



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:57 pm GMT

PDB ID : 1PRC  
Title : CRYSTALLOGRAPHIC REFINEMENT AT 2.3 ANGSTROMS RESOLUTION AND REFINED MODEL OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS  
Authors : Deisenhofer, J.; Epp, O.; Miki, K.; Huber, R.; Michel, H.  
Deposited on : 1988-02-04  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

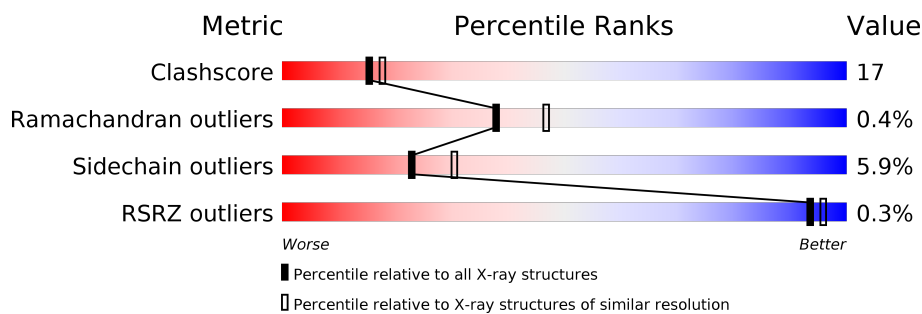
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.30 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 112137                      | 4751 (2.30-2.30)                                      |
| Ramachandran outliers | 110173                      | 4705 (2.30-2.30)                                      |
| Sidechain outliers    | 110143                      | 4704 (2.30-2.30)                                      |
| RSRZ outliers         | 101464                      | 4156 (2.30-2.30)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | C     | 336    | <br>59% 35% 5% .. |
| 2   | L     | 273    | <br>65% 31% .     |
| 3   | M     | 323    | <br>66% 31% .     |
| 4   | H     | 258    | <br>61% 32% 6% .  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | NS1  | M     | 613 | -         | -        | -       | X                |
| 12  | UQ1  | L     | 614 | -         | -        | X       | X                |
| 13  | LDA  | H     | 616 | -         | -        | -       | X                |
| 6   | SO4  | H     | 622 | -         | -        | -       | X                |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | C     | 333      | Total | C    | N   | O   | S  | 54      | 0       | 1     |
|     |       |          | 2603  | 1640 | 467 | 478 | 18 |         |         |       |

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | L     | 273      | Total | C    | N   | O   | S | 13      | 0       | 0     |
|     |       |          | 2171  | 1459 | 350 | 355 | 7 |         |         |       |

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | M     | 323      | Total | C    | N   | O   | S  | 26      | 0       | 0     |
|     |       |          | 2555  | 1702 | 419 | 423 | 11 |         |         |       |

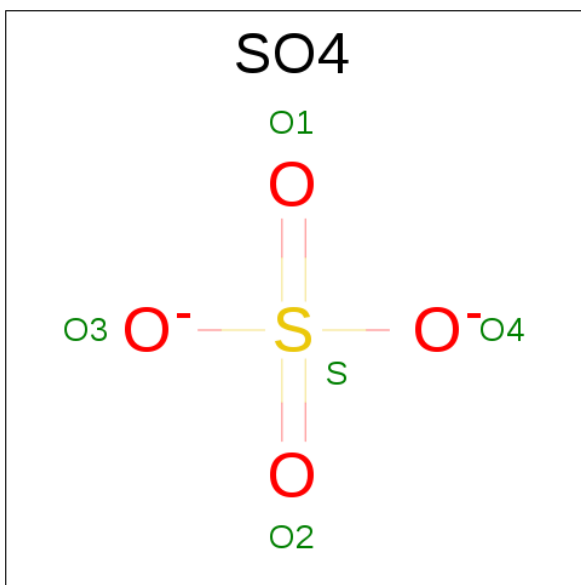
- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | H     | 258      | Total | C    | N   | O   | S | 106     | 0       | 0     |
|     |       |          | 2018  | 1292 | 344 | 380 | 2 |         |         |       |

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

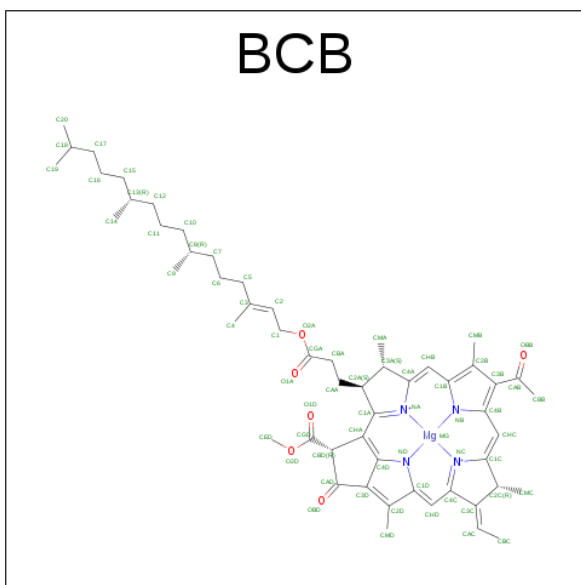
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | M     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



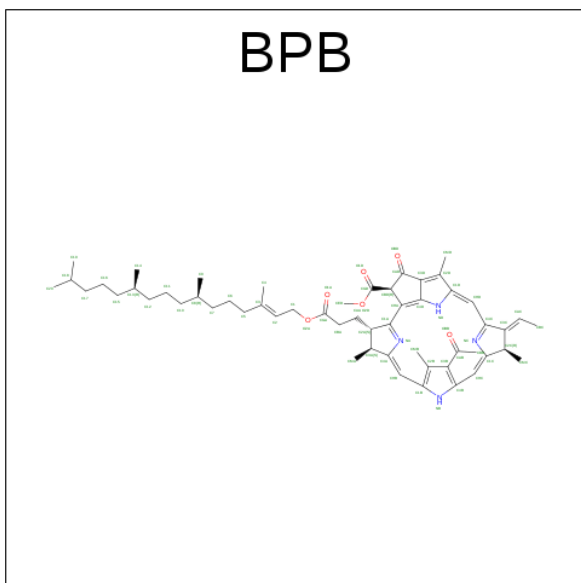
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 6   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 6   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 6   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 6   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 6   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula:  $C_{55}H_{72}MgN_4O_6$ ).



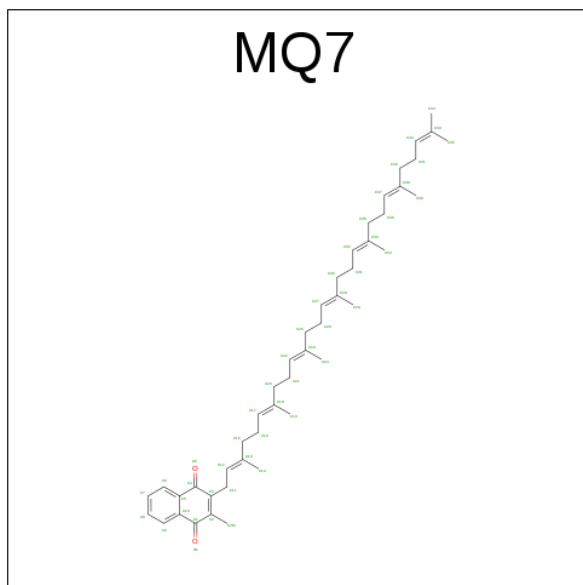
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 7   | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 13      | 0       |
| 7   | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 7   | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 7   | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_6$ ).



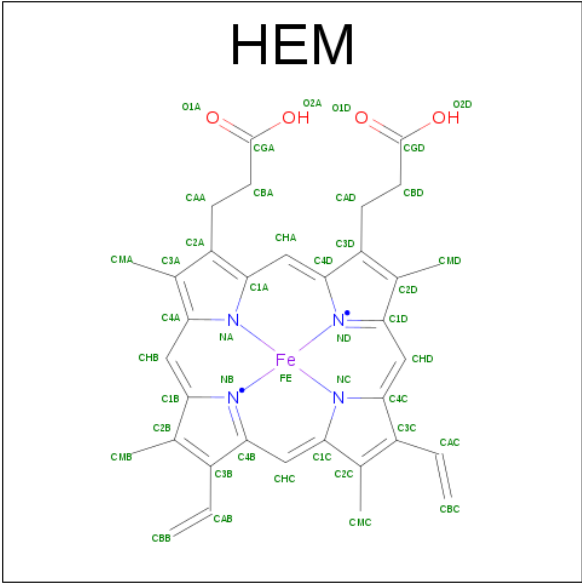
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 8   | M     | 1        | Total | C  | N | O | 7       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |
| 8   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula:  $C_{46}H_{64}O_2$ ).



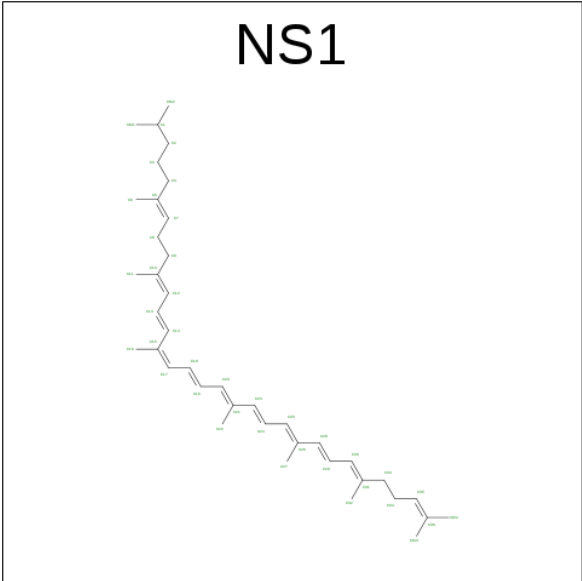
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | M     | 1        | Total | C  | O | 4       | 0       |
|     |       |          | 48    | 46 | 2 |         |         |

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



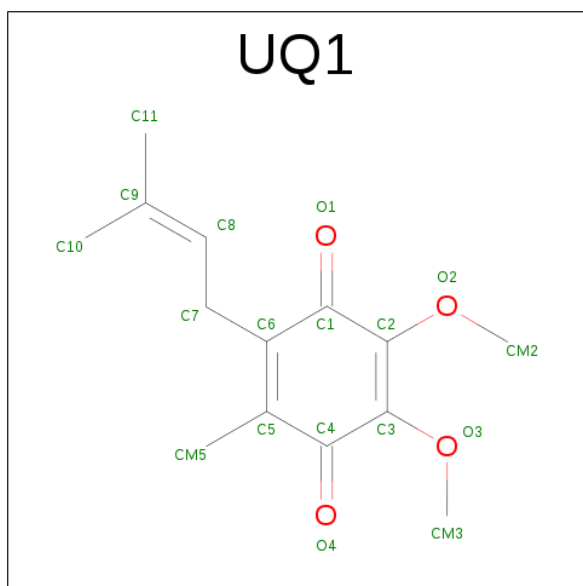
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 11 is 15-TRANS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS1) (formula: C<sub>40</sub>H<sub>60</sub>).



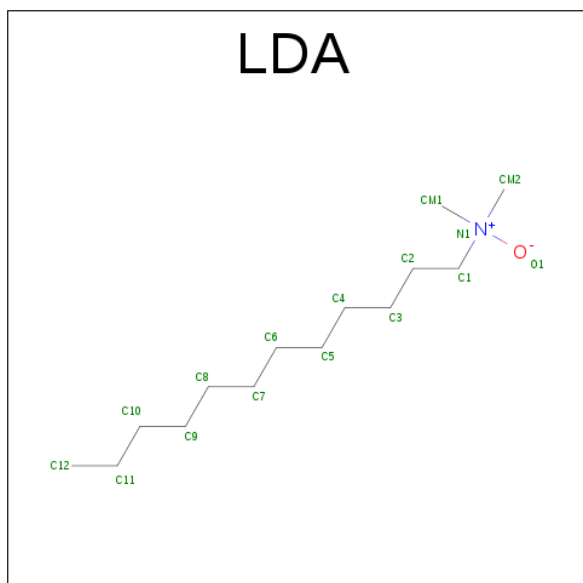
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | M     | 1        | Total | C  | 14      | 0       |
|     |       |          | 40    | 40 |         |         |

- Molecule 12 is UBIQUINONE-1 (three-letter code: UQ1) (formula:  $C_{14}H_{18}O_4$ ).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 12  | L     | 1        | Total | C  | 0       | 0       |
|     |       |          | 18    | 14 | 4       |         |

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 13  | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 13  | H     | 1        | Total | C  | N | O | 6       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

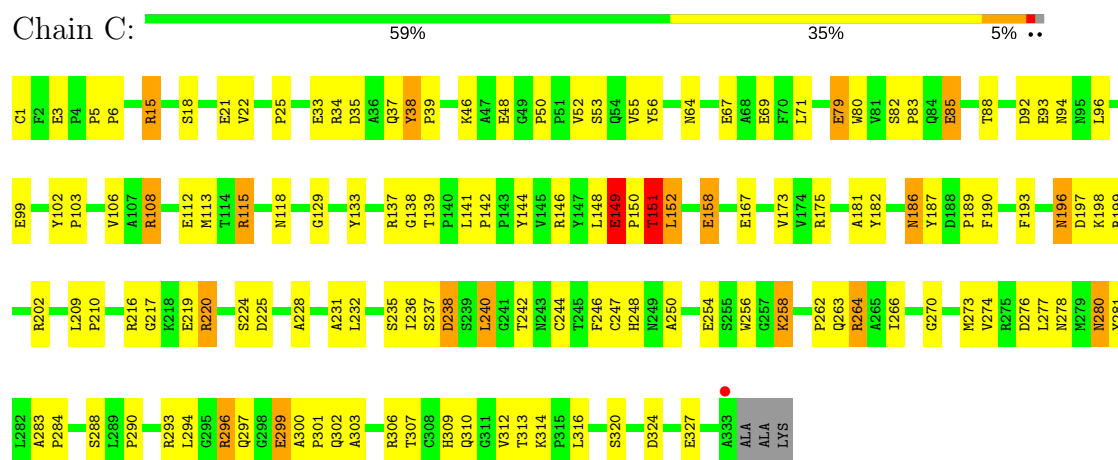
- Molecule 14 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | C     | 66       | Total | O  | 0       | 0       |
|     |       |          | 66    | 66 |         |         |
| 14  | H     | 41       | Total | O  | 0       | 0       |
|     |       |          | 41    | 41 |         |         |
| 14  | L     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 14  | M     | 55       | Total | O  | 0       | 0       |
|     |       |          | 55    | 55 |         |         |

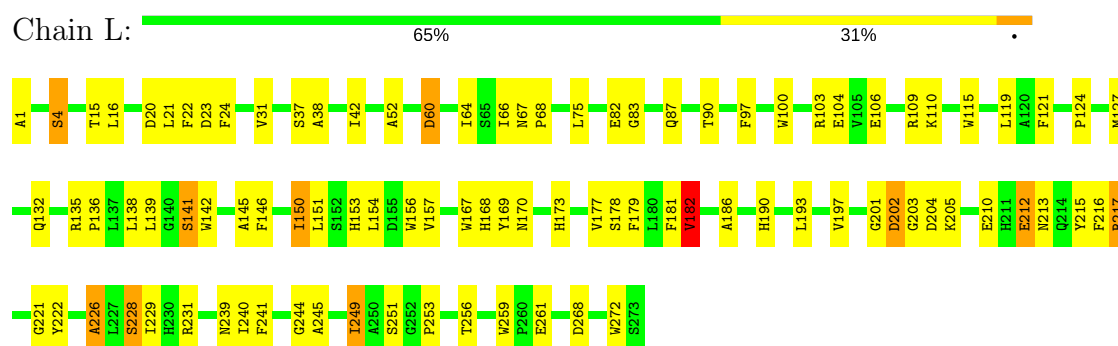
### 3 Residue-property plots

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

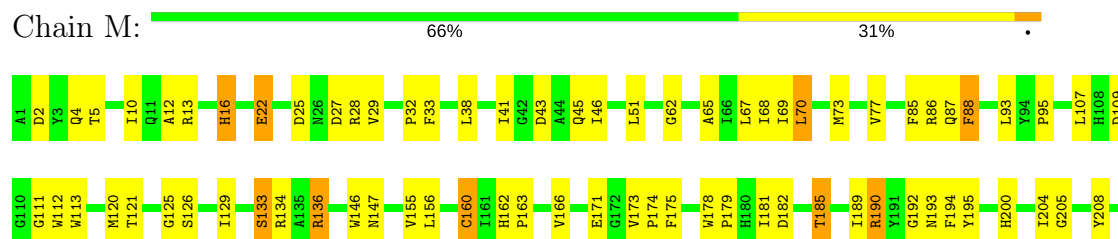
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER

