2 | 49 | TYR | 4.1 |
| 1 | 6 | 84 | ALA | 4.1 |
| 1 | 6 | 88 | SER | 4.1 |
| 1 | 6 | 94 | ASN | 4.1 |
| 1 | 6 | 76 | LEU | 4.0 |
| 1 | 2 | 47 | PRO | 4.0 |
| 1 | K | 86 | LEU | 4.0 |
| 1 | 5 | 36 | ALA | 4.0 |
| 1 | 5 | 41 | ASP | 4.0 |
| 1 | 3 | 40 | ALA | 3.9 |
| 1 | 6 | 60 | ILE | 3.9 |
| 1 | 5 | 53 | LYS | 3.9 |
| 1 | 5 | 102 | LEU | 3.8 |
| 1 | 1 | 69 | ASN | 3.7 |
| 1 | 6 | 56 | ASN | 3.7 |
| 1 | 5 | 49 | TYR | 3.7 |
| 1 | 2 | 75 | GLY | 3.7 |
| 1 | L | 75 | GLY | 3.7 |
| 1 | 5 | 73 | SER | 3.7 |
| 1 | 2 | 41 | ASP | 3.6 |
| 1 | 6 | 97 | ALA | 3.6 |
| 1 | 5 | 43 | ASN | 3.5 |
| 1 | 6 | 47 | PRO | 3.5 |
| 1 | 5 | 77 | ALA | 3.5 |
| 1 | 6 | 58 | GLN | 3.5 |
| 1 | M | 101 | SER | 3.5 |
| 1 | 2 | 90 | ASP | 3.5 |
| 1 | 6 | 61 | VAL | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 5 | 79 | VAL | 3.4 |
| 1 | 6 | 40 | ALA | 3.4 |
| 1 | 5 | 70 | LYS | 3.4 |
| 1 | 3 | 74 | GLY | 3.4 |
| 1 | 5 | 75 | GLY | 3.4 |
| 1 | 6 | 57 | GLU | 3.4 |
| 1 | S | 26 | ALA | 3.3 |
| 1 | 6 | 22 | GLY | 3.3 |
| 1 | 6 | 65 | LYS | 3.3 |
| 1 | 6 | 81 | GLN | 3.3 |
| 1 | N | 47 | PRO | 3.3 |
| 1 | 6 | 80 | MET | 3.3 |
| 1 | 2 | 43 | ASN | 3.3 |
| 1 | 6 | 89 | ASP | 3.2 |
| 1 | 3 | 86 | LEU | 3.2 |
| 1 | S | 22 | GLY | 3.2 |
| 1 | 6 | 25 | ALA | 3.2 |
| 1 | 2 | 74 | GLY | 3.1 |
| 1 | 3 | 47 | PRO | 3.1 |
| 1 | 6 | 32 | ALA | 3.0 |
| 1 | 6 | 64 | ILE | 3.0 |
| 1 | 6 | 43 | ASN | 3.0 |
| 1 | 5 | 101 | SER | 2.9 |
| 1 | R | 45 | THR | 2.9 |
| 1 | K | 70 | LYS | 2.9 |
| 1 | 2 | 46 | ILE | 2.9 |
| 1 | 5 | 66 | ALA | 2.9 |
| 1 | 5 | 54 | GLY | 2.8 |
| 1 | 5 | 84 | ALA | 2.8 |
| 1 | H | 40 | ALA | 2.7 |
| 1 | 6 | 93 | ALA | 2.7 |
| 1 | 6 | 63 | SER | 2.7 |
| 1 | 5 | 51 | ASN | 2.7 |
| 1 | 2 | 89 | ASP | 2.7 |
| 1 | Q | 75 | GLY | 2.7 |
| 1 | 2 | 76 | LEU | 2.7 |
| 1 | 6 | 92 | ILE | 2.7 |
| 1 | 6 | 23 | ASP | 2.7 |
| 1 | 5 | 67 | TYR | 2.7 |
| 1 | 6 | 71 | GLU | 2.6 |
| 1 | W | 75 | GLY | 2.6 |
| 1 | 3 | 22 | GLY | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 6 | 91 | ASP | 2.6 |
| 1 | G | 40 | ALA | 2.6 |
| 1 | H | 41 | ASP | 2.6 |
| 1 | J | 40 | ALA | 2.6 |
| 1 | Z | 75 | GLY | 2.6 |
| 1 | 1 | 56 | ASN | 2.5 |
| 1 | 6 | 52 | LEU | 2.5 |
| 1 | 1 | 45 | THR | 2.5 |
