



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:14 AM GMT

PDB ID : 3HK9  
Title : Crystal structure of uronate isomerase from *Bacillus halodurans* complexed with zinc and D-Glucuronate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Nguyen, T.T.; Raushel, F.M.; Almo, S.C.  
Deposited on : 2009-05-22  
Resolution : 2.10 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

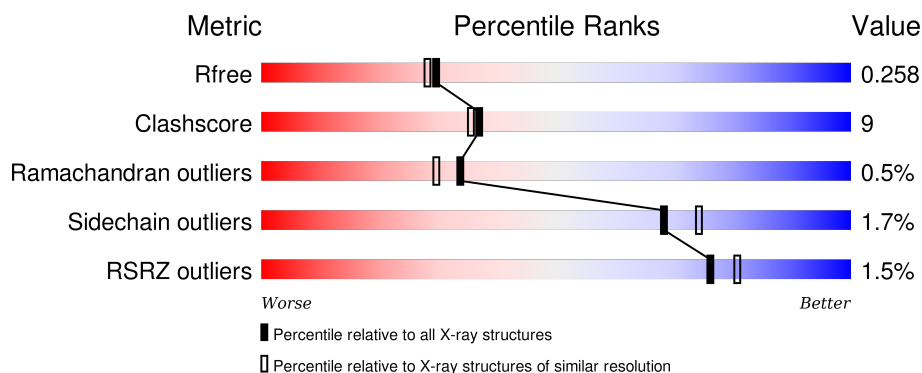
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 3939 (2.10-2.10)                                      |
| Clashscore            | 102246                      | 4460 (2.10-2.10)                                      |
| Ramachandran outliers | 100387                      | 4413 (2.10-2.10)                                      |
| Sidechain outliers    | 100360                      | 4414 (2.10-2.10)                                      |
| RSRZ outliers         | 91569                       | 3948 (2.10-2.10)                                      |

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     | 427    | <div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>  |
| 1   | B     | 427    | <div> <div>4%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>..</div> </div> </div> |
| 1   | C     | 427    | <div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>  |
| 1   | D     | 427    | <div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>  |
| 1   | E     | 427    | <div> <div>2%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | F     | 427    | <div><div><div></div><div></div><div></div></div><div><div>2%</div><div>76%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div> |
| 1   | G     | 427    | <div><div><div></div><div></div><div></div></div><div><div>2%</div><div>74%</div><div>21%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div> |
| 1   | H     | 427    | <div><div><div></div><div></div><div></div></div><div><div>%</div><div>76%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>  |
| 1   | I     | 427    | <div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>  |
| 1   | J     | 427    | <div><div><div></div><div></div><div></div></div><div><div>%</div><div>75%</div><div>20%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>  |
| 1   | K     | 427    | <div><div><div></div><div></div><div></div></div><div><div>2%</div><div>76%</div><div>20%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div> |
| 1   | L     | 427    | <div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>17%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>  |

## 2 Entry composition

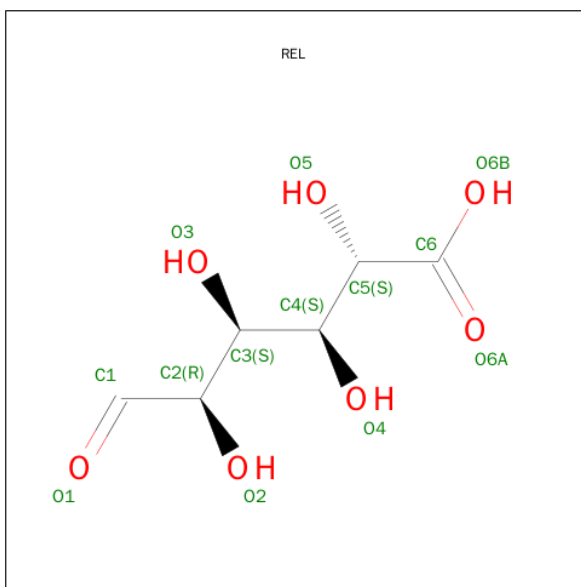
There are 6 unique types of molecules in this entry. The entry contains 42892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uronate isomerase.