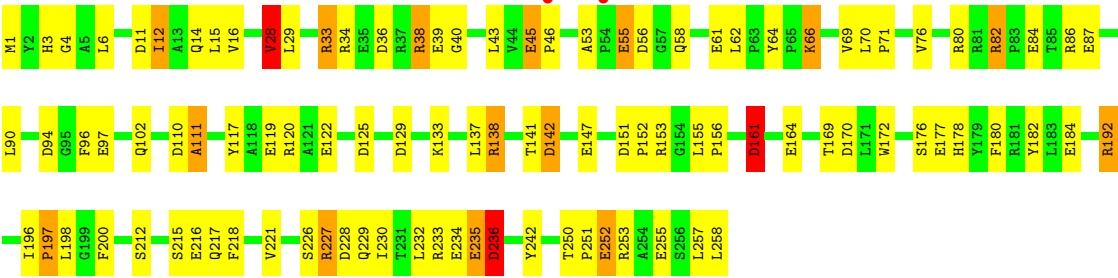


#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER





● Molecule 4: PHOTOSYNTHETIC REACTION CENTER



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 43 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 223.50Å 223.50Å 113.60Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 19.99 – 2.30<br>19.99 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (19.99-2.30)<br>75.5 (19.99-2.30)           | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$   | -   | Xtriage          |
| Refinement program  | TNT   | Depositor        |
| R, $R_{free}$   | 0.193 , (Not available)<br>0.186 , (Not available)          | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.4  | Xtriage          |
| Anisotropy  | 0.098   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 64.5   | EDS              |
| L-test for twinning <sup>1</sup>  | $\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.15$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 10288   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 21.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, BCB, FE, MQ7, HEM, UQ1, NS1, FME, SO4

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | C     | 1.07         | 17/2670 (0.6%) | 1.56        | 36/3639 (1.0%)   |
| 2   | L     | 1.01         | 5/2259 (0.2%)  | 1.42        | 18/3084 (0.6%)   |
| 3   | M     | 0.96         | 3/2659 (0.1%)  | 1.46        | 26/3637 (0.7%)   |
| 4   | H     | 1.13         | 18/2055 (0.9%) | 1.65        | 32/2807 (1.1%)   |
| All | All   | 1.04         | 43/9643 (0.4%) | 1.52        | 112/13167 (0.9%) |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | H     | 255 | GLU  | CD-OE2 | 9.06  | 1.35        | 1.25     |
| 1   | C     | 299 | GLU  | CD-OE2 | 8.31  | 1.34        | 1.25     |
| 3   | M     | 244 | GLU  | CD-OE2 | 8.03  | 1.34        | 1.25     |
| 2   | L     | 261 | GLU  | CD-OE2 | 7.64  | 1.34        | 1.25     |
| 1   | C     | 21  | GLU  | CD-OE2 | 7.48  | 1.33        | 1.25     |
| 4   | H     | 177 | GLU  | CD-OE2 | 7.40  | 1.33        | 1.25     |
| 1   | C     | 33  | GLU  | CD-OE2 | 7.39  | 1.33        | 1.25     |
| 1   | C     | 158 | GLU  | CD-OE2 | 7.36  | 1.33        | 1.25     |
| 1   | C     | 149 | GLU  | CD-OE2 | 7.18  | 1.33        | 1.25     |
| 4   | H     | 234 | GLU  | CD-OE2 | 6.91  | 1.33        | 1.25     |
| 1   | C     | 99  | GLU  | CD-OE2 | 6.86  | 1.33        | 1.25     |
| 4   | H     | 122 | GLU  | CD-OE2 | 6.59  | 1.32        | 1.25     |
| 1   | C     | 112 | GLU  | CD-OE2 | 6.56  | 1.32        | 1.25     |
| 4   | H     | 164 | GLU  | CD-OE2 | 6.56  | 1.32        | 1.25     |
| 4   | H     | 84  | GLU  | CD-OE2 | 6.54  | 1.32        | 1.25     |
| 1   | C     | 167 | GLU  | CD-OE2 | 6.36  | 1.32        | 1.25     |
| 1   | C     | 254 | GLU  | CD-OE1 | -6.23 | 1.18        | 1.25     |
| 1   | C     | 67  | GLU  | CD-OE2 | 6.16  | 1.32        | 1.25     |
| 4   | H     | 119 | GLU  | CD-OE2 | 6.01  | 1.32        | 1.25     |
| 2   | L     | 82  | GLU  | CD-OE2 | 5.94  | 1.32        | 1.25     |
| 4   | H     | 252 | GLU  | CD-OE2 | 5.87  | 1.32        | 1.25     |
| 1   | C     | 85  | GLU  | CD-OE2 | 5.82  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 219 | GLU  | CD-OE1 | -5.77 | 1.19        | 1.25     |
| 1   | C     | 79  | GLU  | CD-OE2 | 5.73  | 1.31        | 1.25     |
| 1   | C     | 69  | GLU  | CD-OE2 | 5.71  | 1.31        | 1.25     |
| 4   | H     | 61  | GLU  | CD-OE2 | 5.67  | 1.31        | 1.25     |
| 2   | L     | 212 | GLU  | CD-OE2 | 5.58  | 1.31        | 1.25     |
| 1   | C     | 3   | GLU  | CD-OE2 | 5.52  | 1.31        | 1.25     |
| 4   | H     | 147 | GLU  | CD-OE2 | 5.48  | 1.31        | 1.25     |
| 4   | H     | 87  | GLU  | CD-OE2 | 5.45  | 1.31        | 1.25     |
| 4   | H     | 235 | GLU  | CD-OE2 | 5.40  | 1.31        | 1.25     |
| 2   | L     | 104 | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |
| 1   | C     | 48  | GLU  | CD-OE2 | 5.37  | 1.31        | 1.25     |
| 4   | H     | 216 | GLU  | CD-OE2 | 5.34  | 1.31        | 1.25     |
| 1   | C     | 93  | GLU  | CD-OE2 | 5.32  | 1.31        | 1.25     |
| 3   | M     | 22  | GLU  | CD-OE2 | 5.31  | 1.31        | 1.25     |
| 4   | H     | 55  | GLU  | CD-OE2 | 5.22  | 1.31        | 1.25     |
| 4   | H     | 97  | GLU  | CD-OE2 | 5.18  | 1.31        | 1.25     |
| 4   | H     | 184 | GLU  | CD-OE2 | 5.10  | 1.31        | 1.25     |
| 3   | M     | 232 | GLU  | CD-OE2 | 5.10  | 1.31        | 1.25     |
| 4   | H     | 45  | GLU  | CD-OE2 | 5.04  | 1.31        | 1.25     |
| 4   | H     | 39  | GLU  | CD-OE1 | -5.03 | 1.20        | 1.25     |
| 2   | L     | 210 | GLU  | CD-OE2 | 5.01  | 1.31        | 1.25     |

