



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:16 PM GMT

PDB ID : 4H0L  
Title : Cytochrome b6f Complex Crystal Structure from *Mastigocladus laminosus* with n-Side Inhibitor NQNO  
Authors : Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.  
Deposited on : 2012-09-08  
Resolution : 3.25 Å(reported)

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

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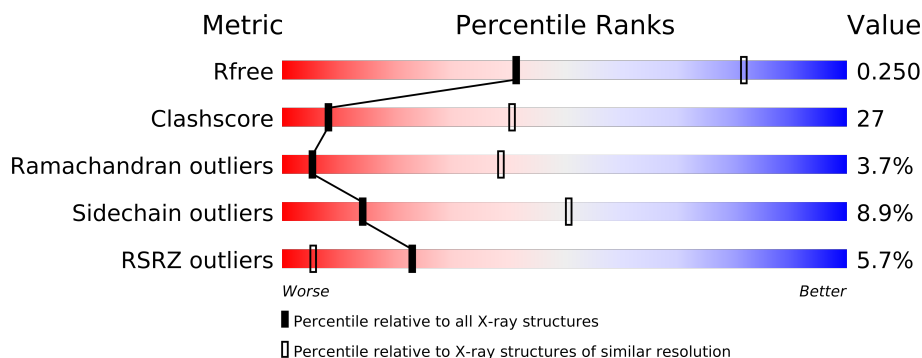
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.25 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 66092                       | 1085 (3.32-3.20)                                      |
| Clashscore            | 79885                       | 1374 (3.32-3.20)                                      |
| Ramachandran outliers | 78287                       | 1348 (3.32-3.20)                                      |
| Sidechain outliers    | 78261                       | 1346 (3.32-3.20)                                      |
| RSRZ outliers         | 66119                       | 1086 (3.32-3.20)                                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 215    |                  |
| 2   | B     | 160    |                  |
| 3   | C     | 289    |                  |
| 4   | D     | 179    |                  |
| 5   | E     | 32     |                  |
| 6   | F     | 35     |                  |
| 7   | G     | 37     |                  |
| 8   | H     | 29     |                  |

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

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 11  | OPC  | A     | 305 | -        | X                |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 11  | OPC  | B     | 203 | -        | X                |
| 12  | UMQ  | A     | 306 | -        | X                |
| 12  | UMQ  | C     | 301 | -        | X                |
| 16  | SQD  | D     | 201 | -        | X                |
| 17  | BCR  | G     | 101 | -        | X                |

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 16219 atoms, of which 8226 are hydrogens and 0 are deuterium.

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

- Molecule 1 is a protein called Cytochrome b6.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 213      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3420  | 1132 | 1722 | 270 | 286 | 10 |         |         |       |

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 160      | Total | C   | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2558  | 841 | 1309 | 193 | 209 | 6 |         |         |       |

- Molecule 3 is a protein called Apocytochrome f.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 286      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4419  | 1406 | 2219 | 366 | 421 | 7 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 11      | PRO      | GLU    | SEE REMARK 999 | UNP P83793 |

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 161      | Total | C   | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2460  | 791 | 1224 | 213 | 225 | 7 |         |         |       |

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 5   | E     | 32       | Total | C   | H   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 179 | 284 | 34 | 34 | 1 |         |         |       |

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 6   | F     | 32       | Total | C   | H   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 502   | 165 | 260 | 35 | 40 | 2 |         |         |       |

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 7   | G     | 37       | Total | C   | H   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 572   | 188 | 289 | 44 | 50 | 1 |         |         |       |

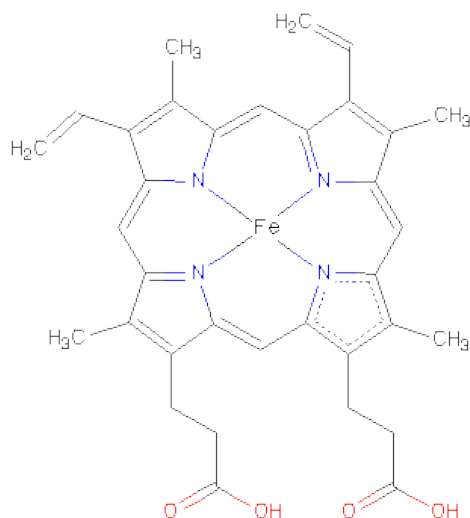
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|---------|-------|
| 8   | H     | 29       | Total | C   | H   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 469   | 156 | 239 | 36 | 36 | 2 |         |         |       |

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

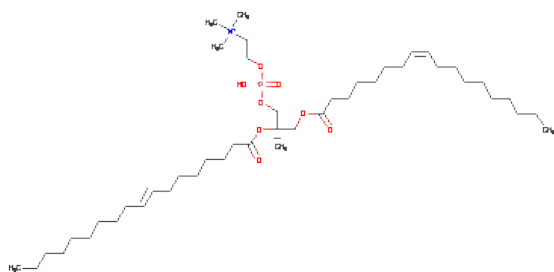
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | B     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | A     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



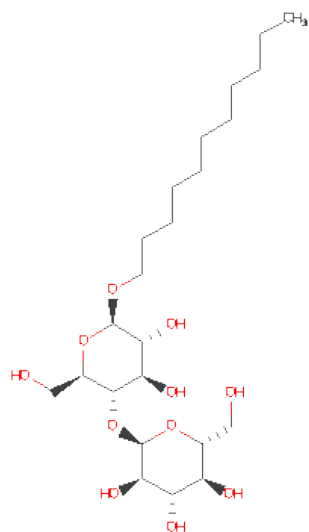
| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 10  | A     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |
| 10  | A     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |
| 10  | A     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |
| 10  | C     | 1        | Total | C  | Fe | H  | N | O | 0       | 0       |
|     |       |          | 73    | 34 | 1  | 30 | 4 | 4 |         |         |

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM4-OXIDE (three-letter code: OPC) (formula: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



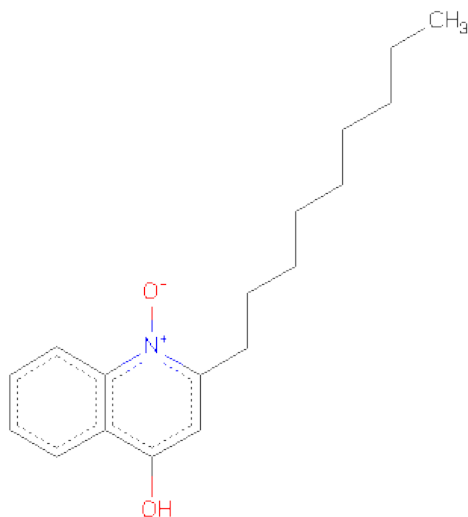
| Mol | Chain | Residues | Atoms |    |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|---------|
| 11  | A     | 1        | Total | C  | H  | N | O | P | 0       | 0       |
|     |       |          | 137   | 44 | 83 | 1 | 8 | 1 |         |         |
| 11  | B     | 1        | Total | C  | H  | N | O | P | 0       | 0       |
|     |       |          | 137   | 44 | 83 | 1 | 8 | 1 |         |         |

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



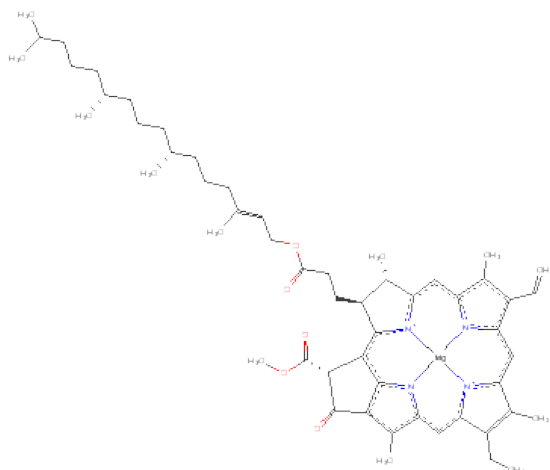
| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 12  | A     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 77    | 23 | 43 | 11 |         |         |
| 12  | A     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 77    | 23 | 43 | 11 |         |         |
| 12  | A     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 77    | 23 | 43 | 11 |         |         |
| 12  | C     | 1        | Total | C  | H  | O  | 0       | 0       |
|     |       |          | 78    | 23 | 44 | 11 |         |         |

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINEN-OXIDE (three-letter code: QNO) (formula: C<sub>18</sub>H<sub>25</sub>NO<sub>2</sub>).



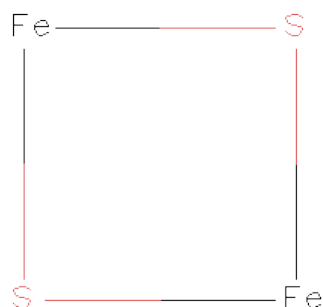
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 13  | A     | 1        | Total | C  | H  | N | O | 0       | 0       |
|     |       |          | 46    | 18 | 25 | 1 | 2 |         |         |

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|
| 14  | B     | 1        | Total | C  | H  | Mg | N | O | 0       | 0       |
|     |       |          | 127   | 55 | 62 | 1  | 4 | 5 |         |         |

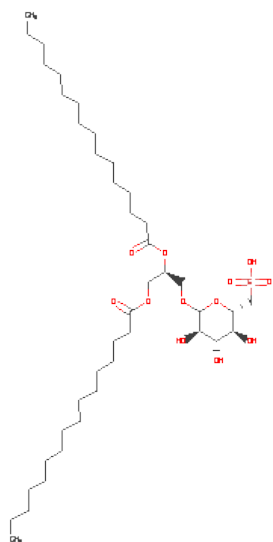
- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).





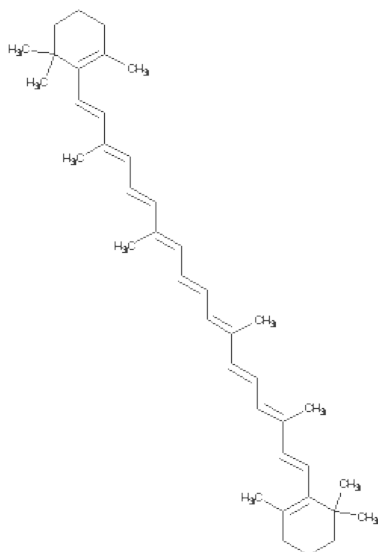
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 15  | D     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 16  | D     | 1        | Total | C  | H  | O  | S | 1       | 0       |
|     |       |          | 131   | 41 | 78 | 11 | 1 |         |         |

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 17  | G     | 1        | Total | C  | H  | 0       | 0       |
|     |       |          | 96    | 40 | 56 |         |         |

- Molecule 18 is water.

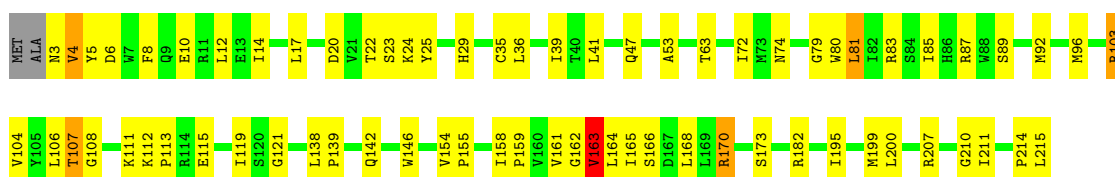
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 18  | A     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 18  | B     | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 18  | C     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots

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

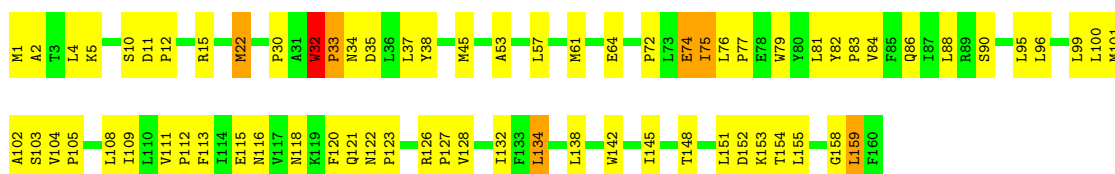
- Molecule 1: Cytochrome b6

Chain A: 



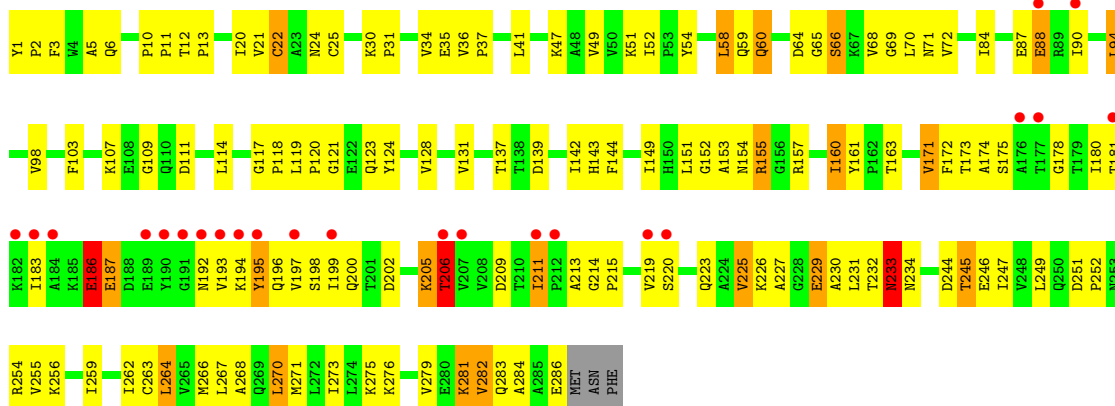
- Molecule 2: Cytochrome b6-f complex subunit 4

Chain B: 



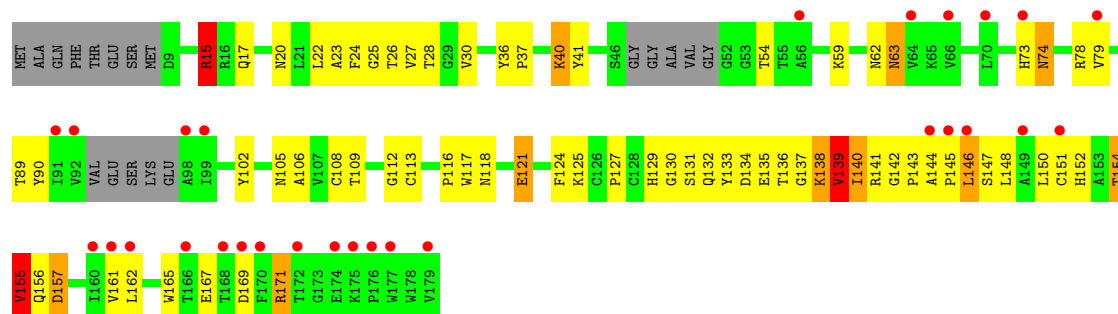
- Molecule 3: Apocytochrome f

Chain C: 



- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit

Chain D: 



- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:



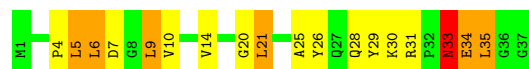
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:



- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 61 2 2                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 159.13Å 159.13Å 362.25Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 48.45 – 3.25<br>48.45 – 3.25                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (48.45-3.25)<br>99.6 (48.45-3.25)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.47 (at 3.25Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.1_1168)                          | Depositor        |
| R, $R_{free}$                                                           | 0.218 , 0.247<br>0.221 , 0.250                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2185 reflections (5.03%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 96.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.106                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 71.3                                                 | EDS              |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| L-test for twinning                                                     | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Outliers                                                                | 2 of 43469 reflections (0.005%)                             | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 16219                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 106.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, CLA, CD, FES, OPC, HEM, QNO, BCR, SQD

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.40         | 0/1750  | 0.55        | 0/2388         |
| 2   | B     | 0.34         | 0/1288  | 0.63        | 1/1765 (0.1%)  |
| 3   | C     | 0.37         | 0/2248  | 0.60        | 0/3061         |
| 4   | D     | 0.29         | 0/1267  | 0.58        | 1/1725 (0.1%)  |
| 5   | E     | 0.47         | 0/253   | 0.94        | 0/340          |
| 6   | F     | 0.40         | 0/246   | 0.52        | 0/331          |
| 7   | G     | 0.42         | 0/289   | 0.75        | 1/391 (0.3%)   |
| 8   | H     | 0.40         | 0/236   | 0.55        | 0/323          |
| All | All   | 0.37         | 0/7577  | 0.61        | 3/10324 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 2                   |
| 5   | E     | 0                   | 1                   |
| 7   | G     | 0                   | 1                   |
| 8   | H     | 0                   | 2                   |
| All | All   | 0                   | 6                   |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 32  | TRP  | C-N-CD    | -8.06 | 102.87      | 120.60   |
| 7   | G     | 35  | LEU  | CA-CB-CG  | 5.34  | 127.58      | 115.30   |
| 4   | D     | 15  | ARG  | NE-CZ-NH1 | -5.03 | 117.78      | 120.30   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 2   | ALA  | Peptide |
| 2   | B     | 32  | TRP  | Peptide |
| 5   | E     | 28  | SER  | Peptide |
| 7   | G     | 33  | ASN  | Peptide |
| 8   | H     | 2   | GLU  | Peptide |
| 8   | H     | 27  | ASN  | Peptide |

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1698  | 1722     | 0        | 73      | 1            |
| 2   | B     | 1249  | 1309     | 0        | 62      | 0            |
| 3   | C     | 2200  | 2219     | 0        | 128     | 1            |
| 4   | D     | 1236  | 1224     | 0        | 92      | 0            |
| 5   | E     | 248   | 284      | 0        | 47      | 0            |
| 6   | F     | 242   | 260      | 0        | 14      | 0            |
| 7   | G     | 283   | 289      | 0        | 24      | 0            |
| 8   | H     | 230   | 239      | 0        | 12      | 0            |
| 9   | A     | 1     | 0        | 0        | 0       | 0            |
| 9   | B     | 1     | 0        | 0        | 0       | 0            |
| 10  | A     | 129   | 90       | 72       | 31      | 0            |
| 10  | C     | 43    | 30       | 24       | 16      | 0            |
| 11  | A     | 54    | 83       | 0        | 12      | 0            |
| 11  | B     | 54    | 83       | 0        | 4       | 0            |
| 12  | A     | 102   | 129      | 0        | 8       | 0            |
| 12  | C     | 34    | 44       | 0        | 4       | 0            |
| 13  | A     | 21    | 25       | 0        | 2       | 0            |
| 14  | B     | 65    | 62       | 7        | 4       | 0            |
| 15  | D     | 4     | 0        | 0        | 1       | 0            |
| 16  | D     | 53    | 78       | 0        | 16      | 0            |
| 17  | G     | 40    | 56       | 0        | 6       | 0            |
| 18  | A     | 2     | 0        | 0        | 0       | 0            |
| 18  | B     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | C     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 7993  | 8226     | 103      | 432     | 1            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (432) close contacts within the same asymmetric unit are listed below.

| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:15:ARG:NH1    | 5:E:30:LYS:O      | 1.87        | 1.07     |
| 3:C:22:CYS:SG     | 10:C:302:HEM:C3B  | 2.51        | 1.04     |
| 4:D:25:GLY:HA3    | 16:D:201:SQD:H342 | 1.40        | 1.00     |
| 3:C:25:CYS:SG     | 10:C:302:HEM:CAC  | 2.51        | 0.99     |
| 4:D:25:GLY:HA2    | 16:D:201:SQD:H312 | 1.53        | 0.91     |
| 4:D:25:GLY:O      | 16:D:201:SQD:H331 | 1.72        | 0.90     |
| 5:E:6:VAL:O       | 5:E:9:ILE:O       | 1.92        | 0.88     |
| 5:E:20:VAL:HG22   | 6:F:29:ILE:HD11   | 1.56        | 0.86     |
| 4:D:25:GLY:HA3    | 16:D:201:SQD:C34  | 2.06        | 0.85     |
| 5:E:20:VAL:HG22   | 6:F:29:ILE:CD1    | 2.05        | 0.85     |
| 1:A:163:VAL:HG12  | 1:A:164:LEU:N     | 1.92        | 0.84     |
| 1:A:39:ILE:HD11   | 17:G:101:BCR:H313 | 1.61        | 0.83     |
| 14:B:202:CLA:HBB1 | 14:B:202:CLA:HHC  | 1.60        | 0.83     |
| 1:A:92:MET:HE3    | 11:A:305:OPC:HBV1 | 1.60        | 0.82     |
| 1:A:39:ILE:CD1    | 17:G:101:BCR:H313 | 2.10        | 0.82     |
| 3:C:22:CYS:SG     | 10:C:302:HEM:CAB  | 2.68        | 0.81     |
| 4:D:134:ASP:OD2   | 4:D:171:ARG:NH2   | 2.15        | 0.79     |
| 1:A:35:CYS:SG     | 10:A:304:HEM:CAB  | 2.71        | 0.79     |
| 3:C:35:GLU:OE1    | 3:C:51:LYS:NZ     | 2.13        | 0.79     |
| 4:D:138:LYS:HD3   | 4:D:171:ARG:CZ    | 2.13        | 0.78     |
| 2:B:109:ILE:O     | 2:B:112:PRO:HD2   | 1.84        | 0.76     |
| 10:A:302:HEM:HMB  | 10:A:302:HEM:HBBA | 1.65        | 0.76     |
| 10:A:302:HEM:HMB  | 10:A:302:HEM:HBB2 | 1.65        | 0.76     |
| 3:C:117:GLY:HA2   | 3:C:119:LEU:HG    | 1.66        | 0.76     |
| 3:C:25:CYS:SG     | 10:C:302:HEM:CBC  | 2.73        | 0.76     |
| 1:A:35:CYS:SG     | 10:A:304:HEM:CBB  | 2.74        | 0.76     |
| 10:C:302:HEM:HBC2 | 10:C:302:HEM:HMC  | 1.68        | 0.76     |
| 3:C:41:LEU:HD22   | 3:C:252:PRO:HG3   | 1.67        | 0.76     |
| 10:C:302:HEM:HBCA | 10:C:302:HEM:HMC  | 1.68        | 0.75     |
| 7:G:4:PRO:O       | 7:G:7:ASP:N       | 2.20        | 0.74     |
| 6:F:22:LEU:O      | 6:F:26:LEU:HD23   | 1.87        | 0.74     |
| 3:C:271:MET:HE1   | 4:D:22:LEU:HD23   | 1.69        | 0.74     |
| 4:D:25:GLY:CA     | 16:D:201:SQD:H342 | 2.18        | 0.73     |
| 4:D:15:ARG:NH2    | 5:E:29:ILE:O      | 2.22        | 0.72     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 10:A:304:HEM:HMB  | 10:A:304:HEM:HBBA | 1.72        | 0.72     |
| 2:B:32:TRP:CD1    | 2:B:33:PRO:HD3    | 2.24        | 0.72     |
| 10:A:304:HEM:HMB  | 10:A:304:HEM:HBB2 | 1.72        | 0.72     |
| 2:B:104:VAL:HB    | 2:B:105:PRO:HD3   | 1.72        | 0.71     |
| 5:E:26:ILE:HG23   | 5:E:31:LEU:HB3    | 1.73        | 0.71     |
| 4:D:136:THR:OG1   | 4:D:171:ARG:NE    | 2.18        | 0.71     |
| 4:D:25:GLY:HA2    | 16:D:201:SQD:C31  | 2.20        | 0.71     |
| 8:H:17:TRP:O      | 8:H:21:MET:HG2    | 1.91        | 0.70     |
| 4:D:102:TYR:OH    | 4:D:136:THR:HA    | 1.91        | 0.70     |
| 4:D:25:GLY:CA     | 16:D:201:SQD:H312 | 2.22        | 0.70     |
| 3:C:65:GLY:O      | 3:C:66:SER:O      | 2.10        | 0.69     |
| 1:A:111:LYS:NZ    | 2:B:120:PHE:O     | 2.25        | 0.69     |
| 4:D:15:ARG:CZ     | 5:E:30:LYS:O      | 2.39        | 0.69     |
| 1:A:41:LEU:HD23   | 10:A:304:HEM:HBC2 | 1.74        | 0.69     |
| 1:A:41:LEU:HD23   | 10:A:304:HEM:HBCA | 1.74        | 0.69     |
| 10:A:303:HEM:HMC  | 10:A:303:HEM:HBCA | 1.74        | 0.69     |
| 4:D:25:GLY:C      | 16:D:201:SQD:H331 | 2.12        | 0.69     |
| 4:D:118:ASN:OD1   | 4:D:121:GLU:HB2   | 1.93        | 0.68     |
| 5:E:8:TYR:CZ      | 5:E:12:ILE:HD11   | 2.29        | 0.68     |
| 10:A:302:HEM:HMB2 | 10:A:302:HEM:HBBA | 1.73        | 0.68     |
| 10:A:302:HEM:HMB2 | 10:A:302:HEM:HBB2 | 1.73        | 0.68     |
| 10:A:303:HEM:HBC2 | 10:A:303:HEM:HMC2 | 1.75        | 0.68     |
| 10:A:303:HEM:HMC2 | 10:A:303:HEM:HBCA | 1.75        | 0.68     |
| 1:A:8:PHE:HB3     | 1:A:14:ILE:HG13   | 1.75        | 0.68     |
| 1:A:92:MET:HE3    | 11:A:305:OPC:HCB3 | 1.75        | 0.68     |
| 4:D:15:ARG:HH12   | 5:E:31:LEU:HA     | 1.59        | 0.68     |
| 17:G:101:BCR:C21  | 17:G:101:BCR:H383 | 2.24        | 0.68     |
| 5:E:22:ILE:O      | 5:E:23:ILE:O      | 2.12        | 0.67     |
| 3:C:232:THR:O     | 3:C:233:ASN:OD1   | 2.11        | 0.67     |
| 3:C:225:VAL:CG1   | 3:C:229:GLU:HG2   | 2.23        | 0.67     |
| 3:C:21:VAL:O      | 3:C:24:ASN:HB2    | 1.95        | 0.67     |
| 3:C:251:ASP:HB3   | 3:C:254:ARG:HD3   | 1.76        | 0.67     |
| 10:A:303:HEM:HMC  | 10:A:303:HEM:HBC2 | 1.74        | 0.67     |
| 4:D:62:ASN:O      | 4:D:63:ASN:ND2    | 2.28        | 0.67     |
| 3:C:283:GLN:O     | 3:C:286:GLU:HG2   | 1.93        | 0.67     |
| 1:A:83:ARG:NH2    | 2:B:61:MET:O      | 2.28        | 0.67     |
| 3:C:271:MET:HE2   | 4:D:22:LEU:HB3    | 1.76        | 0.67     |
| 3:C:268:ALA:HB2   | 4:D:26:THR:HG22   | 1.77        | 0.67     |
| 1:A:24:LYS:NZ     | 12:A:306:UMQ:O3   | 2.27        | 0.67     |
| 3:C:211:ILE:O     | 3:C:211:ILE:HG13  | 1.94        | 0.67     |
| 3:C:276:LYS:HE2   | 8:H:25:GLY:O      | 1.95        | 0.66     |
| 1:A:113:PRO:HG3   | 2:B:22:MET:CE     | 2.25        | 0.66     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:73:HIS:CE1    | 4:D:79:VAL:HG13   | 2.31        | 0.66     |
| 10:A:302:HEM:HMC  | 10:A:302:HEM:HBC2 | 1.76        | 0.66     |
| 1:A:161:VAL:HG12  | 1:A:165:ILE:HG13  | 1.78        | 0.65     |
| 4:D:109:THR:HG22  | 4:D:144:ALA:HB1   | 1.76        | 0.65     |
| 3:C:271:MET:CE    | 4:D:22:LEU:HD23   | 2.26        | 0.65     |
| 1:A:3:ASN:ND2     | 1:A:6:ASP:OD2     | 2.30        | 0.65     |
| 4:D:131:SER:HA    | 4:D:142:GLY:HA3   | 1.78        | 0.65     |
| 2:B:82:TYR:HB2    | 2:B:83:PRO:HD3    | 1.79        | 0.65     |
| 7:G:33:ASN:O      | 7:G:34:GLU:O      | 2.14        | 0.65     |
| 10:A:302:HEM:HMC  | 10:A:302:HEM:HBCA | 1.76        | 0.65     |
| 4:D:129:HIS:HB2   | 15:D:200:FES:S1   | 2.37        | 0.65     |
| 3:C:22:CYS:SG     | 10:C:302:HEM:C4B  | 2.89        | 0.65     |
| 1:A:142:GLN:HG3   | 2:B:72:PRO:HG3    | 1.77        | 0.65     |
| 4:D:136:THR:HG1   | 4:D:171:ARG:HE    | 1.43        | 0.64     |
| 4:D:138:LYS:HD3   | 4:D:171:ARG:NH1   | 2.12        | 0.64     |
| 3:C:219:VAL:HG21  | 3:C:231:LEU:HB2   | 1.80        | 0.64     |
| 4:D:25:GLY:CA     | 16:D:201:SQD:C34  | 2.75        | 0.64     |
| 4:D:139:VAL:O     | 4:D:140:ILE:HB    | 1.97        | 0.64     |
| 3:C:270:LEU:HA    | 8:H:21:MET:HE2    | 1.80        | 0.64     |
| 3:C:64:ASP:OD1    | 3:C:65:GLY:N      | 2.31        | 0.64     |
| 3:C:174:ALA:HB2   | 3:C:231:LEU:HD23  | 1.80        | 0.63     |
| 5:E:9:ILE:O       | 5:E:10:VAL:HG23   | 1.98        | 0.63     |
| 6:F:31:GLY:O      | 6:F:32:ALA:CB     | 2.47        | 0.63     |
| 1:A:20:ASP:OD1    | 12:A:306:UMQ:O3   | 2.15        | 0.63     |
| 4:D:145:PRO:O     | 4:D:146:LEU:HD13  | 1.98        | 0.63     |
| 4:D:137:GLY:O     | 4:D:138:LYS:O     | 2.17        | 0.63     |
| 2:B:128:VAL:O     | 2:B:132:ILE:HD12  | 1.99        | 0.63     |
| 3:C:25:CYS:SG     | 10:C:302:HEM:HAC  | 2.39        | 0.62     |
| 4:D:25:GLY:CA     | 16:D:201:SQD:C33  | 2.78        | 0.62     |
| 1:A:113:PRO:HG3   | 2:B:22:MET:HE2    | 1.81        | 0.62     |
| 2:B:154:THR:HG23  | 2:B:155:LEU:N     | 2.14        | 0.62     |
| 3:C:175:SER:HB2   | 3:C:209:ASP:OD1   | 1.99        | 0.62     |
| 6:F:27:LEU:HD11   | 8:H:27:ASN:HA     | 1.82        | 0.62     |
| 3:C:144:PHE:CZ    | 3:C:251:ASP:HB2   | 2.35        | 0.62     |
| 10:A:303:HEM:HMB2 | 10:A:303:HEM:HBBA | 1.82        | 0.62     |
| 4:D:165:TRP:CD1   | 4:D:167:GLU:O     | 2.52        | 0.62     |
| 10:A:303:HEM:HMB2 | 10:A:303:HEM:HBB2 | 1.82        | 0.61     |
| 4:D:25:GLY:HA2    | 16:D:201:SQD:C32  | 2.31        | 0.61     |
| 3:C:279:VAL:O     | 3:C:283:GLN:HG3   | 1.99        | 0.61     |
| 2:B:142:TRP:CZ2   | 2:B:155:LEU:O     | 2.54        | 0.61     |
| 5:E:14:LEU:O      | 5:E:18:ILE:HG13   | 1.99        | 0.61     |
| 1:A:161:VAL:CG1   | 1:A:165:ILE:HG13  | 2.29        | 0.61     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:193:VAL:HB    | 3:C:213:ALA:HB2   | 1.83        | 0.61     |
| 4:D:73:HIS:O      | 4:D:74:ASN:HB2    | 2.00        | 0.61     |
| 5:E:16:PHE:HZ     | 6:F:25:LEU:HD22   | 1.65        | 0.61     |
| 2:B:74:GLU:OE2    | 2:B:75:ILE:N      | 2.34        | 0.60     |
| 2:B:151:LEU:O     | 2:B:154:THR:HG22  | 2.02        | 0.60     |
| 3:C:144:PHE:CE1   | 3:C:251:ASP:HB2   | 2.36        | 0.60     |
| 1:A:92:MET:HE3    | 11:A:305:OPC:CBY  | 2.29        | 0.60     |
| 10:A:303:HEM:HMB  | 10:A:303:HEM:HBBA | 1.83        | 0.60     |
| 1:A:113:PRO:CG    | 2:B:22:MET:HE2    | 2.32        | 0.60     |
| 3:C:34:VAL:HG22   | 3:C:151:LEU:HD22  | 1.84        | 0.60     |
| 2:B:37:LEU:HD23   | 2:B:38:TYR:CE2    | 2.36        | 0.60     |
| 10:A:303:HEM:HMB  | 10:A:303:HEM:HBB2 | 1.83        | 0.60     |
| 3:C:262:ILE:HG23  | 8:H:14:VAL:HG13   | 1.84        | 0.60     |
| 3:C:3:PHE:HB2     | 3:C:6:GLN:NE2     | 2.16        | 0.60     |
| 3:C:2:PRO:HG3     | 10:C:302:HEM:HMB3 | 1.84        | 0.59     |
| 2:B:32:TRP:CD1    | 2:B:33:PRO:CD     | 2.86        | 0.59     |
| 1:A:142:GLN:OE1   | 1:A:142:GLN:HA    | 2.02        | 0.59     |
| 4:D:152:HIS:CE1   | 4:D:165:TRP:CE3   | 2.90        | 0.59     |
| 2:B:45:MET:HE3    | 4:D:27:VAL:HA     | 1.84        | 0.59     |
| 1:A:103:ARG:O     | 1:A:107:THR:HB    | 2.03        | 0.59     |
| 1:A:121:GLY:O     | 10:A:303:HEM:HMCB | 2.03        | 0.59     |
| 10:A:304:HEM:O2D  | 13:A:308:QNO:H3   | 2.03        | 0.58     |
| 5:E:12:ILE:O      | 5:E:13:ALA:HB2    | 2.04        | 0.58     |
| 3:C:173:THR:O     | 3:C:231:LEU:HG    | 2.03        | 0.58     |
| 5:E:12:ILE:O      | 5:E:13:ALA:CB     | 2.52        | 0.58     |
| 3:C:251:ASP:HB3   | 3:C:254:ARG:CD    | 2.33        | 0.58     |
| 3:C:58:LEU:HD12   | 3:C:59:GLN:N      | 2.18        | 0.58     |
| 4:D:124:PHE:HB2   | 4:D:133:TYR:HB2   | 1.85        | 0.58     |
| 3:C:5:ALA:HB2     | 10:C:302:HEM:HBB2 | 1.83        | 0.58     |
| 3:C:5:ALA:HB2     | 10:C:302:HEM:HBBA | 1.83        | 0.58     |
| 3:C:172:PHE:HB2   | 3:C:232:THR:HG21  | 1.85        | 0.58     |
| 17:G:101:BCR:H21C | 17:G:101:BCR:H383 | 1.84        | 0.58     |
| 4:D:165:TRP:NE1   | 4:D:167:GLU:O     | 2.37        | 0.58     |
| 3:C:171:VAL:HG12  | 3:C:234:ASN:HA    | 1.86        | 0.57     |
| 3:C:173:THR:OG1   | 3:C:174:ALA:N     | 2.37        | 0.57     |
| 5:E:5:ALA:O       | 5:E:9:ILE:HG12    | 2.05        | 0.57     |
| 2:B:84:VAL:HG13   | 2:B:101:MET:CG    | 2.34        | 0.57     |
| 2:B:79:TRP:CD1    | 7:G:6:LEU:CD1     | 2.87        | 0.57     |
| 1:A:35:CYS:HG     | 10:A:304:HEM:CAB  | 2.14        | 0.56     |
| 4:D:118:ASN:OD1   | 4:D:121:GLU:CB    | 2.53        | 0.56     |
| 6:F:13:PHE:CE2    | 6:F:17:PHE:HE1    | 2.24        | 0.56     |
| 5:E:27:LYS:O      | 5:E:30:LYS:N      | 2.39        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 6:F:31:GLY:O      | 6:F:32:ALA:HB2    | 2.06        | 0.56     |
| 12:C:301:UMQ:O5   | 12:C:301:UMQ:H6'1 | 2.06        | 0.56     |
| 3:C:273:ILE:HD12  | 8:H:25:GLY:HA3    | 1.87        | 0.56     |
| 4:D:143:PRO:O     | 4:D:145:PRO:HD3   | 2.06        | 0.56     |
| 6:F:7:TYR:O       | 6:F:11:LEU:HD12   | 2.06        | 0.56     |
| 3:C:197:VAL:O     | 3:C:209:ASP:N     | 2.38        | 0.56     |
| 2:B:95:LEU:O      | 2:B:95:LEU:HD23   | 2.06        | 0.55     |
| 4:D:15:ARG:NH1    | 5:E:31:LEU:HA     | 2.21        | 0.55     |
| 3:C:84:ILE:HD12   | 3:C:103:PHE:CD1   | 2.42        | 0.55     |
| 2:B:123:PRO:HD2   | 7:G:25:ALA:HB1    | 1.87        | 0.55     |
| 4:D:25:GLY:CA     | 16:D:201:SQD:H331 | 2.36        | 0.55     |
| 3:C:194:LYS:O     | 3:C:196:GLN:N     | 2.40        | 0.55     |
| 3:C:187:GLU:O     | 3:C:187:GLU:HG3   | 2.06        | 0.55     |
| 3:C:71:ASN:HB2    | 10:C:302:HEM:O2A  | 2.06        | 0.55     |
| 3:C:52:ILE:HG12   | 3:C:153:ALA:HB1   | 1.87        | 0.55     |
| 4:D:36:TYR:HB3    | 4:D:37:PRO:HD3    | 1.88        | 0.55     |
| 3:C:225:VAL:HG11  | 3:C:229:GLU:HG2   | 1.88        | 0.55     |
| 3:C:225:VAL:HG12  | 3:C:229:GLU:HG2   | 1.88        | 0.55     |
| 4:D:78:ARG:HG3    | 4:D:117:TRP:CD1   | 2.42        | 0.55     |
| 4:D:15:ARG:NH2    | 5:E:30:LYS:O      | 2.39        | 0.54     |
| 4:D:138:LYS:HA    | 4:D:147:SER:OG    | 2.07        | 0.54     |
| 5:E:9:ILE:O       | 5:E:10:VAL:CB     | 2.54        | 0.54     |
| 11:A:305:OPC:HBZ2 | 17:G:101:BCR:H333 | 1.90        | 0.54     |
| 1:A:106:LEU:HD12  | 7:G:21:LEU:HD23   | 1.89        | 0.54     |
| 7:G:26:TYR:O      | 7:G:30:LYS:HG3    | 2.08        | 0.54     |
| 1:A:111:LYS:O     | 1:A:112:LYS:C     | 2.45        | 0.54     |
| 5:E:24:PHE:O      | 5:E:25:ALA:C      | 2.46        | 0.53     |
| 11:A:305:OPC:CBP  | 7:G:5:LEU:HD11    | 2.37        | 0.53     |
| 1:A:8:PHE:HB3     | 1:A:14:ILE:CG1    | 2.37        | 0.53     |
| 5:E:23:ILE:O      | 5:E:26:ILE:N      | 2.42        | 0.53     |
| 1:A:168:LEU:O     | 1:A:182:ARG:NH1   | 2.41        | 0.53     |
| 4:D:116:PRO:HD2   | 4:D:125:LYS:O     | 2.08        | 0.53     |
| 3:C:30:LYS:HB3    | 3:C:31:PRO:HD2    | 1.89        | 0.53     |
| 3:C:160:ILE:O     | 10:C:302:HEM:HMD1 | 2.08        | 0.53     |
| 3:C:273:ILE:HG13  | 8:H:21:MET:HE3    | 1.91        | 0.53     |
| 3:C:90:ILE:HG23   | 3:C:94:LEU:HD13   | 1.91        | 0.53     |
| 7:G:4:PRO:O       | 7:G:5:LEU:C       | 2.46        | 0.52     |
| 2:B:122:ASN:OD1   | 2:B:123:PRO:HD2   | 2.10        | 0.52     |
| 1:A:35:CYS:SG     | 10:A:304:HEM:C3B  | 3.02        | 0.52     |
| 1:A:163:VAL:O     | 1:A:166:SER:N     | 2.42        | 0.52     |
| 2:B:158:GLY:O     | 2:B:159:LEU:HD23  | 2.10        | 0.52     |
| 1:A:35:CYS:O      | 1:A:39:ILE:HD12   | 2.10        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 11:A:305:OPC:CBW  | 7:G:9:LEU:HD21    | 2.39        | 0.52     |
| 2:B:154:THR:CG2   | 2:B:155:LEU:N     | 2.73        | 0.52     |
| 2:B:37:LEU:CD2    | 2:B:38:TYR:CE2    | 2.93        | 0.52     |
| 1:A:92:MET:CE     | 11:A:305:OPC:HBV1 | 2.35        | 0.52     |
| 7:G:29:TYR:CD2    | 7:G:29:TYR:O      | 2.63        | 0.52     |
| 1:A:39:ILE:HG22   | 1:A:96:MET:HG3    | 1.92        | 0.52     |
| 3:C:231:LEU:HD12  | 3:C:232:THR:HG23  | 1.92        | 0.51     |
| 4:D:28:THR:HB     | 16:D:201:SQD:H321 | 1.92        | 0.51     |
| 3:C:194:LYS:O     | 3:C:195:TYR:C     | 2.48        | 0.51     |
| 1:A:103:ARG:NH1   | 1:A:104:VAL:HA    | 2.26        | 0.51     |
| 3:C:84:ILE:HD12   | 3:C:103:PHE:CG    | 2.46        | 0.51     |
| 1:A:215:LEU:HB2   | 7:G:28:GLN:OE1    | 2.11        | 0.51     |
| 3:C:30:LYS:HB2    | 3:C:155:ARG:NH1   | 2.25        | 0.51     |
| 1:A:29:HIS:CG     | 1:A:214:PRO:HA    | 2.46        | 0.51     |
| 1:A:138:LEU:N     | 1:A:139:PRO:CD    | 2.74        | 0.51     |
| 7:G:28:GLN:C      | 7:G:30:LYS:H      | 2.14        | 0.51     |
| 4:D:36:TYR:HB3    | 4:D:37:PRO:CD     | 2.41        | 0.50     |
| 1:A:115:GLU:O     | 1:A:119:ILE:HG13  | 2.11        | 0.50     |
| 3:C:34:VAL:HG22   | 3:C:151:LEU:CD2   | 2.41        | 0.50     |
| 2:B:102:ALA:O     | 2:B:105:PRO:HD2   | 2.10        | 0.50     |
| 1:A:47:GLN:NE2    | 1:A:89:SER:HB3    | 2.27        | 0.50     |
| 3:C:226:LYS:HG2   | 3:C:227:ALA:H     | 1.77        | 0.50     |
| 1:A:146:TRP:CD1   | 2:B:72:PRO:HD3    | 2.46        | 0.50     |
| 7:G:29:TYR:HD2    | 7:G:30:LYS:HG2    | 1.77        | 0.50     |
| 4:D:138:LYS:HD2   | 4:D:171:ARG:HG3   | 1.94        | 0.50     |
| 1:A:103:ARG:HA    | 7:G:21:LEU:HD21   | 1.92        | 0.50     |
| 3:C:84:ILE:HD11   | 3:C:114:LEU:HD13  | 1.93        | 0.50     |
| 1:A:195:ILE:O     | 1:A:199:MET:HG3   | 2.12        | 0.50     |
| 5:E:26:ILE:O      | 5:E:31:LEU:HB2    | 2.12        | 0.49     |
| 3:C:275:LYS:HE2   | 4:D:20:ASN:OD1    | 2.11        | 0.49     |
| 1:A:210:GLY:HA2   | 10:A:304:HEM:O1A  | 2.12        | 0.49     |
| 5:E:22:ILE:HG22   | 5:E:22:ILE:O      | 2.11        | 0.49     |
| 3:C:154:ASN:CG    | 3:C:155:ARG:N     | 2.65        | 0.49     |
| 7:G:31:ARG:HG2    | 7:G:31:ARG:HH11   | 1.77        | 0.49     |
| 3:C:266:MET:HE3   | 5:E:11:PHE:CE2    | 2.47        | 0.49     |
| 2:B:11:ASP:O      | 2:B:15:ARG:HG3    | 2.13        | 0.49     |
| 5:E:16:PHE:CE2    | 6:F:26:LEU:HD22   | 2.48        | 0.49     |
| 10:A:304:HEM:HHD  | 10:A:304:HEM:HBCA | 1.95        | 0.49     |
| 6:F:25:LEU:O      | 6:F:29:ILE:HG23   | 2.13        | 0.49     |
| 10:A:304:HEM:HBC2 | 10:A:304:HEM:HHD  | 1.95        | 0.49     |
| 11:A:305:OPC:HBC2 | 11:A:305:OPC:HAX2 | 1.93        | 0.49     |
| 6:F:13:PHE:CE2    | 6:F:17:PHE:CE1    | 3.00        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 7:G:5:LEU:O       | 7:G:9:LEU:HB2     | 2.13        | 0.49     |
| 3:C:151:LEU:HD12  | 3:C:152:GLY:H     | 1.77        | 0.49     |
| 4:D:138:LYS:HA    | 4:D:147:SER:CB    | 2.43        | 0.48     |
| 3:C:180:ILE:HG13  | 3:C:198:SER:O     | 2.13        | 0.48     |
| 1:A:166:SER:HB3   | 1:A:170:ARG:NH2   | 2.29        | 0.48     |
| 2:B:142:TRP:HZ2   | 2:B:155:LEU:O     | 1.96        | 0.48     |
| 2:B:113:PHE:O     | 2:B:116:ASN:HB2   | 2.13        | 0.48     |
| 7:G:20:GLY:N      | 17:G:101:BCR:H362 | 2.29        | 0.48     |
| 4:D:125:LYS:O     | 4:D:127:PRO:HD3   | 2.12        | 0.48     |
| 7:G:10:VAL:O      | 7:G:14:VAL:HG23   | 2.13        | 0.48     |
| 1:A:113:PRO:HG3   | 2:B:22:MET:HE3    | 1.96        | 0.48     |
| 4:D:156:GLN:HB2   | 4:D:161:VAL:CG2   | 2.44        | 0.48     |
| 3:C:199:ILE:C     | 3:C:200:GLN:HG3   | 2.34        | 0.48     |
| 3:C:180:ILE:CD1   | 3:C:197:VAL:CG1   | 2.92        | 0.48     |
| 14:B:202:CLA:C3C  | 11:B:203:OPC:HBT2 | 2.43        | 0.48     |
| 3:C:180:ILE:HD11  | 3:C:197:VAL:HG13  | 1.95        | 0.47     |
| 1:A:103:ARG:HH11  | 1:A:104:VAL:HA    | 1.78        | 0.47     |
| 5:E:22:ILE:O      | 5:E:22:ILE:CG2    | 2.62        | 0.47     |
| 3:C:281:LYS:O     | 3:C:282:VAL:C     | 2.52        | 0.47     |
| 3:C:88:GLU:HG2    | 3:C:88:GLU:O      | 2.14        | 0.47     |
| 4:D:25:GLY:HA2    | 16:D:201:SQD:C33  | 2.43        | 0.47     |
| 2:B:84:VAL:HG13   | 2:B:101:MET:HG2   | 1.95        | 0.47     |
| 4:D:102:TYR:HA    | 4:D:151:CYS:O     | 2.15        | 0.47     |
| 2:B:99:LEU:O      | 2:B:103:SER:OG    | 2.30        | 0.47     |
| 2:B:142:TRP:CH2   | 2:B:155:LEU:HD23  | 2.49        | 0.47     |
| 2:B:37:LEU:HD23   | 2:B:38:TYR:CD2    | 2.49        | 0.47     |
| 3:C:94:LEU:O      | 3:C:98:VAL:HG23   | 2.14        | 0.47     |
| 4:D:73:HIS:CE1    | 4:D:79:VAL:CG1    | 2.98        | 0.47     |
| 4:D:141:ARG:HG2   | 4:D:142:GLY:H     | 1.79        | 0.47     |
| 4:D:154:THR:C     | 4:D:155:VAL:HG22  | 2.35        | 0.47     |
| 1:A:22:THR:HG21   | 12:A:309:UMQ:H2'1 | 1.97        | 0.47     |
| 2:B:100:LEU:CD2   | 11:B:203:OPC:HBX2 | 2.44        | 0.47     |
| 3:C:59:GLN:HB3    | 3:C:68:VAL:O      | 2.15        | 0.47     |
| 4:D:124:PHE:O     | 4:D:132:GLN:HA    | 2.13        | 0.47     |
| 3:C:60:GLN:OE1    | 3:C:157:ARG:HG3   | 2.15        | 0.47     |
| 10:A:304:HEM:HMB2 | 10:A:304:HEM:HBBA | 1.88        | 0.47     |
| 5:E:9:ILE:HG12    | 5:E:9:ILE:H       | 1.58        | 0.47     |
| 3:C:71:ASN:OD1    | 3:C:120:PRO:HA    | 2.14        | 0.47     |
| 3:C:2:PRO:HG3     | 10:C:302:HEM:HMBA | 1.94        | 0.47     |
| 10:A:304:HEM:HMB2 | 10:A:304:HEM:HBB2 | 1.88        | 0.47     |
| 2:B:104:VAL:O     | 2:B:108:LEU:HB2   | 2.14        | 0.47     |
| 5:E:9:ILE:O       | 5:E:10:VAL:CG2    | 2.61        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:C:301:UMQ:HL2  | 4:D:37:PRO:CG     | 2.45        | 0.46     |
| 2:B:10:SER:O      | 2:B:12:PRO:HD3    | 2.15        | 0.46     |
| 5:E:24:PHE:O      | 5:E:27:LYS:N      | 2.48        | 0.46     |
| 5:E:2:ILE:O       | 5:E:6:VAL:HG23    | 2.14        | 0.46     |
| 4:D:15:ARG:NH1    | 5:E:31:LEU:HG     | 2.30        | 0.46     |
| 1:A:92:MET:HE3    | 11:A:305:OPC:CCB  | 2.43        | 0.46     |
| 2:B:101:MET:HB3   | 14:B:202:CLA:H91  | 1.97        | 0.46     |
| 3:C:281:LYS:HG2   | 3:C:282:VAL:N     | 2.30        | 0.46     |
| 3:C:36:VAL:HG21   | 3:C:247:ILE:HB    | 1.97        | 0.46     |
| 1:A:154:VAL:HB    | 1:A:155:PRO:HD3   | 1.98        | 0.46     |
| 12:C:301:UMQ:H6'1 | 12:C:301:UMQ:C5   | 2.45        | 0.46     |
| 5:E:16:PHE:CZ     | 6:F:25:LEU:HD22   | 2.48        | 0.46     |
| 4:D:156:GLN:HB2   | 4:D:161:VAL:HG23  | 1.96        | 0.46     |
| 2:B:118:ASN:ND2   | 11:B:203:OPC:HAH1 | 2.30        | 0.46     |
| 2:B:45:MET:HE1    | 4:D:30:VAL:HB     | 1.97        | 0.46     |
| 2:B:32:TRP:HE1    | 16:D:201:SQD:HO3  | 1.62        | 0.46     |
| 3:C:36:VAL:HG11   | 3:C:149:ILE:HD13  | 1.97        | 0.46     |
| 3:C:12:THR:OG1    | 3:C:13:PRO:HD2    | 2.16        | 0.46     |
| 5:E:22:ILE:O      | 5:E:26:ILE:HB     | 2.16        | 0.46     |
| 3:C:229:GLU:OE2   | 3:C:230:ALA:N     | 2.48        | 0.46     |
| 4:D:152:HIS:ND1   | 4:D:165:TRP:CE3   | 2.84        | 0.46     |
| 4:D:73:HIS:CE1    | 4:D:79:VAL:HG22   | 2.51        | 0.45     |
| 4:D:130:GLY:C     | 4:D:141:ARG:HH21  | 2.19        | 0.45     |
| 5:E:16:PHE:CE2    | 6:F:26:LEU:CD2    | 3.00        | 0.45     |
| 3:C:54:TYR:OH     | 3:C:121:GLY:HA3   | 2.15        | 0.45     |
| 14:B:202:CLA:O2A  | 14:B:202:CLA:C4   | 2.65        | 0.45     |
| 5:E:26:ILE:CG2    | 5:E:31:LEU:HB3    | 2.45        | 0.45     |
| 2:B:111:VAL:N     | 2:B:112:PRO:HD2   | 2.32        | 0.45     |
| 3:C:3:PHE:O       | 3:C:6:GLN:HG2     | 2.17        | 0.45     |
| 2:B:86:GLN:O      | 2:B:90:SER:OG     | 2.27        | 0.45     |
| 2:B:145:ILE:O     | 2:B:148:THR:HB    | 2.17        | 0.45     |
| 3:C:271:MET:CE    | 4:D:22:LEU:HB3    | 2.45        | 0.45     |
| 4:D:152:HIS:O     | 4:D:162:LEU:HD23  | 2.17        | 0.45     |
| 11:A:305:OPC:HBG3 | 11:A:305:OPC:OAI  | 2.16        | 0.45     |
| 3:C:271:MET:HB3   | 4:D:23:ALA:HA     | 1.99        | 0.45     |
| 2:B:37:LEU:CD2    | 2:B:38:TYR:CZ     | 3.00        | 0.45     |
| 2:B:79:TRP:CD1    | 7:G:6:LEU:HD11    | 2.52        | 0.45     |
| 3:C:139:ASP:CG    | 3:C:142:ILE:HG12  | 2.37        | 0.45     |
| 4:D:169:ASP:OD2   | 4:D:171:ARG:HB3   | 2.16        | 0.45     |
| 4:D:130:GLY:C     | 4:D:141:ARG:NH2   | 2.71        | 0.45     |
| 3:C:180:ILE:HD12  | 3:C:197:VAL:CG1   | 2.47        | 0.45     |
| 3:C:255:VAL:O     | 3:C:259:ILE:HG13  | 2.17        | 0.45     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:D:73:HIS:ND1   | 4:D:79:VAL:CG2    | 2.80        | 0.44     |
| 7:G:29:TYR:CG    | 7:G:29:TYR:O      | 2.69        | 0.44     |
| 7:G:34:GLU:O     | 7:G:35:LEU:HD12   | 2.16        | 0.44     |
| 3:C:151:LEU:HD12 | 3:C:152:GLY:N     | 2.32        | 0.44     |
| 2:B:4:LEU:HG     | 2:B:5:LYS:N       | 2.32        | 0.44     |
| 4:D:78:ARG:HG3   | 4:D:117:TRP:NE1   | 2.33        | 0.44     |
| 2:B:134:LEU:HA   | 2:B:134:LEU:HD12  | 1.75        | 0.44     |
| 1:A:4:VAL:O      | 1:A:5:TYR:C       | 2.55        | 0.44     |
| 4:D:154:THR:C    | 4:D:155:VAL:CG2   | 2.85        | 0.44     |
| 4:D:40:LYS:HA    | 4:D:40:LYS:HD2    | 1.84        | 0.44     |
| 4:D:73:HIS:ND1   | 4:D:79:VAL:HG22   | 2.32        | 0.44     |
| 3:C:200:GLN:HA   | 3:C:205:LYS:HG2   | 2.00        | 0.44     |
| 4:D:108:CYS:HB2  | 4:D:113:CYS:O     | 2.17        | 0.44     |
| 12:A:306:UMQ:O2' | 12:A:306:UMQ:HB1  | 2.17        | 0.44     |
| 3:C:262:ILE:HG23 | 8:H:14:VAL:CG1    | 2.47        | 0.44     |
| 3:C:266:MET:SD   | 8:H:13:VAL:HG12   | 2.58        | 0.44     |
| 3:C:270:LEU:HA   | 8:H:21:MET:CE     | 2.48        | 0.44     |
| 1:A:92:MET:HG3   | 11:A:305:OPC:HCB1 | 2.00        | 0.43     |
| 1:A:35:CYS:C     | 1:A:39:ILE:HD12   | 2.39        | 0.43     |
| 4:D:133:TYR:CD2  | 4:D:148:LEU:HG    | 2.53        | 0.43     |
| 1:A:207:ARG:NH1  | 13:A:308:QNO:H3   | 2.33        | 0.43     |
| 8:H:23:VAL:O     | 8:H:27:ASN:N      | 2.51        | 0.43     |
| 1:A:166:SER:O    | 1:A:170:ARG:HG2   | 2.18        | 0.43     |
| 3:C:219:VAL:HG12 | 3:C:220:SER:N     | 2.33        | 0.43     |
| 4:D:145:PRO:O    | 4:D:146:LEU:CD1   | 2.65        | 0.43     |
| 3:C:251:ASP:OD2  | 3:C:252:PRO:HD2   | 2.19        | 0.43     |
| 3:C:58:LEU:C     | 3:C:58:LEU:HD12   | 2.38        | 0.43     |
| 2:B:53:ALA:O     | 2:B:57:LEU:HG     | 2.17        | 0.43     |
| 1:A:108:GLY:HA3  | 2:B:121:GLN:HA    | 2.00        | 0.43     |
| 1:A:111:LYS:HE2  | 2:B:115:GLU:O     | 2.18        | 0.43     |
| 3:C:262:ILE:HG22 | 3:C:263:CYS:N     | 2.34        | 0.43     |
| 3:C:211:ILE:CG1  | 3:C:211:ILE:O     | 2.65        | 0.43     |
| 3:C:47:LYS:HG3   | 3:C:128:VAL:HG13  | 2.00        | 0.43     |
| 2:B:32:TRP:NE1   | 16:D:201:SQD:O3   | 2.50        | 0.43     |
| 1:A:6:ASP:O      | 1:A:10:GLU:HG3    | 2.19        | 0.43     |
| 4:D:90:TYR:CD1   | 4:D:106:ALA:HB2   | 2.53        | 0.43     |
| 3:C:68:VAL:HG22  | 3:C:69:GLY:N      | 2.33        | 0.43     |
| 3:C:206:THR:O    | 3:C:206:THR:CG2   | 2.65        | 0.43     |
| 3:C:109:GLY:O    | 3:C:111:ASP:N     | 2.50        | 0.43     |
| 3:C:200:GLN:HA   | 3:C:205:LYS:HB3   | 2.00        | 0.43     |
| 2:B:77:PRO:HB2   | 2:B:81:LEU:HD12   | 2.01        | 0.43     |
| 5:E:18:ILE:O     | 5:E:22:ILE:HG13   | 2.19        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 11:B:203:OPC:HAE1 | 11:B:203:OPC:OAI  | 2.17        | 0.42     |
| 3:C:178:GLY:HA3   | 3:C:202:ASP:OD2   | 2.19        | 0.42     |
| 3:C:161:TYR:O     | 3:C:163:THR:N     | 2.52        | 0.42     |
| 3:C:281:LYS:O     | 3:C:284:ALA:N     | 2.47        | 0.42     |
| 3:C:254:ARG:HA    | 12:C:301:UMQ:HB2  | 2.01        | 0.42     |
| 4:D:156:GLN:O     | 4:D:157:ASP:C     | 2.57        | 0.42     |
| 3:C:245:THR:OG1   | 3:C:246:GLU:N     | 2.51        | 0.42     |
| 5:E:26:ILE:HG21   | 5:E:32:ILE:CD1    | 2.49        | 0.42     |
| 3:C:199:ILE:C     | 3:C:200:GLN:CG    | 2.88        | 0.42     |
| 2:B:153:LYS:HB3   | 2:B:153:LYS:HE3   | 1.91        | 0.42     |
| 11:A:305:OPC:HBW1 | 7:G:9:LEU:HD21    | 2.00        | 0.42     |
| 3:C:35:GLU:HB2    | 3:C:49:VAL:HB     | 2.01        | 0.42     |
| 2:B:37:LEU:HD21   | 4:D:24:PHE:HZ     | 1.83        | 0.42     |
| 7:G:21:LEU:HA     | 7:G:21:LEU:HD12   | 1.90        | 0.42     |
| 3:C:36:VAL:HG23   | 3:C:37:PRO:O      | 2.18        | 0.42     |
| 12:A:306:UMQ:CA   | 12:A:306:UMQ:O2'  | 2.68        | 0.42     |
| 3:C:1:TYR:HD2     | 3:C:118:PRO:HG3   | 1.85        | 0.42     |
| 4:D:15:ARG:HH12   | 5:E:31:LEU:CA     | 2.31        | 0.42     |
| 5:E:26:ILE:HG23   | 5:E:31:LEU:CB     | 2.47        | 0.42     |
| 1:A:83:ARG:HD2    | 10:A:302:HEM:O1D  | 2.20        | 0.42     |
| 12:A:306:UMQ:C3'  | 12:A:306:UMQ:O5   | 2.67        | 0.42     |
| 5:E:22:ILE:O      | 5:E:23:ILE:C      | 2.53        | 0.42     |
| 5:E:23:ILE:HB     | 5:E:24:PHE:H      | 1.71        | 0.42     |
| 1:A:161:VAL:HG13  | 1:A:164:LEU:HD12  | 2.02        | 0.42     |
| 3:C:20:ILE:HD13   | 3:C:152:GLY:HA3   | 2.02        | 0.42     |
| 5:E:29:ILE:O      | 5:E:29:ILE:HG22   | 2.20        | 0.42     |
| 2:B:126:ARG:N     | 2:B:127:PRO:HD3   | 2.34        | 0.42     |
| 1:A:154:VAL:HG22  | 2:B:88:LEU:HD21   | 2.02        | 0.41     |
| 1:A:25:TYR:CD2    | 2:B:30:PRO:HA     | 2.54        | 0.41     |
| 4:D:140:ILE:O     | 4:D:140:ILE:HG13  | 2.20        | 0.41     |
| 1:A:74:ASN:HB3    | 3:C:143:HIS:CD2   | 2.55        | 0.41     |
| 3:C:10:PRO:N      | 3:C:11:PRO:CD     | 2.83        | 0.41     |
| 4:D:15:ARG:HH12   | 5:E:30:LYS:C      | 2.12        | 0.41     |
| 5:E:16:PHE:HE1    | 5:E:20:VAL:HG21   | 1.85        | 0.41     |
| 5:E:9:ILE:O       | 5:E:10:VAL:HB     | 2.20        | 0.41     |
| 3:C:223:GLN:HB3   | 3:C:225:VAL:CG2   | 2.50        | 0.41     |
| 3:C:264:LEU:HD13  | 4:D:30:VAL:CG2    | 2.50        | 0.41     |
| 1:A:53:ALA:HB1    | 4:D:41:TYR:CE2    | 2.55        | 0.41     |
| 1:A:5:TYR:CE1     | 12:A:307:UMQ:H1'1 | 2.56        | 0.41     |
| 3:C:10:PRO:N      | 3:C:11:PRO:HD3    | 2.35        | 0.41     |
| 5:E:10:VAL:O      | 5:E:14:LEU:HD12   | 2.19        | 0.41     |
| 1:A:80:TRP:CH2    | 3:C:254:ARG:HG2   | 2.55        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:C:171:VAL:HG12 | 3:C:233:ASN:O     | 2.20        | 0.41     |
| 7:G:29:TYR:HD2   | 7:G:30:LYS:CG     | 2.33        | 0.41     |
| 4:D:89:THR:HG22  | 4:D:105:ASN:HA    | 2.03        | 0.41     |
| 3:C:70:LEU:HD23  | 3:C:70:LEU:H      | 1.86        | 0.41     |
| 1:A:158:ILE:HA   | 1:A:159:PRO:HD3   | 1.78        | 0.41     |
| 2:B:32:TRP:CG    | 2:B:33:PRO:N      | 2.89        | 0.41     |
| 1:A:211:ILE:N    | 10:A:304:HEM:O1A  | 2.54        | 0.41     |
| 3:C:273:ILE:HD12 | 8:H:25:GLY:CA     | 2.51        | 0.41     |
| 3:C:281:LYS:O    | 3:C:283:GLN:N     | 2.54        | 0.41     |
| 1:A:72:ILE:O     | 1:A:79:GLY:HA3    | 2.20        | 0.41     |
| 3:C:72:VAL:HG21  | 3:C:124:TYR:O     | 2.20        | 0.41     |
| 1:A:103:ARG:HD2  | 1:A:103:ARG:O     | 2.21        | 0.40     |
| 10:C:302:HEM:HHC | 10:C:302:HEM:HBB2 | 2.03        | 0.40     |
| 10:C:302:HEM:HHC | 10:C:302:HEM:HBBA | 2.03        | 0.40     |
| 1:A:14:ILE:HG22  | 12:A:307:UMQ:HD1  | 2.03        | 0.40     |
| 2:B:45:MET:HE1   | 4:D:30:VAL:CB     | 2.52        | 0.40     |
| 3:C:186:GLU:O    | 3:C:187:GLU:HB3   | 2.21        | 0.40     |
| 3:C:183:ILE:O    | 3:C:183:ILE:HG22  | 2.21        | 0.40     |
| 1:A:81:LEU:HD22  | 1:A:85:ILE:HG13   | 2.04        | 0.40     |
| 3:C:214:GLY:N    | 3:C:215:PRO:HD2   | 2.37        | 0.40     |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Distance(Å) | Clash(Å) |
|----------------|-----------------------|-------------|----------|
| 1:A:112:LYS:NZ | 3:C:87:GLU:OE1[8_665] | 1.82        | 0.38     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 1   | A     | 211/215 (98%) | 187 (89%) | 19 (9%)  | 5 (2%)   | 9 53        |
| 2   | B     | 158/160 (99%) | 143 (90%) | 11 (7%)  | 4 (2%)   | 9 52        |
| 3   | C     | 284/289 (98%) | 235 (83%) | 41 (14%) | 8 (3%)   | 8 48        |