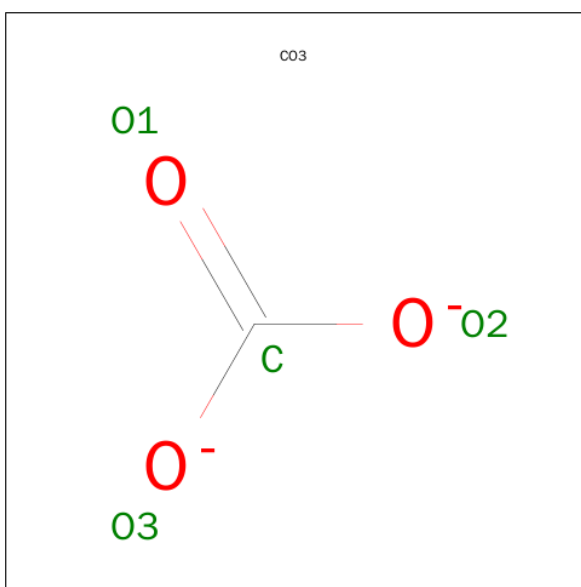
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | B     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | C     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | D     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | E     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | F     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | G     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | H     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | I     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | J     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | K     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |
| 1   | L     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 588 | 626 | 20 |         |         |       |

- Molecule 2 is SUGAR (D-GLUCURONIC ACID) (three-letter code: REL) (formula: C<sub>6</sub>H<sub>10</sub>O<sub>7</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | H     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | A     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | K     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | F     | 1        | Total Cl<br>1 1 | 0       | 0       |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6   | A     | 155      | Total O<br>155 155 | 0       | 0       |
| 6   | B     | 123      | Total O<br>123 123 | 0       | 0       |

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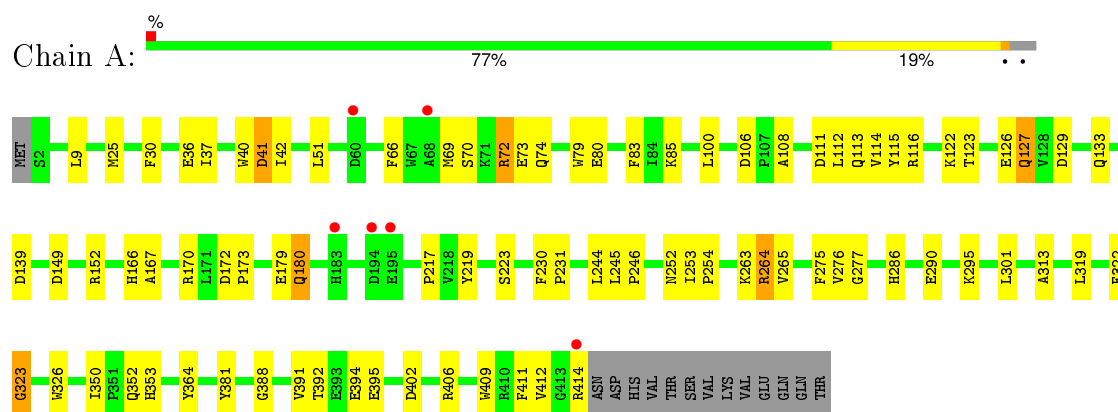
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | C     | 169      | Total<br>169 | O<br>169 | 0       | 0       |
| 6   | D     | 189      | Total<br>189 | O<br>189 | 0       | 0       |
| 6   | E     | 128      | Total<br>128 | O<br>128 | 0       | 0       |
| 6   | F     | 163      | Total<br>163 | O<br>163 | 0       | 0       |
| 6   | G     | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 6   | H     | 143      | Total<br>143 | O<br>143 | 0       | 0       |
| 6   | I     | 141      | Total<br>141 | O<br>141 | 0       | 0       |
| 6   | J     | 160      | Total<br>160 | O<br>160 | 0       | 0       |
| 6   | K     | 135      | Total<br>135 | O<br>135 | 0       | 0       |
| 6   | L     | 182      | Total<br>182 | O<br>182 | 0       | 0       |