All (112) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 4   | H     | 38  | ARG  | NE-CZ-NH2 | -18.45 | 111.08      | 120.30   |
| 3   | M     | 245 | ARG  | NE-CZ-NH2 | -11.45 | 114.57      | 120.30   |
| 3   | M     | 25  | ASP  | CB-CG-OD2 | -10.22 | 109.10      | 118.30   |
| 4   | H     | 153 | ARG  | NE-CZ-NH2 | -9.86  | 115.37      | 120.30   |
| 4   | H     | 153 | ARG  | NE-CZ-NH1 | 9.74   | 125.17      | 120.30   |
| 3   | M     | 245 | ARG  | NE-CZ-NH1 | 9.64   | 125.12      | 120.30   |
| 1   | C     | 216 | ARG  | NE-CZ-NH1 | 9.51   | 125.05      | 120.30   |
| 3   | M     | 239 | ARG  | NE-CZ-NH2 | -9.45  | 115.58      | 120.30   |
| 3   | M     | 27  | ASP  | CB-CG-OD2 | -9.40  | 109.84      | 118.30   |
| 3   | M     | 239 | ARG  | NE-CZ-NH1 | 9.11   | 124.86      | 120.30   |
| 1   | C     | 225 | ASP  | CB-CG-OD2 | -9.02  | 110.18      | 118.30   |
| 2   | L     | 231 | ARG  | NE-CZ-NH1 | 8.96   | 124.78      | 120.30   |
| 1   | C     | 108 | ARG  | NE-CZ-NH1 | 8.68   | 124.64      | 120.30   |
| 2   | L     | 231 | ARG  | NE-CZ-NH2 | -8.44  | 116.08      | 120.30   |
| 3   | M     | 304 | ASP  | CB-CG-OD1 | 8.33   | 125.80      | 118.30   |
| 4   | H     | 38  | ARG  | NE-CZ-NH1 | 8.25   | 124.43      | 120.30   |
| 1   | C     | 35  | ASP  | CB-CG-OD2 | -8.03  | 111.07      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | H     | 236 | ASP  | CB-CG-OD1 | 7.97  | 125.47      | 118.30   |
| 2   | L     | 215 | TYR  | CB-CG-CD2 | -7.83 | 116.30      | 121.00   |
| 1   | C     | 220 | ARG  | NE-CZ-NH2 | -7.79 | 116.41      | 120.30   |
| 3   | M     | 25  | ASP  | CB-CG-OD1 | 7.76  | 125.28      | 118.30   |
| 3   | M     | 190 | ARG  | NE-CZ-NH2 | -7.59 | 116.51      | 120.30   |
| 4   | H     | 161 | ASP  | CB-CG-OD2 | -7.58 | 111.48      | 118.30   |
| 4   | H     | 236 | ASP  | CB-CG-OD2 | -7.47 | 111.58      | 118.30   |
| 2   | L     | 20  | ASP  | CB-CG-OD2 | -7.42 | 111.62      | 118.30   |
| 1   | C     | 313 | THR  | CA-CB-CG2 | -7.38 | 102.07      | 112.40   |
| 1   | C     | 264 | ARG  | NE-CZ-NH2 | -7.24 | 116.68      | 120.30   |
| 3   | M     | 160 | CYS  | CB-CA-C   | -7.06 | 96.28       | 110.40   |
| 1   | C     | 196 | ASN  | CB-CA-C   | -7.05 | 96.29       | 110.40   |
| 1   | C     | 225 | ASP  | CB-CG-OD1 | 7.03  | 124.63      | 118.30   |
| 1   | C     | 324 | ASP  | CB-CG-OD2 | -7.02 | 111.98      | 118.30   |
| 1   | C     | 115 | ARG  | NE-CZ-NH1 | 7.02  | 123.81      | 120.30   |
| 2   | L     | 23  | ASP  | CB-CG-OD1 | 6.88  | 124.50      | 118.30   |
| 4   | H     | 62  | LEU  | CB-CG-CD1 | -6.78 | 99.48       | 111.00   |
| 1   | C     | 115 | ARG  | NE-CZ-NH2 | -6.77 | 116.91      | 120.30   |
| 3   | M     | 251 | ARG  | NE-CZ-NH2 | -6.72 | 116.94      | 120.30   |
| 1   | C     | 146 | ARG  | NE-CZ-NH1 | 6.68  | 123.64      | 120.30   |
| 3   | M     | 304 | ASP  | CB-CG-OD2 | -6.64 | 112.33      | 118.30   |
| 3   | M     | 43  | ASP  | CB-CG-OD2 | -6.59 | 112.37      | 118.30   |
| 4   | H     | 110 | ASP  | CB-CG-OD2 | -6.51 | 112.44      | 118.30   |
| 1   | C     | 296 | ARG  | NE-CZ-NH1 | 6.49  | 123.55      | 120.30   |
| 3   | M     | 85  | PHE  | CB-CA-C   | 6.39  | 123.18      | 110.40   |
| 2   | L     | 215 | TYR  | CB-CG-CD1 | 6.35  | 124.81      | 121.00   |
| 2   | L     | 60  | ASP  | CB-CG-OD2 | -6.34 | 112.59      | 118.30   |
| 3   | M     | 86  | ARG  | NE-CZ-NH1 | 6.31  | 123.45      | 120.30   |
| 3   | M     | 230 | ASP  | CB-CG-OD2 | -6.25 | 112.68      | 118.30   |
| 3   | M     | 27  | ASP  | CB-CG-OD1 | 6.21  | 123.89      | 118.30   |
| 1   | C     | 280 | ASN  | CB-CA-C   | -6.21 | 97.99       | 110.40   |
| 1   | C     | 197 | ASP  | CB-CG-OD2 | -6.19 | 112.73      | 118.30   |
| 2   | L     | 23  | ASP  | CB-CG-OD2 | -6.12 | 112.79      | 118.30   |
| 1   | C     | 149 | GLU  | N-CA-CB   | 6.12  | 121.62      | 110.60   |
| 1   | C     | 216 | ARG  | NE-CZ-NH2 | -6.07 | 117.27      | 120.30   |
| 3   | M     | 134 | ARG  | NE-CZ-NH2 | -5.99 | 117.31      | 120.30   |
| 2   | L     | 202 | ASP  | CB-CG-OD2 | -5.97 | 112.92      | 118.30   |
| 1   | C     | 224 | SER  | CB-CA-C   | -5.96 | 98.78       | 110.10   |
| 2   | L     | 204 | ASP  | CB-CG-OD2 | -5.92 | 112.97      | 118.30   |
| 3   | M     | 28  | ARG  | NE-CZ-NH2 | -5.89 | 117.36      | 120.30   |
| 3   | M     | 231 | ARG  | NE-CZ-NH2 | -5.87 | 117.36      | 120.30   |
| 4   | H     | 11  | ASP  | CB-CG-OD1 | 5.87  | 123.58      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | H     | 33  | ARG  | NE-CZ-NH1  | 5.84  | 123.22      | 120.30   |
| 2   | L     | 217 | ARG  | NE-CZ-NH1  | 5.84  | 123.22      | 120.30   |
| 1   | C     | 151 | THR  | CA-CB-CG2  | -5.78 | 104.31      | 112.40   |
| 3   | M     | 43  | ASP  | CB-CG-OD1  | 5.77  | 123.50      | 118.30   |
| 4   | H     | 34  | ARG  | NE-CZ-NH1  | 5.77  | 123.19      | 120.30   |
| 1   | C     | 33  | GLU  | CB-CA-C    | -5.75 | 98.89       | 110.40   |
| 4   | H     | 151 | ASP  | CB-CG-OD1  | 5.75  | 123.47      | 118.30   |
| 1   | C     | 46  | LYS  | N-CA-CB    | 5.68  | 120.83      | 110.60   |
| 1   | C     | 300 | ALA  | CB-CA-C    | -5.68 | 101.58      | 110.10   |
| 1   | C     | 92  | ASP  | CB-CG-OD1  | 5.65  | 123.38      | 118.30   |
| 1   | C     | 146 | ARG  | NE-CZ-NH2  | -5.65 | 117.48      | 120.30   |
| 1   | C     | 199 | ARG  | NE-CZ-NH1  | 5.62  | 123.11      | 120.30   |
| 3   | M     | 13  | ARG  | NE-CZ-NH1  | 5.62  | 123.11      | 120.30   |
| 3   | M     | 185 | THR  | CA-CB-CG2  | -5.59 | 104.57      | 112.40   |
| 4   | H     | 253 | ARG  | NE-CZ-NH2  | -5.59 | 117.50      | 120.30   |
| 1   | C     | 25  | PRO  | N-CA-CB    | 5.59  | 110.00      | 103.30   |
| 4   | H     | 129 | ASP  | CA-CB-CG   | -5.58 | 101.14      | 113.40   |
| 2   | L     | 186 | ALA  | CB-CA-C    | -5.57 | 101.75      | 110.10   |
| 2   | L     | 268 | ASP  | CB-CG-OD2  | -5.53 | 113.32      | 118.30   |
| 1   | C     | 324 | ASP  | CB-CG-OD1  | 5.51  | 123.26      | 118.30   |
| 3   | M     | 190 | ARG  | NE-CZ-NH1  | 5.48  | 123.04      | 120.30   |
| 4   | H     | 251 | PRO  | N-CA-CB    | 5.46  | 109.85      | 103.30   |
| 4   | H     | 11  | ASP  | CB-CG-OD2  | -5.45 | 113.39      | 118.30   |
| 1   | C     | 238 | ASP  | CB-CG-OD2  | -5.44 | 113.40      | 118.30   |
| 1   | C     | 152 | LEU  | CB-CA-C    | 5.43  | 120.52      | 110.20   |
| 4   | H     | 138 | ARG  | CB-CA-C    | -5.40 | 99.60       | 110.40   |
| 1   | C     | 220 | ARG  | NE-CZ-NH1  | 5.38  | 122.99      | 120.30   |
| 1   | C     | 139 | THR  | N-CA-CB    | 5.34  | 120.44      | 110.30   |
| 3   | M     | 230 | ASP  | CB-CG-OD1  | 5.31  | 123.08      | 118.30   |
| 4   | H     | 227 | ARG  | NE-CZ-NH2  | -5.30 | 117.65      | 120.30   |
| 2   | L     | 182 | VAL  | CB-CA-C    | -5.29 | 101.34      | 111.40   |
| 4   | H     | 64  | TYR  | CB-CG-CD2  | -5.28 | 117.83      | 121.00   |
| 1   | C     | 92  | ASP  | CB-CG-OD2  | -5.27 | 113.56      | 118.30   |
| 4   | H     | 111 | ALA  | CB-CA-C    | 5.26  | 117.99      | 110.10   |
| 4   | H     | 129 | ASP  | CB-CG-OD2  | -5.25 | 113.58      | 118.30   |
| 2   | L     | 60  | ASP  | CB-CG-OD1  | 5.23  | 123.01      | 118.30   |
| 4   | H     | 14  | GLN  | CB-CA-C    | -5.22 | 99.95       | 110.40   |
| 2   | L     | 150 | ILE  | CA-CB-CG1  | -5.20 | 101.12      | 111.00   |
| 4   | H     | 94  | ASP  | CB-CG-OD2  | -5.18 | 113.64      | 118.30   |
| 4   | H     | 80  | ARG  | NE-CZ-NH2  | -5.17 | 117.71      | 120.30   |
| 1   | C     | 152 | LEU  | N-CA-CB    | -5.17 | 100.06      | 110.40   |
| 4   | H     | 28  | VAL  | CG1-CB-CG2 | -5.15 | 102.66      | 110.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | H     | 34  | ARG  | NE-CZ-NH2 | -5.15 | 117.72      | 120.30   |
| 4   | H     | 161 | ASP  | CB-CG-OD1 | 5.15  | 122.93      | 118.30   |
| 4   | H     | 192 | ARG  | NE-CZ-NH2 | -5.14 | 117.73      | 120.30   |
| 2   | L     | 226 | ALA  | N-CA-CB   | -5.14 | 102.91      | 110.10   |
| 4   | H     | 66  | LYS  | N-CA-CB   | -5.12 | 101.39      | 110.60   |
| 2   | L     | 90  | THR  | CA-CB-CG2 | -5.11 | 105.25      | 112.40   |
| 1   | C     | 237 | SER  | CB-CA-C   | -5.09 | 100.43      | 110.10   |
| 1   | C     | 296 | ARG  | NE-CZ-NH2 | -5.07 | 117.76      | 120.30   |
| 3   | M     | 109 | ASP  | CB-CG-OD1 | 5.04  | 122.83      | 118.30   |
| 4   | H     | 197 | PRO  | N-CA-CB   | 5.04  | 109.34      | 103.30   |
| 4   | H     | 141 | THR  | N-CA-CB   | -5.02 | 100.77      | 110.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 2603  | 0        | 2579     | 81      | 0            |
| 2   | L     | 2171  | 0        | 2098     | 83      | 0            |
| 3   | M     | 2555  | 0        | 2452     | 78      | 0            |
| 4   | H     | 2018  | 0        | 2020     | 58      | 0            |
| 5   | M     | 1     | 0        | 0        | 0       | 0            |
| 6   | H     | 15    | 0        | 0        | 0       | 0            |
| 6   | M     | 20    | 0        | 0        | 0       | 0            |
| 7   | L     | 132   | 0        | 144      | 22      | 0            |
| 7   | M     | 132   | 0        | 144      | 22      | 0            |
| 8   | L     | 65    | 0        | 74       | 8       | 0            |
| 8   | M     | 65    | 0        | 74       | 11      | 0            |
| 9   | M     | 48    | 0        | 64       | 1       | 0            |
| 10  | C     | 172   | 0        | 120      | 14      | 0            |
| 11  | M     | 40    | 0        | 59       | 4       | 0            |
| 12  | L     | 18    | 0        | 18       | 10      | 0            |
| 13  | H     | 16    | 0        | 31       | 2       | 0            |
| 13  | M     | 16    | 0        | 31       | 1       | 0            |
| 14  | C     | 66    | 0        | 0        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | H     | 41    | 0        | 0        | 1       | 0            |
| 14  | L     | 39    | 0        | 0        | 3       | 0            |
| 14  | M     | 55    | 0        | 0        | 3       | 0            |
| All | All   | 10288 | 0        | 9908     | 321     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:120:MET:HE2  | 7:M:603:BCB:H172  | 1.41                     | 1.00              |
| 3:M:136:ARG:HE   | 3:M:136:ARG:HA    | 1.31                     | 0.93              |
| 1:C:152:LEU:HD22 | 1:C:175:ARG:HA    | 1.53                     | 0.90              |
| 8:L:606:BPB:HHC  | 8:L:606:BPB:HBBB  | 1.52                     | 0.90              |
| 7:L:602:BCB:H61  | 7:L:604:BCB:HBB3  | 1.55                     | 0.88              |
| 4:H:152:PRO:HA   | 4:H:155:LEU:CD1   | 2.04                     | 0.86              |
| 3:M:318:LEU:HB3  | 3:M:319:PRO:HD2   | 1.57                     | 0.86              |
| 3:M:275:MET:HG2  | 8:M:605:BPB:HBCA  | 1.58                     | 0.84              |
| 7:L:604:BCB:HBB2 | 7:L:604:BCB:HHC   | 1.57                     | 0.84              |
| 2:L:139:LEU:HD21 | 2:L:253:PRO:HD3   | 1.59                     | 0.82              |
| 7:L:604:BCB:HMB2 | 8:L:606:BPB:HMBA  | 1.62                     | 0.82              |
| 7:M:603:BCB:HBB3 | 7:M:603:BCB:HMB1  | 1.61                     | 0.82              |
| 1:C:202:ARG:HG2  | 10:C:611:HEM:CGA  | 2.12                     | 0.80              |
| 1:C:270:GLY:O    | 1:C:274:VAL:HG12  | 1.81                     | 0.79              |
| 3:M:120:MET:HE3  | 7:M:603:BCB:H193  | 1.63                     | 0.79              |
| 7:L:602:BCB:H61  | 7:L:604:BCB:CBB   | 2.13                     | 0.79              |
| 2:L:190:HIS:HA   | 12:L:614:UQ1:O4   | 1.81                     | 0.79              |
| 4:H:82:ARG:HG2   | 4:H:82:ARG:HH11   | 1.47                     | 0.78              |
| 8:L:606:BPB:HHC  | 8:L:606:BPB:CBB   | 2.14                     | 0.77              |
| 4:H:152:PRO:HA   | 4:H:155:LEU:HD11  | 1.67                     | 0.77              |
| 2:L:181:PHE:HB3  | 8:M:605:BPB:HBBA  | 1.67                     | 0.76              |
| 1:C:102:TYR:CG   | 1:C:103:PRO:HD3   | 2.19                     | 0.76              |
| 1:C:196:ASN:HB3  | 1:C:198:LYS:H     | 1.49                     | 0.76              |
| 3:M:190:ARG:HD2  | 3:M:190:ARG:O     | 1.85                     | 0.76              |
| 2:L:202:ASP:CG   | 2:L:203:GLY:H     | 1.90                     | 0.74              |
| 8:M:605:BPB:H55  | 8:M:605:BPB:HMC   | 1.70                     | 0.74              |
| 4:H:133:LYS:HG3  | 4:H:176:SER:HB2   | 1.69                     | 0.73              |
| 3:M:185:THR:O    | 3:M:189:ILE:HG13  | 1.90                     | 0.72              |
| 2:L:212:GLU:OE1  | 12:L:614:UQ1:HM33 | 1.90                     | 0.72              |
| 1:C:148:LEU:HG   | 1:C:299:GLU:HG3   | 1.72                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:141:LEU:HD12 | 1:C:142:PRO:HD2   | 1.72                     | 0.71              |
| 4:H:45:GLU:HB3   | 4:H:46:PRO:HD2    | 1.72                     | 0.70              |
| 4:H:152:PRO:HA   | 4:H:155:LEU:HD12  | 1.71                     | 0.70              |
| 1:C:220:ARG:NH2  | 14:C:637:HOH:O    | 2.22                     | 0.70              |
| 4:H:55:GLU:HB3   | 4:H:58:GLN:HG3    | 1.73                     | 0.70              |
| 8:M:605:BPB:HBBB | 8:M:605:BPB:HHC   | 1.73                     | 0.70              |
| 4:H:138:ARG:NH1  | 4:H:228:ASP:OD1   | 2.25                     | 0.70              |
| 3:M:5:THR:CG2    | 3:M:222:LEU:HB3   | 2.21                     | 0.69              |
| 3:M:136:ARG:NE   | 3:M:136:ARG:HA    | 2.07                     | 0.69              |
| 7:M:603:BCB:CBD  | 7:M:603:BCB:HAA2  | 2.23                     | 0.68              |
| 7:L:602:BCB:C6   | 7:L:604:BCB:HBB3  | 2.23                     | 0.68              |
| 8:L:606:BPB:HBB  | 3:M:208:TYR:CD2   | 2.28                     | 0.68              |
| 7:M:603:BCB:HBD  | 7:M:603:BCB:HAA2  | 1.75                     | 0.67              |
| 1:C:102:TYR:CD2  | 1:C:103:PRO:HD3   | 2.30                     | 0.67              |
| 7:M:603:BCB:CBB  | 7:M:603:BCB:HMB1  | 2.24                     | 0.67              |
| 7:M:601:BCB:CBB  | 11:M:613:NS1:H223 | 2.25                     | 0.67              |
| 2:L:38:ALA:O     | 2:L:42:ILE:HG13   | 1.95                     | 0.67              |
| 3:M:288:PHE:CD1  | 4:H:12:ILE:HD11   | 2.31                     | 0.66              |
| 2:L:151:LEU:HD21 | 13:H:616:LDA:H111 | 1.78                     | 0.66              |
| 2:L:151:LEU:CD2  | 13:H:616:LDA:H111 | 2.26                     | 0.65              |
| 1:C:149:GLU:OE1  | 1:C:296:ARG:NH1   | 2.27                     | 0.65              |
| 4:H:197:PRO:HG2  | 4:H:200:PHE:CD1   | 2.32                     | 0.65              |
| 1:C:80:TRP:CD1   | 1:C:133:TYR:HB2   | 2.31                     | 0.65              |
| 3:M:70:LEU:HD23  | 3:M:73:MET:CE     | 2.27                     | 0.65              |
| 3:M:160:CYS:SG   | 11:M:613:NS1:H322 | 2.36                     | 0.64              |
| 4:H:125:ASP:HB2  | 4:H:232:LEU:HD21  | 1.78                     | 0.64              |
| 2:L:167:TRP:HE1  | 2:L:173:HIS:CD2   | 2.16                     | 0.63              |
| 2:L:22:PHE:HA    | 2:L:24:PHE:CE1    | 2.33                     | 0.63              |
| 2:L:226:ALA:HA   | 12:L:614:UQ1:HM32 | 1.80                     | 0.62              |
| 4:H:218:PHE:O    | 4:H:221:VAL:HG23  | 1.99                     | 0.62              |
