



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:56 am GMT

PDB ID : 3Q9F  
Title : Crystal Structure of APAH complexed with CAPS  
Authors : Lombardi, P.M.; Christianson, D.W.  
Deposited on : 2011-01-07  
Resolution : 2.35 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

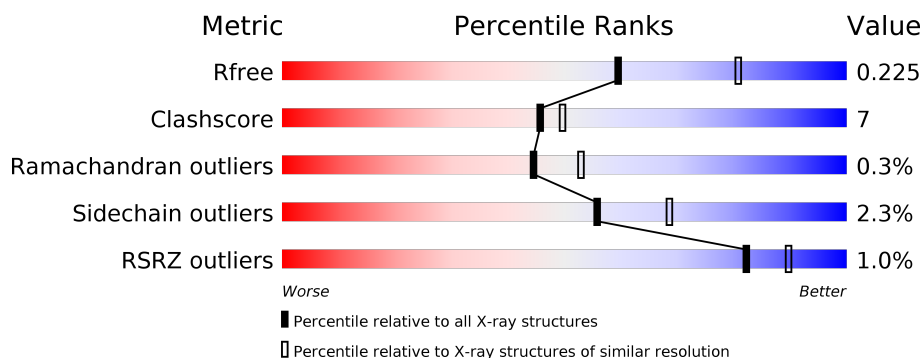
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1522 (2.38-2.34)                                      |
| Clashscore            | 112137                      | 1626 (2.38-2.34)                                      |
| Ramachandran outliers | 110173                      | 1605 (2.38-2.34)                                      |
| Sidechain outliers    | 110143                      | 1606 (2.38-2.34)                                      |
| RSRZ outliers         | 101464                      | 1528 (2.38-2.34)                                      |

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   | A     | 341    | <div> <div style="width: 81%;"></div> <div style="width: 18%;"></div> <div style="width: 1%;"></div> </div> <div>81% 18% .</div> |
| 1   | B     | 341    | <div> <div style="width: 83%;"></div> <div style="width: 16%;"></div> <div style="width: 1%;"></div> </div> <div>83% 16% .</div> |
| 1   | C     | 341    | <div> <div style="width: 83%;"></div> <div style="width: 16%;"></div> <div style="width: 1%;"></div> </div> <div>83% 16% .</div> |
| 1   | D     | 341    | <div> <div style="width: 82%;"></div> <div style="width: 16%;"></div> <div style="width: 2%;"></div> </div> <div>82% 16% .</div> |
| 1   | E     | 341    | <div> <div style="width: 79%;"></div> <div style="width: 20%;"></div> <div style="width: 1%;"></div> </div> <div>79% 20% .</div> |
| 1   | F     | 341    | <div> <div style="width: 84%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> <div>84% 15% .</div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 341    | <br>81% 19%      |
| 1   | H     | 341    | <br>84% 15%      |
| 1   | I     | 341    | <br>80% 19%      |
| 1   | J     | 341    | <br>81% 18%      |
| 1   | K     | 341    | <br>82% 18%      |
| 1   | L     | 341    | <br>81% 18%      |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CXS  | A     | 401 | -         | -        | -       | X                |
| 2   | CXS  | B     | 402 | -         | -        | -       | X                |
| 2   | CXS  | C     | 403 | -         | -        | -       | X                |
| 2   | CXS  | D     | 404 | -         | -        | -       | X                |
| 2   | CXS  | F     | 406 | -         | -        | -       | X                |
| 2   | CXS  | G     | 407 | -         | -        | -       | X                |
| 2   | CXS  | H     | 408 | -         | -        | -       | X                |
| 2   | CXS  | I     | 409 | -         | -        | -       | X                |
| 2   | CXS  | J     | 410 | -         | -        | -       | X                |
| 2   | CXS  | K     | 411 | -         | -        | -       | X                |
| 2   | CXS  | L     | 412 | -         | -        | -       | X                |
| 5   | NA   | A     | 343 | -         | -        | -       | X                |
| 5   | NA   | B     | 343 | -         | -        | -       | X                |
| 5   | NA   | C     | 343 | -         | -        | -       | X                |
| 5   | NA   | D     | 343 | -         | -        | -       | X                |
| 5   | NA   | E     | 343 | -         | -        | -       | X                |
| 5   | NA   | G     | 343 | -         | -        | -       | X                |
| 5   | NA   | I     | 343 | -         | -        | -       | X                |
| 5   | NA   | K     | 343 | -         | -        | -       | X                |

## 2 Entry composition

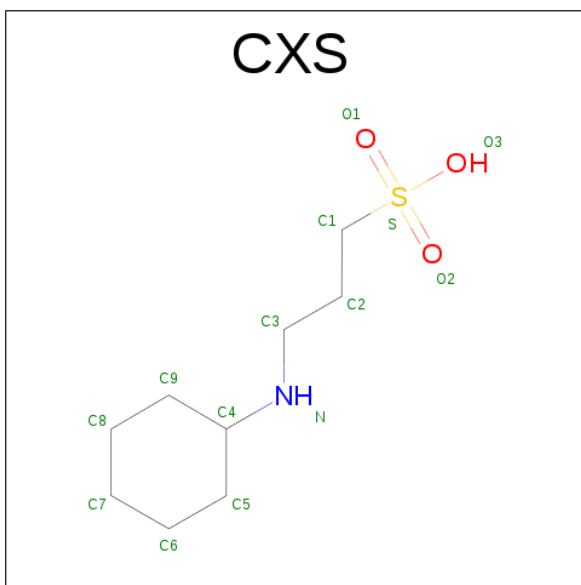
There are 7 unique types of molecules in this entry. The entry contains 32471 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylpolysamine amidohydrolase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | B     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | C     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | D     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | E     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | F     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | G     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | H     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | I     | 340      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2563  | 1642 | 434 | 478 | 9 |         |         |       |
| 1   | J     | 340      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2563  | 1642 | 434 | 478 | 9 |         |         |       |
| 1   | K     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |
| 1   | L     | 341      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2568  | 1644 | 435 | 480 | 9 |         |         |       |

- Molecule 2 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | B     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | E     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | F     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | G     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | H     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | I     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | J     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | K     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |
| 2   | L     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 14    | 9 | 1 | 3 | 1 |         |         |

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | I     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | K     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | L     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | G     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | J     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | D     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | K     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | E     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | H     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | B     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | I     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | C     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | A     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | L     | 2        | Total K<br>2 2 | 0       | 0       |
| 4   | F     | 2        | Total K<br>2 2 | 0       | 0       |

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | G     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | J     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | D     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | K     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | E     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | H     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | B     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | I     | 1        | Total Na<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 5   | C     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 5   | A     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 5   | L     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 5   | F     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 6   | G     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | J     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | D     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | K     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | E     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | H     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | B     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | I     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | C     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | A     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | L     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | F     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7   | A     | 129      | Total<br>129 | O<br>129 | 0       | 0       |

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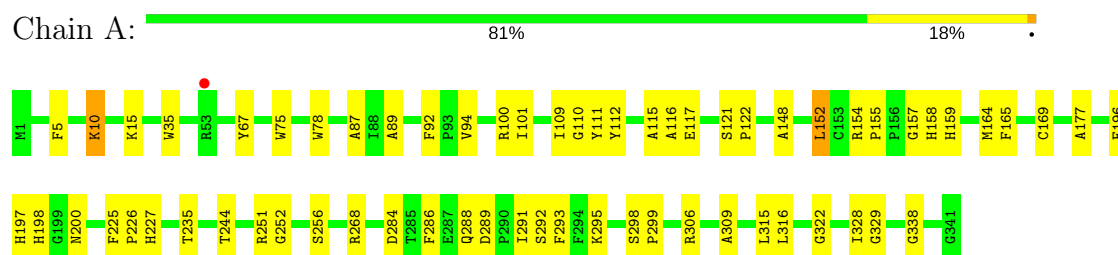
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7   | B     | 117      | Total<br>117 | O<br>117 | 0       | 0       |
| 7   | C     | 124      | Total<br>124 | O<br>124 | 0       | 0       |
| 7   | D     | 125      | Total<br>125 | O<br>125 | 0       | 0       |
| 7   | E     | 115      | Total<br>115 | O<br>115 | 0       | 0       |
| 7   | F     | 107      | Total<br>107 | O<br>107 | 0       | 0       |
| 7   | G     | 106      | Total<br>106 | O<br>106 | 0       | 0       |
| 7   | H     | 112      | Total<br>112 | O<br>112 | 0       | 0       |
| 7   | I     | 132      | Total<br>132 | O<br>132 | 0       | 0       |
| 7   | J     | 98       | Total<br>98  | O<br>98  | 0       | 0       |
| 7   | K     | 113      | Total<br>113 | O<br>113 | 0       | 0       |
| 7   | L     | 115      | Total<br>115 | O<br>115 | 0       | 0       |

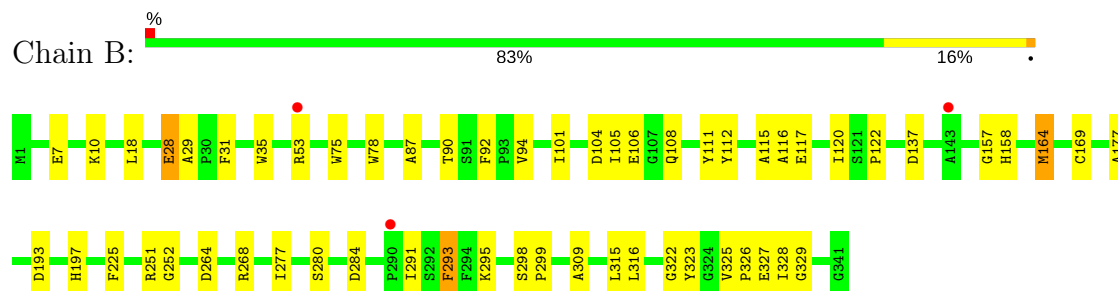
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

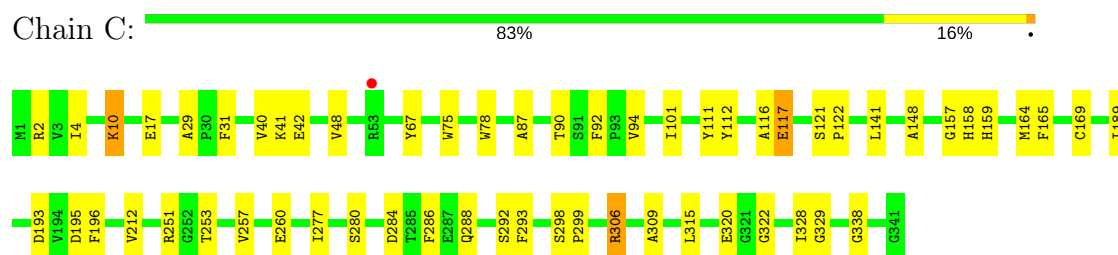
#### • Molecule 1: Acetypolyamine amidohydrolase



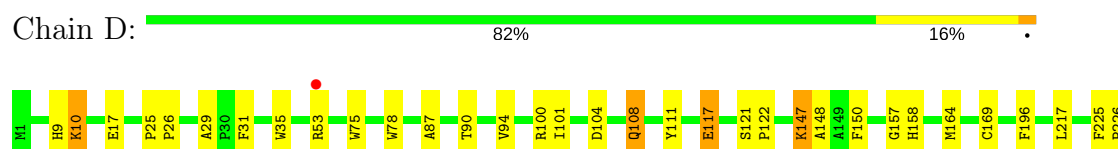
#### • Molecule 1: Acetypolyamine amidohydrolase



#### • Molecule 1: Acetypolyamine amidohydrolase

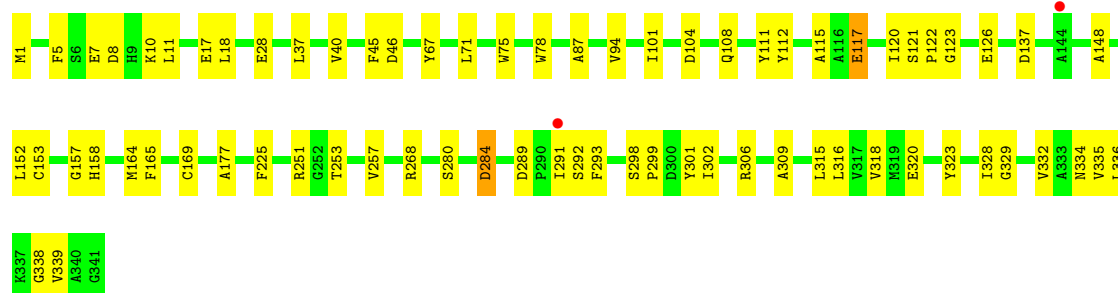
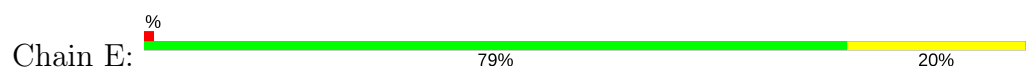


#### • Molecule 1: Acetypolyamine amidohydrolase

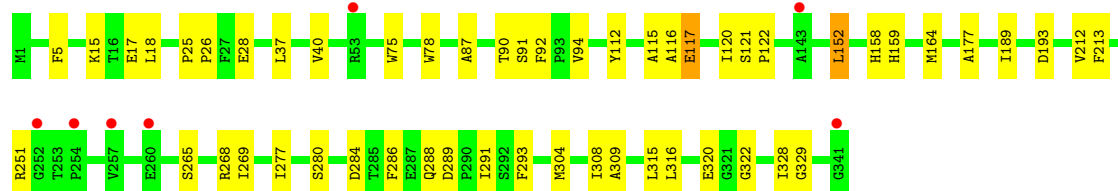
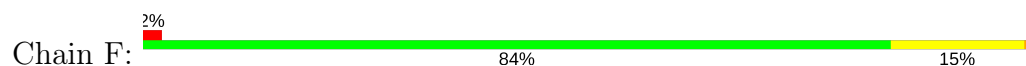