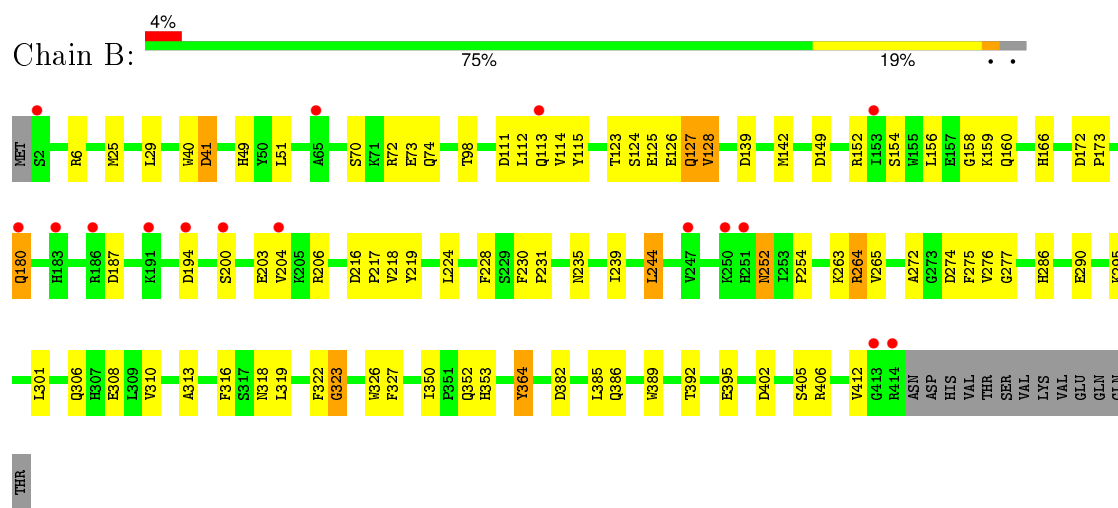
### 3 Residue-property plots

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

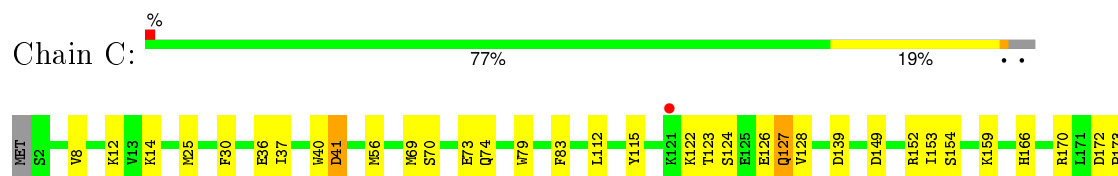
#### • Molecule 1: Uronate isomerase

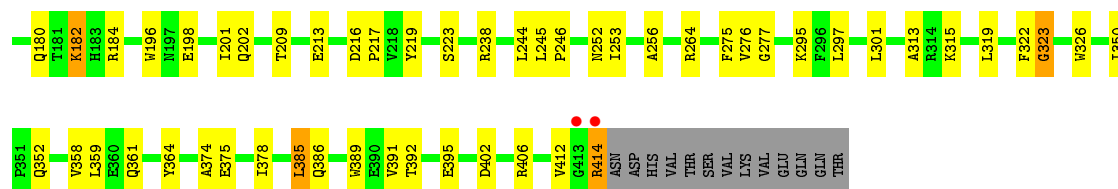


#### • Molecule 1: Uronate isomerase

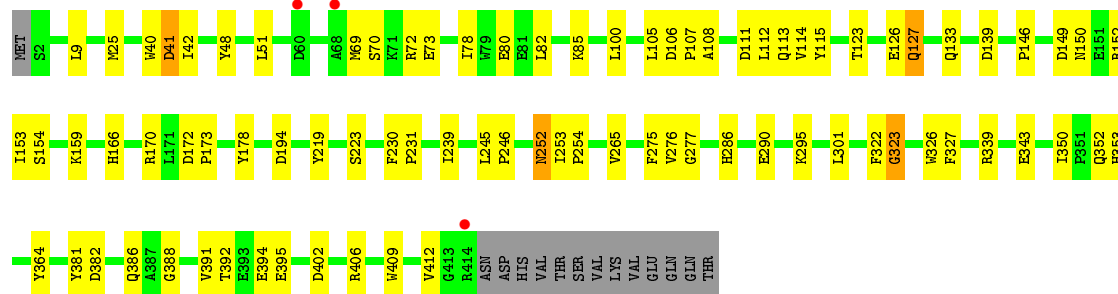
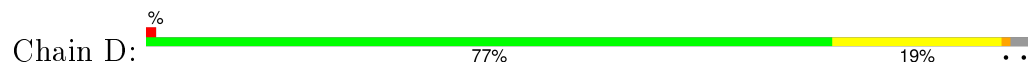