| 4:H:250:THR:HG22 | 4:H:252:GLU:H     | 1.63                     | 0.62              |
| 3:M:70:LEU:HD23  | 3:M:73:MET:HE2    | 1.79                     | 0.62              |
| 1:C:248:HIS:HB3  | 14:C:635:HOH:O    | 2.00                     | 0.62              |
| 8:L:606:BPB:HBBA | 3:M:208:TYR:HB3   | 1.82                     | 0.61              |
| 1:C:278:ASN:OD1  | 1:C:302:GLN:HB3   | 2.00                     | 0.61              |
| 2:L:226:ALA:O    | 2:L:229:ILE:HG22  | 2.01                     | 0.61              |
| 1:C:56:TYR:HB3   | 10:C:609:HEM:O2A  | 2.01                     | 0.61              |
| 2:L:22:PHE:HA    | 2:L:24:PHE:HE1    | 1.66                     | 0.61              |
| 7:L:602:BCB:CBB  | 7:L:602:BCB:HMB1  | 2.31                     | 0.61              |
| 2:L:124:PRO:HB2  | 7:L:602:BCB:H93   | 1.83                     | 0.61              |
| 1:C:173:VAL:HB   | 3:M:87:GLN:OE1    | 2.01                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:C:611:HEM:HHA | 10:C:611:HEM:HBA1 | 1.83                     | 0.60              |
| 2:L:213:ASN:O    | 2:L:217:ARG:HG3   | 2.02                     | 0.60              |
| 3:M:205:GLY:HA3  | 13:M:615:LDA:H121 | 1.84                     | 0.60              |
| 1:C:247:CYS:HB2  | 10:C:611:HEM:C2C  | 2.36                     | 0.60              |
| 1:C:5:PRO:CB     | 1:C:6:PRO:HA      | 2.32                     | 0.60              |
| 7:M:601:BCB:OBB  | 7:M:601:BCB:HMB1  | 2.01                     | 0.60              |
| 1:C:309:HIS:HE1  | 10:C:612:HEM:NA   | 1.99                     | 0.60              |
| 1:C:102:TYR:CD1  | 1:C:103:PRO:HD3   | 2.37                     | 0.60              |
| 2:L:178:SER:O    | 2:L:182:VAL:HG22  | 2.02                     | 0.60              |
| 8:M:605:BPB:HMC  | 8:M:605:BPB:CBC   | 2.32                     | 0.59              |
| 3:M:120:MET:CE   | 7:M:603:BCB:H193  | 2.32                     | 0.59              |
| 7:M:601:BCB:HBB1 | 11:M:613:NS1:H223 | 1.83                     | 0.59              |
| 1:C:15:ARG:HG2   | 14:L:629:HOH:O    | 2.03                     | 0.59              |
| 1:C:108:ARG:NH1  | 10:C:609:HEM:O2D  | 2.35                     | 0.59              |
| 2:L:154:LEU:HD23 | 2:L:154:LEU:N     | 2.18                     | 0.59              |
| 7:L:602:BCB:NA   | 7:M:603:BCB:HBB2  | 2.18                     | 0.59              |
| 2:L:139:LEU:HD21 | 2:L:253:PRO:CD    | 2.32                     | 0.58              |
| 4:H:4:GLY:HA2    | 4:H:12:ILE:HD11   | 1.84                     | 0.58              |
| 1:C:244:CYS:HA   | 10:C:611:HEM:HHC  | 1.86                     | 0.57              |
| 4:H:86:ARG:NH2   | 4:H:111:ALA:O     | 2.38                     | 0.57              |
| 7:L:604:BCB:CBB  | 7:L:604:BCB:HHC   | 2.30                     | 0.57              |
| 3:M:227:PHE:HB2  | 3:M:242:ALA:HB2   | 1.87                     | 0.57              |
| 3:M:258:ALA:HA   | 4:H:36:ASP:HB3    | 1.85                     | 0.57              |
| 3:M:107:LEU:HA   | 3:M:111:GLY:HA3   | 1.87                     | 0.57              |
| 3:M:107:LEU:HD22 | 3:M:112:TRP:CE2   | 2.40                     | 0.57              |
| 2:L:216:PHE:CE2  | 12:L:614:UQ1:HM53 | 2.40                     | 0.56              |
| 7:L:604:BCB:HMB2 | 8:L:606:BPB:CMB   | 2.33                     | 0.56              |
| 1:C:283:ALA:HB3  | 1:C:284:PRO:HD3   | 1.86                     | 0.56              |
| 2:L:4:SER:HB3    | 4:H:40:GLY:HA2    | 1.85                     | 0.56              |
| 3:M:93:LEU:HD21  | 3:M:113:TRP:HA    | 1.88                     | 0.56              |
| 1:C:256:TRP:CH2  | 1:C:264:ARG:HG2   | 2.40                     | 0.56              |
| 3:M:226:ARG:HG3  | 14:M:646:HOH:O    | 2.06                     | 0.56              |
| 4:H:38:ARG:NH1   | 4:H:66:LYS:HB2    | 2.21                     | 0.56              |
| 7:L:602:BCB:HBB3 | 7:L:602:BCB:HMB1  | 1.88                     | 0.56              |
| 2:L:181:PHE:CD2  | 8:M:605:BPB:HBB   | 2.41                     | 0.55              |
| 3:M:240:GLY:O    | 3:M:244:GLU:HG3   | 2.07                     | 0.55              |
| 4:H:137:LEU:HB2  | 4:H:170:ASP:OD2   | 2.06                     | 0.55              |
| 2:L:202:ASP:CG   | 2:L:203:GLY:N     | 2.59                     | 0.55              |
| 2:L:179:PHE:HA   | 2:L:182:VAL:HG23  | 1.89                     | 0.55              |
| 2:L:193:LEU:HD22 | 2:L:216:PHE:HE2   | 1.72                     | 0.55              |
| 1:C:301:PRO:HG2  | 10:C:610:HEM:HBD1 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:202:ARG:HG2  | 10:C:611:HEM:O2A  | 2.07                     | 0.55              |
| 3:M:162:HIS:O    | 3:M:166:VAL:HG22  | 2.07                     | 0.55              |
| 1:C:244:CYS:HA   | 10:C:611:HEM:CHC  | 2.37                     | 0.55              |
| 1:C:148:LEU:HD12 | 1:C:299:GLU:HB3   | 1.88                     | 0.55              |
| 1:C:144:TYR:CD1  | 1:C:310:GLN:HG2   | 2.42                     | 0.54              |
| 1:C:150:PRO:O    | 1:C:175:ARG:HD2   | 2.07                     | 0.54              |
| 3:M:200:HIS:CE1  | 3:M:204:ILE:HD11  | 2.41                     | 0.54              |
| 2:L:244:GLY:O    | 7:L:602:BCB:HED3  | 2.07                     | 0.54              |
| 3:M:195:TYR:CZ   | 7:M:603:BCB:HMC2  | 2.42                     | 0.54              |
| 2:L:170:ASN:HB2  | 2:L:259:TRP:CD1   | 2.43                     | 0.53              |
| 7:L:602:BCB:C5   | 7:L:604:BCB:HBB3  | 2.38                     | 0.53              |
| 2:L:181:PHE:CB   | 8:M:605:BPB:HBBA  | 2.38                     | 0.53              |
| 4:H:155:LEU:HB3  | 4:H:156:PRO:HD2   | 1.90                     | 0.53              |
| 4:H:82:ARG:HH11  | 4:H:82:ARG:CG     | 2.20                     | 0.53              |
| 2:L:124:PRO:HB2  | 7:L:602:BCB:C9    | 2.39                     | 0.53              |
| 4:H:70:LEU:HB3   | 4:H:71:PRO:HD2    | 1.91                     | 0.53              |
| 2:L:193:LEU:HD22 | 2:L:216:PHE:CE2   | 2.43                     | 0.53              |
| 3:M:318:LEU:HB3  | 3:M:319:PRO:CD    | 2.34                     | 0.52              |
| 1:C:37:GLN:O     | 1:C:39:PRO:HD3    | 2.08                     | 0.52              |
| 4:H:6:LEU:HD12   | 4:H:15:LEU:HD11   | 1.91                     | 0.52              |
| 2:L:153:HIS:O    | 2:L:157:VAL:HG23  | 2.10                     | 0.52              |
| 3:M:69:ILE:O     | 3:M:73:MET:HG3    | 2.09                     | 0.52              |
| 3:M:29:VAL:HG23  | 3:M:51:LEU:HD13   | 1.90                     | 0.52              |
| 3:M:195:TYR:CE2  | 7:M:603:BCB:HMC2  | 2.44                     | 0.52              |
| 1:C:52:VAL:HA    | 1:C:55:VAL:HB     | 1.92                     | 0.52              |
| 2:L:16:LEU:HB2   | 2:L:106:GLU:HG2   | 1.91                     | 0.52              |
| 2:L:1:ALA:H2     | 4:H:43:LEU:HB3    | 1.74                     | 0.52              |
| 2:L:127:MET:O    | 2:L:127:MET:HG3   | 2.10                     | 0.52              |
| 2:L:138:LEU:HD12 | 2:L:249:ILE:CD1   | 2.40                     | 0.52              |
| 4:H:192:ARG:NH1  | 4:H:221:VAL:O     | 2.43                     | 0.51              |
| 1:C:80:TRP:O     | 1:C:138:GLY:HA2   | 2.10                     | 0.51              |
| 2:L:168:HIS:CE1  | 7:L:602:BCB:HMC2  | 2.45                     | 0.51              |
| 2:L:150:ILE:HG13 | 14:L:633:HOH:O    | 2.10                     | 0.51              |
| 12:L:614:UQ1:C8  | 12:L:614:UQ1:HM51 | 2.39                     | 0.51              |
| 1:C:22:VAL:HG12  | 2:L:256:THR:HB    | 1.92                     | 0.51              |
| 1:C:290:PRO:HG2  | 1:C:293:ARG:HG2   | 1.92                     | 0.51              |
| 1:C:96:LEU:O     | 10:C:609:HEM:HBA1 | 2.11                     | 0.51              |
| 2:L:217:ARG:NH1  | 14:L:647:HOH:O    | 2.43                     | 0.51              |
| 4:H:90:LEU:HD23  | 4:H:102:GLN:C     | 2.32                     | 0.50              |
| 4:H:161:ASP:OD2  | 4:H:161:ASP:N     | 2.33                     | 0.50              |
| 2:L:21:LEU:HD23  | 2:L:22:PHE:CE2    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:M:155:VAL:CG2   | 7:M:603:BCB:H62  | 2.42                     | 0.50              |
| 3:M:212:LEU:C     | 3:M:212:LEU:HD23 | 2.32                     | 0.50              |
| 1:C:309:HIS:HE1   | 10:C:612:HEM:C1A | 2.29                     | 0.50              |
| 1:C:238:ASP:OD1   | 1:C:306:ARG:NH2  | 2.45                     | 0.50              |
| 2:L:167:TRP:NE1   | 2:L:173:HIS:CD2  | 2.79                     | 0.50              |
| 2:L:60:ASP:O      | 2:L:64:ILE:HG13  | 2.10                     | 0.50              |
| 3:M:155:VAL:HG21  | 7:M:603:BCB:H8   | 1.94                     | 0.49              |
| 1:C:277:LEU:O     | 1:C:281:TYR:HB2  | 2.12                     | 0.49              |
| 4:H:196:ILE:HD12  | 4:H:242:TYR:CE1  | 2.48                     | 0.49              |
| 3:M:70:LEU:CD2    | 3:M:73:MET:HE3   | 2.42                     | 0.49              |
| 4:H:152:PRO:CA    | 4:H:155:LEU:HD12 | 2.41                     | 0.49              |
| 1:C:273:MET:O     | 1:C:277:LEU:HG   | 2.12                     | 0.49              |
| 3:M:224:VAL:O     | 3:M:225:ALA:C    | 2.50                     | 0.49              |
| 1:C:15:ARG:NH2    | 14:C:667:HOH:O   | 2.45                     | 0.48              |
| 3:M:318:LEU:CB    | 3:M:319:PRO:HD2  | 2.35                     | 0.48              |
| 3:M:51:LEU:HD12   | 3:M:51:LEU:N     | 2.28                     | 0.48              |
| 3:M:162:HIS:HD2   | 14:M:626:HOH:O   | 1.96                     | 0.48              |
| 1:C:18:SER:HB2    | 2:L:156:TRP:CD1  | 2.48                     | 0.48              |
| 12:L:614:UQ1:HM22 | 12:L:614:UQ1:O1  | 2.14                     | 0.48              |
| 3:M:192:GLY:O     | 3:M:193:ASN:HB3  | 2.13                     | 0.48              |
| 3:M:160:CYS:C     | 3:M:163:PRO:HD2  | 2.33                     | 0.48              |
| 3:M:2:ASP:OD2     | 3:M:4:GLN:HB2    | 2.14                     | 0.48              |
| 7:L:604:BCB:H192  | 7:L:604:BCB:H161 | 1.63                     | 0.48              |
| 3:M:120:MET:CE    | 7:M:603:BCB:H172 | 2.28                     | 0.48              |
| 1:C:189:PRO:CB    | 1:C:232:LEU:HA   | 2.43                     | 0.47              |
| 4:H:133:LYS:HG3   | 4:H:176:SER:CB   | 2.40                     | 0.47              |
| 3:M:5:THR:HG21    | 3:M:222:LEU:HB3  | 1.93                     | 0.47              |
| 3:M:266:TRP:CH2   | 4:H:28:VAL:CG2   | 2.97                     | 0.47              |
| 8:M:605:BPB:CBB   | 8:M:605:BPB:HHC  | 2.42                     | 0.47              |
| 4:H:125:ASP:HB2   | 4:H:232:LEU:CD2  | 2.42                     | 0.47              |
| 1:C:189:PRO:O     | 1:C:193:PHE:HB2  | 2.15                     | 0.47              |
| 4:H:120:ARG:HB2   | 4:H:233:ARG:HA   | 1.97                     | 0.47              |
| 4:H:70:LEU:HD11   | 4:H:76:VAL:HG23  | 1.96                     | 0.47              |
| 3:M:234:GLU:HB2   | 14:H:632:HOH:O   | 2.14                     | 0.47              |
| 4:H:226:SER:HB3   | 4:H:229:GLN:HG2  | 1.95                     | 0.47              |
| 3:M:10:ILE:O      | 4:H:180:PHE:HD2  | 1.98                     | 0.47              |
| 2:L:153:HIS:CE1   | 2:L:154:LEU:HD21 | 2.50                     | 0.47              |
| 2:L:75:LEU:HA     | 2:L:75:LEU:HD23  | 1.70                     | 0.47              |
| 2:L:249:ILE:O     | 2:L:253:PRO:HG2  | 2.15                     | 0.47              |
| 4:H:138:ARG:NH1   | 4:H:227:ARG:NE   | 2.62                     | 0.47              |
| 4:H:142:ASP:OD2   | 4:H:142:ASP:N    | 2.40                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:L:135:ARG:NH2  | 2:L:251:SER:O     | 2.41                     | 0.46              |
| 7:L:602:BCB:C3   | 7:L:604:BCB:HBB3  | 2.46                     | 0.46              |
| 3:M:129:ILE:O    | 3:M:133:SER:HB3   | 2.15                     | 0.46              |
| 1:C:181:ALA:O    | 1:C:182:TYR:HB2   | 2.15                     | 0.46              |
| 1:C:240:LEU:HD23 | 1:C:240:LEU:N     | 2.30                     | 0.46              |
| 1:C:262:PRO:O    | 1:C:266:ILE:HG12  | 2.14                     | 0.46              |
| 3:M:5:THR:HG22   | 3:M:222:LEU:HB3   | 1.96                     | 0.46              |
| 4:H:45:GLU:HB3   | 4:H:46:PRO:CD     | 2.41                     | 0.46              |
| 2:L:216:PHE:CD2  | 12:L:614:UQ1:H71  | 2.51                     | 0.46              |
| 1:C:52:VAL:HB    | 1:C:56:TYR:HD2    | 1.80                     | 0.46              |
| 3:M:121:THR:HG23 | 3:M:156:LEU:HD21  | 1.98                     | 0.46              |
| 4:H:161:ASP:OD1  | 4:H:215:SER:OG    | 2.33                     | 0.46              |
| 2:L:205:LYS:HA   | 4:H:69:VAL:HG22   | 1.96                     | 0.46              |
| 4:H:172:TRP:N    | 4:H:172:TRP:CD1   | 2.84                     | 0.46              |
| 1:C:246:PHE:CE2  | 1:C:263:GLN:HG2   | 2.51                     | 0.46              |
| 1:C:276:ASP:O    | 1:C:280:ASN:HB2   | 2.16                     | 0.45              |
| 2:L:216:PHE:CE2  | 12:L:614:UQ1:CM5  | 2.98                     | 0.45              |
| 1:C:38:TYR:CD2   | 1:C:316:LEU:HD13  | 2.51                     | 0.45              |
| 2:L:245:ALA:O    | 2:L:249:ILE:HB    | 2.15                     | 0.45              |
| 3:M:87:GLN:O     | 3:M:88:PHE:C      | 2.55                     | 0.45              |
| 1:C:151:THR:O    | 1:C:152:LEU:HB2   | 2.17                     | 0.45              |
| 1:C:242:THR:HA   | 14:C:675:HOH:O    | 2.17                     | 0.45              |
| 1:C:309:HIS:O    | 1:C:310:GLN:C     | 2.54                     | 0.45              |
| 4:H:33:ARG:HD2   | 4:H:33:ARG:HA     | 1.90                     | 0.45              |
| 2:L:110:LYS:HB2  | 2:L:110:LYS:HE2   | 1.73                     | 0.45              |
| 2:L:193:LEU:HD12 | 2:L:193:LEU:HA    | 1.58                     | 0.45              |
| 3:M:224:VAL:HG23 | 3:M:229:GLY:HA3   | 1.99                     | 0.45              |
| 4:H:197:PRO:HG2  | 4:H:200:PHE:HD1   | 1.76                     | 0.45              |
| 2:L:228:SER:HB3  | 3:M:41:ILE:O      | 2.17                     | 0.45              |
| 8:M:605:BPB:CMC  | 8:M:605:BPB:H55   | 2.44                     | 0.45              |
| 1:C:137:ARG:HG3  | 1:C:310:GLN:HE22  | 1.82                     | 0.45              |
| 8:L:606:BPB:CBB  | 3:M:208:TYR:CD2   | 2.98                     | 0.45              |
| 2:L:240:ILE:HG22 | 2:L:241:PHE:CD1   | 2.52                     | 0.44              |
| 3:M:155:VAL:HG22 | 7:M:603:BCB:H62   | 1.98                     | 0.44              |
| 3:M:70:LEU:CD2   | 3:M:73:MET:CE     | 2.94                     | 0.44              |
| 3:M:146:TRP:HA   | 3:M:146:TRP:CE3   | 2.52                     | 0.44              |
| 8:M:605:BPB:H6A  | 8:M:605:BPB:H4    | 1.86                     | 0.44              |
| 1:C:56:TYR:HB3   | 10:C:609:HEM:CGA  | 2.48                     | 0.44              |
| 2:L:226:ALA:N    | 12:L:614:UQ1:HM21 | 2.32                     | 0.44              |
| 3:M:38:LEU:CD2   | 3:M:46:ILE:HD11   | 2.47                     | 0.44              |
| 2:L:121:PHE:O    | 2:L:124:PRO:HD2   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:132:GLN:OE1  | 2:L:145:ALA:HB1  | 2.18                     | 0.44              |