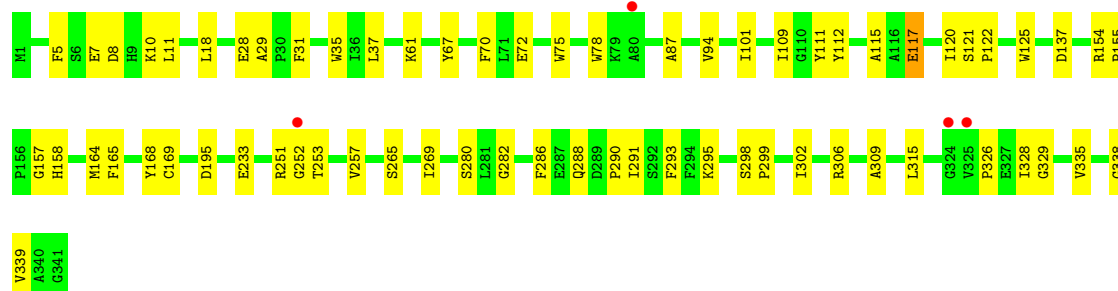
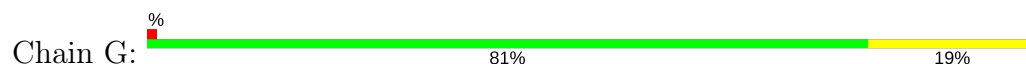
• Molecule 1: Acetylpolyamine amidohydrolase



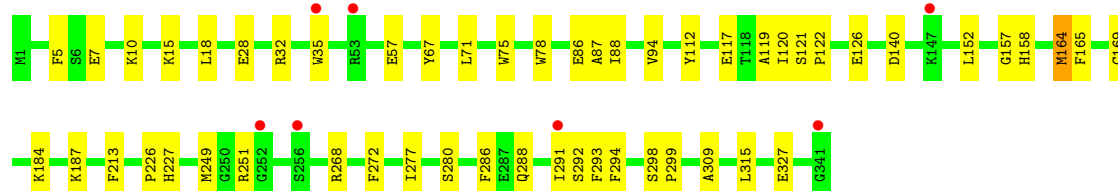
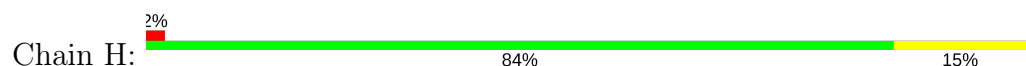
• Molecule 1: Acetylpolyamine amidohydrolase



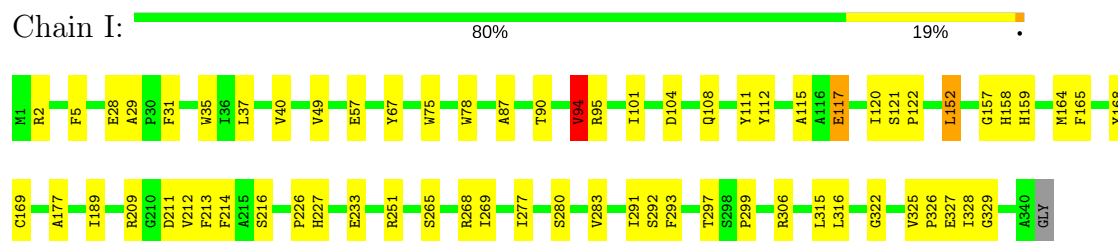
• Molecule 1: Acetylpolyamine amidohydrolase



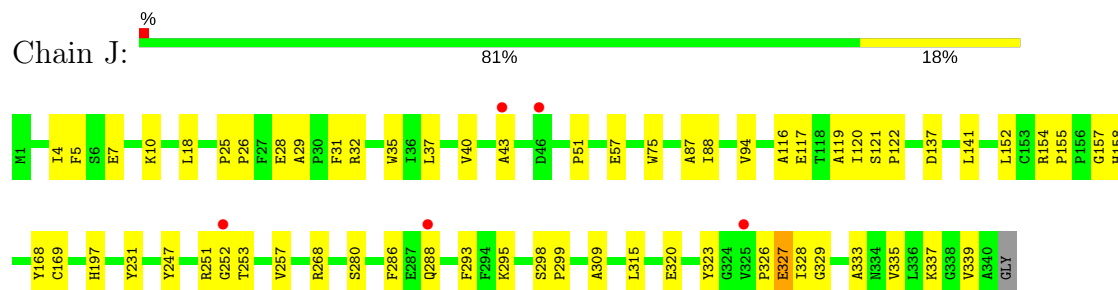
• Molecule 1: Acetylpolyamine amidohydrolase



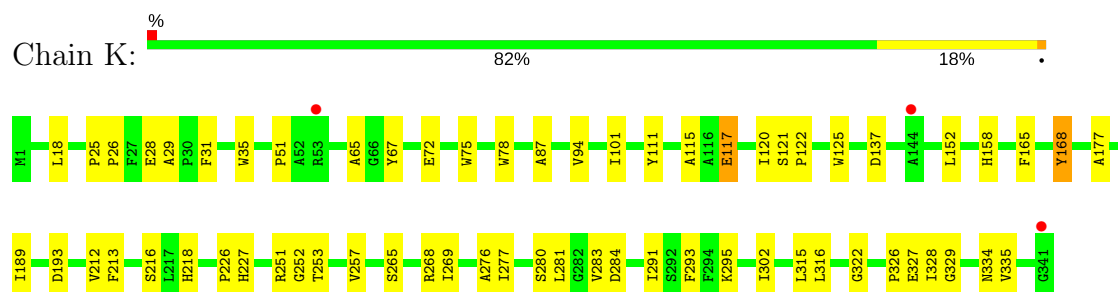
- Molecule 1: Acetylpolyamine amidohydrolase



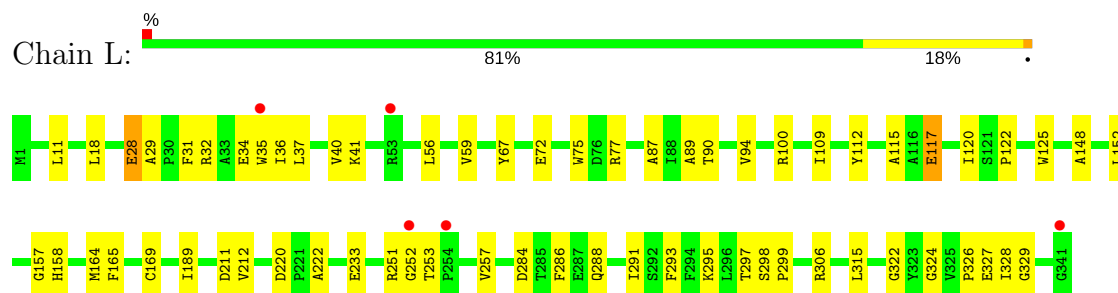
- Molecule 1: Acetylpolyamine amidohydrolase



- Molecule 1: Acetylpolyamine amidohydrolase



- Molecule 1: Acetylpolyamine amidohydrolase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 118.25Å 119.65Å 119.57Å<br>98.34° 94.94° 114.95°            | Depositor        |
| Resolution (Å)  | 50.00 – 2.35<br>46.62 – 2.35                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.1 (50.00-2.35)<br>85.3 (46.62-2.35)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | 0.10  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.54 (at 2.34Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.189 , 0.225<br>0.189 , 0.225                              | Depositor<br>DCC |
| $R_{free}$ test set   | 11007 reflections (5.00%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 32.1  | Xtriage          |
| Anisotropy  | 0.139   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 39.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | 0.001 for -k,-h,-l  | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 32471   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, NA, ZN, CXS, PO4

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.41         | 0/2636  | 0.59        | 0/3582  |
| 1   | B     | 0.39         | 0/2636  | 0.58        | 0/3582  |
| 1   | C     | 0.41         | 0/2636  | 0.59        | 0/3582  |
| 1   | D     | 0.41         | 0/2636  | 0.59        | 0/3582  |
| 1   | E     | 0.39         | 0/2636  | 0.58        | 0/3582  |
| 1   | F     | 0.39         | 0/2636  | 0.57        | 0/3582  |
| 1   | G     | 0.39         | 0/2636  | 0.59        | 0/3582  |
| 1   | H     | 0.39         | 0/2636  | 0.56        | 0/3582  |
| 1   | I     | 0.41         | 0/2631  | 0.58        | 0/3577  |
| 1   | J     | 0.37         | 0/2631  | 0.56        | 0/3577  |
| 1   | K     | 0.40         | 0/2636  | 0.58        | 0/3582  |
| 1   | L     | 0.39         | 0/2636  | 0.58        | 0/3582  |
| All | All   | 0.40         | 0/31622 | 0.58        | 0/42974 |

There are no bond length outliers.

There are no bond angle outliers.