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| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|-----------|----------|-------------|-----|
| 4   | D     | 155/179 (87%) | 123 (79%) | 22 (14%)  | 10 (6%)  | 2           | 19  |
| 5   | E     | 30/32 (94%)   | 16 (53%)  | 11 (37%)  | 3 (10%)  | 1           | 8   |
| 6   | F     | 30/35 (86%)   | 29 (97%)  | 1 (3%)    | 0        | 100         | 100 |
| 7   | G     | 35/37 (95%)   | 26 (74%)  | 6 (17%)   | 3 (9%)   | 1           | 11  |
| 8   | H     | 27/29 (93%)   | 26 (96%)  | 0         | 1 (4%)   | 5           | 39  |
| All | All   | 930/976 (95%) | 785 (84%) | 111 (12%) | 34 (4%)  | 5           | 39  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 162 | GLY  |
| 2   | B     | 33  | PRO  |
| 2   | B     | 34  | ASN  |
| 2   | B     | 75  | ILE  |
| 3   | C     | 66  | SER  |
| 3   | C     | 186 | GLU  |
| 3   | C     | 192 | ASN  |
| 3   | C     | 195 | TYR  |
| 4   | D     | 138 | LYS  |
| 4   | D     | 139 | VAL  |
| 4   | D     | 140 | ILE  |
| 5   | E     | 10  | VAL  |
| 5   | E     | 13  | ALA  |
| 5   | E     | 23  | ILE  |
| 7   | G     | 34  | GLU  |
| 1   | A     | 23  | SER  |
| 2   | B     | 22  | MET  |
| 3   | C     | 233 | ASN  |
| 4   | D     | 63  | ASN  |
| 4   | D     | 121 | GLU  |
| 4   | D     | 171 | ARG  |
| 1   | A     | 4   | VAL  |
| 3   | C     | 187 | GLU  |
| 3   | C     | 282 | VAL  |
| 4   | D     | 74  | ASN  |
| 4   | D     | 112 | GLY  |
| 4   | D     | 155 | VAL  |
| 1   | A     | 170 | ARG  |
| 3   | C     | 206 | THR  |
| 4   | D     | 157 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 5   | LEU  |
| 7   | G     | 33  | ASN  |
| 8   | H     | 2   | GLU  |
| 1   | A     | 163 | 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   | A     | 183/184 (100%) | 172 (94%) | 11 (6%)  | 27          | 72 |
| 2   | B     | 137/137 (100%) | 127 (93%) | 10 (7%)  | 20          | 63 |
| 3   | C     | 240/243 (99%)  | 212 (88%) | 28 (12%) | 8           | 36 |
| 4   | D     | 133/146 (91%)  | 122 (92%) | 11 (8%)  | 16          | 56 |
| 5   | E     | 25/25 (100%)   | 20 (80%)  | 5 (20%)  | 2           | 9  |
| 6   | F     | 24/27 (89%)    | 22 (92%)  | 2 (8%)   | 16          | 56 |
| 7   | G     | 28/28 (100%)   | 25 (89%)  | 3 (11%)  | 10          | 40 |
| 8   | H     | 24/24 (100%)   | 23 (96%)  | 1 (4%)   | 40          | 82 |
| All | All   | 794/814 (98%)  | 723 (91%) | 71 (9%)  | 14          | 51 |