| 7:M:601:BCB:HBB2 | 7:M:601:BCB:HHC  | 1.98                     | 0.44              |
| 4:H:197:PRO:HG2  | 4:H:200:PHE:CE1  | 2.52                     | 0.44              |
| 1:C:88:THR:O     | 1:C:88:THR:HG22  | 2.17                     | 0.44              |
| 1:C:258:LYS:HD3  | 3:M:305:TYR:O    | 2.17                     | 0.44              |
| 2:L:217:ARG:O    | 2:L:221:GLY:HA2  | 2.17                     | 0.44              |
| 1:C:106:VAL:HG11 | 10:C:610:HEM:CAA | 2.48                     | 0.44              |
| 1:C:297:GLN:HB2  | 1:C:297:GLN:HE21 | 1.46                     | 0.44              |
| 1:C:50:PRO:HG2   | 1:C:55:VAL:CG2   | 2.47                     | 0.44              |
| 2:L:136:PRO:HB3  | 2:L:141:SER:O    | 2.18                     | 0.44              |
| 1:C:118:ASN:OD1  | 1:C:129:GLY:HA2  | 2.17                     | 0.43              |
| 1:C:299:GLU:N    | 1:C:299:GLU:OE2  | 2.41                     | 0.43              |
| 1:C:82:SER:HB2   | 1:C:85:GLU:HB2   | 2.00                     | 0.43              |
| 2:L:135:ARG:HD3  | 2:L:135:ARG:HH11 | 1.69                     | 0.43              |
| 3:M:173:VAL:HG12 | 3:M:174:PRO:O    | 2.18                     | 0.43              |
| 1:C:228:ALA:O    | 1:C:231:ALA:HB3  | 2.18                     | 0.43              |
| 4:H:16:VAL:O     | 4:H:16:VAL:HG12  | 2.19                     | 0.43              |
| 2:L:239:ASN:HD22 | 2:L:239:ASN:HA   | 1.67                     | 0.43              |
| 3:M:178:TRP:N    | 3:M:179:PRO:CD   | 2.81                     | 0.43              |
| 7:M:601:BCB:HBB2 | 11:M:613:NS1:C22 | 2.48                     | 0.43              |
| 4:H:230:ILE:HD13 | 4:H:235:GLU:HG2  | 2.00                     | 0.43              |
| 2:L:37:SER:O     | 2:L:38:ALA:C     | 2.57                     | 0.43              |
| 3:M:69:ILE:HD13  | 3:M:175:PHE:CD1  | 2.54                     | 0.43              |
| 1:C:186:ASN:C    | 1:C:187:TYR:CD1  | 2.91                     | 0.43              |
| 4:H:12:ILE:H     | 4:H:12:ILE:HG12  | 1.48                     | 0.43              |
| 7:M:601:BCB:C4A  | 7:M:601:BCB:CBA  | 2.97                     | 0.43              |
| 7:L:602:BCB:C4A  | 7:M:603:BCB:HBB2 | 2.49                     | 0.43              |
| 1:C:186:ASN:ND2  | 14:C:649:HOH:O   | 2.51                     | 0.43              |
| 2:L:83:GLY:O     | 2:L:87:GLN:HG3   | 2.19                     | 0.43              |
| 1:C:312:VAL:HG12 | 1:C:314:LYS:O    | 2.19                     | 0.43              |
| 8:M:605:BPB:H11A | 8:M:605:BPB:H9   | 1.78                     | 0.43              |
| 1:C:210:PRO:HB2  | 4:H:3:HIS:HD2    | 1.84                     | 0.42              |
| 2:L:100:TRP:O    | 2:L:103:ARG:HB3  | 2.19                     | 0.42              |
| 2:L:67:ASN:HB3   | 2:L:68:PRO:HD2   | 2.00                     | 0.42              |
| 3:M:12:ALA:HB2   | 4:H:180:PHE:CE2  | 2.54                     | 0.42              |
| 3:M:67:LEU:O     | 3:M:68:ILE:C     | 2.53                     | 0.42              |
| 1:C:217:GLY:O    | 1:C:220:ARG:HB2  | 2.19                     | 0.42              |
| 1:C:283:ALA:N    | 1:C:284:PRO:HD2  | 2.34                     | 0.42              |
| 2:L:52:ALA:HB3   | 2:L:66:ILE:CD1   | 2.49                     | 0.42              |
| 1:C:71:LEU:HD23  | 1:C:71:LEU:HA    | 1.96                     | 0.42              |
| 4:H:1:FME:HB3    | 4:H:1:FME:HE2    | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:115:TRP:CD1  | 2:L:115:TRP:N    | 2.88                     | 0.42              |
| 7:M:601:BCB:HBA1 | 7:M:601:BCB:C4A  | 2.50                     | 0.42              |
| 1:C:102:TYR:O    | 1:C:103:PRO:C    | 2.58                     | 0.42              |
| 3:M:259:THR:HG23 | 4:H:36:ASP:O     | 2.20                     | 0.42              |
| 4:H:29:LEU:HD23  | 4:H:29:LEU:HA    | 1.82                     | 0.42              |
| 3:M:125:GLY:O    | 3:M:129:ILE:HG13 | 2.19                     | 0.42              |
| 2:L:229:ILE:O    | 2:L:229:ILE:HG13 | 2.20                     | 0.42              |
| 3:M:289:VAL:HG21 | 3:M:292:TRP:CH2  | 2.55                     | 0.42              |
| 1:C:79:GLU:O     | 1:C:83:PRO:HG3   | 2.19                     | 0.41              |
| 3:M:293:TYR:O    | 3:M:297:VAL:HG23 | 2.19                     | 0.41              |
| 2:L:156:TRP:O    | 2:L:157:VAL:C    | 2.57                     | 0.41              |
| 2:L:146:PHE:HB3  | 2:L:156:TRP:CD2  | 2.55                     | 0.41              |
| 2:L:201:GLY:O    | 2:L:202:ASP:HB3  | 2.20                     | 0.41              |
| 1:C:190:PHE:HE1  | 1:C:303:ALA:O    | 2.03                     | 0.41              |
| 4:H:4:GLY:HA2    | 4:H:12:ILE:CD1   | 2.49                     | 0.41              |
| 2:L:139:LEU:HA   | 2:L:139:LEU:HD23 | 1.81                     | 0.41              |
| 2:L:229:ILE:HD13 | 12:L:614:UQ1:H8  | 2.02                     | 0.41              |
| 3:M:282:ILE:HD13 | 3:M:282:ILE:HA   | 1.88                     | 0.41              |
| 7:L:602:BCB:H193 | 9:M:608:MQ7:H292 | 2.02                     | 0.41              |
| 3:M:62:GLY:O     | 3:M:65:ALA:HB3   | 2.21                     | 0.41              |
| 4:H:117:TYR:HB2  | 4:H:236:ASP:HB3  | 2.02                     | 0.41              |
| 2:L:177:VAL:HG13 | 7:L:602:BCB:HMB3 | 2.02                     | 0.41              |
| 3:M:95:PRO:HG2   | 14:M:629:HOH:O   | 2.20                     | 0.41              |
| 1:C:236:ILE:O    | 1:C:240:LEU:HG   | 2.20                     | 0.41              |
| 4:H:257:LEU:HA   | 4:H:257:LEU:HD23 | 1.72                     | 0.41              |
| 7:L:604:BCB:H13  | 7:L:604:BCB:H172 | 1.82                     | 0.41              |
| 1:C:102:TYR:CG   | 1:C:103:PRO:CD   | 2.96                     | 0.41              |
| 3:M:231:ARG:HH22 | 4:H:235:GLU:CD   | 2.24                     | 0.41              |
| 2:L:222:TYR:HD1  | 3:M:45:GLN:O     | 2.03                     | 0.41              |
| 2:L:97:PHE:CZ    | 7:L:602:BCB:H112 | 2.55                     | 0.41              |
| 2:L:169:TYR:OH   | 3:M:182:ASP:OD2  | 2.31                     | 0.41              |
| 2:L:87:GLN:NE2   | 2:L:142:TRP:CD1  | 2.89                     | 0.41              |
| 2:L:52:ALA:HB3   | 2:L:66:ILE:HD11  | 2.03                     | 0.41              |
| 2:L:67:ASN:OD1   | 2:L:67:ASN:N     | 2.53                     | 0.41              |
| 3:M:258:ALA:HB1  | 3:M:262:SER:OG   | 2.21                     | 0.40              |
| 1:C:113:MET:HB2  | 1:C:281:TYR:CD1  | 2.56                     | 0.40              |
| 4:H:138:ARG:HG3  | 4:H:170:ASP:OD1  | 2.21                     | 0.40              |
| 3:M:16:HIS:HD2   | 3:M:32:PRO:HG3   | 1.85                     | 0.40              |
| 3:M:312:THR:HA   | 3:M:313:PRO:HD2  | 1.90                     | 0.40              |
| 1:C:102:TYR:CE2  | 1:C:103:PRO:HD3  | 2.57                     | 0.40              |
| 1:C:144:TYR:O    | 1:C:307:THR:HG23 | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:109:ARG:HD2  | 2:L:109:ARG:HH11 | 1.77                     | 0.40              |
| 2:L:241:PHE:CE2  | 8:L:606:BPB:H43  | 2.56                     | 0.40              |
| 1:C:149:GLU:HB3  | 1:C:150:PRO:HD2  | 2.03                     | 0.40              |
| 2:L:197:VAL:HG21 | 2:L:212:GLU:HG2  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | C     | 331/336 (98%)   | 306 (92%)  | 24 (7%) | 1 (0%)   | 44          | 55 |
| 2   | L     | 271/273 (99%)   | 252 (93%)  | 18 (7%) | 1 (0%)   | 38          | 47 |
| 3   | M     | 321/323 (99%)   | 300 (94%)  | 19 (6%) | 2 (1%)   | 28          | 34 |
| 4   | H     | 256/258 (99%)   | 239 (93%)  | 16 (6%) | 1 (0%)   | 38          | 47 |
| All | All   | 1179/1190 (99%) | 1097 (93%) | 77 (6%) | 5 (0%)   | 38          | 47 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | M     | 22  | GLU  |
| 4   | H     | 53  | ALA  |
| 3   | M     | 88  | PHE  |
| 1   | C     | 250 | ALA  |
| 2   | L     | 31  | VAL  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | C     | 281/282 (100%) | 261 (93%) | 20 (7%)  | 17          | 22 |
| 2   | L     | 218/218 (100%) | 210 (96%) | 8 (4%)   | 39          | 53 |
| 3   | M     | 249/249 (100%) | 235 (94%) | 14 (6%)  | 25          | 33 |
| 4   | H     | 212/212 (100%) | 197 (93%) | 15 (7%)  | 17          | 22 |
| All | All   | 960/961 (100%) | 903 (94%) | 57 (6%)  | 23          | 30 |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 1   | CYS  |
| 1   | C     | 15  | ARG  |
| 1   | C     | 34  | ARG  |
| 1   | C     | 38  | TYR  |
| 1   | C     | 53  | SER  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 94  | ASN  |
| 1   | C     | 115 | ARG  |
| 1   | C     | 149 | GLU  |
| 1   | C     | 151 | THR  |
| 1   | C     | 158 | GLU  |
| 1   | C     | 186 | ASN  |
| 1   | C     | 209 | LEU  |
| 1   | C     | 235 | SER  |
| 1   | C     | 240 | LEU  |
| 1   | C     | 258 | LYS  |
| 1   | C     | 288 | SER  |
| 1   | C     | 294 | LEU  |
| 1   | C     | 320 | SER  |
| 1   | C     | 327 | GLU  |
| 2   | L     | 4   | SER  |
| 2   | L     | 15  | THR  |
| 2   | L     | 119 | LEU  |
| 2   | L     | 141 | SER  |
| 2   | L     | 182 | VAL  |
| 2   | L     | 228 | SER  |
| 2   | L     | 249 | ILE  |
| 2   | L     | 272 | TRP  |
| 3   | M     | 16  | HIS  |
| 3   | M     | 33  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | M     | 70  | LEU  |
| 3   | M     | 77  | VAL  |
| 3   | M     | 126 | SER  |
| 3   | M     | 133 | SER  |
| 3   | M     | 136 | ARG  |
| 3   | M     | 147 | ASN  |
| 3   | M     | 171 | GLU  |
| 3   | M     | 181 | ILE  |
| 3   | M     | 194 | PHE  |
| 3   | M     | 214 | PHE  |
| 3   | M     | 249 | PHE  |
| 3   | M     | 279 | SER  |
| 4   | H     | 12  | ILE  |
| 4   | H     | 28  | VAL  |
| 4   | H     | 56  | ASP  |
| 4   | H     | 82  | ARG  |
| 4   | H     | 96  | PHE  |
| 4   | H     | 142 | ASP  |
| 4   | H     | 161 | ASP  |
| 4   | H     | 169 | THR  |
| 4   | H     | 178 | HIS  |
| 4   | H     | 182 | TYR  |
| 4   | H     | 198 | LEU  |
| 4   | H     | 212 | SER  |
| 4   | H     | 217 | GLN  |
| 4   | H     | 236 | ASP  |
| 4   | H     | 258 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 196 | ASN  |
| 1   | C     | 297 | GLN  |
| 1   | C     | 302 | GLN  |
| 1   | C     | 310 | GLN  |
| 2   | L     | 144 | HIS  |
| 2   | L     | 183 | ASN  |
| 2   | L     | 214 | GLN  |
| 2   | L     | 239 | ASN  |
| 4   | H     | 3   | HIS  |
| 4   | H     | 225 | GLN  |
| 4   | H     | 229 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | FME  | H     | 1   | 4    | 9,9,10       | 1.08 | 1 (11%)     | 7,9,11      | 2.67 | 3 (42%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 4   | FME  | H     | 1   | 4    | -       | 1/6/9/11 | 0/0/0/0 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | H     | 1   | FME  | CA-N  | -2.29 | 1.43        | 1.46     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | H     | 1   | FME  | CA-N-CN | -4.40 | 116.05      | 122.82   |
| 4   | H     | 1   | FME  | O1-CN-N | -3.76 | 114.72      | 125.20   |
| 4   | H     | 1   | FME  | CB-CA-C | 3.57  | 117.53      | 111.65   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 4   | H     | 1   | FME  | O1-CN-N-CA |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | H     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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  | C     | 609 | 1    | 28,50,50     | 1.41 | 4 (14%)     | 17,82,82    | 1.80 | 5 (29%)     |
| 10  | HEM  | C     | 610 | 1    | 28,50,50     | 1.42 | 3 (10%)     | 17,82,82    | 1.53 | 2 (11%)     |
| 10  | HEM  | C     | 611 | 1    | 28,50,50     | 1.54 | 6 (21%)     | 17,82,82    | 1.84 | 4 (23%)     |
| 10  | HEM  | C     | 612 | 1    | 28,50,50     | 1.71 | 6 (21%)     | 17,82,82    | 2.25 | 5 (29%)     |
| 13  | LDA  | H     | 616 | -    | 13,15,15     | 2.88 | 2 (15%)     | 14,17,17    | 0.93 | 1 (7%)      |
| 6   | SO4  | H     | 617 | -    | 4,4,4        | 1.05 | 0           | 6,6,6       | 0.21 | 0           |
| 6   | SO4  | H     | 622 | -    | 4,4,4        | 1.06 | 0           | 6,6,6       | 0.29 | 0           |
| 6   | SO4  | H     | 623 | -    | 4,4,4        | 1.00 | 0           | 6,6,6       | 0.43 | 0           |
| 7   | BCB  | L     | 602 | 2    | 63,74,74     | 4.44 | 24 (38%)    | 50,115,115  | 2.63 | 22 (44%)    |
| 7   | BCB  | L     | 604 | 2    | 63,74,74     | 4.26 | 25 (39%)    | 50,115,115  | 2.50 | 19 (38%)    |
| 8   | BPB  | L     | 606 | -    | 63,70,70     | 1.41 | 7 (11%)     | 67,101,101  | 1.72 | 20 (29%)    |
| 12  | UQ1  | L     | 614 | -    | 18,18,18     | 0.78 | 1 (5%)      | 22,25,25    | 1.17 | 3 (13%)     |
| 7   | BCB  | M     | 601 | 3    | 63,74,74     | 3.95 | 26 (41%)    | 50,115,115  | 2.65 | 20 (40%)    |
| 7   | BCB  | M     | 603 | 3    | 63,74,74     | 4.61 | 32 (50%)    | 50,115,115  | 2.63 | 20 (40%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | BPB  | M     | 605 | -    | 63,70,70     | 1.35 | 8 (12%)  | 67,101,101  | 1.42 | 9 (13%)  |
| 9   | MQ7  | M     | 608 | -    | 49,49,49     | 1.36 | 5 (10%)  | 61,63,63    | 2.32 | 22 (36%) |
| 11  | NS1  | M     | 613 | -    | 39,39,39     | 2.69 | 12 (30%) | 44,46,46    | 2.15 | 16 (36%) |
| 13  | LDA  | M     | 615 | -    | 13,15,15     | 2.94 | 1 (7%)   | 14,17,17    | 2.58 | 6 (42%)  |
| 6   | SO4  | M     | 618 | -    | 4,4,4        | 0.80 | 0        | 6,6,6       | 0.27 | 0        |
| 6   | SO4  | M     | 619 | -    | 4,4,4        | 0.82 | 0        | 6,6,6       | 0.24 | 0        |
| 6   | SO4  | M     | 620 | -    | 4,4,4        | 0.69 | 0        | 6,6,6       | 0.13 | 0        |
| 6   | SO4  | M     | 621 | -    | 4,4,4        | 1.05 | 0        | 6,6,6       | 0.30 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 10  | HEM  | C     | 609 | 1    | -       | 0/6/54/54    | 0/0/8/8 |
| 10  | HEM  | C     | 610 | 1    | -       | 0/6/54/54    | 0/0/8/8 |
| 10  | HEM  | C     | 611 | 1    | -       | 0/6/54/54    | 0/0/8/8 |
| 10  | HEM  | C     | 612 | 1    | -       | 0/6/54/54    | 0/0/8/8 |
| 13  | LDA  | H     | 616 | -    | -       | 0/13/13/13   | 0/0/0/0 |
| 6   | SO4  | H     | 617 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 6   | SO4  | H     | 622 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 6   | SO4  | H     | 623 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 7   | BCB  | L     | 602 | 2    | -       | 0/41/177/177 | 0/0/9/9 |
| 7   | BCB  | L     | 604 | 2    | -       | 0/41/177/177 | 0/0/9/9 |
| 8   | BPB  | L     | 606 | -    | -       | 0/47/105/105 | 0/1/6/6 |
| 12  | UQ1  | L     | 614 | -    | -       | 0/9/33/33    | 0/1/1/1 |
| 7   | BCB  | M     | 601 | 3    | -       | 0/41/177/177 | 0/0/9/9 |
| 7   | BCB  | M     | 603 | 3    | -       | 0/41/177/177 | 0/0/9/9 |
| 8   | BPB  | M     | 605 | -    | -       | 0/47/105/105 | 0/1/6/6 |
| 9   | MQ7  | M     | 608 | -    | -       | 0/41/61/61   | 0/2/2/2 |
| 11  | NS1  | M     | 613 | -    | -       | 0/43/43/43   | 0/0/0/0 |
| 13  | LDA  | M     | 615 | -    | -       | 0/13/13/13   | 0/0/0/0 |
| 6   | SO4  | M     | 618 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 6   | SO4  | M     | 619 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 6   | SO4  | M     | 620 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 6   | SO4  | M     | 621 | -    | -       | 0/0/0/0      | 0/0/0/0 |