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   | A     | 2568  | 0        | 2490     | 40      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 2568  | 0        | 2492     | 37      | 0            |
| 1   | C     | 2568  | 0        | 2491     | 37      | 0            |
| 1   | D     | 2568  | 0        | 2491     | 44      | 0            |
| 1   | E     | 2568  | 0        | 2491     | 44      | 0            |
| 1   | F     | 2568  | 0        | 2490     | 36      | 0            |
| 1   | G     | 2568  | 0        | 2492     | 38      | 0            |
| 1   | H     | 2568  | 0        | 2492     | 34      | 0            |
| 1   | I     | 2563  | 0        | 2488     | 40      | 0            |
| 1   | J     | 2563  | 0        | 2488     | 38      | 0            |
| 1   | K     | 2568  | 0        | 2491     | 36      | 0            |
| 1   | L     | 2568  | 0        | 2492     | 41      | 0            |
| 2   | A     | 14    | 0        | 19       | 1       | 0            |
| 2   | B     | 14    | 0        | 18       | 4       | 0            |
| 2   | C     | 14    | 0        | 18       | 1       | 0            |
| 2   | D     | 14    | 0        | 18       | 6       | 0            |
| 2   | E     | 14    | 0        | 18       | 3       | 0            |
| 2   | F     | 14    | 0        | 19       | 1       | 0            |
| 2   | G     | 14    | 0        | 18       | 1       | 0            |
| 2   | H     | 14    | 0        | 19       | 0       | 0            |
| 2   | I     | 14    | 0        | 18       | 4       | 0            |
| 2   | J     | 14    | 0        | 18       | 1       | 0            |
| 2   | K     | 14    | 0        | 18       | 3       | 0            |
| 2   | L     | 14    | 0        | 18       | 1       | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 3   | B     | 5     | 0        | 0        | 0       | 0            |
| 3   | C     | 5     | 0        | 0        | 0       | 0            |
| 3   | D     | 5     | 0        | 0        | 0       | 0            |
| 3   | E     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 5     | 0        | 0        | 0       | 0            |
| 3   | G     | 5     | 0        | 0        | 0       | 0            |
| 3   | H     | 5     | 0        | 0        | 0       | 0            |
| 3   | I     | 5     | 0        | 0        | 0       | 0            |
| 3   | J     | 5     | 0        | 0        | 0       | 0            |
| 3   | K     | 5     | 0        | 0        | 0       | 0            |
| 3   | L     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 2     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 2     | 0        | 0        | 0       | 0            |
| 4   | E     | 2     | 0        | 0        | 0       | 0            |
| 4   | F     | 2     | 0        | 0        | 0       | 0            |
| 4   | G     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | H     | 2     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | E     | 1     | 0        | 0        | 0       | 0            |
| 5   | F     | 1     | 0        | 0        | 0       | 0            |
| 5   | G     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 1     | 0        | 0        | 0       | 0            |
| 5   | I     | 1     | 0        | 0        | 0       | 0            |
| 5   | J     | 1     | 0        | 0        | 0       | 0            |
| 5   | K     | 1     | 0        | 0        | 0       | 0            |
| 5   | L     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 1     | 0        | 0        | 0       | 0            |
| 6   | H     | 1     | 0        | 0        | 0       | 0            |
| 6   | I     | 1     | 0        | 0        | 0       | 0            |
| 6   | J     | 1     | 0        | 0        | 0       | 0            |
| 6   | K     | 1     | 0        | 0        | 0       | 0            |
| 6   | L     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 129   | 0        | 0        | 1       | 0            |
| 7   | B     | 117   | 0        | 0        | 1       | 0            |
| 7   | C     | 124   | 0        | 0        | 1       | 0            |
| 7   | D     | 125   | 0        | 0        | 0       | 0            |
| 7   | E     | 115   | 0        | 0        | 3       | 0            |
| 7   | F     | 107   | 0        | 0        | 1       | 0            |
| 7   | G     | 106   | 0        | 0        | 1       | 0            |
| 7   | H     | 112   | 0        | 0        | 1       | 0            |
| 7   | I     | 132   | 0        | 0        | 2       | 0            |
| 7   | J     | 98    | 0        | 0        | 1       | 0            |
| 7   | K     | 113   | 0        | 0        | 0       | 0            |
| 7   | L     | 115   | 0        | 0        | 2       | 0            |
| All | All   | 32471 | 0        | 30107    | 449     | 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 7.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:157:GLY:HA2  | 1:L:169:CYS:HB3  | 1.63                     | 0.79              |
| 1:E:306:ARG:HD2  | 1:E:338:GLY:O    | 1.87                     | 0.75              |
| 1:D:289:ASP:OD1  | 1:D:291:ILE:HG12 | 1.88                     | 0.74              |
| 1:I:291:ILE:HD12 | 2:I:409:CXS:H51  | 1.71                     | 0.73              |
| 1:H:157:GLY:HA2  | 1:H:169:CYS:HB3  | 1.70                     | 0.72              |
| 1:J:157:GLY:HA2  | 1:J:169:CYS:HB3  | 1.70                     | 0.72              |
| 1:A:15:LYS:HE2   | 1:A:15:LYS:HA    | 1.73                     | 0.70              |
| 1:L:75:TRP:CE2   | 1:L:122:PRO:HG3  | 2.25                     | 0.70              |
| 1:A:286:PHE:CE2  | 1:A:288:GLN:HB2  | 2.27                     | 0.69              |
| 1:G:306:ARG:HD2  | 1:G:338:GLY:O    | 1.91                     | 0.69              |
| 1:L:72:GLU:HG3   | 1:L:125:TRP:NE1  | 2.07                     | 0.69              |
| 1:I:159:HIS:CD2  | 2:I:409:CXS:H11  | 2.28                     | 0.68              |
| 1:G:328:ILE:HG13 | 1:G:329:GLY:N    | 2.09                     | 0.67              |
| 1:D:225:PHE:CE2  | 2:D:404:CXS:H31  | 2.30                     | 0.67              |
| 1:K:302:ILE:HG13 | 1:K:334:ASN:HB3  | 1.78                     | 0.66              |
| 1:E:157:GLY:HA2  | 1:E:169:CYS:HB3  | 1.78                     | 0.66              |
| 1:E:251:ARG:HA   | 1:E:293:PHE:CD2  | 2.31                     | 0.66              |
| 1:C:251:ARG:HA   | 1:C:293:PHE:CD2  | 2.30                     | 0.66              |
| 1:L:31:PHE:HA    | 1:L:34:GLU:HG2   | 1.77                     | 0.65              |
| 1:E:291:ILE:HD12 | 2:E:405:CXS:H51  | 1.77                     | 0.65              |
| 1:B:75:TRP:CE2   | 1:B:122:PRO:HG3  | 2.32                     | 0.65              |
| 1:A:306:ARG:HD2  | 1:A:338:GLY:O    | 1.97                     | 0.65              |
| 1:L:36:ILE:O     | 1:L:40:VAL:HG13  | 1.97                     | 0.64              |
| 1:A:289:ASP:OD1  | 1:A:291:ILE:HG12 | 1.99                     | 0.62              |
| 1:I:159:HIS:HD2  | 2:I:409:CXS:H11  | 1.64                     | 0.62              |
| 2:E:405:CXS:H52  | 7:E:1003:HOH:O   | 2.00                     | 0.62              |
| 1:J:29:ALA:HB3   | 1:J:31:PHE:CE1   | 2.35                     | 0.62              |
| 1:K:168:TYR:CE2  | 2:K:411:CXS:H32  | 2.34                     | 0.62              |
| 1:F:251:ARG:HA   | 1:F:293:PHE:CD2  | 2.34                     | 0.62              |
| 1:F:286:PHE:CE2  | 1:F:288:GLN:HB2  | 2.34                     | 0.62              |
| 1:B:87:ALA:HB3   | 1:B:120:ILE:HB   | 1.83                     | 0.61              |
| 1:F:121:SER:HB2  | 1:F:122:PRO:CD   | 2.31                     | 0.61              |
| 1:F:159:HIS:CD2  | 2:F:406:CXS:H11  | 2.37                     | 0.60              |
| 1:D:286:PHE:CE2  | 1:D:288:GLN:HB2  | 2.37                     | 0.60              |
| 1:H:309:ALA:HA   | 1:H:315:LEU:HD11 | 1.83                     | 0.60              |
| 1:J:87:ALA:HB3   | 1:J:120:ILE:HB   | 1.84                     | 0.60              |
| 1:G:115:ALA:HB1  | 1:G:117:GLU:OE1  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:251:ARG:HA   | 1:J:293:PHE:CD2  | 2.37                     | 0.59              |
| 1:D:284:ASP:HB3  | 1:D:322:GLY:HA2  | 1.84                     | 0.59              |
| 1:C:4:ILE:HD12   | 1:C:4:ILE:N      | 2.18                     | 0.59              |
| 1:J:75:TRP:CE2   | 1:J:122:PRO:HG3  | 2.38                     | 0.59              |
| 1:A:268:ARG:HB3  | 1:A:268:ARG:NH1  | 2.18                     | 0.59              |
| 1:E:302:ILE:HG13 | 1:E:334:ASN:HB3  | 1.85                     | 0.59              |
| 1:C:309:ALA:HA   | 1:C:315:LEU:HD11 | 1.83                     | 0.58              |
| 1:B:309:ALA:HA   | 1:B:315:LEU:HD11 | 1.84                     | 0.58              |
| 1:F:75:TRP:NE1   | 1:F:122:PRO:HG3  | 2.19                     | 0.58              |
| 1:L:117:GLU:HG3  | 2:L:412:CXS:H92  | 1.84                     | 0.58              |
| 1:L:35:TRP:CZ3   | 1:L:326:PRO:HA   | 2.39                     | 0.58              |
| 1:E:75:TRP:CE2   | 1:E:122:PRO:HG3  | 2.39                     | 0.58              |
| 1:E:323:TYR:HB3  | 7:E:864:HOH:O    | 2.03                     | 0.58              |
| 1:K:251:ARG:HA   | 1:K:293:PHE:CD2  | 2.39                     | 0.58              |
| 1:K:35:TRP:CE3   | 1:K:326:PRO:HA   | 2.39                     | 0.57              |
| 1:E:8:ASP:HB3    | 1:E:11:LEU:HD12  | 1.86                     | 0.57              |
| 1:L:286:PHE:CE2  | 1:L:288:GLN:HB2  | 2.40                     | 0.57              |
| 1:I:117:GLU:HG3  | 2:I:409:CXS:H92  | 1.87                     | 0.57              |
| 1:C:92:PHE:HZ    | 1:C:116:ALA:HB2  | 1.70                     | 0.57              |
| 2:G:407:CXS:H71  | 7:G:1004:HOH:O   | 2.02                     | 0.57              |
| 1:A:251:ARG:HA   | 1:A:293:PHE:CD2  | 2.39                     | 0.56              |
| 1:D:225:PHE:HB2  | 2:D:404:CXS:H81  | 1.86                     | 0.56              |
| 1:A:309:ALA:HA   | 1:A:315:LEU:HD11 | 1.86                     | 0.56              |
| 1:B:225:PHE:CD2  | 2:B:402:CXS:H31  | 2.40                     | 0.56              |
| 1:K:213:PHE:HZ   | 1:K:268:ARG:HD2  | 1.70                     | 0.56              |
| 1:A:75:TRP:NE1   | 1:A:122:PRO:HG3  | 2.21                     | 0.56              |
| 1:A:35:TRP:HA    | 1:A:35:TRP:CE3   | 2.40                     | 0.56              |
| 1:E:309:ALA:HA   | 1:E:315:LEU:HD11 | 1.86                     | 0.56              |
| 1:D:298:SER:HB2  | 1:D:299:PRO:HD3  | 1.87                     | 0.56              |
| 1:I:115:ALA:HB1  | 1:I:117:GLU:OE1  | 2.05                     | 0.56              |
| 1:G:72:GLU:HG3   | 1:G:125:TRP:NE1  | 2.21                     | 0.56              |
| 1:I:328:ILE:HG13 | 1:I:329:GLY:N    | 2.21                     | 0.56              |
| 1:L:87:ALA:HB3   | 1:L:120:ILE:HB   | 1.88                     | 0.56              |
| 1:A:35:TRP:HE3   | 1:A:35:TRP:HA    | 1.71                     | 0.56              |
| 1:G:35:TRP:CE3   | 1:G:326:PRO:HA   | 2.41                     | 0.56              |
| 1:L:306:ARG:HH11 | 1:L:306:ARG:HG3  | 1.71                     | 0.55              |
| 1:E:115:ALA:HB1  | 1:E:117:GLU:OE1  | 2.06                     | 0.55              |
| 1:C:2:ARG:HD2    | 1:C:141:LEU:HD11 | 1.87                     | 0.55              |
| 1:G:87:ALA:HB3   | 1:G:120:ILE:HB   | 1.88                     | 0.55              |
| 1:D:225:PHE:CG   | 2:D:404:CXS:H4   | 2.42                     | 0.55              |
| 1:A:75:TRP:CE2   | 1:A:122:PRO:HG3  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:284:ASP:HB3  | 1:B:322:GLY:HA2  | 1.88                     | 0.55              |
| 1:H:112:TYR:O    | 1:H:164:MET:HA   | 2.07                     | 0.55              |
| 1:C:284:ASP:HB3  | 1:C:322:GLY:HA2  | 1.88                     | 0.55              |
| 1:C:298:SER:HB2  | 1:C:299:PRO:HD3  | 1.89                     | 0.55              |