All (71) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | LEU  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 63  | THR  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 87  | ARG  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 107 | THR  |
| 1   | A     | 163 | VAL  |
| 1   | A     | 173 | SER  |
| 1   | A     | 200 | LEU  |
| 2   | B     | 1   | MET  |
| 2   | B     | 35  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 64  | GLU  |
| 2   | B     | 74  | GLU  |
| 2   | B     | 76  | LEU  |
| 2   | B     | 96  | LEU  |
| 2   | B     | 134 | LEU  |
| 2   | B     | 138 | LEU  |
| 2   | B     | 152 | ASP  |
| 2   | B     | 159 | LEU  |
| 3   | C     | 22  | CYS  |
| 3   | C     | 58  | LEU  |
| 3   | C     | 60  | GLN  |
| 3   | C     | 88  | GLU  |
| 3   | C     | 94  | LEU  |
| 3   | C     | 107 | LYS  |
| 3   | C     | 123 | GLN  |
| 3   | C     | 131 | VAL  |
| 3   | C     | 137 | THR  |
| 3   | C     | 155 | ARG  |
| 3   | C     | 160 | ILE  |
| 3   | C     | 171 | VAL  |
| 3   | C     | 181 | THR  |
| 3   | C     | 186 | GLU  |
| 3   | C     | 205 | LYS  |
| 3   | C     | 206 | THR  |
| 3   | C     | 211 | ILE  |
| 3   | C     | 225 | VAL  |
| 3   | C     | 229 | GLU  |
| 3   | C     | 233 | ASN  |
| 3   | C     | 244 | ASP  |
| 3   | C     | 245 | THR  |
| 3   | C     | 249 | LEU  |
| 3   | C     | 256 | LYS  |
| 3   | C     | 264 | LEU  |
| 3   | C     | 267 | LEU  |
| 3   | C     | 270 | LEU  |
| 3   | C     | 281 | LYS  |
| 4   | D     | 15  | ARG  |
| 4   | D     | 17  | GLN  |
| 4   | D     | 40  | LYS  |
| 4   | D     | 54  | THR  |
| 4   | D     | 59  | LYS  |
| 4   | D     | 135 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 139 | VAL  |
| 4   | D     | 146 | LEU  |
| 4   | D     | 150 | LEU  |
| 4   | D     | 154 | THR  |
| 4   | D     | 155 | VAL  |
| 5   | E     | 9   | ILE  |
| 5   | E     | 11  | PHE  |
| 5   | E     | 12  | ILE  |
| 5   | E     | 14  | LEU  |
| 5   | E     | 31  | LEU  |
| 6   | F     | 5   | MET  |
| 6   | F     | 7   | TYR  |
| 7   | G     | 6   | LEU  |
| 7   | G     | 9   | LEU  |
| 7   | G     | 21  | LEU  |
| 8   | H     | 2   | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | GLN  |
| 3   | C     | 154 | ASN  |
| 3   | C     | 233 | ASN  |
| 4   | D     | 63  | ASN  |
| 4   | D     | 159 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 10  | HEM  | A     | 302 | 1     | 49,50,50     | 2.16 | 13 (26%)    | 46,82,82    | 2.03 | 11 (23%)    |
| 10  | HEM  | A     | 303 | 1     | 49,50,50     | 2.71 | 15 (30%)    | 46,82,82    | 1.85 | 9 (19%)     |
| 10  | HEM  | A     | 304 | 18,13 | 49,50,50     | 2.64 | 15 (30%)    | 46,82,82    | 1.99 | 9 (19%)     |
| 11  | OPC  | A     | 305 | -     | 51,53,54     | 1.25 | 3 (5%)      | 55,61,64    | 1.04 | 3 (5%)      |
| 12  | UMQ  | A     | 306 | -     | 35,35,35     | 1.14 | 4 (11%)     | 46,46,46    | 1.80 | 8 (17%)     |
| 12  | UMQ  | A     | 307 | -     | 35,35,35     | 1.25 | 5 (14%)     | 46,46,46    | 2.12 | 13 (28%)    |
| 13  | QNO  | A     | 308 | 10    | 22,22,22     | 2.54 | 5 (22%)     | 28,28,28    | 3.02 | 7 (25%)     |
| 12  | UMQ  | A     | 309 | -     | 35,35,35     | 1.22 | 5 (14%)     | 46,46,46    | 2.77 | 17 (36%)    |
| 14  | CLA  | B     | 202 | 18    | 73,73,73     | 1.93 | 11 (15%)    | 95,113,113  | 1.32 | 15 (15%)    |
| 11  | OPC  | B     | 203 | -     | 51,53,54     | 1.26 | 3 (5%)      | 55,61,64    | 1.03 | 5 (9%)      |
| 12  | UMQ  | C     | 301 | -     | 35,35,35     | 1.28 | 5 (14%)     | 46,46,46    | 2.15 | 10 (21%)    |
| 10  | HEM  | C     | 302 | 3     | 49,50,50     | 2.25 | 15 (30%)    | 46,82,82    | 2.23 | 12 (26%)    |
| 15  | FES  | D     | 200 | 4     | 0,4,4        | 0.00 | -           | 0,4,4       | 0.00 | -           |
| 16  | SQD  | D     | 201 | -     | 53,53,54     | 3.38 | 15 (28%)    | 58,63,65    | 2.06 | 15 (25%)    |
| 17  | BCR  | G     | 101 | -     | 41,41,41     | 2.29 | 22 (53%)    | 56,56,56    | 2.43 | 25 (44%)    |