All (162) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 7   | L     | 604 | BCB  | C3D-C4D | -14.76 | 1.37        | 1.54     |
| 7   | L     | 602 | BCB  | C3D-C4D | -12.70 | 1.40        | 1.54     |
| 7   | M     | 603 | BCB  | C3D-C4D | -11.86 | 1.41        | 1.54     |
| 7   | M     | 603 | BCB  | C1A-CHA | -11.73 | 1.35        | 1.53     |
| 7   | M     | 601 | BCB  | CHC-C4B | -11.39 | 1.35        | 1.53     |
| 7   | M     | 601 | BCB  | C1A-CHA | -11.38 | 1.35        | 1.53     |
| 7   | M     | 601 | BCB  | C3D-C4D | -11.37 | 1.41        | 1.54     |
| 7   | L     | 604 | BCB  | CHC-C4B | -11.23 | 1.35        | 1.53     |
| 7   | M     | 603 | BCB  | CHB-C1B | -10.46 | 1.36        | 1.53     |
| 7   | L     | 604 | BCB  | CHB-C1B | -10.45 | 1.36        | 1.53     |
| 7   | L     | 602 | BCB  | CHD-C4C | -10.34 | 1.35        | 1.53     |
| 13  | M     | 615 | LDA  | O1-N1   | -10.34 | 1.21        | 1.42     |
| 7   | M     | 603 | BCB  | CHC-C4B | -10.31 | 1.36        | 1.53     |
| 7   | L     | 604 | BCB  | C1A-CHA | -10.30 | 1.37        | 1.53     |
| 7   | L     | 602 | BCB  | C1A-CHA | -10.21 | 1.37        | 1.53     |
| 13  | H     | 616 | LDA  | O1-N1   | -9.84  | 1.22        | 1.42     |
| 7   | L     | 602 | BCB  | CHC-C4B | -9.72  | 1.37        | 1.53     |
| 7   | L     | 602 | BCB  | C3B-C4B | -9.31  | 1.43        | 1.54     |
| 7   | L     | 604 | BCB  | CHD-C4C | -8.81  | 1.37        | 1.53     |
| 7   | M     | 601 | BCB  | CHD-C4C | -8.73  | 1.37        | 1.53     |
| 7   | M     | 603 | BCB  | C3B-CAB | -8.64  | 1.43        | 1.52     |
| 7   | L     | 602 | BCB  | CHB-C1B | -8.58  | 1.39        | 1.53     |
| 7   | M     | 603 | BCB  | CHD-C4C | -8.51  | 1.38        | 1.53     |
| 7   | L     | 602 | BCB  | CHD-C1D | -8.36  | 1.40        | 1.53     |
| 7   | M     | 601 | BCB  | CHB-C1B | -7.86  | 1.40        | 1.53     |
| 7   | L     | 602 | BCB  | C3D-CAD | -7.73  | 1.36        | 1.51     |
| 7   | L     | 602 | BCB  | C4D-ND  | -7.72  | 1.33        | 1.50     |
| 7   | M     | 603 | BCB  | C3B-C2B | -7.68  | 1.34        | 1.55     |
| 7   | M     | 603 | BCB  | CHD-C1D | -7.64  | 1.41        | 1.53     |
| 7   | L     | 602 | BCB  | C2B-C1B | -7.63  | 1.38        | 1.53     |
| 7   | M     | 601 | BCB  | C3B-C2B | -7.29  | 1.35        | 1.55     |
| 7   | M     | 601 | BCB  | C4D-ND  | -7.17  | 1.34        | 1.50     |
| 7   | L     | 604 | BCB  | CHD-C1D | -7.16  | 1.42        | 1.53     |
| 7   | M     | 603 | BCB  | C4B-NB  | -7.01  | 1.35        | 1.50     |
| 7   | M     | 603 | BCB  | C4D-ND  | -6.99  | 1.35        | 1.50     |
| 7   | L     | 604 | BCB  | C4D-ND  | -6.98  | 1.35        | 1.50     |
| 7   | L     | 602 | BCB  | C3B-C2B | -6.95  | 1.36        | 1.55     |
| 7   | M     | 603 | BCB  | C3B-C4B | -6.84  | 1.46        | 1.54     |
| 7   | M     | 603 | BCB  | C2D-C1D | -6.78  | 1.40        | 1.53     |
| 7   | M     | 601 | BCB  | CHD-C1D | -6.75  | 1.42        | 1.53     |
| 7   | M     | 603 | BCB  | C2B-C1B | -6.66  | 1.40        | 1.53     |
| 7   | M     | 603 | BCB  | CHB-C4A | -6.50  | 1.37        | 1.52     |
| 7   | L     | 602 | BCB  | CHB-C4A | -6.40  | 1.37        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | M     | 603 | BCB  | C1B-NB  | -6.31 | 1.36        | 1.50     |
| 7   | L     | 604 | BCB  | C3B-CAB | -6.28 | 1.45        | 1.52     |
| 7   | L     | 604 | BCB  | C2D-C1D | -6.28 | 1.41        | 1.53     |
| 7   | L     | 602 | BCB  | C3D-C2D | -6.16 | 1.38        | 1.55     |
| 7   | L     | 602 | BCB  | C1B-NB  | -6.07 | 1.37        | 1.50     |
| 7   | L     | 604 | BCB  | C4B-NB  | -6.06 | 1.37        | 1.50     |
| 7   | L     | 602 | BCB  | C4B-NB  | -6.05 | 1.37        | 1.50     |
| 7   | L     | 604 | BCB  | C1D-ND  | -6.02 | 1.37        | 1.50     |
| 7   | M     | 601 | BCB  | C4B-NB  | -5.88 | 1.37        | 1.50     |
| 7   | L     | 602 | BCB  | C2D-C1D | -5.70 | 1.42        | 1.53     |
| 7   | L     | 604 | BCB  | CHB-C4A | -5.54 | 1.39        | 1.52     |
| 7   | M     | 601 | BCB  | CHB-C4A | -5.29 | 1.40        | 1.52     |
| 7   | M     | 601 | BCB  | C3D-C2D | -5.21 | 1.41        | 1.55     |
| 7   | L     | 602 | BCB  | C1D-ND  | -5.17 | 1.39        | 1.50     |
| 7   | L     | 604 | BCB  | C3D-C2D | -5.10 | 1.41        | 1.55     |
| 7   | M     | 603 | BCB  | C1D-ND  | -5.06 | 1.39        | 1.50     |
| 7   | M     | 603 | BCB  | C3D-C2D | -5.05 | 1.41        | 1.55     |
| 7   | M     | 603 | BCB  | C3D-CAD | -4.94 | 1.42        | 1.51     |
| 7   | M     | 601 | BCB  | C2D-C1D | -4.86 | 1.43        | 1.53     |
| 7   | M     | 601 | BCB  | CHC-C1C | -4.84 | 1.41        | 1.52     |
| 7   | L     | 604 | BCB  | C3B-C2B | -4.79 | 1.42        | 1.55     |
| 7   | M     | 601 | BCB  | C1D-ND  | -4.68 | 1.40        | 1.50     |
| 7   | M     | 603 | BCB  | CAA-C2A | -4.58 | 1.44        | 1.53     |
| 7   | L     | 604 | BCB  | C2B-C1B | -4.51 | 1.44        | 1.53     |
| 7   | L     | 604 | BCB  | CHC-C1C | -4.47 | 1.42        | 1.52     |
| 7   | L     | 602 | BCB  | C3B-CAB | -4.45 | 1.47        | 1.52     |
| 7   | L     | 604 | BCB  | O1A-CGA | -4.42 | 1.09        | 1.22     |
| 7   | L     | 602 | BCB  | CHC-C1C | -4.39 | 1.42        | 1.52     |
| 10  | C     | 611 | HEM  | CAA-C2A | -4.23 | 1.44        | 1.52     |
| 7   | M     | 603 | BCB  | CHC-C1C | -4.22 | 1.42        | 1.52     |
| 7   | M     | 601 | BCB  | C1B-NB  | -4.21 | 1.41        | 1.50     |
| 7   | M     | 601 | BCB  | C3D-CAD | -4.20 | 1.43        | 1.51     |
| 7   | M     | 601 | BCB  | C1A-C2A | -3.95 | 1.49        | 1.53     |
| 8   | L     | 606 | BPB  | O2D-CED | -3.90 | 1.35        | 1.45     |
| 7   | M     | 601 | BCB  | O1D-CGD | -3.73 | 1.11        | 1.21     |
| 7   | L     | 604 | BCB  | C1B-NB  | -3.66 | 1.42        | 1.50     |
| 10  | C     | 610 | HEM  | CAA-C2A | -3.64 | 1.45        | 1.52     |
| 7   | L     | 602 | BCB  | O2D-CED | -3.63 | 1.36        | 1.45     |
| 11  | M     | 613 | NS1  | C14-C15 | -3.60 | 1.38        | 1.45     |
| 9   | M     | 608 | MQ7  | C10-C1  | -3.58 | 1.41        | 1.48     |
| 7   | M     | 601 | BCB  | C2B-C1B | -3.41 | 1.46        | 1.53     |
| 7   | M     | 603 | BCB  | O1A-CGA | -3.39 | 1.12        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | L     | 604 | BCB  | C3B-C4B | -3.33 | 1.50        | 1.54     |
| 7   | L     | 604 | BCB  | C4A-C3A | -3.31 | 1.49        | 1.53     |
| 7   | M     | 603 | BCB  | C2A-C3A | -3.23 | 1.48        | 1.55     |
| 9   | M     | 608 | MQ7  | C10-C5  | -3.21 | 1.35        | 1.40     |
| 7   | L     | 604 | BCB  | C3D-CAD | -3.15 | 1.45        | 1.51     |
| 10  | C     | 609 | HEM  | C4C-NC  | -3.02 | 1.33        | 1.36     |
| 13  | H     | 616 | LDA  | C1-N1   | -2.73 | 1.45        | 1.51     |
| 9   | M     | 608 | MQ7  | C6-C5   | -2.70 | 1.35        | 1.39     |
| 11  | M     | 613 | NS1  | C2-C1   | -2.58 | 1.33        | 1.51     |
| 9   | M     | 608 | MQ7  | C9-C10  | -2.53 | 1.35        | 1.39     |
| 7   | M     | 601 | BCB  | C3B-C4B | -2.51 | 1.51        | 1.54     |
| 10  | C     | 609 | HEM  | C3B-C2B | -2.42 | 1.37        | 1.40     |
| 7   | M     | 601 | BCB  | CMD-C2D | -2.36 | 1.48        | 1.53     |
| 7   | M     | 603 | BCB  | OBB-CAB | -2.28 | 1.15        | 1.21     |
| 8   | L     | 606 | BPB  | CMA-C3A | -2.28 | 1.48        | 1.53     |
| 7   | M     | 603 | BCB  | O1D-CGD | -2.25 | 1.15        | 1.21     |
| 7   | M     | 603 | BCB  | CAA-CBA | -2.20 | 1.45        | 1.52     |
| 7   | M     | 601 | BCB  | C3B-CAB | -2.16 | 1.49        | 1.52     |
| 10  | C     | 611 | HEM  | C3C-C2C | -2.12 | 1.37        | 1.40     |
| 7   | L     | 602 | BCB  | C2A-C3A | -2.10 | 1.50        | 1.55     |
| 7   | M     | 603 | BCB  | O2D-CGD | -2.08 | 1.27        | 1.33     |
| 8   | M     | 605 | BPB  | C3B-C2B | -2.08 | 1.35        | 1.39     |
| 10  | C     | 611 | HEM  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 7   | L     | 602 | BCB  | CMD-C2D | -2.02 | 1.49        | 1.53     |
| 7   | M     | 601 | BCB  | CBD-CAD | 2.02  | 1.56        | 1.53     |
| 8   | M     | 605 | BPB  | CBC-CAC | 2.03  | 1.57        | 1.49     |
| 9   | M     | 608 | MQ7  | C36-C37 | 2.03  | 1.57        | 1.50     |
| 7   | L     | 602 | BCB  | CBB-CAB | 2.06  | 1.55        | 1.49     |
| 10  | C     | 612 | HEM  | C3D-C2D | 2.07  | 1.43        | 1.37     |
| 7   | L     | 604 | BCB  | C2A-C3A | 2.09  | 1.59        | 1.55     |
| 7   | M     | 603 | BCB  | O2A-C1  | 2.09  | 1.52        | 1.46     |
| 8   | L     | 606 | BPB  | C5-C3   | 2.10  | 1.55        | 1.51     |
| 7   | M     | 603 | BCB  | C5-C3   | 2.14  | 1.56        | 1.51     |
| 12  | L     | 614 | UQ1  | C7-C8   | 2.15  | 1.54        | 1.50     |
| 10  | C     | 612 | HEM  | CAD-C3D | 2.16  | 1.56        | 1.52     |
| 7   | M     | 601 | BCB  | OBD-CAD | 2.17  | 1.25        | 1.21     |
| 8   | M     | 605 | BPB  | O2A-C1  | 2.20  | 1.52        | 1.46     |
| 11  | M     | 613 | NS1  | C22-C21 | 2.26  | 1.55        | 1.50     |
| 7   | M     | 601 | BCB  | CBA-CGA | 2.27  | 1.57        | 1.50     |
| 11  | M     | 613 | NS1  | C19-C18 | 2.29  | 1.41        | 1.35     |
| 10  | C     | 611 | HEM  | C3C-CAC | 2.35  | 1.52        | 1.47     |
| 7   | M     | 603 | BCB  | CBC-CAC | 2.38  | 1.59        | 1.49     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 8   | M     | 605 | BPB  | CHC-C1C | 2.38 | 1.43        | 1.37     |
| 8   | M     | 605 | BPB  | C2-C3   | 2.39 | 1.38        | 1.33     |
| 7   | L     | 604 | BCB  | O2A-C1  | 2.43 | 1.53        | 1.46     |
| 8   | L     | 606 | BPB  | C4C-C3C | 2.45 | 1.51        | 1.45     |
| 7   | M     | 603 | BCB  | OBD-CAD | 2.53 | 1.25        | 1.21     |
| 11  | M     | 613 | NS1  | C29-C28 | 2.54 | 1.41        | 1.34     |
| 8   | M     | 605 | BPB  | C2A-C1A | 2.56 | 1.54        | 1.50     |
| 7   | M     | 601 | BCB  | C5-C3   | 2.60 | 1.57        | 1.51     |
| 8   | L     | 606 | BPB  | CBC-CAC | 2.64 | 1.60        | 1.49     |
| 10  | C     | 611 | HEM  | CBB-CAB | 2.83 | 1.48        | 1.28     |
| 7   | L     | 602 | BCB  | CBD-CAD | 2.98 | 1.57        | 1.53     |
| 10  | C     | 611 | HEM  | CBC-CAC | 3.07 | 1.50        | 1.28     |
| 10  | C     | 609 | HEM  | CBB-CAB | 3.19 | 1.51        | 1.28     |
| 11  | M     | 613 | NS1  | C24-C23 | 3.22 | 1.42        | 1.34     |
| 7   | L     | 604 | BCB  | C5-C3   | 3.22 | 1.58        | 1.51     |
| 8   | L     | 606 | BPB  | CAA-C2A | 3.25 | 1.60        | 1.54     |
| 10  | C     | 612 | HEM  | CBC-CAC | 3.25 | 1.51        | 1.28     |
| 10  | C     | 610 | HEM  | CBC-CAC | 3.42 | 1.53        | 1.28     |
| 10  | C     | 609 | HEM  | CBC-CAC | 3.49 | 1.53        | 1.28     |
| 10  | C     | 610 | HEM  | CBB-CAB | 3.54 | 1.53        | 1.28     |
| 7   | M     | 603 | BCB  | CBD-CGD | 3.67 | 1.58        | 1.52     |
| 10  | C     | 612 | HEM  | CBB-CAB | 3.80 | 1.55        | 1.28     |
| 11  | M     | 613 | NS1  | C17-C15 | 3.81 | 1.40        | 1.35     |
| 8   | M     | 605 | BPB  | C1-C2   | 3.93 | 1.61        | 1.49     |
| 10  | C     | 612 | HEM  | C3B-CAB | 4.13 | 1.56        | 1.47     |
| 8   | L     | 606 | BPB  | C3B-C4B | 4.30 | 1.46        | 1.41     |
| 11  | M     | 613 | NS1  | C20-C21 | 4.33 | 1.41        | 1.35     |
| 7   | L     | 604 | BCB  | CBD-CAD | 4.45 | 1.59        | 1.53     |
| 10  | C     | 612 | HEM  | C3C-CAC | 4.49 | 1.56        | 1.47     |
| 8   | M     | 605 | BPB  | C3B-C4B | 4.81 | 1.47        | 1.41     |
| 11  | M     | 613 | NS1  | C12-C10 | 4.82 | 1.39        | 1.34     |
| 11  | M     | 613 | NS1  | C25-C26 | 5.29 | 1.42        | 1.35     |
| 7   | M     | 603 | BCB  | CBD-CAD | 6.81 | 1.63        | 1.53     |
| 11  | M     | 613 | NS1  | C30-C31 | 7.40 | 1.42        | 1.34     |
| 11  | M     | 613 | NS1  | C35-C36 | 7.66 | 1.54        | 1.32     |