| 1:F:121:SER:HB2  | 1:F:122:PRO:HD2  | 1.89                     | 0.55              |
| 1:A:78:TRP:CE2   | 1:A:87:ALA:HA    | 2.41                     | 0.54              |
| 1:B:157:GLY:HA2  | 1:B:169:CYS:HB3  | 1.89                     | 0.54              |
| 1:G:75:TRP:CE2   | 1:G:122:PRO:HG3  | 2.42                     | 0.54              |
| 1:K:328:ILE:HG13 | 1:K:329:GLY:N    | 2.22                     | 0.54              |
| 1:G:298:SER:HB2  | 1:G:299:PRO:HD3  | 1.90                     | 0.54              |
| 1:D:150:PHE:CZ   | 1:D:319:MET:HG2  | 2.42                     | 0.54              |
| 1:G:251:ARG:HA   | 1:G:293:PHE:CD2  | 2.42                     | 0.54              |
| 1:B:78:TRP:CE2   | 1:B:87:ALA:HA    | 2.43                     | 0.54              |
| 1:D:277:ILE:HB   | 1:D:315:LEU:HD23 | 1.89                     | 0.54              |
| 1:D:225:PHE:CD1  | 2:D:404:CXS:H61  | 2.43                     | 0.54              |
| 1:K:67:TYR:OH    | 1:K:165:PHE:HB3  | 2.08                     | 0.54              |
| 1:K:75:TRP:CE2   | 1:K:122:PRO:HG3  | 2.43                     | 0.54              |
| 1:E:101:ILE:HG12 | 1:E:111:TYR:CZ   | 2.43                     | 0.53              |
| 1:I:5:PHE:CD1    | 1:I:152:LEU:HD13 | 2.43                     | 0.53              |
| 1:I:78:TRP:CE2   | 1:I:87:ALA:HA    | 2.44                     | 0.53              |
| 1:K:291:ILE:HD12 | 2:K:411:CXS:H51  | 1.89                     | 0.53              |
| 1:C:121:SER:HB2  | 1:C:122:PRO:HD2  | 1.90                     | 0.53              |
| 1:L:112:TYR:O    | 1:L:164:MET:HA   | 2.08                     | 0.53              |
| 1:D:196:PHE:CD1  | 1:D:292:SER:HB2  | 2.43                     | 0.53              |
| 1:H:75:TRP:NE1   | 1:H:122:PRO:HG3  | 2.24                     | 0.53              |
| 1:I:75:TRP:CE2   | 1:I:122:PRO:HG3  | 2.44                     | 0.53              |
| 1:L:298:SER:HB2  | 1:L:299:PRO:HD3  | 1.91                     | 0.53              |
| 1:J:309:ALA:HA   | 1:J:315:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:112:TYR:O    | 1:A:164:MET:HA   | 2.09                     | 0.52              |
| 1:F:309:ALA:HA   | 1:F:315:LEU:HD11 | 1.92                     | 0.52              |
| 1:H:75:TRP:CE2   | 1:H:122:PRO:HG3  | 2.45                     | 0.52              |
| 1:B:328:ILE:HG13 | 1:B:329:GLY:N    | 2.24                     | 0.52              |
| 1:G:157:GLY:HA2  | 1:G:169:CYS:HB3  | 1.92                     | 0.52              |
| 1:G:29:ALA:HB3   | 1:G:31:PHE:CE1   | 2.44                     | 0.52              |
| 1:K:72:GLU:HG3   | 1:K:125:TRP:NE1  | 2.25                     | 0.52              |
| 1:D:121:SER:HB2  | 1:D:122:PRO:CD   | 2.40                     | 0.52              |
| 1:J:43:ALA:HB1   | 1:J:337:LYS:HE2  | 1.90                     | 0.52              |
| 1:K:117:GLU:HG3  | 2:K:411:CXS:H92  | 1.91                     | 0.52              |
| 1:J:298:SER:HB2  | 1:J:299:PRO:HD3  | 1.91                     | 0.52              |
| 1:I:157:GLY:HA2  | 1:I:169:CYS:HB3  | 1.92                     | 0.52              |
| 1:K:277:ILE:HB   | 1:K:315:LEU:CD2  | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:88:ILE:HG12  | 1:H:119:ALA:HB2  | 1.92                     | 0.52              |
| 1:B:298:SER:HB2  | 1:B:299:PRO:HD3  | 1.92                     | 0.52              |
| 1:E:280:SER:HB3  | 1:E:320:GLU:HG3  | 1.91                     | 0.52              |
| 1:E:328:ILE:HG13 | 1:E:329:GLY:N    | 2.25                     | 0.51              |
| 1:G:252:GLY:HA2  | 1:G:295:LYS:HG3  | 1.92                     | 0.51              |
| 1:A:268:ARG:HB3  | 1:A:268:ARG:HH11 | 1.76                     | 0.51              |
| 1:C:121:SER:HB2  | 1:C:122:PRO:CD   | 2.40                     | 0.51              |
| 1:G:35:TRP:CZ3   | 1:G:326:PRO:HA   | 2.45                     | 0.51              |
| 1:B:53:ARG:HH11  | 1:B:53:ARG:HG2   | 1.76                     | 0.51              |
| 1:H:226:PRO:O    | 1:H:227:HIS:HB2  | 2.11                     | 0.51              |
| 1:C:280:SER:HB3  | 1:C:320:GLU:HG3  | 1.93                     | 0.51              |
| 1:E:87:ALA:HB3   | 1:E:120:ILE:HB   | 1.93                     | 0.51              |
| 1:H:35:TRP:HA    | 1:H:35:TRP:CE3   | 2.45                     | 0.51              |
| 1:B:7:GLU:O      | 1:B:10:LYS:HG2   | 2.10                     | 0.50              |
| 1:C:112:TYR:O    | 1:C:164:MET:HA   | 2.11                     | 0.50              |
| 1:I:29:ALA:HB3   | 1:I:31:PHE:CE1   | 2.47                     | 0.50              |
| 1:D:104:ASP:O    | 1:D:108:GLN:HB2  | 2.12                     | 0.50              |
| 1:F:15:LYS:HE2   | 1:F:15:LYS:HA    | 1.93                     | 0.50              |
| 1:J:333:ALA:O    | 1:J:337:LYS:HG3  | 2.11                     | 0.50              |
| 1:J:326:PRO:HG2  | 1:J:327:GLU:OE1  | 2.12                     | 0.50              |
| 1:C:29:ALA:HB3   | 1:C:31:PHE:CE1   | 2.46                     | 0.50              |
| 1:A:252:GLY:O    | 1:A:295:LYS:HE2  | 2.12                     | 0.50              |
| 1:D:302:ILE:HG13 | 1:D:334:ASN:HB3  | 1.94                     | 0.50              |
| 1:D:78:TRP:CE2   | 1:D:87:ALA:HA    | 2.47                     | 0.50              |
| 1:F:5:PHE:CD1    | 1:F:152:LEU:HD13 | 2.46                     | 0.50              |
| 1:D:29:ALA:HB3   | 1:D:31:PHE:CE1   | 2.47                     | 0.49              |
| 1:G:112:TYR:O    | 1:G:164:MET:HA   | 2.11                     | 0.49              |
| 1:H:298:SER:HB2  | 1:H:299:PRO:HD3  | 1.94                     | 0.49              |
| 1:I:326:PRO:HG2  | 1:I:327:GLU:OE2  | 2.12                     | 0.49              |
| 1:L:115:ALA:HB1  | 1:L:117:GLU:OE1  | 2.11                     | 0.49              |
| 1:B:264:ASP:O    | 1:B:268:ARG:HG2  | 2.13                     | 0.49              |
| 1:L:37:LEU:O     | 1:L:41:LYS:HG3   | 2.12                     | 0.49              |
| 1:E:123:GLY:HA2  | 1:E:126:GLU:OE1  | 2.12                     | 0.49              |
| 1:F:78:TRP:CE2   | 1:F:87:ALA:HA    | 2.48                     | 0.49              |
| 1:D:277:ILE:HB   | 1:D:315:LEU:CD2  | 2.42                     | 0.49              |
| 1:A:196:PHE:CD1  | 1:A:292:SER:HB2  | 2.48                     | 0.49              |
| 1:H:87:ALA:HB3   | 1:H:120:ILE:HB   | 1.94                     | 0.49              |
| 1:K:78:TRP:CE2   | 1:K:87:ALA:HA    | 2.48                     | 0.49              |
| 1:D:35:TRP:CE3   | 1:D:35:TRP:HA    | 2.47                     | 0.49              |
| 1:I:214:PHE:CZ   | 1:I:216:SER:HB2  | 2.48                     | 0.49              |
| 1:I:87:ALA:HB3   | 1:I:120:ILE:HB   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:10:LYS:HB3   | 1:C:10:LYS:NZ    | 2.28                     | 0.49              |
| 1:J:5:PHE:CD1    | 1:J:152:LEU:HD13 | 2.48                     | 0.49              |
| 1:L:189:ILE:O    | 1:L:212:VAL:HA   | 2.13                     | 0.49              |
| 1:D:225:PHE:CD1  | 2:D:404:CXS:H4   | 2.48                     | 0.49              |
| 1:E:225:PHE:HB2  | 2:E:405:CXS:H91  | 1.95                     | 0.49              |
| 1:C:328:ILE:HG23 | 1:C:329:GLY:N    | 2.28                     | 0.48              |
| 1:H:67:TYR:CZ    | 1:H:71:LEU:HD11  | 2.48                     | 0.48              |
| 1:A:10:LYS:NZ    | 1:A:10:LYS:HB3   | 2.27                     | 0.48              |
| 1:A:157:GLY:HA2  | 1:A:169:CYS:HB3  | 1.95                     | 0.48              |
| 1:K:189:ILE:O    | 1:K:212:VAL:HA   | 2.13                     | 0.48              |
| 1:A:101:ILE:HG12 | 1:A:111:TYR:CZ   | 2.48                     | 0.48              |
| 1:A:121:SER:HB2  | 1:A:122:PRO:CD   | 2.44                     | 0.48              |
| 1:A:284:ASP:HB3  | 1:A:322:GLY:HA2  | 1.94                     | 0.48              |
| 1:B:112:TYR:O    | 1:B:164:MET:HA   | 2.13                     | 0.48              |
| 1:H:121:SER:HB2  | 1:H:122:PRO:CD   | 2.44                     | 0.48              |
| 1:I:209:ARG:HB3  | 1:I:211:ASP:OD1  | 2.13                     | 0.48              |
| 1:A:121:SER:HB2  | 1:A:122:PRO:HD2  | 1.95                     | 0.48              |
| 1:G:72:GLU:HG3   | 1:G:125:TRP:CD1  | 2.48                     | 0.48              |
| 1:K:101:ILE:HG12 | 1:K:111:TYR:CZ   | 2.49                     | 0.48              |
| 1:L:284:ASP:HB3  | 1:L:322:GLY:HA2  | 1.95                     | 0.48              |
| 1:B:277:ILE:HB   | 1:B:315:LEU:HD23 | 1.95                     | 0.48              |
| 1:E:18:LEU:HD22  | 1:H:18:LEU:HD12  | 1.95                     | 0.48              |
| 1:F:115:ALA:HB1  | 1:F:117:GLU:OE1  | 2.13                     | 0.48              |
| 1:G:67:TYR:OH    | 1:G:165:PHE:HB3  | 2.14                     | 0.48              |
| 1:D:256:SER:O    | 1:D:260:GLU:HG3  | 2.14                     | 0.48              |
| 1:F:328:ILE:HG23 | 1:F:329:GLY:N    | 2.29                     | 0.48              |
| 1:J:247:TYR:OH   | 1:J:268:ARG:HD2  | 2.14                     | 0.47              |
| 1:C:159:HIS:CD2  | 2:C:403:CXS:H11  | 2.49                     | 0.47              |
| 1:I:189:ILE:O    | 1:I:212:VAL:HA   | 2.14                     | 0.47              |
| 1:J:7:GLU:O      | 1:J:10:LYS:HG2   | 2.14                     | 0.47              |
| 1:A:67:TYR:OH    | 1:A:165:PHE:HB3  | 2.14                     | 0.47              |
| 1:F:75:TRP:CE2   | 1:F:122:PRO:HG3  | 2.49                     | 0.47              |
| 1:G:328:ILE:HG13 | 1:G:329:GLY:H    | 1.76                     | 0.47              |
| 1:G:5:PHE:CE2    | 1:G:37:LEU:HD22  | 2.50                     | 0.47              |
| 1:J:328:ILE:HG13 | 1:J:329:GLY:N    | 2.28                     | 0.47              |
| 1:F:280:SER:HB3  | 1:F:320:GLU:HG3  | 1.95                     | 0.47              |
| 1:I:277:ILE:HB   | 1:I:315:LEU:CD2  | 2.45                     | 0.47              |
| 1:L:56:LEU:O     | 1:L:59:VAL:HG12  | 2.14                     | 0.47              |
| 1:B:104:ASP:O    | 1:B:108:GLN:HG3  | 2.14                     | 0.47              |
| 1:B:299:PRO:HB2  | 1:E:306:ARG:CG   | 2.45                     | 0.47              |
| 1:G:233:GLU:OE2  | 1:L:100:ARG:NH2  | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:35:TRP:CE3   | 1:I:326:PRO:HA   | 2.50                     | 0.47              |
| 1:D:90:THR:O     | 1:J:116:ALA:N    | 2.47                     | 0.47              |
| 1:J:4:ILE:HD11   | 1:J:141:LEU:HD11 | 1.95                     | 0.47              |
| 1:L:253:THR:HG23 | 1:L:257:VAL:HB   | 1.96                     | 0.47              |
| 1:B:35:TRP:CE3   | 1:B:326:PRO:HA   | 2.50                     | 0.47              |
| 1:D:147:LYS:HD2  | 1:D:148:ALA:N    | 2.30                     | 0.47              |
| 1:K:87:ALA:HB3   | 1:K:120:ILE:HB   | 1.96                     | 0.47              |
| 1:E:67:TYR:CZ    | 1:E:71:LEU:HD11  | 2.50                     | 0.47              |
| 1:A:159:HIS:CD2  | 2:A:401:CXS:H11  | 2.50                     | 0.47              |
| 1:F:92:PHE:HZ    | 1:F:116:ALA:HB2  | 1.79                     | 0.47              |
| 1:G:101:ILE:HG12 | 1:G:111:TYR:CZ   | 2.50                     | 0.47              |
| 1:A:268:ARG:NH2  | 7:A:360:HOH:O    | 2.47                     | 0.47              |
| 1:D:121:SER:HB2  | 1:D:122:PRO:HD2  | 1.97                     | 0.47              |
| 1:F:117:GLU:HG2  | 1:F:117:GLU:O    | 2.15                     | 0.46              |
| 1:H:268:ARG:HG2  | 1:H:268:ARG:HH11 | 1.80                     | 0.46              |
| 1:L:28:GLU:OE2   | 1:L:32:ARG:NH1   | 2.41                     | 0.46              |
| 1:L:148:ALA:HA   | 1:L:315:LEU:O    | 2.14                     | 0.46              |
| 1:B:29:ALA:HB3   | 1:B:31:PHE:CE1   | 2.50                     | 0.46              |
| 1:J:29:ALA:HB3   | 1:J:31:PHE:CD1   | 2.50                     | 0.46              |