#### • Molecule 1: Uronate isomerase

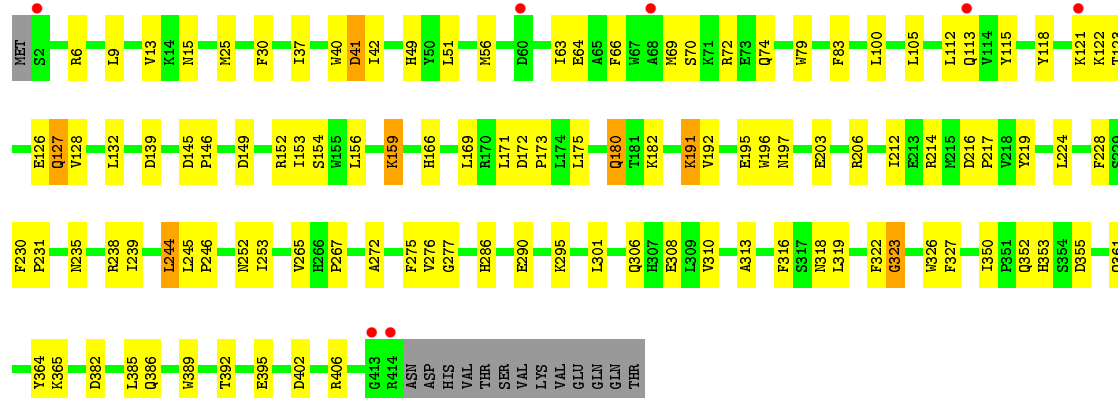




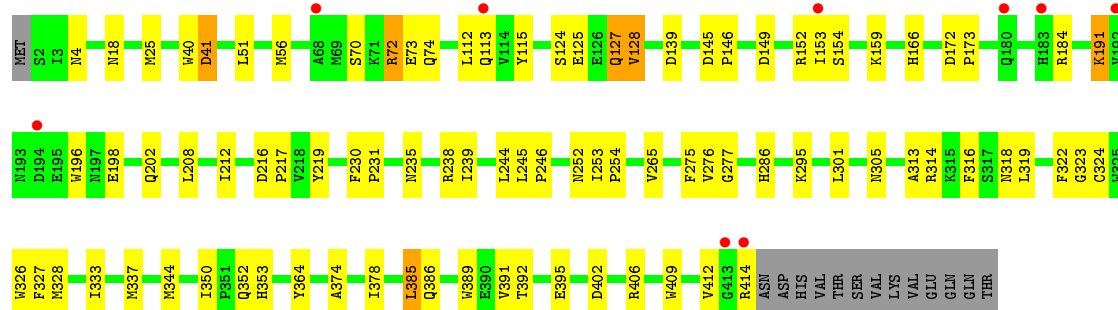
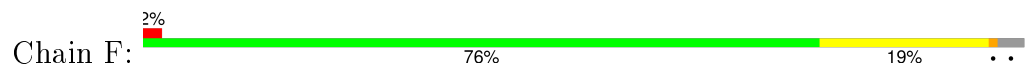
• Molecule 1: Uronate isomerase