All (174) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | M     | 608 | MQ7  | C11-C3-C4   | -8.87 | 108.61      | 118.50   |
| 13  | M     | 615 | LDA  | CM2-N1-CM1  | -7.30 | 97.01       | 110.99   |
| 11  | M     | 613 | NS1  | C34-C35-C36 | -4.98 | 110.04      | 127.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | M     | 603 | BCB  | C1-O2A-CGA  | -4.79 | 105.29      | 116.77   |
| 7   | M     | 601 | BCB  | OBB-CAB-CBB | -4.72 | 112.41      | 121.09   |
| 7   | L     | 602 | BCB  | C1-C2-C3    | -4.69 | 117.31      | 125.96   |
| 7   | L     | 602 | BCB  | CBC-CAC-C3C | -4.43 | 116.56      | 126.49   |
| 11  | M     | 613 | NS1  | CM4-C36-C35 | -4.30 | 109.67      | 122.65   |
| 9   | M     | 608 | MQ7  | C21-C22-C23 | -4.23 | 117.06      | 127.68   |
| 9   | M     | 608 | MQ7  | C36-C37-C38 | -4.19 | 117.17      | 127.68   |
| 11  | M     | 613 | NS1  | CM3-C36-C35 | -4.16 | 110.09      | 122.65   |
| 10  | C     | 611 | HEM  | CAA-C2A-C3A | -4.15 | 117.16      | 129.00   |
| 7   | L     | 604 | BCB  | C1-C2-C3    | -4.13 | 118.35      | 125.96   |
| 8   | L     | 606 | BPB  | C1-O2A-CGA  | -4.10 | 106.93      | 116.77   |
| 9   | M     | 608 | MQ7  | O1-C1-C10   | -4.09 | 114.83      | 121.55   |
| 8   | M     | 605 | BPB  | C2C-C3C-C4C | -3.88 | 103.59      | 107.35   |
| 10  | C     | 609 | HEM  | CBD-CAD-C3D | -3.79 | 105.24      | 112.47   |
| 8   | M     | 605 | BPB  | CBC-CAC-C3C | -3.60 | 119.06      | 127.00   |
| 7   | M     | 603 | BCB  | O2D-CGD-O1D | -3.55 | 116.69      | 123.82   |
| 7   | M     | 603 | BCB  | OBB-CAB-CBB | -3.52 | 114.60      | 121.09   |
| 7   | M     | 603 | BCB  | CAA-CBA-CGA | -3.52 | 102.75      | 113.35   |
| 8   | M     | 605 | BPB  | OBB-CAB-CBB | -3.37 | 112.48      | 120.16   |
| 11  | M     | 613 | NS1  | C8-C7-C5    | -3.35 | 119.27      | 127.68   |
| 7   | L     | 604 | BCB  | C16-C15-C13 | -3.22 | 105.16      | 115.73   |
| 7   | L     | 604 | BCB  | OBB-CAB-CBB | -3.20 | 115.20      | 121.09   |
| 9   | M     | 608 | MQ7  | C2M-C2-C1   | -3.03 | 111.15      | 116.23   |
| 7   | L     | 602 | BCB  | CMA-C3A-C2A | -3.00 | 105.87      | 115.84   |
| 7   | L     | 602 | BCB  | C11-C10-C8  | -2.91 | 106.19      | 115.73   |
| 8   | L     | 606 | BPB  | CED-O2D-CGD | -2.90 | 109.16      | 115.97   |
| 8   | L     | 606 | BPB  | CBD-CHA-C4D | -2.90 | 105.27      | 108.54   |
| 7   | M     | 601 | BCB  | O2D-CGD-O1D | -2.89 | 118.00      | 123.82   |
| 7   | M     | 601 | BCB  | CBA-CAA-C2A | -2.87 | 111.80      | 115.76   |
| 7   | L     | 602 | BCB  | C14-C13-C15 | -2.86 | 100.91      | 111.36   |
| 8   | L     | 606 | BPB  | CHD-C1D-ND  | -2.86 | 119.03      | 124.64   |
| 11  | M     | 613 | NS1  | C18-C17-C15 | -2.83 | 123.27      | 127.31   |
| 11  | M     | 613 | NS1  | C13-C14-C15 | -2.82 | 118.48      | 126.42   |
| 11  | M     | 613 | NS1  | C27-C26-C25 | -2.76 | 119.06      | 122.92   |
| 7   | M     | 601 | BCB  | CAA-CBA-CGA | -2.75 | 105.06      | 113.35   |
| 9   | M     | 608 | MQ7  | C30-C31-C32 | -2.75 | 102.53      | 111.97   |
| 7   | M     | 603 | BCB  | O2A-CGA-O1A | -2.74 | 116.73      | 123.55   |
| 8   | L     | 606 | BPB  | C7-C6-C5    | -2.74 | 105.49      | 113.11   |
| 9   | M     | 608 | MQ7  | O4-C4-C3    | -2.71 | 116.53      | 120.63   |
| 7   | M     | 601 | BCB  | C6-C7-C8    | -2.66 | 107.00      | 115.73   |
| 8   | L     | 606 | BPB  | CMA-C3A-C2A | -2.64 | 103.04      | 113.77   |
| 9   | M     | 608 | MQ7  | C39-C38-C37 | -2.64 | 116.64      | 123.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | M     | 601 | BCB  | CMA-C3A-C2A | -2.63 | 107.09      | 115.84   |
| 10  | C     | 609 | HEM  | CAD-C3D-C2D | -2.63 | 121.49      | 129.00   |
| 13  | M     | 615 | LDA  | C9-C8-C7    | -2.61 | 101.02      | 114.45   |
| 10  | C     | 612 | HEM  | C4C-C3C-C2C | -2.56 | 105.11      | 106.90   |
| 7   | M     | 603 | BCB  | C11-C10-C8  | -2.56 | 107.32      | 115.73   |
| 7   | M     | 601 | BCB  | C7-C6-C5    | -2.55 | 106.03      | 113.11   |
| 9   | M     | 608 | MQ7  | C31-C32-C33 | -2.53 | 121.31      | 127.68   |
| 8   | L     | 606 | BPB  | CBC-CAC-C3C | -2.48 | 121.54      | 127.00   |
| 7   | L     | 604 | BCB  | C11-C12-C13 | -2.45 | 107.67      | 115.73   |
| 7   | L     | 602 | BCB  | C4-C3-C2    | -2.43 | 117.21      | 123.69   |
| 8   | M     | 605 | BPB  | CBD-CHA-C4D | -2.43 | 105.80      | 108.54   |
| 7   | M     | 603 | BCB  | C7-C6-C5    | -2.42 | 106.38      | 113.11   |
| 7   | L     | 602 | BCB  | OBD-CAD-CBD | -2.40 | 121.72      | 127.52   |
| 11  | M     | 613 | NS1  | C22-C21-C20 | -2.36 | 119.62      | 122.92   |
| 8   | L     | 606 | BPB  | C14-C13-C12 | -2.35 | 102.79      | 111.36   |
| 7   | L     | 602 | BCB  | CAA-CBA-CGA | -2.35 | 106.28      | 113.35   |
| 11  | M     | 613 | NS1  | C19-C18-C17 | -2.33 | 118.48      | 123.46   |
| 7   | L     | 604 | BCB  | OBD-CAD-CBD | -2.27 | 122.02      | 127.52   |
| 12  | L     | 614 | UQ1  | C7-C8-C9    | -2.27 | 119.30      | 127.13   |
| 12  | L     | 614 | UQ1  | CM5-C5-C6   | -2.27 | 119.60      | 124.20   |
| 8   | L     | 606 | BPB  | C2C-C3C-C4C | -2.27 | 105.16      | 107.35   |
| 7   | L     | 602 | BCB  | CED-O2D-CGD | -2.25 | 110.69      | 115.97   |
| 8   | L     | 606 | BPB  | C9-C8-C10   | -2.25 | 103.16      | 111.36   |
| 11  | M     | 613 | NS1  | C24-C23-C21 | -2.25 | 120.10      | 126.42   |
| 10  | C     | 611 | HEM  | CMA-C3A-C2A | -2.23 | 120.74      | 124.94   |
| 10  | C     | 610 | HEM  | CAD-CBD-CGD | -2.21 | 108.89      | 112.66   |
| 7   | L     | 604 | BCB  | CMA-C3A-C2A | -2.19 | 108.56      | 115.84   |
| 8   | L     | 606 | BPB  | O2D-CGD-O1D | -2.16 | 119.48      | 123.82   |
| 9   | M     | 608 | MQ7  | C11-C12-C13 | -2.15 | 123.11      | 126.71   |
| 11  | M     | 613 | NS1  | CM4-C36-CM3 | -2.14 | 109.61      | 114.60   |
| 7   | M     | 601 | BCB  | C11-C10-C8  | -2.13 | 108.74      | 115.73   |
| 13  | M     | 615 | LDA  | CM1-N1-C1   | -2.13 | 105.77      | 110.23   |
| 7   | L     | 604 | BCB  | CBA-CAA-C2A | -2.11 | 112.85      | 115.76   |
| 11  | M     | 613 | NS1  | C16-C15-C17 | -2.09 | 119.99      | 122.92   |
| 7   | M     | 603 | BCB  | C4A-C3A-C2A | -2.09 | 100.67      | 103.86   |
| 7   | L     | 602 | BCB  | C6-C7-C8    | -2.08 | 108.89      | 115.73   |
| 8   | L     | 606 | BPB  | C20-C18-C19 | -2.07 | 100.70      | 110.50   |
| 9   | M     | 608 | MQ7  | C16-C17-C18 | -2.06 | 122.51      | 127.68   |
| 13  | M     | 615 | LDA  | C6-C5-C4    | -2.05 | 103.88      | 114.45   |
| 13  | H     | 616 | LDA  | CM2-N1-CM1  | -2.05 | 107.07      | 110.99   |
| 7   | M     | 603 | BCB  | C1-C2-C3    | -2.05 | 122.18      | 125.96   |
| 7   | M     | 603 | BCB  | C4-C3-C2    | -2.05 | 118.23      | 123.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | M     | 605 | BPB  | C16-C15-C13 | -2.05 | 109.02      | 115.73   |
| 7   | L     | 604 | BCB  | C4-C3-C2    | -2.03 | 118.27      | 123.69   |
| 7   | M     | 601 | BCB  | OBD-CAD-CBD | -2.03 | 122.60      | 127.52   |
| 7   | M     | 601 | BCB  | C5-C3-C2    | -2.02 | 116.97      | 121.10   |
| 9   | M     | 608 | MQ7  | C41-C42-C43 | -2.02 | 120.61      | 127.80   |
| 7   | L     | 602 | BCB  | C9-C8-C7    | -2.01 | 104.02      | 111.36   |
| 10  | C     | 612 | HEM  | CMD-C2D-C1D | -2.00 | 125.39      | 128.46   |
| 10  | C     | 609 | HEM  | CAD-CBD-CGD | 2.06  | 116.18      | 112.66   |
| 9   | M     | 608 | MQ7  | C45-C43-C44 | 2.07  | 119.44      | 114.60   |
| 9   | M     | 608 | MQ7  | C2M-C2-C3   | 2.09  | 128.44      | 124.20   |
| 7   | L     | 602 | BCB  | O1D-CGD-CBD | 2.10  | 128.88      | 124.53   |
| 7   | M     | 603 | BCB  | C3B-C4B-NB  | 2.13  | 107.44      | 103.57   |
| 12  | L     | 614 | UQ1  | C11-C9-C10  | 2.14  | 119.60      | 114.60   |
| 8   | M     | 605 | BPB  | CAA-C2A-C1A | 2.15  | 119.24      | 112.19   |
| 7   | L     | 604 | BCB  | O2A-CGA-CBA | 2.17  | 118.20      | 111.90   |
| 8   | L     | 606 | BPB  | OBD-CAD-C3D | 2.18  | 133.79      | 128.43   |
| 7   | L     | 602 | BCB  | O2A-CGA-CBA | 2.19  | 118.27      | 111.90   |
| 8   | L     | 606 | BPB  | C3A-C2A-C1A | 2.22  | 104.67      | 101.34   |
| 8   | L     | 606 | BPB  | C2D-C1D-ND  | 2.23  | 113.12      | 109.82   |
| 8   | M     | 605 | BPB  | C4D-C3D-CAD | 2.30  | 109.67      | 105.41   |
| 8   | L     | 606 | BPB  | C3D-C4D-CHA | 2.31  | 115.95      | 109.97   |
| 8   | M     | 605 | BPB  | OBB-CAB-C3B | 2.34  | 124.41      | 119.95   |
| 11  | M     | 613 | NS1  | C14-C15-C17 | 2.35  | 122.55      | 118.94   |
| 8   | M     | 605 | BPB  | C3C-C2C-C1C | 2.38  | 103.93      | 100.59   |
| 8   | L     | 606 | BPB  | C4B-CHC-C1C | 2.39  | 131.64      | 128.53   |
| 7   | L     | 604 | BCB  | C3B-C4B-NB  | 2.40  | 107.91      | 103.57   |
| 7   | M     | 601 | BCB  | C6-C5-C3    | 2.42  | 118.14      | 112.66   |
| 13  | M     | 615 | LDA  | O1-N1-C1    | 2.44  | 115.25      | 109.27   |
| 9   | M     | 608 | MQ7  | C14-C13-C15 | 2.53  | 119.68      | 115.29   |
| 7   | L     | 604 | BCB  | CED-O2D-CGD | 2.56  | 121.98      | 115.97   |
| 10  | C     | 612 | HEM  | CMC-C2C-C3C | 2.58  | 129.67      | 124.89   |
| 11  | M     | 613 | NS1  | C6-C5-C4    | 2.59  | 119.79      | 115.29   |
| 10  | C     | 612 | HEM  | CAA-CBA-CGA | 2.60  | 117.11      | 112.66   |
| 7   | L     | 602 | BCB  | OBD-CAD-C3D | 2.61  | 131.30      | 126.75   |
| 10  | C     | 611 | HEM  | CMB-C2B-C3B | 2.61  | 129.74      | 124.89   |
| 9   | M     | 608 | MQ7  | C29-C28-C30 | 2.62  | 119.84      | 115.29   |
| 7   | L     | 604 | BCB  | CHB-C1B-C2B | 2.63  | 124.27      | 116.99   |
| 10  | C     | 609 | HEM  | C4C-C3C-C2C | 2.75  | 108.82      | 106.90   |
| 7   | L     | 604 | BCB  | C4-C3-C5    | 2.76  | 120.08      | 115.29   |
| 7   | M     | 603 | BCB  | CHB-C1B-C2B | 2.87  | 124.93      | 116.99   |
| 7   | L     | 602 | BCB  | CHB-C1B-C2B | 2.90  | 125.02      | 116.99   |
| 11  | M     | 613 | NS1  | C11-C10-C9  | 2.91  | 120.33      | 115.29   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 9   | M     | 608 | MQ7  | O1-C1-C2    | 3.02 | 124.00      | 120.31   |
| 7   | M     | 601 | BCB  | C3B-C4B-NB  | 3.09 | 109.16      | 103.57   |
| 8   | L     | 606 | BPB  | CAA-C2A-C1A | 3.11 | 122.42      | 112.19   |
| 7   | M     | 601 | BCB  | CHC-C4B-C3B | 3.12 | 125.81      | 118.09   |
| 9   | M     | 608 | MQ7  | C24-C23-C25 | 3.12 | 120.71      | 115.29   |
| 10  | C     | 611 | HEM  | CAD-CBD-CGD | 3.19 | 118.10      | 112.66   |
| 7   | M     | 603 | BCB  | O2A-CGA-CBA | 3.23 | 121.30      | 111.90   |
| 9   | M     | 608 | MQ7  | C9-C10-C5   | 3.30 | 123.00      | 119.26   |
| 10  | C     | 609 | HEM  | CMC-C2C-C3C | 3.37 | 131.15      | 124.89   |
| 13  | M     | 615 | LDA  | CM2-N1-C1   | 3.38 | 117.34      | 110.23   |
| 8   | L     | 606 | BPB  | O1D-CGD-CBD | 3.46 | 130.82      | 124.60   |
| 7   | M     | 601 | BCB  | CMB-C2B-C3B | 3.50 | 123.12      | 114.27   |
| 7   | M     | 603 | BCB  | C4-C3-C5    | 3.63 | 121.59      | 115.29   |
| 7   | L     | 604 | BCB  | CHC-C4B-C3B | 3.69 | 127.21      | 118.09   |
| 7   | M     | 601 | BCB  | CHB-C1B-C2B | 3.69 | 127.22      | 116.99   |
| 9   | M     | 608 | MQ7  | C34-C33-C35 | 3.70 | 121.71      | 115.29   |
| 7   | L     | 602 | BCB  | CHC-C4B-C3B | 3.72 | 127.28      | 118.09   |
| 7   | M     | 603 | BCB  | CHD-C1D-C2D | 3.82 | 127.58      | 116.99   |
| 8   | L     | 606 | BPB  | C2A-C1A-NA  | 3.87 | 111.11      | 107.83   |
| 7   | L     | 602 | BCB  | CHD-C1D-C2D | 3.89 | 127.76      | 116.99   |
| 9   | M     | 608 | MQ7  | C39-C38-C40 | 4.03 | 122.28      | 115.29   |
| 7   | M     | 601 | BCB  | CHD-C1D-C2D | 4.07 | 128.27      | 116.99   |
| 7   | L     | 602 | BCB  | C4-C3-C5    | 4.12 | 122.45      | 115.29   |
| 7   | M     | 601 | BCB  | C4-C3-C5    | 4.24 | 122.64      | 115.29   |
| 10  | C     | 610 | HEM  | CBD-CAD-C3D | 4.26 | 120.59      | 112.47   |
| 7   | L     | 604 | BCB  | CBB-CAB-C3B | 4.33 | 121.26      | 116.82   |
| 7   | M     | 603 | BCB  | CHC-C4B-C3B | 4.42 | 129.01      | 118.09   |
| 7   | L     | 604 | BCB  | CHD-C1D-C2D | 4.45 | 129.33      | 116.99   |
| 9   | M     | 608 | MQ7  | C11-C3-C2   | 4.56 | 132.45      | 123.47   |
| 11  | M     | 613 | NS1  | C19-C20-C21 | 4.83 | 134.21      | 127.31   |
| 7   | L     | 602 | BCB  | CBB-CAB-C3B | 5.50 | 122.46      | 116.82   |
| 7   | M     | 601 | BCB  | CMD-C2D-C3D | 5.71 | 128.72      | 114.27   |
| 7   | L     | 604 | BCB  | CMB-C2B-C3B | 5.88 | 129.15      | 114.27   |
| 7   | M     | 603 | BCB  | CBB-CAB-C3B | 5.92 | 122.89      | 116.82   |
| 7   | L     | 602 | BCB  | CMB-C2B-C3B | 5.96 | 129.35      | 114.27   |
| 7   | L     | 602 | BCB  | CMD-C2D-C3D | 6.03 | 129.52      | 114.27   |
| 7   | M     | 603 | BCB  | C1D-CHD-C4C | 6.05 | 125.25      | 112.37   |
| 7   | M     | 603 | BCB  | CMB-C2B-C3B | 6.12 | 129.75      | 114.27   |
| 7   | M     | 603 | BCB  | CMD-C2D-C3D | 6.47 | 130.66      | 114.27   |
| 7   | L     | 602 | BCB  | C1D-CHD-C4C | 6.69 | 126.62      | 112.37   |
| 7   | L     | 604 | BCB  | CMD-C2D-C3D | 6.82 | 131.53      | 114.27   |
| 7   | M     | 601 | BCB  | C1D-CHD-C4C | 6.83 | 126.92      | 112.37   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 10  | C     | 612 | HEM  | CBD-CAD-C3D | 6.95 | 125.73      | 112.47   |
| 7   | L     | 604 | BCB  | C1D-CHD-C4C | 7.01 | 127.30      | 112.37   |
| 7   | M     | 601 | BCB  | CBB-CAB-C3B | 8.40 | 125.43      | 116.82   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 87 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 10  | C     | 609 | HEM  | 4       | 0            |
| 10  | C     | 610 | HEM  | 2       | 0            |
| 10  | C     | 611 | HEM  | 6       | 0            |
| 10  | C     | 612 | HEM  | 2       | 0            |
| 13  | H     | 616 | LDA  | 2       | 0            |
| 7   | L     | 602 | BCB  | 16      | 0            |
| 7   | L     | 604 | BCB  | 11      | 0            |
| 8   | L     | 606 | BPB  | 8       | 0            |
| 12  | L     | 614 | UQ1  | 10      | 0            |
| 7   | M     | 601 | BCB  | 7       | 0            |
| 7   | M     | 603 | BCB  | 15      | 0            |
| 8   | M     | 605 | BPB  | 11      | 0            |
| 9   | M     | 608 | MQ7  | 1       | 0            |
| 11  | M     | 613 | NS1  | 4       | 0            |
| 13  | M     | 615 | LDA  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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   | C     | 333/336 (99%)   | -1.02  | 1 (0%) 93 96 | 7, 21, 46, 73         | 17 (5%) |
| 2   | L     | 273/273 (100%)  | -1.15  | 0 100 100    | 6, 16, 36, 53         | 6 (2%)  |
| 3   | M     | 323/323 (100%)  | -1.08  | 0 100 100    | 4, 18, 41, 58         | 8 (2%)  |
| 4   | H     | 250/258 (96%)   | -0.95  | 2 (0%) 86 89 | 8, 23, 51, 78         | 17 (6%) |
| All | All   | 1179/1190 (99%) | -1.05  | 3 (0%) 93 96 | 4, 19, 44, 78         | 48 (4%) |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | H     | 46  | PRO  | 3.7  |
| 4   | H     | 54  | PRO  | 3.2  |
| 1   | C     | 333 | ALA  | 3.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 4   | FME  | H     | 1   | 10/11 | 0.98 | 0.06 | -    | 21,32,41,45                | 0     |