| 1:L:291:ILE:HG13 | 1:L:291:ILE:O    | 2.15                     | 0.46              |
| 1:D:302:ILE:HD13 | 1:G:302:ILE:HD13 | 1.96                     | 0.46              |
| 1:F:265:SER:O    | 1:F:269:ILE:HG13 | 2.15                     | 0.46              |
| 1:L:252:GLY:O    | 1:L:295:LYS:HE2  | 2.15                     | 0.46              |
| 1:I:213:PHE:HZ   | 1:I:268:ARG:HD2  | 1.80                     | 0.46              |
| 1:A:235:THR:HA   | 1:A:244:THR:O    | 2.15                     | 0.46              |
| 1:C:157:GLY:HA2  | 1:C:169:CYS:HB3  | 1.98                     | 0.46              |
| 1:K:193:ASP:HA   | 1:K:280:SER:HB2  | 1.96                     | 0.46              |
| 1:I:67:TYR:OH    | 1:I:165:PHE:HB3  | 2.15                     | 0.46              |
| 1:J:121:SER:HB2  | 1:J:122:PRO:CD   | 2.46                     | 0.46              |
| 1:K:281:LEU:HD11 | 1:K:335:VAL:HG21 | 1.96                     | 0.46              |
| 1:K:252:GLY:HA2  | 1:K:295:LYS:HE2  | 1.98                     | 0.46              |
| 1:B:197:HIS:CE1  | 2:B:402:CXS:H22  | 2.51                     | 0.46              |
| 1:H:251:ARG:HA   | 1:H:293:PHE:CD2  | 2.51                     | 0.46              |
| 1:J:37:LEU:O     | 1:J:40:VAL:HG22  | 2.16                     | 0.46              |
| 1:K:226:PRO:O    | 1:K:227:HIS:HB2  | 2.15                     | 0.46              |
| 1:H:187:LYS:HA   | 1:H:187:LYS:HD3  | 1.79                     | 0.46              |
| 1:E:253:THR:HG23 | 1:E:257:VAL:HB   | 1.98                     | 0.45              |
| 1:J:35:TRP:CE3   | 1:J:326:PRO:HA   | 2.51                     | 0.45              |
| 1:J:51:PRO:HA    | 1:J:137:ASP:OD1  | 2.16                     | 0.45              |
| 1:L:251:ARG:HA   | 1:L:293:PHE:CD2  | 2.51                     | 0.45              |
| 1:B:197:HIS:ND1  | 2:B:402:CXS:H22  | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:32:ARG:HD2   | 1:J:323:TYR:HD1  | 1.80                     | 0.45              |
| 1:J:57:GLU:HB2   | 7:J:474:HOH:O    | 2.15                     | 0.45              |
| 1:K:277:ILE:HB   | 1:K:315:LEU:HD23 | 1.98                     | 0.45              |
| 1:G:78:TRP:CE2   | 1:G:87:ALA:HA    | 2.51                     | 0.45              |
| 1:C:75:TRP:NE1   | 1:C:122:PRO:HG3  | 2.31                     | 0.45              |
| 1:D:306:ARG:HE   | 1:D:306:ARG:HA   | 1.81                     | 0.45              |
| 1:H:7:GLU:O      | 1:H:10:LYS:HG2   | 2.16                     | 0.45              |
| 1:J:4:ILE:HG22   | 1:J:51:PRO:HG3   | 1.98                     | 0.45              |
| 1:A:148:ALA:HA   | 1:A:315:LEU:O    | 2.17                     | 0.45              |
| 1:B:325:VAL:HB   | 1:B:327:GLU:OE2  | 2.16                     | 0.45              |
| 1:D:280:SER:HB3  | 1:D:320:GLU:HG3  | 1.98                     | 0.45              |
| 1:F:284:ASP:OD1  | 1:F:284:ASP:N    | 2.50                     | 0.45              |
| 1:G:195:ASP:HA   | 1:G:282:GLY:HA3  | 1.99                     | 0.45              |
| 1:D:225:PHE:CD2  | 2:D:404:CXS:H31  | 2.52                     | 0.45              |
| 1:H:67:TYR:OH    | 1:H:165:PHE:HB3  | 2.16                     | 0.45              |
| 1:H:78:TRP:CE2   | 1:H:87:ALA:HA    | 2.52                     | 0.45              |
| 1:I:121:SER:HB2  | 1:I:122:PRO:CD   | 2.47                     | 0.45              |
| 1:G:70:PHE:CZ    | 1:G:109:ILE:HA   | 2.52                     | 0.45              |
| 1:A:177:ALA:HB1  | 1:A:316:LEU:HD23 | 1.98                     | 0.45              |
| 1:G:121:SER:HB2  | 1:G:122:PRO:CD   | 2.47                     | 0.45              |
| 1:I:283:VAL:HG23 | 1:I:322:GLY:HA3  | 1.97                     | 0.45              |
| 1:B:323:TYR:HB3  | 7:B:695:HOH:O    | 2.16                     | 0.45              |
| 1:B:18:LEU:HD22  | 1:F:18:LEU:HD22  | 1.99                     | 0.45              |
| 1:C:306:ARG:HG2  | 1:C:338:GLY:O    | 2.17                     | 0.45              |
| 1:G:335:VAL:O    | 1:G:339:VAL:HG23 | 2.17                     | 0.45              |
| 1:H:213:PHE:HB2  | 1:H:272:PHE:CD2  | 2.52                     | 0.45              |
| 1:L:72:GLU:HG3   | 1:L:125:TRP:CD1  | 2.52                     | 0.45              |
| 1:L:77:ARG:HD3   | 7:L:355:HOH:O    | 2.15                     | 0.45              |
| 1:G:7:GLU:O      | 1:G:10:LYS:HG2   | 2.17                     | 0.44              |
| 1:D:75:TRP:CE2   | 1:D:122:PRO:HG3  | 2.52                     | 0.44              |
| 1:K:216:SER:OG   | 1:K:218:HIS:ND1  | 2.47                     | 0.44              |
| 1:F:284:ASP:HB3  | 1:F:322:GLY:HA2  | 1.98                     | 0.44              |
| 1:G:61:LYS:HD3   | 1:K:65:ALA:HB1   | 1.99                     | 0.44              |
| 1:L:37:LEU:HG    | 1:L:41:LYS:HE3   | 1.98                     | 0.44              |
| 1:C:4:ILE:HD11   | 1:C:141:LEU:CD1  | 2.47                     | 0.44              |
| 1:L:67:TYR:OH    | 1:L:165:PHE:HB3  | 2.17                     | 0.44              |
| 1:B:28:GLU:HG2   | 1:B:323:TYR:HE1  | 1.82                     | 0.44              |
| 1:E:284:ASP:HA   | 1:E:289:ASP:OD2  | 2.17                     | 0.44              |
| 1:E:298:SER:HB2  | 1:E:299:PRO:HD3  | 2.00                     | 0.44              |
| 1:F:91:SER:HB2   | 7:F:988:HOH:O    | 2.15                     | 0.44              |
| 1:J:327:GLU:N    | 1:J:327:GLU:OE1  | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:25:PRO:HA    | 1:K:26:PRO:HD3   | 1.91                     | 0.44              |
| 1:B:101:ILE:HG12 | 1:B:111:TYR:CZ   | 2.53                     | 0.44              |
| 1:E:17:GLU:HG3   | 1:E:117:GLU:O    | 2.17                     | 0.44              |
| 1:F:17:GLU:HG3   | 1:F:117:GLU:O    | 2.17                     | 0.44              |
| 1:J:88:ILE:HG12  | 1:J:119:ALA:HB2  | 2.00                     | 0.44              |
| 1:B:105:ILE:HG23 | 1:B:106:GLU:N    | 2.33                     | 0.44              |
| 1:B:29:ALA:HB3   | 1:B:31:PHE:CD1   | 2.53                     | 0.44              |
| 1:C:101:ILE:HG12 | 1:C:111:TYR:CZ   | 2.53                     | 0.44              |
| 1:E:148:ALA:HA   | 1:E:315:LEU:O    | 2.18                     | 0.44              |
| 1:E:153:CYS:SG   | 1:E:318:VAL:HG13 | 2.57                     | 0.44              |
| 1:F:112:TYR:O    | 1:F:164:MET:HA   | 2.18                     | 0.44              |
| 1:C:90:THR:O     | 1:K:115:ALA:HA   | 2.18                     | 0.44              |
| 1:F:304:MET:O    | 1:F:308:ILE:HG13 | 2.18                     | 0.44              |
| 1:I:325:VAL:HB   | 1:I:327:GLU:OE1  | 2.18                     | 0.44              |
| 1:E:5:PHE:CE2    | 1:E:37:LEU:HD22  | 2.53                     | 0.43              |
| 1:I:251:ARG:HA   | 1:I:293:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:298:SER:HB2  | 1:A:299:PRO:HD3  | 1.99                     | 0.43              |
| 1:K:121:SER:HB2  | 1:K:122:PRO:CD   | 2.48                     | 0.43              |
| 1:K:177:ALA:HB1  | 1:K:316:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:40:VAL:HG23  | 1:C:41:LYS:N     | 2.32                     | 0.43              |
| 1:E:40:VAL:O     | 1:E:45:PHE:HB2   | 2.18                     | 0.43              |
| 1:I:226:PRO:O    | 1:I:227:HIS:HB2  | 2.18                     | 0.43              |
| 1:L:37:LEU:O     | 1:L:40:VAL:HG22  | 2.18                     | 0.43              |
| 1:J:252:GLY:HA2  | 1:J:295:LYS:HG2  | 2.00                     | 0.43              |
| 1:E:1:MET:SD     | 1:E:336:LEU:HD22 | 2.58                     | 0.43              |
| 1:E:78:TRP:CE2   | 1:E:87:ALA:HA    | 2.53                     | 0.43              |
| 1:B:115:ALA:HA   | 1:F:90:THR:O     | 2.17                     | 0.43              |
| 1:H:5:PHE:CD1    | 1:H:152:LEU:HD13 | 2.53                     | 0.43              |
| 1:I:265:SER:O    | 1:I:269:ILE:HG13 | 2.19                     | 0.43              |
| 1:I:297:THR:OG1  | 1:I:299:PRO:HD2  | 2.18                     | 0.43              |
| 1:D:251:ARG:HA   | 1:D:293:PHE:CD2  | 2.53                     | 0.43              |
| 1:E:301:TYR:HB3  | 1:E:335:VAL:HG23 | 1.98                     | 0.43              |
| 1:F:284:ASP:HA   | 1:F:289:ASP:OD2  | 2.19                     | 0.43              |
| 1:G:8:ASP:HB3    | 1:G:11:LEU:HD12  | 2.01                     | 0.43              |
| 1:H:140:ASP:OD1  | 1:H:184:LYS:HE3  | 2.19                     | 0.43              |
| 1:L:328:ILE:HG23 | 1:L:329:GLY:N    | 2.34                     | 0.43              |
| 1:A:328:ILE:HG23 | 1:A:329:GLY:N    | 2.33                     | 0.43              |
| 1:E:121:SER:HB2  | 1:E:122:PRO:HD2  | 2.00                     | 0.43              |
| 1:F:193:ASP:HA   | 1:F:280:SER:HB2  | 2.01                     | 0.43              |
| 1:H:286:PHE:CE2  | 1:H:288:GLN:HB2  | 2.53                     | 0.43              |
| 1:A:226:PRO:O    | 1:A:227:HIS:HB2  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:291:ILE:HB   | 2:B:402:CXS:H82  | 2.01                     | 0.43              |
| 1:D:148:ALA:HA   | 1:D:315:LEU:O    | 2.18                     | 0.43              |
| 1:E:7:GLU:O      | 1:E:10:LYS:HG2   | 2.18                     | 0.43              |
| 1:A:100:ARG:NE   | 1:I:233:GLU:OE2  | 2.48                     | 0.43              |
| 1:K:302:ILE:CG1  | 1:K:334:ASN:HB3  | 2.47                     | 0.43              |
| 1:B:251:ARG:HA   | 1:B:293:PHE:CD2  | 2.53                     | 0.43              |
| 1:C:286:PHE:CE2  | 1:C:288:GLN:HB2  | 2.54                     | 0.43              |
| 1:H:121:SER:HB2  | 1:H:122:PRO:HD2  | 2.00                     | 0.43              |
| 1:H:15:LYS:HG2   | 1:H:86:GLU:OE2   | 2.19                     | 0.43              |
| 1:I:112:TYR:O    | 1:I:164:MET:HA   | 2.19                     | 0.43              |
| 1:D:101:ILE:HG12 | 1:D:111:TYR:CZ   | 2.54                     | 0.43              |
| 1:E:104:ASP:O    | 1:E:108:GLN:HG3  | 2.19                     | 0.43              |
| 1:C:148:ALA:HA   | 1:C:315:LEU:O    | 2.19                     | 0.42              |
| 1:D:299:PRO:HB2  | 1:G:306:ARG:HD3  | 2.01                     | 0.42              |
| 1:E:268:ARG:HH11 | 1:E:268:ARG:HG3  | 1.84                     | 0.42              |
| 1:J:121:SER:HB2  | 1:J:122:PRO:HD2  | 2.00                     | 0.42              |
| 1:K:51:PRO:HA    | 1:K:137:ASP:OD1  | 2.18                     | 0.42              |
| 1:A:92:PHE:HZ    | 1:A:116:ALA:HB2  | 1.84                     | 0.42              |
| 1:B:252:GLY:HA2  | 1:B:295:LYS:HG2  | 2.01                     | 0.42              |
| 1:C:41:LYS:CE    | 1:C:48:VAL:HG21  | 2.48                     | 0.42              |
| 1:L:211:ASP:OD1  | 1:L:212:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:197:HIS:CD2  | 1:A:225:PHE:HB3  | 2.54                     | 0.42              |
| 1:C:17:GLU:HG3   | 1:C:117:GLU:O    | 2.20                     | 0.42              |
| 1:C:75:TRP:CE2   | 1:C:122:PRO:HG3  | 2.55                     | 0.42              |
| 1:D:309:ALA:HA   | 1:D:315:LEU:HD11 | 2.01                     | 0.42              |
| 1:F:189:ILE:O    | 1:F:212:VAL:HA   | 2.18                     | 0.42              |
| 1:I:101:ILE:HG12 | 1:I:111:TYR:CZ   | 2.54                     | 0.42              |
| 1:B:92:PHE:HZ    | 1:B:116:ALA:HB2  | 1.84                     | 0.42              |
| 1:C:189:ILE:O    | 1:C:212:VAL:HA   | 2.19                     | 0.42              |
| 1:E:67:TYR:OH    | 1:E:165:PHE:HB3  | 2.20                     | 0.42              |
| 1:B:193:ASP:HA   | 1:B:280:SER:HB2  | 2.01                     | 0.42              |
| 1:D:150:PHE:HZ   | 1:D:319:MET:HG2  | 1.84                     | 0.42              |
| 1:G:121:SER:HB2  | 1:G:122:PRO:HD2  | 2.01                     | 0.42              |
| 1:I:2:ARG:HD3    | 1:I:49:VAL:HG11  | 2.01                     | 0.42              |