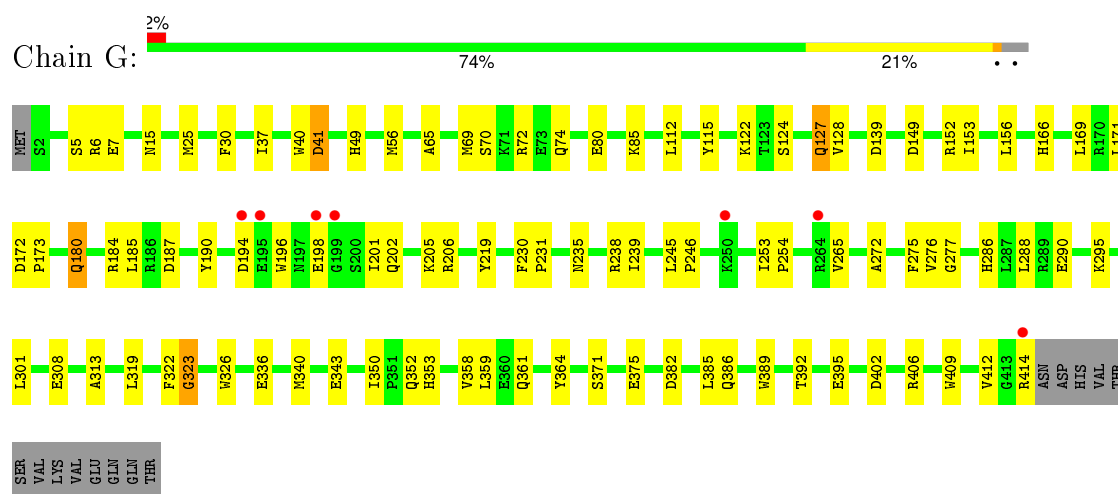
• Molecule 1: Uronate isomerase

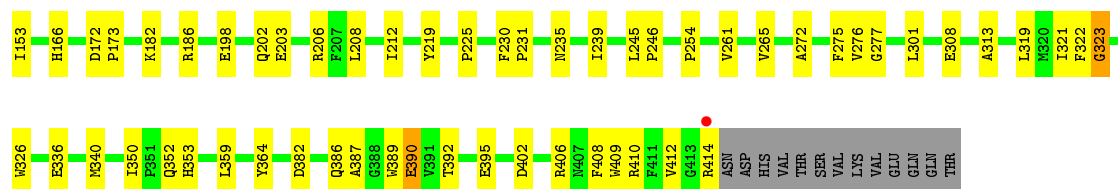


• Molecule 1: Uronate isomerase

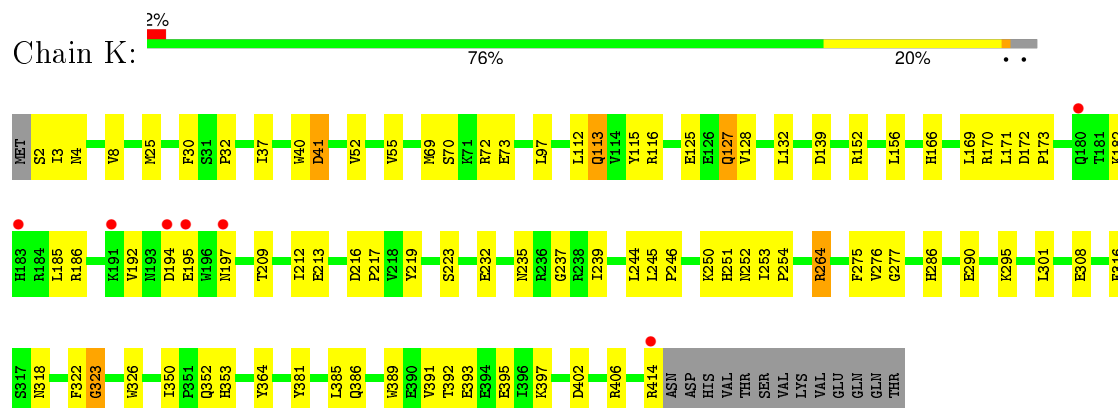


• Molecule 1: Uronate isomerase

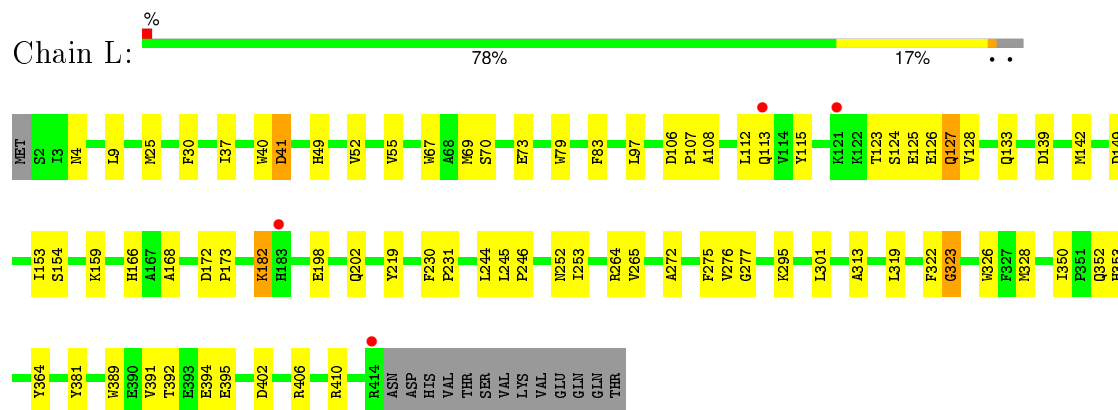




• Molecule 1: Uronate isomerase



• Molecule 1: Uronate isomerase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 274.09Å 156.88Å 185.21Å<br>90.00° 115.78° 90.00°            | Depositor        |
| Resolution (Å)  | 24.95 – 2.10<br>39.46 – 2.09                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.7 (24.95-2.10)<br>97.9 (39.46-2.09)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.40 (at 2.08Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.227 , 0.258<br>0.227 , 0.258                              | Depositor<br>DCC |
| $R_{free}$ test set   | 20316 reflections (5.03%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 26.5  | Xtriage          |
| Anisotropy  | 0.207   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 43.6   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Outliers  | 2 of 407624 reflections (0.000%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 42892   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 29.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, ZN, REL, CL

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     | 0.34         | 0/3488      | 0.60        | 0/4726      |
| 1   | B     | 0.33         | 0/3488      | 0.60        | 0/4726      |
| 1   | C     | 0.34         | 0/3488      | 0.61        | 0/4726      |
| 1   | D     | 0.35         | 0/3488      | 0.62        | 0/4726      |
| 1   | E     | 0.34         | 0/3488      | 0.61        | 0/4726      |
| 1   | F     | 0.34         | 0/3488      | 0.61        | 0/4726      |
| 1   | G     | 0.33         | 0/3488      | 0.61        | 0/4726      |
| 1   | H     | 0.34         | 0/3488      | 0.60        | 0/4726      |
| 1   | I     | 0.33         | 0/3488      | 0.61        | 0/4726      |
| 1   | J     | 0.34         | 0/3488      | 0.61        | 0/4726      |
| 1   | K     | 0.33         | 0/3488      | 0.60        | 0/4726      |
| 1   | L     | 0.34         | 0/3488      | 0.61        | 0/4726      |
| All | All   | 0.34         | 0/41856     | 0.61        | 0/56712     |

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 [i](#)