### 6.3 Carbohydrates [i](#)

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 | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 12  | UQ1  | L     | 614 | 18/18 | 0.84 | 0.57 | 46.70 | 19,26,29,30                | 18    |
| 6   | SO4  | H     | 622 | 5/5   | 0.92 | 0.22 | 11.58 | 73,74,85,89                | 0     |
| 13  | LDA  | H     | 616 | 16/16 | 0.91 | 0.17 | 7.37  | 0,27,42,46                 | 6     |
| 11  | NS1  | M     | 613 | 40/40 | 0.96 | 0.11 | 4.14  | 0,25,39,49                 | 14    |
| 8   | BPB  | M     | 605 | 65/65 | 0.96 | 0.10 | 1.48  | 0,21,62,71                 | 7     |
| 10  | HEM  | C     | 611 | 43/43 | 0.99 | 0.09 | 0.94  | 5,16,25,38                 | 0     |
| 6   | SO4  | M     | 618 | 5/5   | 1.00 | 0.07 | 0.63  | 22,23,35,37                | 0     |
| 10  | HEM  | C     | 610 | 43/43 | 0.99 | 0.09 | 0.60  | 3,21,29,37                 | 0     |
| 8   | BPB  | L     | 606 | 65/65 | 0.99 | 0.07 | 0.54  | 3,10,19,22                 | 0     |
| 6   | SO4  | H     | 617 | 5/5   | 0.98 | 0.07 | 0.53  | 47,50,59,61                | 0     |
| 10  | HEM  | C     | 612 | 43/43 | 0.98 | 0.08 | 0.24  | 3,22,31,46                 | 0     |
| 10  | HEM  | C     | 609 | 43/43 | 0.99 | 0.08 | 0.20  | 7,22,32,36                 | 0     |
| 7   | BCB  | L     | 602 | 66/66 | 0.99 | 0.07 | 0.05  | 3,10,19,21                 | 0     |
| 13  | LDA  | M     | 615 | 16/16 | 0.97 | 0.07 | -0.17 | 17,25,36,37                | 0     |
| 9   | MQ7  | M     | 608 | 48/48 | 0.98 | 0.06 | -0.49 | 0,10,20,32                 | 4     |
| 7   | BCB  | L     | 604 | 66/66 | 0.98 | 0.06 | -0.52 | 3,10,27,35                 | 0     |
| 7   | BCB  | M     | 603 | 66/66 | 0.99 | 0.06 | -0.62 | 3,10,20,21                 | 0     |
| 7   | BCB  | M     | 601 | 66/66 | 0.98 | 0.06 | -1.15 | 0,12,40,61                 | 13    |
| 5   | FE   | M     | 607 | 1/1   | 1.00 | 0.04 | -1.20 | 19,19,19,19                | 0     |
| 6   | SO4  | M     | 620 | 5/5   | 0.99 | 0.05 | -1.25 | 31,34,40,41                | 0     |
| 6   | SO4  | H     | 623 | 5/5   | 0.94 | 0.13 | -     | 58,59,62,64                | 5     |
| 6   | SO4  | M     | 619 | 5/5   | 0.99 | 0.11 | -     | 39,43,50,59                | 0     |
| 6   | SO4  | M     | 621 | 5/5   | 0.97 | 0.20 | -     | 68,78,81,82                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.