| 1:J:335:VAL:O    | 1:J:339:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:5:PHE:CD1    | 1:A:152:LEU:HD13 | 2.54                     | 0.42              |
| 1:A:198:HIS:CE1  | 1:A:200:ASN:HA   | 2.54                     | 0.42              |
| 1:D:17:GLU:HG3   | 1:D:117:GLU:O    | 2.20                     | 0.42              |
| 1:E:121:SER:HB2  | 1:E:122:PRO:CD   | 2.50                     | 0.42              |
| 1:E:335:VAL:O    | 1:E:339:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:309:ALA:HA   | 1:G:315:LEU:HD11 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:277:ILE:HB   | 1:H:315:LEU:CD2  | 2.50                     | 0.42              |
| 1:L:233:GLU:HG2  | 7:L:504:HOH:O    | 2.20                     | 0.42              |
| 1:B:90:THR:O     | 1:F:116:ALA:N    | 2.53                     | 0.42              |
| 1:I:177:ALA:HB1  | 1:I:316:LEU:HD23 | 2.02                     | 0.42              |
| 1:I:94:VAL:HB    | 1:I:95:ARG:H     | 1.62                     | 0.42              |
| 1:A:115:ALA:HA   | 1:I:90:THR:O     | 2.20                     | 0.41              |
| 1:F:87:ALA:HB3   | 1:F:120:ILE:HB   | 2.02                     | 0.41              |
| 1:I:104:ASP:O    | 1:I:108:GLN:HG3  | 2.20                     | 0.41              |
| 1:K:253:THR:HG23 | 1:K:257:VAL:HB   | 2.02                     | 0.41              |
| 1:K:265:SER:O    | 1:K:269:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:53:ARG:NH1   | 1:B:53:ARG:HG2   | 2.36                     | 0.41              |
| 1:G:265:SER:O    | 1:G:269:ILE:HG13 | 2.20                     | 0.41              |
| 1:C:90:THR:HG22  | 1:K:18:LEU:HD23  | 2.02                     | 0.41              |
| 1:K:189:ILE:HD12 | 1:K:276:ALA:HB3  | 2.02                     | 0.41              |
| 1:K:29:ALA:HB3   | 1:K:31:PHE:CE1   | 2.55                     | 0.41              |
| 1:C:67:TYR:OH    | 1:C:165:PHE:HB3  | 2.20                     | 0.41              |
| 1:C:78:TRP:CE2   | 1:C:87:ALA:HA    | 2.55                     | 0.41              |
| 1:G:154:ARG:HA   | 1:G:155:PRO:C    | 2.41                     | 0.41              |
| 1:J:154:ARG:HA   | 1:J:155:PRO:C    | 2.41                     | 0.41              |
| 1:J:286:PHE:CE2  | 1:J:288:GLN:HB2  | 2.56                     | 0.41              |
| 1:L:157:GLY:HA2  | 1:L:169:CYS:CB   | 2.43                     | 0.41              |
| 1:E:292:SER:HB2  | 7:E:1288:HOH:O   | 2.20                     | 0.41              |
| 1:F:25:PRO:HA    | 1:F:26:PRO:HD3   | 1.96                     | 0.41              |
| 1:G:253:THR:HG23 | 1:G:257:VAL:HB   | 2.00                     | 0.41              |
| 1:J:25:PRO:HA    | 1:J:26:PRO:HD3   | 1.91                     | 0.41              |
| 1:A:154:ARG:HA   | 1:A:155:PRO:C    | 2.41                     | 0.41              |
| 1:C:257:VAL:HA   | 1:C:260:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:255:TYR:CD1  | 1:D:300:ASP:HB3  | 2.55                     | 0.41              |
| 1:E:177:ALA:HB1  | 1:E:316:LEU:HD23 | 2.02                     | 0.41              |
| 1:H:291:ILE:HG13 | 1:H:291:ILE:O    | 2.20                     | 0.41              |
| 1:B:299:PRO:HB2  | 1:E:306:ARG:HG3  | 2.00                     | 0.41              |
| 1:C:193:ASP:OD1  | 1:C:195:ASP:HB3  | 2.20                     | 0.41              |
| 1:C:253:THR:HG23 | 1:C:257:VAL:HB   | 2.02                     | 0.41              |
| 1:C:277:ILE:HB   | 1:C:315:LEU:CD2  | 2.51                     | 0.41              |
| 1:D:217:LEU:HD23 | 1:D:249:MET:HE1  | 2.03                     | 0.41              |
| 1:I:37:LEU:O     | 1:I:40:VAL:HG22  | 2.20                     | 0.41              |
| 1:I:57:GLU:HB2   | 7:I:479:HOH:O    | 2.19                     | 0.41              |
| 1:L:220:ASP:OD2  | 1:L:222:ALA:HB3  | 2.20                     | 0.41              |
| 1:G:115:ALA:HA   | 1:L:90:THR:O     | 2.21                     | 0.41              |
| 1:E:7:GLU:O      | 1:E:10:LYS:HE3   | 2.21                     | 0.41              |
| 1:H:57:GLU:HB2   | 7:H:359:HOH:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:252:GLY:HA2  | 1:J:295:LYS:CG   | 2.51                     | 0.41              |
| 1:A:89:ALA:HB1   | 1:A:110:GLY:HA2  | 2.03                     | 0.41              |
| 1:B:177:ALA:HB1  | 1:B:316:LEU:HD23 | 2.03                     | 0.41              |
| 1:E:284:ASP:N    | 1:E:284:ASP:OD1  | 2.50                     | 0.41              |
| 1:I:306:ARG:HG2  | 1:I:306:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:89:ALA:HB2   | 1:A:109:ILE:HG12 | 2.02                     | 0.41              |
| 1:H:35:TRP:HA    | 1:H:35:TRP:HE3   | 1.85                     | 0.41              |
| 1:L:11:LEU:HD23  | 1:L:11:LEU:HA    | 1.93                     | 0.41              |
| 1:L:89:ALA:HB2   | 1:L:109:ILE:HG12 | 2.02                     | 0.41              |
| 1:H:213:PHE:HB2  | 1:H:272:PHE:CE2  | 2.56                     | 0.41              |
| 1:J:32:ARG:HD2   | 1:J:323:TYR:CD1  | 2.56                     | 0.41              |
| 1:D:157:GLY:HA2  | 1:D:169:CYS:HB3  | 2.03                     | 0.40              |
| 1:D:225:PHE:CG   | 1:D:226:PRO:HA   | 2.56                     | 0.40              |
| 1:D:25:PRO:HA    | 1:D:26:PRO:HD3   | 1.96                     | 0.40              |
| 1:F:291:ILE:H    | 1:F:291:ILE:HG13 | 1.70                     | 0.40              |
| 1:C:196:PHE:CD1  | 1:C:292:SER:HB2  | 2.57                     | 0.40              |
| 1:E:112:TYR:O    | 1:E:164:MET:HA   | 2.20                     | 0.40              |
| 1:F:213:PHE:HZ   | 1:F:268:ARG:HD2  | 1.86                     | 0.40              |
| 1:F:177:ALA:HB1  | 1:F:316:LEU:HD23 | 2.04                     | 0.40              |
| 1:F:37:LEU:O     | 1:F:40:VAL:HG22  | 2.22                     | 0.40              |
| 1:H:249:MET:HB2  | 1:H:294:PHE:CZ   | 2.55                     | 0.40              |
| 1:H:327:GLU:OE1  | 1:H:327:GLU:N    | 2.54                     | 0.40              |
| 1:J:253:THR:HG23 | 1:J:257:VAL:HB   | 2.03                     | 0.40              |
| 1:D:287:GLU:OE1  | 1:D:297:THR:HG22 | 2.21                     | 0.40              |
| 1:F:277:ILE:HB   | 1:F:315:LEU:HD23 | 2.03                     | 0.40              |
| 1:G:286:PHE:CE2  | 1:G:288:GLN:HB2  | 2.57                     | 0.40              |
| 1:L:297:THR:OG1  | 1:L:299:PRO:HD2  | 2.21                     | 0.40              |
| 1:C:164:MET:HE2  | 7:C:359:HOH:O    | 2.20                     | 0.40              |
| 1:D:100:ARG:HD2  | 1:J:231:TYR:CD2  | 2.56                     | 0.40              |
| 1:D:9:HIS:CG     | 1:D:10:LYS:N     | 2.90                     | 0.40              |
| 1:D:35:TRP:HA    | 1:D:35:TRP:HE3   | 1.86                     | 0.40              |
| 1:E:328:ILE:O    | 1:E:332:VAL:HG23 | 2.22                     | 0.40              |
| 1:H:126:GLU:CD   | 1:H:126:GLU:H    | 2.24                     | 0.40              |
| 1:H:28:GLU:OE2   | 1:H:32:ARG:NH1   | 2.52                     | 0.40              |
| 1:I:292:SER:HB2  | 7:I:1279:HOH:O   | 2.20                     | 0.40              |
| 1:G:18:LEU:HD22  | 1:L:18:LEU:HD22  | 2.03                     | 0.40              |
| 1:L:29:ALA:HB3   | 1:L:31:PHE:CD2   | 2.57                     | 0.40              |
| 1:L:31:PHE:CZ    | 1:L:324:GLY:HA3  | 2.56                     | 0.40              |
| 1:I:5:PHE:CE2    | 1:I:37:LEU:HD22  | 2.56                     | 0.40              |
| 1:J:280:SER:HB3  | 1:J:320:GLU:HG3  | 2.03                     | 0.40              |
| 1:J:197:HIS:CE1  | 2:J:410:CXS:H12  | 2.57                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:283:VAL:CG2 | 1:K:322:GLY:HA3 | 2.51                     | 0.40              |
| 1:K:327:GLU:N   | 1:K:327:GLU:OE1 | 2.54                     | 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   | A     | 339/341 (99%)   | 322 (95%)  | 16 (5%)  | 1 (0%)   | 44          | 53 |
| 1   | B     | 339/341 (99%)   | 321 (95%)  | 17 (5%)  | 1 (0%)   | 44          | 53 |
| 1   | C     | 339/341 (99%)   | 322 (95%)  | 16 (5%)  | 1 (0%)   | 44          | 53 |
| 1   | D     | 339/341 (99%)   | 323 (95%)  | 15 (4%)  | 1 (0%)   | 44          | 53 |
| 1   | E     | 339/341 (99%)   | 323 (95%)  | 15 (4%)  | 1 (0%)   | 44          | 53 |
| 1   | F     | 339/341 (99%)   | 318 (94%)  | 20 (6%)  | 1 (0%)   | 44          | 53 |
| 1   | G     | 339/341 (99%)   | 319 (94%)  | 17 (5%)  | 3 (1%)   | 20          | 21 |
| 1   | H     | 339/341 (99%)   | 322 (95%)  | 16 (5%)  | 1 (0%)   | 44          | 53 |
| 1   | I     | 338/341 (99%)   | 324 (96%)  | 13 (4%)  | 1 (0%)   | 44          | 53 |
| 1   | J     | 338/341 (99%)   | 319 (94%)  | 18 (5%)  | 1 (0%)   | 44          | 53 |
| 1   | K     | 339/341 (99%)   | 326 (96%)  | 12 (4%)  | 1 (0%)   | 44          | 53 |
| 1   | L     | 339/341 (99%)   | 319 (94%)  | 19 (6%)  | 1 (0%)   | 44          | 53 |
| All | All   | 4066/4092 (99%) | 3858 (95%) | 194 (5%) | 14 (0%)  | 44          | 53 |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 94  | VAL  |
| 1   | G     | 290 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 291 | ILE  |
| 1   | D     | 94  | VAL  |
| 1   | A     | 94  | VAL  |
| 1   | H     | 94  | VAL  |
| 1   | B     | 94  | VAL  |
| 1   | I     | 94  | VAL  |
| 1   | K     | 94  | VAL  |
| 1   | C     | 94  | VAL  |
| 1   | J     | 94  | VAL  |
| 1   | L     | 94  | VAL  |
| 1   | E     | 94  | VAL  |
| 1   | G     | 94  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | A     | 253/253 (100%)   | 248 (98%)  | 5 (2%)   | 60          | 73 |
| 1   | B     | 253/253 (100%)   | 247 (98%)  | 6 (2%)   | 54          | 67 |
| 1   | C     | 253/253 (100%)   | 248 (98%)  | 5 (2%)   | 60          | 73 |
| 1   | D     | 253/253 (100%)   | 244 (96%)  | 9 (4%)   | 40          | 51 |
| 1   | E     | 253/253 (100%)   | 246 (97%)  | 7 (3%)   | 49          | 61 |
| 1   | F     | 253/253 (100%)   | 249 (98%)  | 4 (2%)   | 68          | 79 |
| 1   | G     | 253/253 (100%)   | 247 (98%)  | 6 (2%)   | 54          | 67 |
| 1   | H     | 253/253 (100%)   | 248 (98%)  | 5 (2%)   | 60          | 73 |
| 1   | I     | 253/253 (100%)   | 246 (97%)  | 7 (3%)   | 49          | 61 |
| 1   | J     | 253/253 (100%)   | 247 (98%)  | 6 (2%)   | 54          | 67 |
| 1   | K     | 253/253 (100%)   | 247 (98%)  | 6 (2%)   | 54          | 67 |
| 1   | L     | 253/253 (100%)   | 248 (98%)  | 5 (2%)   | 60          | 73 |
| All | All   | 3036/3036 (100%) | 2965 (98%) | 71 (2%)  | 56          | 68 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | LYS  |
| 1   | A     | 117 | GLU  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 158 | HIS  |
| 1   | A     | 256 | SER  |
| 1   | B     | 28  | GLU  |
| 1   | B     | 117 | GLU  |
| 1   | B     | 137 | ASP  |
| 1   | B     | 158 | HIS  |
| 1   | B     | 164 | MET  |
| 1   | B     | 293 | PHE  |
| 1   | C     | 10  | LYS  |
| 1   | C     | 42  | GLU  |
| 1   | C     | 117 | GLU  |
| 1   | C     | 158 | HIS  |
| 1   | C     | 306 | ARG  |
| 1   | D     | 10  | LYS  |
| 1   | D     | 53  | ARG  |
| 1   | D     | 108 | GLN  |
| 1   | D     | 117 | GLU  |
| 1   | D     | 147 | LYS  |
| 1   | D     | 158 | HIS  |
| 1   | D     | 164 | MET  |
| 1   | D     | 288 | GLN  |
| 1   | D     | 293 | PHE  |
| 1   | E     | 28  | GLU  |
| 1   | E     | 46  | ASP  |
| 1   | E     | 117 | GLU  |
| 1   | E     | 137 | ASP  |
| 1   | E     | 152 | LEU  |
| 1   | E     | 158 | HIS  |
| 1   | E     | 284 | ASP  |
| 1   | F     | 28  | GLU  |
| 1   | F     | 117 | GLU  |
| 1   | F     | 152 | LEU  |
| 1   | F     | 158 | HIS  |
| 1   | G     | 28  | GLU  |
| 1   | G     | 117 | GLU  |
| 1   | G     | 137 | ASP  |
| 1   | G     | 158 | HIS  |
| 1   | G     | 168 | TYR  |
| 1   | G     | 280 | SER  |
| 1   | H     | 117 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 158 | HIS  |
| 1   | H     | 164 | MET  |
| 1   | H     | 280 | SER  |
| 1   | H     | 292 | SER  |
| 1   | I     | 28  | GLU  |