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     | 3404  | 0        | 3328     | 63      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 3404  | 0        | 3328     | 65      | 0            |
| 1   | C     | 3404  | 0        | 3328     | 59      | 0            |
| 1   | D     | 3404  | 0        | 3328     | 59      | 0            |
| 1   | E     | 3404  | 0        | 3328     | 77      | 0            |
| 1   | F     | 3404  | 0        | 3328     | 67      | 0            |
| 1   | G     | 3404  | 0        | 3328     | 66      | 0            |
| 1   | H     | 3404  | 0        | 3328     | 67      | 0            |
| 1   | I     | 3404  | 0        | 3328     | 55      | 0            |
| 1   | J     | 3404  | 0        | 3328     | 67      | 0            |
| 1   | K     | 3404  | 0        | 3328     | 58      | 0            |
| 1   | L     | 3404  | 0        | 3328     | 56      | 0            |
| 2   | A     | 13    | 0        | 8        | 1       | 0            |
| 2   | B     | 13    | 0        | 8        | 0       | 0            |
| 2   | C     | 13    | 0        | 8        | 1       | 0            |
| 2   | D     | 13    | 0        | 8        | 1       | 0            |
| 2   | E     | 13    | 0        | 8        | 0       | 0            |
| 2   | F     | 13    | 0        | 8        | 1       | 0            |
| 2   | G     | 13    | 0        | 8        | 1       | 0            |
| 2   | H     | 13    | 0        | 8        | 1       | 0            |
| 2   | I     | 13    | 0        | 8        | 0       | 0            |
| 2   | J     | 13    | 0        | 8        | 0       | 0            |
| 2   | K     | 13    | 0        | 8        | 1       | 0            |
| 2   | L     | 13    | 0        | 8        | 1       | 0            |
| 3   | A     | 8     | 0        | 0        | 0       | 0            |
| 3   | C     | 4     | 0        | 0        | 0       | 0            |
| 3   | D     | 8     | 0        | 0        | 0       | 0            |
| 3   | F     | 4     | 0        | 0        | 0       | 0            |
| 3   | G     | 4     | 0        | 0        | 0       | 0            |
| 3   | H     | 4     | 0        | 0        | 0       | 0            |
| 3   | I     | 4     | 0        | 0        | 0       | 0            |
| 3   | J     | 4     | 0        | 0        | 0       | 0            |
| 3   | K     | 4     | 0        | 0        | 0       | 0            |
| 3   | L     | 4     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | F     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 1     | 0        | 0        | 0       | 0            |
| 5   | K     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 155   | 0        | 0        | 4       | 0            |
| 6   | B     | 123   | 0        | 0        | 1       | 0            |
| 6   | C     | 169   | 0        | 0        | 4       | 0            |
| 6   | D     | 189   | 0        | 0        | 4       | 0            |
| 6   | E     | 128   | 0        | 0        | 5       | 0            |
| 6   | F     | 163   | 0        | 0        | 2       | 0            |
| 6   | G     | 136   | 0        | 0        | 6       | 0            |
| 6   | H     | 143   | 0        | 0        | 6       | 0            |
| 6   | I     | 141   | 0        | 0        | 3       | 0            |
| 6   | J     | 160   | 0        | 0        | 5       | 0            |
| 6   | K     | 135   | 0        | 0        | 3       | 0            |
| 6   | L     | 182   | 0        | 0        | 7       | 0            |
| All | All   | 42892 | 0        | 40032    | 759     | 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 9.