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   |
|-----|------|-------|-----|-------|-----------|--------------|---------|
| 10  | HEM  | A     | 302 | 1     | -         | 0/14/114/114 | 0/0/8/8 |
| 10  | HEM  | A     | 303 | 1     | -         | 0/14/114/114 | 0/0/8/8 |
| 10  | HEM  | A     | 304 | 18,13 | -         | 0/14/114/114 | 0/0/8/8 |
| 11  | OPC  | A     | 305 | -     | -         | 1/55/57/60   | 0/0/0/0 |
| 12  | UMQ  | A     | 306 | -     | 1/1/10/10 | 0/20/60/60   | 0/2/2/2 |
| 12  | UMQ  | A     | 307 | -     | 2/2/10/10 | 0/20/60/60   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 13  | QNO  | A     | 308 | 10   | 1/1/0/0   | 0/9/9/9      | 0/0/2/2 |
| 12  | UMQ  | A     | 309 | -    | 4/4/10/10 | 0/20/60/60   | 0/2/2/2 |
| 14  | CLA  | B     | 202 | 18   | 1/1/22/25 | 0/37/135/135 | 0/0/9/9 |
| 11  | OPC  | B     | 203 | -    | -         | 0/55/57/60   | 0/0/0/0 |
| 12  | UMQ  | C     | 301 | -    | 1/1/10/10 | 0/20/60/60   | 0/2/2/2 |
| 10  | HEM  | C     | 302 | 3    | -         | 0/14/114/114 | 0/0/8/8 |
| 15  | FES  | D     | 200 | 4    | -         | 0/0/4/4      | 0/0/1/1 |
| 16  | SQD  | D     | 201 | -    | 3/3/9/9   | 0/49/65/69   | 0/1/1/1 |
| 17  | BCR  | G     | 101 | -    | -         | 0/29/63/63   | 0/2/2/2 |

All (136) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | D     | 201 | SQD  | C6-S    | 12.40 | 1.91        | 1.77     |
| 16  | D     | 201 | SQD  | O5-C1   | 10.29 | 1.57        | 1.41     |
| 10  | A     | 303 | HEM  | C2B-C1B | 9.77  | 1.47        | 1.44     |
| 16  | D     | 201 | SQD  | O6-C44  | 8.75  | 1.60        | 1.43     |
| 10  | A     | 304 | HEM  | C2D-C1D | 7.70  | 1.46        | 1.44     |
| 16  | D     | 201 | SQD  | C8-C7   | 7.37  | 1.73        | 1.50     |
| 14  | B     | 202 | CLA  | C1B-C2B | 7.37  | 1.49        | 1.40     |
| 10  | A     | 303 | HEM  | C3D-C4D | 7.14  | 1.46        | 1.44     |
| 13  | A     | 308 | QNO  | C6-N1   | -6.78 | 1.32        | 1.40     |
| 11  | A     | 305 | OPC  | OAK-CAL | -6.52 | 1.38        | 1.43     |
| 14  | B     | 202 | CLA  | C4B-NB  | 6.41  | 1.42        | 1.34     |
| 14  | B     | 202 | CLA  | C3B-C4B | 6.37  | 1.50        | 1.40     |
| 11  | B     | 203 | OPC  | OAK-CAL | -6.20 | 1.38        | 1.43     |
| 10  | A     | 304 | HEM  | C3D-C2D | 6.15  | 1.54        | 1.43     |
| 10  | A     | 304 | HEM  | C3C-C2C | -6.08 | 1.33        | 1.43     |
| 16  | D     | 201 | SQD  | C4-C5   | -6.06 | 1.39        | 1.53     |
| 10  | C     | 302 | HEM  | C3B-C2B | -5.69 | 1.33        | 1.43     |
| 10  | A     | 303 | HEM  | C3C-C2C | -5.63 | 1.33        | 1.43     |
| 16  | D     | 201 | SQD  | O47-C7  | 5.53  | 1.51        | 1.34     |
| 13  | A     | 308 | QNO  | C4-C5   | -5.52 | 1.31        | 1.43     |
| 10  | C     | 302 | HEM  | C3D-C2D | 5.47  | 1.53        | 1.43     |
| 10  | A     | 302 | HEM  | C3D-C2D | 5.46  | 1.53        | 1.43     |
| 14  | B     | 202 | CLA  | C3B-CAB | -5.46 | 1.44        | 1.49     |
| 14  | B     | 202 | CLA  | C4D-C3D | 5.35  | 1.48        | 1.41     |
| 10  | A     | 303 | HEM  | C3D-C2D | 5.28  | 1.53        | 1.43     |
| 10  | A     | 303 | HEM  | C3B-C2B | -5.27 | 1.34        | 1.43     |
| 10  | A     | 302 | HEM  | C3C-C2C | -5.20 | 1.34        | 1.43     |
| 10  | A     | 304 | HEM  | C3B-C2B | -5.19 | 1.34        | 1.43     |
| 10  | C     | 302 | HEM  | C3C-C2C | -5.18 | 1.34        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 304 | HEM  | C2B-C1B | 5.06  | 1.45        | 1.44     |
| 10  | A     | 302 | HEM  | C3B-C2B | -5.05 | 1.34        | 1.43     |
| 13  | A     | 308 | QNO  | C5-C6   | -5.03 | 1.33        | 1.42     |
| 10  | A     | 304 | HEM  | C3B-CAB | 4.97  | 1.56        | 1.40     |
| 16  | D     | 201 | SQD  | C6-C5   | 4.94  | 1.57        | 1.52     |
| 16  | D     | 201 | SQD  | C46-C45 | -4.93 | 1.37        | 1.50     |
| 10  | C     | 302 | HEM  | C3B-CAB | 4.83  | 1.55        | 1.40     |
| 10  | A     | 303 | HEM  | C3B-CAB | 4.80  | 1.55        | 1.40     |
| 10  | A     | 304 | HEM  | C3C-CAC | 4.71  | 1.55        | 1.40     |
| 10  | C     | 302 | HEM  | C3C-CAC | 4.64  | 1.55        | 1.40     |
| 16  | D     | 201 | SQD  | O47-C45 | 4.64  | 1.58        | 1.46     |
| 10  | A     | 302 | HEM  | C2B-C1B | 4.63  | 1.45        | 1.44     |
| 10  | A     | 302 | HEM  | C3C-CAC | 4.56  | 1.54        | 1.40     |
| 10  | A     | 302 | HEM  | C3B-CAB | 4.51  | 1.54        | 1.40     |
| 10  | A     | 303 | HEM  | C3C-CAC | 4.45  | 1.54        | 1.40     |
| 13  | A     | 308 | QNO  | C2-N1   | 4.42  | 1.43        | 1.36     |
| 10  | A     | 303 | HEM  | C4A-C3A | 4.29  | 1.45        | 1.40     |
| 10  | A     | 304 | HEM  | C4A-C3A | 4.20  | 1.45        | 1.40     |
| 13  | A     | 308 | QNO  | C3-C2   | 4.17  | 1.47        | 1.38     |
| 10  | A     | 304 | HEM  | FE-ND   | 3.95  | 2.12        | 1.97     |
| 10  | C     | 302 | HEM  | C2D-C1D | 3.72  | 1.45        | 1.44     |
| 14  | B     | 202 | CLA  | C1A-NA  | 3.72  | 1.40        | 1.32     |
| 17  | G     | 101 | BCR  | C26-C25 | 3.65  | 1.40        | 1.34     |
| 10  | C     | 302 | HEM  | C4A-C3A | 3.58  | 1.44        | 1.40     |
| 17  | G     | 101 | BCR  | C17-C18 | 3.52  | 1.40        | 1.35     |
| 10  | A     | 304 | HEM  | FE-NB   | 3.51  | 2.10        | 1.97     |
| 10  | A     | 302 | HEM  | C4A-C3A | 3.51  | 1.44        | 1.40     |
| 10  | C     | 302 | HEM  | FE-NB   | 3.50  | 2.10        | 1.97     |
| 17  | G     | 101 | BCR  | C14-C13 | 3.45  | 1.40        | 1.35     |
| 10  | A     | 302 | HEM  | FE-ND   | 3.44  | 2.10        | 1.97     |
| 17  | G     | 101 | BCR  | C20-C21 | 3.43  | 1.53        | 1.43     |
| 10  | A     | 304 | HEM  | FE-NC   | 3.43  | 2.10        | 1.97     |
| 17  | G     | 101 | BCR  | C21-C22 | 3.41  | 1.40        | 1.35     |
| 17  | G     | 101 | BCR  | C15-C14 | 3.40  | 1.53        | 1.43     |
| 17  | G     | 101 | BCR  | C23-C22 | 3.39  | 1.53        | 1.45     |
| 17  | G     | 101 | BCR  | C11-C10 | 3.32  | 1.53        | 1.43     |
| 17  | G     | 101 | BCR  | C16-C17 | 3.22  | 1.53        | 1.43     |
| 17  | G     | 101 | BCR  | C12-C13 | 3.16  | 1.52        | 1.45     |
| 17  | G     | 101 | BCR  | C19-C18 | 3.12  | 1.52        | 1.45     |
| 16  | D     | 201 | SQD  | O5-C5   | 3.11  | 1.52        | 1.44     |
| 10  | A     | 302 | HEM  | C3D-C4D | 3.03  | 1.45        | 1.44     |
| 10  | C     | 302 | HEM  | C3B-C4B | 2.98  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | A     | 307 | UMQ  | C4-C5   | -2.88 | 1.46        | 1.53     |
| 16  | D     | 201 | SQD  | C4-C3   | 2.85  | 1.59        | 1.52     |
| 12  | A     | 306 | UMQ  | C4-C5   | -2.80 | 1.46        | 1.53     |
| 17  | G     | 101 | BCR  | C8-C9   | 2.75  | 1.52        | 1.45     |
| 12  | C     | 301 | UMQ  | O2'-C2' | -2.75 | 1.36        | 1.43     |
| 10  | A     | 302 | HEM  | CMB-C2B | 2.75  | 1.55        | 1.47     |
| 12  | C     | 301 | UMQ  | C4-C5   | -2.72 | 1.47        | 1.53     |
| 10  | C     | 302 | HEM  | C3D-C4D | 2.69  | 1.45        | 1.44     |
| 12  | C     | 301 | UMQ  | O5'-C5' | -2.68 | 1.37        | 1.44     |
| 10  | A     | 303 | HEM  | FE-NB   | 2.65  | 2.07        | 1.97     |
| 11  | B     | 203 | OPC  | OBJ-CBK | 2.64  | 1.41        | 1.33     |
| 17  | G     | 101 | BCR  | C10-C9  | 2.63  | 1.39        | 1.35     |
| 10  | A     | 302 | HEM  | CMC-C2C | 2.63  | 1.55        | 1.47     |
| 12  | A     | 309 | UMQ  | C4-C5   | -2.62 | 1.47        | 1.53     |
| 16  | D     | 201 | SQD  | O48-C46 | -2.62 | 1.39        | 1.45     |
| 10  | C     | 302 | HEM  | CMB-C2B | 2.61  | 1.55        | 1.47     |
| 17  | G     | 101 | BCR  | C24-C23 | 2.57  | 1.40        | 1.32     |
| 14  | B     | 202 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 12  | A     | 309 | UMQ  | O5'-C5' | -2.46 | 1.38        | 1.44     |
| 17  | G     | 101 | BCR  | C31-C1  | -2.46 | 1.48        | 1.53     |
| 12  | A     | 306 | UMQ  | O2'-C2' | -2.45 | 1.37        | 1.43     |
| 12  | A     | 309 | UMQ  | O2'-C2' | -2.45 | 1.37        | 1.43     |
| 16  | D     | 201 | SQD  | C9-C8   | 2.44  | 1.61        | 1.52     |
| 12  | A     | 307 | UMQ  | O3'-C3' | -2.41 | 1.37        | 1.43     |
| 10  | A     | 303 | HEM  | CMB-C2B | 2.40  | 1.54        | 1.47     |
| 12  | A     | 307 | UMQ  | O5'-C5' | -2.40 | 1.38        | 1.44     |
| 10  | C     | 302 | HEM  | CMD-C2D | 2.40  | 1.54        | 1.47     |
| 10  | A     | 304 | HEM  | CMD-C2D | 2.39  | 1.54        | 1.47     |
| 12  | A     | 309 | UMQ  | C3-C4   | -2.38 | 1.46        | 1.52     |
| 12  | A     | 307 | UMQ  | O2'-C2' | -2.36 | 1.37        | 1.43     |
| 10  | A     | 304 | HEM  | FE-NA   | 2.35  | 2.02        | 1.92     |
| 10  | C     | 302 | HEM  | CMC-C2C | 2.33  | 1.54        | 1.47     |
| 10  | A     | 302 | HEM  | CMD-C2D | 2.32  | 1.54        | 1.47     |
| 14  | B     | 202 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 10  | C     | 302 | HEM  | FE-NA   | 2.31  | 2.02        | 1.92     |
| 10  | A     | 303 | HEM  | CMD-C2D | 2.30  | 1.54        | 1.47     |
| 14  | B     | 202 | CLA  | C3B-C2B | -2.29 | 1.37        | 1.41     |
| 17  | G     | 101 | BCR  | C32-C1  | -2.29 | 1.48        | 1.53     |
| 10  | A     | 303 | HEM  | CMC-C2C | 2.28  | 1.54        | 1.47     |
| 11  | A     | 305 | OPC  | CAV-CAW | 2.28  | 1.44        | 1.31     |
| 12  | A     | 306 | UMQ  | O5'-C5' | -2.28 | 1.38        | 1.44     |
| 11  | B     | 203 | OPC  | CAV-CAW | 2.28  | 1.44        | 1.31     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 304 | HEM  | CMB-C2B | 2.27  | 1.54        | 1.47     |
| 17  | G     | 101 | BCR  | C20-C19 | 2.26  | 1.40        | 1.34     |
| 12  | A     | 307 | UMQ  | C3-C4   | -2.26 | 1.46        | 1.52     |
| 10  | A     | 304 | HEM  | CMC-C2C | 2.25  | 1.54        | 1.47     |
| 11  | A     | 305 | OPC  | OBJ-CBK | 2.25  | 1.40        | 1.33     |
| 12  | A     | 306 | UMQ  | O3'-C3' | -2.24 | 1.37        | 1.43     |
| 12  | C     | 301 | UMQ  | C3-C4   | -2.23 | 1.46        | 1.52     |
| 10  | A     | 303 | HEM  | FE-ND   | 2.20  | 2.05        | 1.97     |
| 16  | D     | 201 | SQD  | C10-C9  | 2.20  | 1.64        | 1.51     |
| 12  | C     | 301 | UMQ  | O3'-C3' | -2.20 | 1.37        | 1.43     |
| 17  | G     | 101 | BCR  | C11-C12 | 2.19  | 1.40        | 1.34     |
| 10  | A     | 302 | HEM  | FE-NC   | 2.19  | 2.06        | 1.97     |
| 10  | A     | 303 | HEM  | FE-NA   | 2.14  | 2.01        | 1.92     |
| 17  | G     | 101 | BCR  | C5-C6   | 2.14  | 1.37        | 1.34     |
| 16  | D     | 201 | SQD  | O6-C1   | 2.13  | 1.46        | 1.42     |
| 12  | A     | 309 | UMQ  | O3'-C3' | -2.10 | 1.37        | 1.43     |
| 17  | G     | 101 | BCR  | C40-C30 | -2.06 | 1.49        | 1.53     |
| 10  | C     | 302 | HEM  | CHC-C1C | 2.06  | 1.40        | 1.36     |
| 17  | G     | 101 | BCR  | C1-C6   | -2.06 | 1.50        | 1.53     |
| 14  | B     | 202 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.51     |
| 10  | A     | 303 | HEM  | CHB-C1B | 2.04  | 1.38        | 1.35     |
| 17  | G     | 101 | BCR  | C24-C25 | 2.04  | 1.53        | 1.46     |
| 14  | B     | 202 | CLA  | C1D-ND  | 2.03  | 1.42        | 1.36     |