| 1 | 3 | 70 | LYS | 2.5 |
| 1 | Z | 40 | ALA | 2.5 |
| 1 | 2 | 32 | ALA | 2.5 |
| 1 | J | 47 | PRO | 2.5 |
| 1 | J | 90 | ASP | 2.5 |
| 1 | 2 | 73 | SER | 2.5 |
| 1 | J | 25 | ALA | 2.5 |
| 1 | 2 | 35 | ALA | 2.5 |
| 1 | 4 | 22 | GLY | 2.5 |
| 1 | N | 85 | SER | 2.4 |
| 1 | X | 90 | ASP | 2.4 |
| 1 | L | 74 | GLY | 2.4 |
| 1 | 6 | 33 | VAL | 2.4 |
| 1 | Z | 86 | LEU | 2.4 |
| 1 | 1 | 75 | GLY | 2.4 |
| 1 | 6 | 70 | LYS | 2.4 |
| 1 | S | 45 | THR | 2.4 |
| 1 | 5 | 35 | ALA | 2.4 |
| 1 | X | 45 | THR | 2.4 |
| 1 | M | 97 | ALA | 2.4 |
| 1 | R | 47 | PRO | 2.4 |
| 1 | S | 41 | ASP | 2.4 |
| 1 | 6 | 72 | ARG | 2.4 |
| 1 | 6 | 96 | ALA | 2.4 |
| 1 | J | 41 | ASP | 2.3 |
| 1 | 4 | 90 | ASP | 2.3 |
| 1 | 3 | 49 | TYR | 2.3 |
| 1 | 6 | 28 | GLN | 2.3 |
| 1 | 4 | 69 | ASN | 2.3 |
| 1 | 1 | 89 | ASP | 2.3 |
| 1 | 5 | 80 | MET | 2.3 |
| 1 | Z | 41 | ASP | 2.3 |
| 1 | J | 89 | ASP | 2.3 |
| 1 | 5 | 99 | TYR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 5 | 72 | ARG | 2.2 |
| 1 | 4 | 81 | GLN | 2.2 |
| 1 | 5 | 42 | GLY | 2.2 |
| 1 | 6 | 46 | ILE | 2.2 |
| 1 | 6 | 85 | SER | 2.2 |
| 1 | Y | 41 | ASP | 2.2 |
| 1 | 5 | 45 | THR | 2.2 |
| 1 | M | 96 | ALA | 2.2 |
| 1 | 3 | 46 | ILE | 2.2 |
| 1 | M | 100 | SER | 2.2 |
| 1 | T | 41 | ASP | 2.1 |
| 1 | 6 | 53 | LYS | 2.1 |
| 1 | Q | 41 | ASP | 2.1 |
| 1 | 1 | 36 | ALA | 2.1 |
| 1 | 6 | 66 | ALA | 2.1 |
| 1 | F | 40 | ALA | 2.1 |
| 1 | K | 45 | THR | 2.1 |
| 1 | 4 | 58 | GLN | 2.1 |
| 1 | 4 | 88 | SER | 2.1 |
| 1 | S | 29 | ALA | 2.1 |
| 1 | 1 | 90 | ASP | 2.1 |
| 1 | 4 | 60 | ILE | 2.1 |
| 1 | J | 23 | ASP | 2.1 |
| 1 | 6 | 59 | TYR | 2.0 |
| 1 | 6 | 90 | ASP | 2.0 |
| 1 | 6 | 62 | SER | 2.0 |
| 1 | 1 | 46 | ILE | 2.0 |
| 1 | K | 69 | ASN | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no 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 | GOL | P | 104 | 6/6 | 0.90 | 0.17 | 2.59 | 24,32,34,37 | 0 |
| 3 | GOL | E | 104 | 6/6 | 0.92 | 0.15 | 1.84 | 18,26,29,34 | 0 |
| 2 | HEC | U | 220 | 43/43 | 0.98 | 0.13 | 1.43 | 10,14,19,22 | 0 |
| 2 | HEC | F | 220 | 43/43 | 0.99 | 0.13 | 1.37 | 7,12,17,19 | 0 |
| 3 | GOL | R | 104 | 6/6 | 0.93 | 0.17 | 1.16 | 32,36,37,41 | 0 |