| 1   | I     | 94  | VAL  |
| 1   | I     | 117 | GLU  |
| 1   | I     | 152 | LEU  |
| 1   | I     | 158 | HIS  |
| 1   | I     | 168 | TYR  |
| 1   | I     | 280 | SER  |
| 1   | J     | 18  | LEU  |
| 1   | J     | 28  | GLU  |
| 1   | J     | 117 | GLU  |
| 1   | J     | 158 | HIS  |
| 1   | J     | 168 | TYR  |
| 1   | J     | 327 | GLU  |
| 1   | K     | 28  | GLU  |
| 1   | K     | 117 | GLU  |
| 1   | K     | 152 | LEU  |
| 1   | K     | 158 | HIS  |
| 1   | K     | 168 | TYR  |
| 1   | K     | 284 | ASP  |
| 1   | L     | 28  | GLU  |
| 1   | L     | 117 | GLU  |
| 1   | L     | 152 | LEU  |
| 1   | L     | 158 | HIS  |
| 1   | L     | 327 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 197 | HIS  |
| 1   | C     | 197 | HIS  |
| 1   | F     | 198 | HIS  |
| 1   | H     | 69  | ASN  |
| 1   | J     | 69  | ASN  |
| 1   | L     | 13  | ASN  |
| 1   | L     | 331 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 68 ligands modelled in this entry, 44 are monoatomic - leaving 24 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | PO4  | A     | 353 | -    | 4,4,4        | 1.32 | 0           | 6,6,6       | 0.40 | 0           |
| 2   | CXS  | A     | 401 | 6    | 14,14,14     | 1.54 | 2 (14%)     | 16,18,18    | 2.68 | 4 (25%)     |
| 3   | PO4  | B     | 352 | -    | 4,4,4        | 1.39 | 0           | 6,6,6       | 0.41 | 0           |
| 2   | CXS  | B     | 402 | 6    | 14,14,14     | 1.44 | 2 (14%)     | 16,18,18    | 2.59 | 4 (25%)     |
| 3   | PO4  | C     | 353 | -    | 4,4,4        | 1.34 | 0           | 6,6,6       | 0.39 | 0           |
| 2   | CXS  | C     | 403 | 6    | 14,14,14     | 1.54 | 2 (14%)     | 16,18,18    | 2.59 | 4 (25%)     |
| 3   | PO4  | D     | 352 | -    | 4,4,4        | 1.38 | 0           | 6,6,6       | 0.41 | 0           |
| 2   | CXS  | D     | 404 | 6    | 14,14,14     | 1.67 | 1 (7%)      | 16,18,18    | 2.60 | 4 (25%)     |
| 3   | PO4  | E     | 353 | -    | 4,4,4        | 1.47 | 0           | 6,6,6       | 0.38 | 0           |
| 2   | CXS  | E     | 405 | 6    | 14,14,14     | 1.40 | 2 (14%)     | 16,18,18    | 2.71 | 4 (25%)     |
| 3   | PO4  | F     | 352 | -    | 4,4,4        | 1.34 | 0           | 6,6,6       | 0.40 | 0           |
| 2   | CXS  | F     | 406 | 6    | 14,14,14     | 1.56 | 1 (7%)      | 16,18,18    | 2.58 | 3 (18%)     |
| 3   | PO4  | G     | 353 | -    | 4,4,4        | 1.34 | 0           | 6,6,6       | 0.39 | 0           |
| 2   | CXS  | G     | 407 | 6    | 14,14,14     | 1.56 | 2 (14%)     | 16,18,18    | 2.74 | 4 (25%)     |
| 3   | PO4  | H     | 352 | -    | 4,4,4        | 1.31 | 0           | 6,6,6       | 0.41 | 0           |
| 2   | CXS  | H     | 408 | 6    | 14,14,14     | 1.74 | 2 (14%)     | 16,18,18    | 2.62 | 3 (18%)     |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PO4  | I     | 353 | -    | 4,4,4        | 1.39 | 0        | 6,6,6       | 0.41 | 0        |
| 2   | CXS  | I     | 409 | 6    | 14,14,14     | 1.42 | 2 (14%)  | 16,18,18    | 2.61 | 4 (25%)  |
| 3   | PO4  | J     | 352 | -    | 4,4,4        | 1.29 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | CXS  | J     | 410 | 6    | 14,14,14     | 1.48 | 2 (14%)  | 16,18,18    | 2.83 | 4 (25%)  |
| 3   | PO4  | K     | 353 | -    | 4,4,4        | 1.35 | 0        | 6,6,6       | 0.41 | 0        |
| 2   | CXS  | K     | 411 | 6    | 14,14,14     | 1.47 | 1 (7%)   | 16,18,18    | 2.64 | 3 (18%)  |
| 3   | PO4  | L     | 352 | -    | 4,4,4        | 1.36 | 0        | 6,6,6       | 0.41 | 0        |
| 2   | CXS  | L     | 412 | 6    | 14,14,14     | 1.55 | 1 (7%)   | 16,18,18    | 2.74 | 4 (25%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | PO4  | A     | 353 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | A     | 401 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | B     | 352 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | B     | 402 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | C     | 353 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | C     | 403 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | D     | 352 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | D     | 404 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | E     | 353 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | E     | 405 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | F     | 352 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | F     | 406 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | G     | 353 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | G     | 407 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | H     | 352 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | H     | 408 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | I     | 353 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | I     | 409 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | J     | 352 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | J     | 410 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | K     | 353 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | K     | 411 | 6    | -       | 0/8/16/16 | 0/1/1/1 |
| 3   | PO4  | L     | 352 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | CXS  | L     | 412 | 6    | -       | 0/8/16/16 | 0/1/1/1 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | H     | 408 | CXS  | C1-S  | -5.05 | 1.69        | 1.77     |
| 2   | D     | 404 | CXS  | C1-S  | -4.96 | 1.70        | 1.77     |
| 2   | F     | 406 | CXS  | C1-S  | -4.43 | 1.70        | 1.77     |
| 2   | L     | 412 | CXS  | C1-S  | -4.43 | 1.70        | 1.77     |
| 2   | K     | 411 | CXS  | C1-S  | -4.23 | 1.71        | 1.77     |
| 2   | C     | 403 | CXS  | C1-S  | -4.22 | 1.71        | 1.77     |
| 2   | B     | 402 | CXS  | C1-S  | -4.07 | 1.71        | 1.77     |
| 2   | A     | 401 | CXS  | C1-S  | -4.07 | 1.71        | 1.77     |
| 2   | G     | 407 | CXS  | C1-S  | -3.89 | 1.71        | 1.77     |
| 2   | J     | 410 | CXS  | C1-S  | -3.83 | 1.71        | 1.77     |
| 2   | I     | 409 | CXS  | C1-S  | -3.75 | 1.71        | 1.77     |
| 2   | E     | 405 | CXS  | C1-S  | -3.65 | 1.72        | 1.77     |
| 2   | E     | 405 | CXS  | C9-C4 | 2.01  | 1.56        | 1.51     |
| 2   | B     | 402 | CXS  | C9-C4 | 2.08  | 1.57        | 1.51     |
| 2   | I     | 409 | CXS  | C9-C4 | 2.29  | 1.57        | 1.51     |
| 2   | J     | 410 | CXS  | C9-C4 | 2.35  | 1.57        | 1.51     |
| 2   | H     | 408 | CXS  | C9-C4 | 2.47  | 1.58        | 1.51     |
| 2   | C     | 403 | CXS  | C9-C4 | 2.49  | 1.58        | 1.51     |
| 2   | G     | 407 | CXS  | C9-C4 | 2.49  | 1.58        | 1.51     |
| 2   | A     | 401 | CXS  | C9-C4 | 2.53  | 1.58        | 1.51     |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | L     | 412 | CXS  | O1-S-C1  | -5.11 | 102.41      | 106.79   |
| 2   | A     | 401 | CXS  | O1-S-C1  | -5.08 | 102.43      | 106.79   |
| 2   | G     | 407 | CXS  | O1-S-C1  | -4.71 | 102.75      | 106.79   |
| 2   | H     | 408 | CXS  | O1-S-C1  | -4.70 | 102.75      | 106.79   |
| 2   | I     | 409 | CXS  | O1-S-C1  | -4.62 | 102.82      | 106.79   |
| 2   | C     | 403 | CXS  | O1-S-C1  | -4.55 | 102.89      | 106.79   |
| 2   | K     | 411 | CXS  | O1-S-C1  | -4.54 | 102.89      | 106.79   |
| 2   | J     | 410 | CXS  | O1-S-C1  | -4.52 | 102.91      | 106.79   |
| 2   | F     | 406 | CXS  | O1-S-C1  | -4.47 | 102.95      | 106.79   |
| 2   | E     | 405 | CXS  | O1-S-C1  | -4.34 | 103.06      | 106.79   |
| 2   | B     | 402 | CXS  | O1-S-C1  | -4.09 | 103.28      | 106.79   |
| 2   | D     | 404 | CXS  | O1-S-C1  | -3.84 | 103.49      | 106.79   |
| 2   | E     | 405 | CXS  | C9-C4-C5 | -2.56 | 106.73      | 110.85   |
| 2   | G     | 407 | CXS  | C9-C4-C5 | -2.55 | 106.75      | 110.85   |
| 2   | J     | 410 | CXS  | C9-C4-C5 | -2.50 | 106.83      | 110.85   |
| 2   | H     | 408 | CXS  | C9-C4-C5 | -2.50 | 106.83      | 110.85   |
| 2   | B     | 402 | CXS  | C9-C4-C5 | -2.44 | 106.91      | 110.85   |
| 2   | K     | 411 | CXS  | C9-C4-C5 | -2.31 | 107.13      | 110.85   |
| 2   | F     | 406 | CXS  | C9-C4-C5 | -2.27 | 107.20      | 110.85   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | A     | 401 | CXS  | C9-C4-C5 | -2.22 | 107.27      | 110.85   |
| 2   | D     | 404 | CXS  | C9-C4-C5 | -2.19 | 107.32      | 110.85   |
| 2   | C     | 403 | CXS  | C9-C4-C5 | -2.18 | 107.34      | 110.85   |
| 2   | L     | 412 | CXS  | C9-C4-C5 | -2.16 | 107.37      | 110.85   |
| 2   | I     | 409 | CXS  | C9-C4-C5 | -2.13 | 107.42      | 110.85   |
| 2   | G     | 407 | CXS  | C8-C9-C4 | 2.07  | 114.14      | 111.11   |
| 2   | J     | 410 | CXS  | C8-C9-C4 | 2.13  | 114.24      | 111.11   |
| 2   | L     | 412 | CXS  | C8-C9-C4 | 2.18  | 114.31      | 111.11   |
| 2   | C     | 403 | CXS  | C8-C9-C4 | 2.20  | 114.33      | 111.11   |
| 2   | D     | 404 | CXS  | C8-C9-C4 | 2.23  | 114.38      | 111.11   |
| 2   | A     | 401 | CXS  | C8-C9-C4 | 2.30  | 114.49      | 111.11   |
| 2   | I     | 409 | CXS  | C8-C9-C4 | 2.31  | 114.50      | 111.11   |
| 2   | E     | 405 | CXS  | C8-C9-C4 | 2.36  | 114.58      | 111.11   |
| 2   | B     | 402 | CXS  | C8-C9-C4 | 2.52  | 114.81      | 111.11   |
| 2   | H     | 408 | CXS  | O3-S-C1  | 8.27  | 116.23      | 106.06   |
| 2   | C     | 403 | CXS  | O3-S-C1  | 8.28  | 116.24      | 106.06   |
| 2   | I     | 409 | CXS  | O3-S-C1  | 8.30  | 116.27      | 106.06   |
| 2   | B     | 402 | CXS  | O3-S-C1  | 8.37  | 116.36      | 106.06   |
| 2   | A     | 401 | CXS  | O3-S-C1  | 8.39  | 116.38      | 106.06   |
| 2   | F     | 406 | CXS  | O3-S-C1  | 8.40  | 116.39      | 106.06   |
| 2   | D     | 404 | CXS  | O3-S-C1  | 8.53  | 116.55      | 106.06   |
| 2   | K     | 411 | CXS  | O3-S-C1  | 8.59  | 116.61      | 106.06   |
| 2   | L     | 412 | CXS  | O3-S-C1  | 8.75  | 116.82      | 106.06   |
| 2   | E     | 405 | CXS  | O3-S-C1  | 8.83  | 116.91      | 106.06   |
| 2   | G     | 407 | CXS  | O3-S-C1  | 8.85  | 116.94      | 106.06   |
| 2   | J     | 410 | CXS  | O3-S-C1  | 9.26  | 117.44      | 106.06   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 26 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 401 | CXS  | 1       | 0            |
| 2   | B     | 402 | CXS  | 4       | 0            |
| 2   | C     | 403 | CXS  | 1       | 0            |
| 2   | D     | 404 | CXS  | 6       | 0            |
| 2   | E     | 405 | CXS  | 3       | 0            |
| 2   | F     | 406 | CXS  | 1       | 0            |
| 2   | G     | 407 | CXS  | 1       | 0            |
| 2   | I     | 409 | CXS  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | J     | 410 | CXS  | 1       | 0            |
| 2   | K     | 411 | CXS  | 3       | 0            |
| 2   | L     | 412 | CXS  | 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 341/341 (100%)  | -0.51  | 1 (0%) 93 97  | 22, 33, 46, 63        | 0     |
| 1   | B     | 341/341 (100%)  | -0.40  | 3 (0%) 84 91  | 24, 36, 52, 60        | 0     |
| 1   | C     | 341/341 (100%)  | -0.39  | 1 (0%) 93 97  | 21, 34, 47, 66        | 0     |
| 1   | D     | 341/341 (100%)  | -0.50  | 1 (0%) 93 97  | 23, 34, 46, 60        | 0     |
| 1   | E     | 341/341 (100%)  | -0.35  | 2 (0%) 89 94  | 25, 36, 52, 61        | 0     |
| 1   | F     | 341/341 (100%)  | -0.16  | 7 (2%) 64 74  | 23, 38, 57, 65        | 0     |
| 1   | G     | 341/341 (100%)  | -0.33  | 4 (1%) 79 87  | 24, 36, 52, 65        | 0     |
| 1   | H     | 341/341 (100%)  | -0.24  | 7 (2%) 64 74  | 23, 38, 53, 66        | 0     |
| 1   | I     | 340/341 (99%)   | -0.46  | 0 100 100     | 24, 36, 48, 66        | 0     |
| 1   | J     | 340/341 (99%)   | -0.20  | 5 (1%) 74 83  | 26, 41, 64, 76        | 0     |
| 1   | K     | 341/341 (100%)  | -0.42  | 3 (0%) 84 91  | 26, 36, 49, 66        | 0     |
| 1   | L     | 341/341 (100%)  | -0.30  | 5 (1%) 74 83  | 26, 38, 52, 67        | 0     |
| All | All   | 4090/4092 (99%) | -0.36  | 39 (0%) 82 90 | 21, 36, 52, 76        | 0     |