All (159) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 13  | A     | 308 | QNO  | C3-C2-N1    | -10.60 | 108.97      | 119.42   |
| 10  | C     | 302 | HEM  | C3B-C4B-NB  | -9.72  | 107.04      | 114.00   |
| 12  | A     | 309 | UMQ  | O1'-C1'-C2' | 7.83   | 118.15      | 108.18   |
| 13  | A     | 308 | QNO  | C21-C2-N1   | 7.80   | 129.10      | 117.91   |
| 12  | C     | 301 | UMQ  | O1'-C1'-C2' | 7.79   | 118.10      | 108.18   |
| 10  | A     | 302 | HEM  | C3B-C4B-NB  | -7.44  | 108.67      | 114.00   |
| 12  | A     | 309 | UMQ  | O5'-C1'-C2' | 6.60   | 123.84      | 110.31   |
| 10  | A     | 304 | HEM  | C4D-ND-C1D  | 6.50   | 111.81      | 105.16   |
| 10  | C     | 302 | HEM  | C4D-ND-C1D  | 6.18   | 111.49      | 105.16   |
| 17  | G     | 101 | BCR  | C7-C8-C9    | -6.05  | 117.17      | 126.22   |
| 16  | D     | 201 | SQD  | C5-C4-C3    | 5.89   | 119.63      | 109.98   |
| 10  | A     | 303 | HEM  | C3B-C4B-NB  | -5.80  | 109.85      | 114.00   |
| 16  | D     | 201 | SQD  | C1-O5-C5    | 5.74   | 121.42      | 113.50   |
| 10  | A     | 304 | HEM  | C3B-C4B-NB  | -5.64  | 109.97      | 114.00   |
| 10  | A     | 303 | HEM  | C4D-ND-C1D  | 5.61   | 110.90      | 105.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | C     | 301 | UMQ  | O1-C1-O5    | 5.44  | 124.27      | 110.69   |
| 12  | A     | 307 | UMQ  | O2'-C2'-C1' | 5.42  | 121.85      | 110.04   |
| 10  | A     | 302 | HEM  | C4D-ND-C1D  | 5.25  | 110.53      | 105.16   |
| 12  | A     | 306 | UMQ  | CA-O1'-C1'  | 5.00  | 122.96      | 113.96   |
| 12  | A     | 307 | UMQ  | O2'-C2'-C3' | 4.94  | 121.42      | 110.35   |
| 12  | A     | 309 | UMQ  | C2'-C3'-C4' | 4.88  | 120.22      | 109.61   |
| 17  | G     | 101 | BCR  | C16-C17-C18 | -4.88 | 120.27      | 127.29   |
| 12  | C     | 301 | UMQ  | C1'-C2'-C3' | -4.83 | 100.61      | 110.00   |
| 12  | A     | 307 | UMQ  | O2-C2-C1    | 4.81  | 120.54      | 110.04   |
| 12  | A     | 306 | UMQ  | O1-C4'-C5'  | 4.80  | 121.81      | 109.33   |
| 17  | G     | 101 | BCR  | C20-C21-C22 | -4.76 | 120.43      | 127.29   |
| 12  | A     | 309 | UMQ  | O3-C3-C4    | 4.72  | 120.94      | 110.35   |
| 10  | A     | 302 | HEM  | CBA-CAA-C2A | -4.72 | 104.39      | 112.69   |
| 17  | G     | 101 | BCR  | C15-C14-C13 | -4.71 | 120.51      | 127.29   |
| 13  | A     | 308 | QNO  | C4-C3-C2    | -4.67 | 112.89      | 120.62   |
| 12  | A     | 309 | UMQ  | O2-C2-C1    | 4.67  | 120.22      | 110.04   |
| 16  | D     | 201 | SQD  | O4-C4-C5    | 4.62  | 121.45      | 109.28   |
| 16  | D     | 201 | SQD  | O4-C4-C3    | 4.57  | 118.29      | 109.94   |
| 12  | A     | 309 | UMQ  | O3-C3-C2    | 4.48  | 120.39      | 110.35   |
| 12  | A     | 307 | UMQ  | C1-C2-C3    | 4.46  | 118.67      | 110.00   |
| 17  | G     | 101 | BCR  | C24-C23-C22 | -4.44 | 119.57      | 126.22   |
| 12  | A     | 309 | UMQ  | O2-C2-C3    | 4.44  | 120.30      | 110.35   |
| 12  | C     | 301 | UMQ  | O1-C1-C2    | 4.43  | 118.75      | 108.12   |
| 12  | A     | 309 | UMQ  | O3'-C3'-C4' | 4.43  | 120.18      | 109.85   |
| 10  | A     | 304 | HEM  | C2D-C1D-ND  | -4.42 | 107.72      | 112.93   |
| 16  | D     | 201 | SQD  | O3-C3-C4    | 4.35  | 119.57      | 110.18   |
| 12  | A     | 309 | UMQ  | CA-O1'-C1'  | 4.33  | 121.75      | 113.96   |
| 12  | A     | 307 | UMQ  | O2-C2-C3    | 4.28  | 119.96      | 110.35   |
| 17  | G     | 101 | BCR  | C33-C5-C6   | -4.26 | 119.68      | 124.51   |
| 17  | G     | 101 | BCR  | C1-C6-C5    | -4.24 | 116.46      | 122.60   |
| 12  | A     | 307 | UMQ  | CA-O1'-C1'  | 4.23  | 121.57      | 113.96   |
| 10  | A     | 304 | HEM  | CHC-C1C-NC  | 4.21  | 128.39      | 124.73   |
| 12  | A     | 309 | UMQ  | C1-C2-C3    | 4.20  | 118.17      | 110.00   |
| 12  | A     | 306 | UMQ  | C3'-C4'-C5' | 4.17  | 120.22      | 110.85   |
| 12  | A     | 309 | UMQ  | C4-C3-C2    | 4.04  | 118.28      | 110.82   |
| 10  | A     | 304 | HEM  | CBA-CAA-C2A | -3.99 | 105.67      | 112.69   |
| 13  | A     | 308 | QNO  | C2-N1-C6    | 3.92  | 123.65      | 119.64   |
| 11  | A     | 305 | OPC  | OAN-CAO-CAP | 3.91  | 122.62      | 110.51   |
| 17  | G     | 101 | BCR  | C33-C5-C4   | 3.87  | 120.44      | 113.34   |
| 16  | D     | 201 | SQD  | C44-O6-C1   | 3.83  | 120.53      | 113.06   |
| 12  | A     | 309 | UMQ  | O3'-C3'-C2' | 3.82  | 118.92      | 110.35   |
| 12  | A     | 306 | UMQ  | O1-C4'-C3'  | 3.76  | 116.81      | 107.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | D     | 201 | SQD  | O47-C7-C8   | 3.65  | 119.55      | 111.56   |
| 14  | B     | 202 | CLA  | O2D-CGD-O1D | -3.46 | 116.76      | 123.79   |
| 17  | G     | 101 | BCR  | C23-C24-C25 | -3.43 | 117.18      | 127.32   |
| 12  | C     | 301 | UMQ  | C1-C2-C3    | -3.43 | 103.32      | 110.00   |
| 16  | D     | 201 | SQD  | O9-S-O7     | -3.41 | 101.09      | 113.26   |
| 12  | A     | 307 | UMQ  | O1'-C1'-C2' | 3.37  | 112.47      | 108.18   |
| 13  | A     | 308 | QNO  | C5-C6-N1    | 3.37  | 122.18      | 120.25   |
| 12  | C     | 301 | UMQ  | C1'-O5'-C5' | -3.29 | 107.34      | 113.73   |
| 10  | C     | 302 | HEM  | CHD-C4C-NC  | 3.28  | 127.58      | 124.73   |
| 10  | A     | 304 | HEM  | C4A-CHB-C1B | -3.24 | 123.20      | 127.47   |
| 10  | C     | 302 | HEM  | CBD-CAD-C3D | -3.23 | 107.32      | 114.37   |
| 17  | G     | 101 | BCR  | C38-C26-C25 | -3.20 | 120.88      | 124.51   |
| 16  | D     | 201 | SQD  | O9-S-C6     | 3.19  | 112.63      | 107.03   |
| 13  | A     | 308 | QNO  | OH-N1-C6    | -3.18 | 114.40      | 118.83   |
| 12  | A     | 307 | UMQ  | C1'-C2'-C3' | 3.17  | 116.15      | 110.00   |
| 10  | A     | 303 | HEM  | CAD-C3D-C4D | 3.14  | 130.17      | 124.53   |
| 17  | G     | 101 | BCR  | C38-C26-C27 | 3.14  | 119.10      | 113.34   |
| 12  | C     | 301 | UMQ  | C1-O5-C5    | -3.13 | 107.64      | 113.73   |
| 12  | A     | 307 | UMQ  | C1'-O5'-C5' | -3.11 | 107.69      | 113.73   |
| 17  | G     | 101 | BCR  | C20-C19-C18 | -3.09 | 117.56      | 126.38   |
| 14  | B     | 202 | CLA  | CMB-C2B-C1B | -3.09 | 123.87      | 128.62   |
| 10  | A     | 303 | HEM  | CBD-CAD-C3D | -3.09 | 107.63      | 114.37   |
| 12  | A     | 309 | UMQ  | O5'-C1'-O1' | 3.08  | 117.22      | 109.98   |
| 10  | C     | 302 | HEM  | C2D-C1D-ND  | -3.08 | 109.29      | 112.93   |
| 17  | G     | 101 | BCR  | C37-C22-C21 | -3.08 | 118.54      | 122.92   |
| 10  | A     | 303 | HEM  | C3A-C4A-NA  | -3.06 | 107.10      | 109.41   |
| 12  | A     | 306 | UMQ  | C1-O1-C4'   | -3.06 | 110.19      | 117.99   |
| 11  | B     | 203 | OPC  | OAI-PAJ-OAK | 3.06  | 113.39      | 104.68   |
| 12  | A     | 307 | UMQ  | O5'-C1'-C2' | -3.05 | 104.06      | 110.31   |
| 14  | B     | 202 | CLA  | CHB-C4A-NA  | 3.03  | 128.17      | 124.58   |
| 16  | D     | 201 | SQD  | C5-C6-S     | -3.02 | 110.00      | 114.45   |
| 10  | A     | 303 | HEM  | CHC-C4B-NB  | 3.01  | 127.08      | 124.58   |
| 17  | G     | 101 | BCR  | C3-C4-C5    | 3.00  | 118.29      | 113.74   |
| 10  | A     | 302 | HEM  | CHD-C4C-NC  | 3.00  | 127.34      | 124.73   |
| 10  | C     | 302 | HEM  | CHC-C4B-NB  | -2.97 | 122.12      | 124.58   |
| 14  | B     | 202 | CLA  | CAA-C2A-C1A | -2.95 | 104.27      | 111.62   |
| 17  | G     | 101 | BCR  | C31-C1-C6   | -2.94 | 105.45      | 110.33   |
| 12  | A     | 306 | UMQ  | O1-C1-C2    | 2.90  | 115.08      | 108.12   |
| 16  | D     | 201 | SQD  | O7-S-C6     | 2.90  | 112.11      | 107.03   |
| 12  | A     | 306 | UMQ  | C1-C2-C3    | 2.89  | 115.61      | 110.00   |
| 10  | A     | 302 | HEM  | C2D-C1D-ND  | -2.85 | 109.57      | 112.93   |
| 12  | A     | 306 | UMQ  | O1'-C1'-C2' | 2.83  | 111.78      | 108.18   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | G     | 101 | BCR  | C34-C9-C10  | -2.76 | 119.00      | 122.92   |
| 11  | B     | 203 | OPC  | OBJ-CBK-CBL | 2.73  | 120.52      | 111.94   |
| 17  | G     | 101 | BCR  | C8-C9-C10   | 2.72  | 123.16      | 118.97   |
| 14  | B     | 202 | CLA  | CAA-CBA-CGA | -2.71 | 104.52      | 113.27   |
| 11  | B     | 203 | OPC  | OAN-CAO-CAP | 2.69  | 118.85      | 110.51   |
| 16  | D     | 201 | SQD  | O8-S-C6     | 2.68  | 109.09      | 105.64   |
| 17  | G     | 101 | BCR  | C29-C30-C25 | 2.68  | 114.89      | 110.44   |
| 10  | C     | 302 | HEM  | C4C-NC-C1C  | 2.67  | 108.31      | 105.53   |
| 14  | B     | 202 | CLA  | C9-C8-C10   | 2.65  | 120.74      | 111.02   |
| 10  | C     | 302 | HEM  | C1B-NB-C4B  | 2.55  | 107.77      | 105.16   |
| 13  | A     | 308 | QNO  | C4-C5-C6    | -2.53 | 116.35      | 119.08   |
| 10  | A     | 302 | HEM  | CHC-C4B-NB  | 2.53  | 126.68      | 124.58   |
| 10  | A     | 303 | HEM  | C2D-C1D-ND  | -2.52 | 109.96      | 112.93   |
| 14  | B     | 202 | CLA  | CBD-CHA-C1A | 2.50  | 132.04      | 128.77   |
| 14  | B     | 202 | CLA  | CMB-C2B-C3B | 2.50  | 128.90      | 124.97   |
| 10  | A     | 303 | HEM  | C4A-C3A-C2A | 2.47  | 108.71      | 107.00   |
| 11  | B     | 203 | OPC  | CBI-OBJ-CBK | 2.47  | 121.66      | 116.04   |
| 12  | C     | 301 | UMQ  | O5-C1-C2    | 2.45  | 115.33      | 110.31   |
| 14  | B     | 202 | CLA  | CAA-C2A-C3A | -2.43 | 107.29      | 113.04   |
| 14  | B     | 202 | CLA  | C1B-CHB-C4A | -2.41 | 125.04      | 130.06   |
| 12  | A     | 309 | UMQ  | O5-C5-C4    | 2.41  | 114.23      | 109.76   |
| 14  | B     | 202 | CLA  | C4A-NA-C1A  | 2.41  | 109.85      | 106.52   |
| 10  | A     | 303 | HEM  | CHD-C1D-ND  | 2.40  | 126.58      | 124.58   |
| 12  | A     | 309 | UMQ  | C1-O5-C5    | 2.40  | 118.39      | 113.73   |
| 17  | G     | 101 | BCR  | C1-C6-C7    | 2.37  | 122.25      | 115.69   |
| 10  | A     | 302 | HEM  | CBD-CAD-C3D | -2.34 | 109.26      | 114.37   |
| 12  | C     | 301 | UMQ  | C4-C3-C2    | -2.34 | 106.50      | 110.82   |
| 12  | A     | 307 | UMQ  | O5'-C5'-C4' | 2.33  | 114.57      | 109.70   |
| 17  | G     | 101 | BCR  | C35-C13-C14 | -2.33 | 119.61      | 122.92   |
| 17  | G     | 101 | BCR  | C11-C10-C9  | -2.31 | 123.96      | 127.29   |
| 14  | B     | 202 | CLA  | C3A-C2A-C1A | 2.31  | 104.35      | 101.08   |
| 10  | C     | 302 | HEM  | CHB-C1B-NB  | 2.31  | 127.48      | 124.31   |
| 12  | C     | 301 | UMQ  | O5'-C1'-C2' | -2.31 | 105.58      | 110.31   |
| 12  | A     | 309 | UMQ  | O5'-C5'-C4' | 2.28  | 114.47      | 109.70   |
| 12  | A     | 307 | UMQ  | C1-O5-C5    | -2.28 | 109.30      | 113.73   |
| 11  | A     | 305 | OPC  | OBJ-CBK-CBL | 2.27  | 119.08      | 111.94   |
| 10  | C     | 302 | HEM  | C1A-CHA-C4D | -2.27 | 124.48      | 127.47   |
| 10  | C     | 302 | HEM  | CBA-CAA-C2A | -2.26 | 108.72      | 112.69   |
| 12  | A     | 309 | UMQ  | O5-C5-C6    | 2.22  | 111.81      | 106.34   |
| 17  | G     | 101 | BCR  | C4-C5-C6    | -2.22 | 119.89      | 122.84   |
| 16  | D     | 201 | SQD  | C45-O47-C7  | 2.21  | 123.36      | 117.92   |
| 14  | B     | 202 | CLA  | CMD-C2D-C3D | 2.20  | 128.44      | 124.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | B     | 202 | CLA  | C3A-C4A-CHB | -2.18 | 119.80      | 124.33   |
| 16  | D     | 201 | SQD  | O48-C23-C24 | 2.17  | 118.76      | 111.94   |
| 10  | A     | 304 | HEM  | C3A-C4A-NA  | -2.15 | 107.79      | 109.41   |
| 11  | A     | 305 | OPC  | OAN-CAO-OAD | -2.15 | 118.15      | 122.95   |
| 10  | A     | 304 | HEM  | C4C-NC-C1C  | 2.13  | 107.75      | 105.53   |
| 10  | A     | 304 | HEM  | CMA-C3A-C4A | -2.13 | 125.35      | 128.62   |
| 11  | B     | 203 | OPC  | OAN-CAO-OAD | -2.12 | 118.21      | 122.95   |
| 16  | D     | 201 | SQD  | C13-C12-C11 | 2.11  | 126.04      | 114.61   |
| 17  | G     | 101 | BCR  | C27-C26-C25 | -2.11 | 120.03      | 122.84   |
| 10  | A     | 302 | HEM  | CMA-C3A-C4A | -2.09 | 125.41      | 128.62   |
| 10  | A     | 302 | HEM  | C4A-CHB-C1B | -2.07 | 124.75      | 127.47   |
| 12  | A     | 307 | UMQ  | C6-C5-C4    | -2.06 | 108.03      | 113.00   |
| 10  | C     | 302 | HEM  | CMA-C3A-C4A | -2.05 | 125.47      | 128.62   |
| 14  | B     | 202 | CLA  | O1D-CGD-CBD | 2.03  | 128.58      | 124.42   |
| 17  | G     | 101 | BCR  | C8-C7-C6    | -2.02 | 121.37      | 127.32   |
| 10  | A     | 302 | HEM  | C1A-C2A-C3A | 2.01  | 109.00      | 106.92   |
| 17  | G     | 101 | BCR  | C40-C30-C25 | -2.00 | 107.01      | 110.33   |
| 10  | A     | 302 | HEM  | CHA-C1A-NA  | 2.00  | 127.93      | 124.58   |