| 2 | HEC | T | 220 | 43/43 | 0.98 | 0.13 | 1.16 | 8,14,18,22 | 0 |
| 2 | HEC | C | 220 | 43/43 | 0.98 | 0.12 | 1.14 | 9,13,18,20 | 0 |
| 2 | HEC | A | 220 | 43/43 | 0.98 | 0.12 | 1.02 | 4,11,16,17 | 0 |
| 2 | HEC | G | 220 | 43/43 | 0.98 | 0.12 | 1.01 | 12,16,19,22 | 0 |
| 2 | HEC | B | 220 | 43/43 | 0.99 | 0.12 | 0.76 | 8,11,15,17 | 0 |
| 2 | HEC | V | 220 | 43/43 | 0.98 | 0.12 | 0.75 | 10,14,18,19 | 0 |
| 2 | HEC | D | 220 | 43/43 | 0.98 | 0.12 | 0.73 | 11,15,18,19 | 0 |
| 2 | HEC | 5 | 220 | 43/43 | 0.85 | 0.24 | 0.67 | 26,35,43,48 | 0 |
| 2 | HEC | K | 220 | 43/43 | 0.98 | 0.13 | 0.64 | 12,16,19,21 | 0 |
| 2 | HEC | E | 220 | 43/43 | 0.99 | 0.11 | 0.63 | 7,11,16,19 | 0 |
| 2 | HEC | I | 220 | 43/43 | 0.98 | 0.11 | 0.61 | 13,16,22,24 | 0 |
| 2 | HEC | Q | 220 | 43/43 | 0.98 | 0.11 | 0.54 | 10,14,18,22 | 0 |
| 2 | HEC | O | 220 | 43/43 | 0.98 | 0.11 | 0.54 | 7,12,19,20 | 0 |
| 2 | HEC | J | 220 | 43/43 | 0.96 | 0.13 | 0.48 | 11,21,24,32 | 0 |
| 2 | HEC | H | 220 | 43/43 | 0.98 | 0.11 | 0.40 | 11,14,20,21 | 0 |
| 2 | HEC | L | 220 | 43/43 | 0.98 | 0.11 | 0.30 | 11,16,19,23 | 0 |
| 2 | HEC | Y | 220 | 43/43 | 0.96 | 0.10 | 0.26 | 12,16,20,22 | 0 |
| 2 | HEC | Z | 220 | 43/43 | 0.97 | 0.11 | 0.25 | 10,15,20,25 | 0 |
| 2 | HEC | S | 220 | 43/43 | 0.97 | 0.12 | 0.24 | 12,20,23,26 | 0 |
| 2 | HEC | W | 220 | 43/43 | 0.98 | 0.12 | 0.23 | 14,19,23,24 | 0 |
| 2 | HEC | 6 | 220 | 43/43 | 0.84 | 0.24 | 0.22 | 19,38,44,48 | 0 |
| 2 | HEC | X | 220 | 43/43 | 0.97 | 0.11 | 0.21 | 16,21,25,27 | 0 |
| 2 | HEC | P | 220 | 43/43 | 0.98 | 0.11 | 0.04 | 10,15,19,21 | 0 |
| 2 | HEC | R | 220 | 43/43 | 0.98 | 0.12 | 0.00 | 9,14,18,20 | 0 |
| 2 | HEC | 1 | 220 | 43/43 | 0.98 | 0.12 | -0.05 | 12,19,24,28 | 0 |
| 2 | HEC | 2 | 220 | 43/43 | 0.93 | 0.13 | -0.07 | 17,31,35,36 | 0 |
| 3 | GOL | C | 104 | 6/6 | 0.91 | 0.10 | -0.14 | 26,31,33,34 | 0 |
| 2 | HEC | 4 | 220 | 43/43 | 0.95 | 0.12 | -0.19 | 19,25,30,31 | 0 |
| 2 | HEC | M | 220 | 43/43 | 0.98 | 0.11 | -0.19 | 11,15,18,24 | 0 |
| 2 | HEC | N | 220 | 43/43 | 0.95 | 0.12 | -0.32 | 14,23,28,33 | 0 |
| 2 | HEC | 3 | 220 | 43/43 | 0.95 | 0.11 | -0.65 | 21,29,32,34 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.