All (39) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 341 | GLY  | 4.4  |
| 1   | F     | 341 | GLY  | 3.7  |
| 1   | F     | 254 | PRO  | 3.4  |
| 1   | F     | 257 | VAL  | 3.3  |
| 1   | L     | 341 | GLY  | 3.2  |
| 1   | A     | 53  | ARG  | 3.2  |
| 1   | L     | 53  | ARG  | 3.2  |
| 1   | G     | 325 | VAL  | 3.2  |
| 1   | F     | 252 | GLY  | 3.2  |
| 1   | C     | 53  | ARG  | 3.0  |
| 1   | F     | 53  | ARG  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 143 | ALA  | 3.0  |
| 1   | H     | 291 | ILE  | 2.8  |
| 1   | J     | 325 | VAL  | 2.7  |
| 1   | D     | 53  | ARG  | 2.7  |
| 1   | G     | 324 | GLY  | 2.7  |
| 1   | K     | 144 | ALA  | 2.6  |
| 1   | H     | 53  | ARG  | 2.6  |
| 1   | J     | 43  | ALA  | 2.6  |
| 1   | G     | 252 | GLY  | 2.6  |
| 1   | J     | 252 | GLY  | 2.5  |
| 1   | G     | 80  | ALA  | 2.4  |
| 1   | J     | 288 | GLN  | 2.4  |
| 1   | E     | 291 | ILE  | 2.4  |
| 1   | H     | 256 | SER  | 2.4  |
| 1   | L     | 252 | GLY  | 2.4  |
| 1   | F     | 260 | GLU  | 2.3  |
| 1   | H     | 147 | LYS  | 2.3  |
| 1   | H     | 35  | TRP  | 2.3  |
| 1   | B     | 290 | PRO  | 2.2  |
| 1   | L     | 254 | PRO  | 2.2  |
| 1   | K     | 341 | GLY  | 2.2  |
| 1   | K     | 53  | ARG  | 2.2  |
| 1   | L     | 35  | TRP  | 2.2  |
| 1   | H     | 252 | GLY  | 2.1  |
| 1   | J     | 46  | ASP  | 2.1  |
| 1   | E     | 144 | ALA  | 2.1  |
| 1   | B     | 53  | ARG  | 2.0  |
| 1   | F     | 143 | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 5   | NA   | C     | 343 | 1/1   | 0.99 | 0.18 | 9.63  | 14,14,14,14                | 0     |
| 5   | NA   | D     | 343 | 1/1   | 1.00 | 0.17 | 9.01  | 14,14,14,14                | 0     |
| 2   | CXS  | A     | 401 | 14/14 | 0.92 | 0.23 | 8.08  | 89,95,98,98                | 0     |
| 2   | CXS  | K     | 411 | 14/14 | 0.95 | 0.23 | 7.88  | 92,96,100,101              | 0     |
| 2   | CXS  | C     | 403 | 14/14 | 0.92 | 0.30 | 7.84  | 85,92,97,97                | 0     |
| 5   | NA   | E     | 343 | 1/1   | 0.99 | 0.14 | 5.32  | 16,16,16,16                | 0     |
| 5   | NA   | I     | 343 | 1/1   | 0.97 | 0.15 | 5.11  | 20,20,20,20                | 0     |
| 2   | CXS  | J     | 410 | 14/14 | 0.87 | 0.26 | 5.01  | 88,93,99,99                | 0     |
| 5   | NA   | A     | 343 | 1/1   | 0.99 | 0.16 | 4.98  | 14,14,14,14                | 0     |
| 2   | CXS  | F     | 406 | 14/14 | 0.90 | 0.27 | 4.87  | 97,102,106,106             | 0     |
| 5   | NA   | B     | 343 | 1/1   | 0.99 | 0.15 | 4.60  | 13,13,13,13                | 0     |
| 2   | CXS  | D     | 404 | 14/14 | 0.92 | 0.24 | 4.47  | 78,84,88,88                | 0     |
| 2   | CXS  | I     | 409 | 14/14 | 0.95 | 0.20 | 3.68  | 80,87,91,91                | 0     |
| 5   | NA   | G     | 343 | 1/1   | 0.99 | 0.19 | 3.61  | 16,16,16,16                | 0     |
| 2   | CXS  | B     | 402 | 14/14 | 0.94 | 0.20 | 3.32  | 85,92,96,96                | 0     |
| 2   | CXS  | L     | 412 | 14/14 | 0.93 | 0.23 | 3.24  | 85,90,96,96                | 0     |
| 5   | NA   | K     | 343 | 1/1   | 0.98 | 0.16 | 2.84  | 19,19,19,19                | 0     |
| 2   | CXS  | H     | 408 | 14/14 | 0.93 | 0.26 | 2.75  | 94,98,103,103              | 0     |
| 2   | CXS  | G     | 407 | 14/14 | 0.94 | 0.19 | 2.03  | 76,80,86,86                | 0     |
| 2   | CXS  | E     | 405 | 14/14 | 0.92 | 0.20 | 1.93  | 78,85,90,90                | 0     |
| 5   | NA   | J     | 343 | 1/1   | 0.97 | 0.13 | 1.77  | 22,22,22,22                | 0     |
| 5   | NA   | H     | 343 | 1/1   | 0.99 | 0.11 | 1.42  | 24,24,24,24                | 0     |
| 5   | NA   | L     | 343 | 1/1   | 0.92 | 0.12 | 0.56  | 25,25,25,25                | 0     |
| 3   | PO4  | K     | 353 | 5/5   | 0.91 | 0.16 | 0.26  | 87,87,88,89                | 0     |
| 3   | PO4  | L     | 352 | 5/5   | 0.83 | 0.17 | 0.20  | 102,102,103,103            | 0     |
| 5   | NA   | F     | 343 | 1/1   | 0.91 | 0.11 | 0.13  | 27,27,27,27                | 0     |
| 3   | PO4  | I     | 353 | 5/5   | 0.92 | 0.15 | 0.10  | 87,87,88,88                | 0     |
| 4   | K    | G     | 344 | 1/1   | 0.83 | 0.16 | 0.07  | 120,120,120,120            | 0     |
| 4   | K    | C     | 342 | 1/1   | 0.98 | 0.09 | 0.06  | 29,29,29,29                | 0     |
| 3   | PO4  | E     | 353 | 5/5   | 0.97 | 0.13 | 0.02  | 74,74,75,76                | 0     |
| 4   | K    | H     | 344 | 1/1   | 0.93 | 0.15 | 0.01  | 72,72,72,72                | 0     |
| 4   | K    | E     | 342 | 1/1   | 0.99 | 0.09 | -0.17 | 33,33,33,33                | 0     |
| 3   | PO4  | A     | 353 | 5/5   | 0.94 | 0.12 | -0.26 | 71,73,73,74                | 0     |
| 4   | K    | G     | 342 | 1/1   | 0.99 | 0.08 | -0.32 | 30,30,30,30                | 0     |
| 3   | PO4  | D     | 352 | 5/5   | 0.91 | 0.11 | -0.39 | 78,79,79,79                | 0     |
| 4   | K    | E     | 344 | 1/1   | 0.78 | 0.13 | -0.56 | 96,96,96,96                | 0     |
| 4   | K    | B     | 342 | 1/1   | 0.98 | 0.08 | -0.64 | 32,32,32,32                | 0     |
| 4   | K    | A     | 342 | 1/1   | 0.99 | 0.08 | -0.71 | 29,29,29,29                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 4   | K    | K     | 342 | 1/1   | 0.99 | 0.09 | -0.75 | 33,33,33,33                 | 0     |
| 4   | K    | C     | 344 | 1/1   | 0.93 | 0.10 | -0.88 | 77,77,77,77                 | 0     |
| 6   | ZN   | C     | 345 | 1/1   | 0.98 | 0.09 | -1.21 | 51,51,51,51                 | 0     |
| 4   | K    | L     | 344 | 1/1   | 0.90 | 0.09 | -1.23 | 84,84,84,84                 | 0     |
| 4   | K    | J     | 342 | 1/1   | 1.00 | 0.10 | -1.24 | 39,39,39,39                 | 0     |
| 4   | K    | A     | 344 | 1/1   | 0.97 | 0.07 | -1.39 | 73,73,73,73                 | 0     |
| 4   | K    | F     | 344 | 1/1   | 0.34 | 0.10 | -1.40 | 100,100,100,100             | 0     |
| 6   | ZN   | G     | 345 | 1/1   | 0.99 | 0.04 | -1.71 | 48,48,48,48                 | 0     |
| 6   | ZN   | D     | 345 | 1/1   | 0.99 | 0.04 | -1.78 | 46,46,46,46                 | 0     |
| 4   | K    | I     | 342 | 1/1   | 1.00 | 0.05 | -1.99 | 32,32,32,32                 | 0     |
| 6   | ZN   | I     | 344 | 1/1   | 0.96 | 0.05 | -2.30 | 51,51,51,51                 | 0     |
| 6   | ZN   | J     | 344 | 1/1   | 0.99 | 0.07 | -2.30 | 58,58,58,58                 | 0     |
| 6   | ZN   | H     | 345 | 1/1   | 0.97 | 0.05 | -2.54 | 51,51,51,51                 | 0     |
| 4   | K    | D     | 344 | 1/1   | 0.97 | 0.05 | -2.64 | 69,69,69,69                 | 0     |
| 4   | K    | D     | 342 | 1/1   | 0.99 | 0.04 | -2.78 | 29,29,29,29                 | 0     |
| 4   | K    | H     | 342 | 1/1   | 0.99 | 0.07 | -2.91 | 34,34,34,34                 | 0     |
| 6   | ZN   | E     | 345 | 1/1   | 0.99 | 0.05 | -3.04 | 50,50,50,50                 | 0     |
| 4   | K    | F     | 342 | 1/1   | 0.99 | 0.04 | -3.10 | 31,31,31,31                 | 0     |
| 6   | ZN   | B     | 344 | 1/1   | 0.98 | 0.05 | -3.22 | 53,53,53,53                 | 0     |
| 6   | ZN   | F     | 345 | 1/1   | 0.98 | 0.04 | -3.53 | 58,58,58,58                 | 0     |
| 6   | ZN   | A     | 345 | 1/1   | 0.99 | 0.04 | -3.84 | 52,52,52,52                 | 0     |
| 4   | K    | L     | 342 | 1/1   | 0.99 | 0.04 | -4.26 | 31,31,31,31                 | 0     |
| 6   | ZN   | K     | 344 | 1/1   | 0.96 | 0.05 | -4.59 | 53,53,53,53                 | 0     |
| 6   | ZN   | L     | 345 | 1/1   | 0.99 | 0.04 | -5.62 | 49,49,49,49                 | 0     |
| 3   | PO4  | C     | 353 | 5/5   | 0.95 | 0.08 | -     | 75,76,77,77                 | 0     |
| 3   | PO4  | G     | 353 | 5/5   | 0.95 | 0.13 | -     | 77,77,79,79                 | 0     |
| 3   | PO4  | H     | 352 | 5/5   | 0.89 | 0.12 | -     | 97,97,98,98                 | 0     |
| 3   | PO4  | J     | 352 | 5/5   | 0.96 | 0.08 | -     | 84,84,85,85                 | 0     |
| 3   | PO4  | B     | 352 | 5/5   | 0.97 | 0.11 | -     | 65,66,67,68                 | 0     |
| 3   | PO4  | F     | 352 | 5/5   | 0.91 | 0.11 | -     | 90,91,92,92                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.