All (13) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12  | A     | 307 | UMQ  | C2'  |
| 12  | A     | 307 | UMQ  | C2   |
| 12  | A     | 309 | UMQ  | C3   |
| 12  | A     | 309 | UMQ  | C1'  |
| 12  | A     | 309 | UMQ  | C2   |
| 12  | A     | 309 | UMQ  | C3'  |
| 12  | C     | 301 | UMQ  | C1   |
| 16  | D     | 201 | SQD  | C4   |
| 16  | D     | 201 | SQD  | C3   |
| 16  | D     | 201 | SQD  | C5   |
| 13  | A     | 308 | QNO  | C2   |
| 12  | A     | 306 | UMQ  | C4'  |
| 14  | B     | 202 | CLA  | C8   |

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | A     | 305 | OPC  | CAO-OAN-CAM-CBI |

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|--------------|-----------------------|--------|
| 1   | A     | 213/215 (99%)  | -0.08  | 0 100 100    | 44, 63, 92, 143       | 0      |
| 2   | B     | 160/160 (100%) | -0.06  | 0 100 100    | 53, 81, 125, 155      | 0      |
| 3   | C     | 286/289 (98%)  | 0.41   | 23 (8%) 12 4 | 57, 93, 192, 230      | 1 (0%) |
| 4   | D     | 161/179 (89%)  | 0.88   | 28 (17%) 2 1 | 56, 143, 183, 200     | 0      |
| 5   | E     | 32/32 (100%)   | 0.29   | 2 (6%) 19 5  | 75, 97, 134, 148      | 0      |
| 6   | F     | 32/35 (91%)    | 0.19   | 0 100 100    | 67, 87, 146, 154      | 0      |
| 7   | G     | 37/37 (100%)   | 0.05   | 0 100 100    | 61, 80, 151, 154      | 0      |
| 8   | H     | 29/29 (100%)   | 0.21   | 1 (3%) 43 10 | 65, 80, 101, 130      | 0      |
| All | All   | 950/976 (97%)  | 0.27   | 54 (5%) 23 5 | 44, 85, 178, 230      | 1 (0%) |

All (54) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 160 | ILE  | 4.2  |
| 4   | D     | 179 | VAL  | 4.1  |
| 4   | D     | 175 | LYS  | 3.9  |
| 4   | D     | 70  | LEU  | 3.8  |
| 4   | D     | 91  | ILE  | 3.7  |
| 4   | D     | 99  | ILE  | 3.5  |
| 3   | C     | 190 | TYR  | 3.5  |
| 3   | C     | 194 | LYS  | 3.5  |
| 4   | D     | 98  | ALA  | 3.4  |
| 3   | C     | 199 | ILE  | 3.1  |
| 3   | C     | 195 | TYR  | 3.1  |
| 3   | C     | 184 | ALA  | 3.0  |
| 4   | D     | 145 | PRO  | 2.9  |
| 4   | D     | 177 | TRP  | 2.9  |
| 4   | D     | 56  | ALA  | 2.8  |
| 4   | D     | 161 | VAL  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 149 | ALA  | 2.7  |
| 3   | C     | 193 | VAL  | 2.7  |
| 5   | E     | 32  | ILE  | 2.7  |
| 4   | D     | 79  | VAL  | 2.7  |
| 3   | C     | 220 | SER  | 2.7  |
| 4   | D     | 73  | HIS  | 2.6  |
| 3   | C     | 191 | GLY  | 2.6  |
| 3   | C     | 182 | LYS  | 2.6  |
| 3   | C     | 219 | VAL  | 2.6  |
| 3   | C     | 176 | ALA  | 2.5  |
| 4   | D     | 162 | LEU  | 2.5  |
| 3   | C     | 206 | THR  | 2.5  |
| 4   | D     | 151 | CYS  | 2.5  |
| 3   | C     | 177 | THR  | 2.4  |
| 4   | D     | 176 | PRO  | 2.4  |
| 4   | D     | 146 | LEU  | 2.4  |
| 3   | C     | 211 | ILE  | 2.4  |
| 4   | D     | 144 | ALA  | 2.4  |
| 4   | D     | 170 | PHE  | 2.4  |
| 3   | C     | 189 | GLU  | 2.4  |
| 4   | D     | 92  | VAL  | 2.4  |
| 4   | D     | 174 | GLU  | 2.3  |
| 4   | D     | 64  | VAL  | 2.3  |
| 4   | D     | 168 | THR  | 2.3  |
| 3   | C     | 192 | ASN  | 2.3  |
| 3   | C     | 88  | GLU  | 2.3  |
| 3   | C     | 183 | ILE  | 2.3  |
| 4   | D     | 166 | THR  | 2.3  |
| 3   | C     | 90  | ILE  | 2.3  |
| 4   | D     | 66  | VAL  | 2.2  |
| 3   | C     | 181 | THR  | 2.2  |
| 4   | D     | 172 | THR  | 2.2  |
| 3   | C     | 207 | VAL  | 2.1  |
| 3   | C     | 197 | VAL  | 2.0  |
| 5   | E     | 2   | ILE  | 2.0  |
| 3   | C     | 212 | PRO  | 2.0  |
| 4   | D     | 169 | ASP  | 2.0  |
| 8   | H     | 1   | MET  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|----------------------------|-------|
| 11  | OPC  | A     | 305 | 54/55 | 0.60 | 5.41  | 62,118,206,229             | 0     |
| 12  | UMQ  | A     | 306 | 34/34 | 0.56 | 5.27  | 61,148,192,198             | 0     |
| 17  | BCR  | G     | 101 | 40/40 | 0.56 | 4.23  | 51,97,180,199              | 0     |
| 11  | OPC  | B     | 203 | 54/55 | 0.66 | 4.13  | 66,126,180,198             | 0     |
| 12  | UMQ  | C     | 301 | 34/34 | 0.51 | 3.63  | 51,119,203,224             | 0     |
| 16  | SQD  | D     | 201 | 53/54 | 0.60 | 2.78  | 83,150,191,196             | 1     |
| 14  | CLA  | B     | 202 | 65/65 | 0.37 | 1.70  | 59,90,133,153              | 0     |
| 13  | QNO  | A     | 308 | 21/21 | 0.35 | 1.52  | 83,113,154,167             | 0     |
| 9   | CD   | B     | 201 | 1/1   | 0.27 | 1.52  | 186,186,186,186            | 0     |
| 12  | UMQ  | A     | 307 | 34/34 | 0.34 | 1.09  | 81,138,182,186             | 0     |
| 10  | HEM  | A     | 303 | 43/43 | 0.29 | 1.01  | 39,58,82,83                | 0     |
| 12  | UMQ  | A     | 309 | 34/34 | 0.37 | 0.78  | 87,162,229,238             | 0     |
| 10  | HEM  | A     | 304 | 43/43 | 0.28 | 0.74  | 54,80,107,112              | 0     |
| 10  | HEM  | A     | 302 | 43/43 | 0.27 | 0.44  | 35,58,79,112               | 0     |
| 10  | HEM  | C     | 302 | 43/43 | 0.27 | 0.25  | 52,81,118,122              | 0     |
| 9   | CD   | A     | 301 | 1/1   | 0.20 | 0.19  | 83,83,83,83                | 0     |
| 15  | FES  | D     | 200 | 4/4   | 0.08 | -1.16 | 108,129,130,138            | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.