All (759) 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:F:333:ILE:HG22 | 1:F:337:MET:HE2  | 1.21                     | 1.10              |
| 1:F:72:ARG:HB2   | 1:F:72:ARG:HH11  | 1.20                     | 1.05              |
| 1:G:127:GLN:HE21 | 1:G:127:GLN:HA   | 1.34                     | 0.92              |
| 1:H:4:ASN:HB3    | 6:H:1604:HOH:O   | 1.72                     | 0.90              |
| 1:J:127:GLN:HA   | 1:J:127:GLN:HE21 | 1.35                     | 0.90              |
| 1:C:385:LEU:HD11 | 1:C:391:VAL:HG12 | 1.54                     | 0.89              |
| 1:A:127:GLN:HA   | 1:A:127:GLN:HE21 | 1.37                     | 0.88              |
| 1:B:72:ARG:HB2   | 1:B:72:ARG:HH11  | 1.40                     | 0.86              |
| 1:D:127:GLN:HE21 | 1:D:127:GLN:HA   | 1.41                     | 0.86              |
| 1:F:127:GLN:HA   | 1:F:127:GLN:HE21 | 1.40                     | 0.86              |
| 1:K:32:PRO:HG3   | 1:K:128:VAL:HG11 | 1.58                     | 0.86              |
| 1:I:127:GLN:HA   | 1:I:127:GLN:HE21 | 1.42                     | 0.85              |
| 1:L:127:GLN:HA   | 1:L:127:GLN:HE21 | 1.42                     | 0.84              |
| 1:C:127:GLN:HA   | 1:C:127:GLN:HE21 | 1.42                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:72:ARG:HH11  | 1:E:72:ARG:HB2   | 1.41                     | 0.84              |
| 1:F:72:ARG:NH1   | 1:F:72:ARG:HB2   | 1.93                     | 0.83              |
| 1:C:36:GLU:HG2   | 6:C:1956:HOH:O   | 1.79                     | 0.82              |
| 1:B:111:ASP:O    | 1:B:114:VAL:HG12 | 1.79                     | 0.81              |
| 1:H:127:GLN:HE21 | 1:H:127:GLN:HA   | 1.44                     | 0.81              |
| 1:D:72:ARG:HB2   | 1:D:72:ARG:HH11  | 1.47                     | 0.79              |
| 1:F:324:CYS:HB3  | 1:F:337:MET:HE1  | 1.65                     | 0.79              |
| 1:H:40:TRP:O     | 1:H:41:ASP:HB3   | 1.81                     | 0.78              |
| 1:D:113:GLN:HA   | 1:D:113:GLN:HE21 | 1.49                     | 0.78              |
| 1:B:72:ARG:NH1   | 1:B:72:ARG:HB2   | 1.99                     | 0.78              |
| 1:B:392:THR:OG1  | 1:B:395:GLU:HG3  | 1.85                     | 0.77              |
| 1:E:72:ARG:NH1   | 1:E:72:ARG:HB2   | 1.98                     | 0.77              |
| 1:J:2:SER:OG     | 1:J:390:GLU:HG3  | 1.85                     | 0.77              |
| 1:K:127:GLN:HA   | 1:K:127:GLN:HE21 | 1.49                     | 0.76              |
| 1:F:124:SER:O    | 1:F:128:VAL:HG12 | 1.86                     | 0.76              |
| 1:E:195:GLU:HG2  | 6:E:453:HOH:O    | 1.85                     | 0.75              |
| 1:J:72:ARG:HH11  | 1:J:72:ARG:HB2   | 1.52                     | 0.74              |
| 1:B:127:GLN:HA   | 1:B:127:GLN:HE21 | 1.53                     | 0.74              |
| 1:J:410:ARG:HD3  | 6:J:436:HOH:O    | 1.86                     | 0.74              |
| 1:J:72:ARG:NH1   | 1:J:72:ARG:HB2   | 2.02                     | 0.74              |
| 1:L:410:ARG:HD3  | 6:L:866:HOH:O    | 1.87                     | 0.73              |
| 1:C:402:ASP:HA   | 1:C:406:ARG:HB2  | 1.71                     | 0.73              |
| 1:A:394:GLU:HG2  | 6:A:553:HOH:O    | 1.90                     | 0.72              |
| 1:E:127:GLN:HA   | 1:E:127:GLN:HE21 | 1.55                     | 0.71              |
| 1:F:252:ASN:HD21 | 1:F:295:LYS:HE3  | 1.54                     | 0.71              |
| 1:H:32:PRO:HG3   | 1:H:128:VAL:HG11 | 1.73                     | 0.71              |
| 1:D:72:ARG:HB2   | 1:D:72:ARG:NH1   | 2.06                     | 0.70              |
| 1:K:381:TYR:O    | 1:K:385:LEU:HD23 | 1.91                     | 0.70              |
| 6:G:1153:HOH:O   | 1:H:321:ILE:HG12 | 1.91                     | 0.69              |
| 1:B:323:GLY:HA2  | 1:B:352:GLN:HA   | 1.73                     | 0.69              |
| 1:K:264:ARG:HB2  | 1:K:264:ARG:HH11 | 1.58                     | 0.69              |
| 1:A:127:GLN:HA   | 1:A:127:GLN:NE2  | 2.08                     | 0.69              |
| 1:C:392:THR:OG1  | 1:C:395:GLU:HG3  | 1.93                     | 0.69              |
| 1:C:152:ARG:HH22 | 1:C:184:ARG:HH22 | 1.42                     | 0.68              |
| 1:F:113:GLN:HA   | 1:F:113:GLN:HE21 | 1.58                     | 0.68              |
| 1:L:113:GLN:HE21 | 1:L:113:GLN:HA   | 1.58                     | 0.68              |
| 1:E:25:MET:HG3   | 6:E:450:HOH:O    | 1.92                     | 0.68              |
| 1:E:182:LYS:HB2  | 1:E:192:VAL:HG21 | 1.75                     | 0.68              |
| 1:B:124:SER:O    | 1:B:128:VAL:HG12 | 1.93                     | 0.68              |
| 1:I:72:ARG:NH2   | 1:I:116:ARG:HD3  | 2.09                     | 0.68              |
| 1:F:402:ASP:HA   | 1:F:406:ARG:HB2  | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:180:GLN:H    | 1:B:180:GLN:NE2  | 1.92                     | 0.68              |
| 1:B:402:ASP:HA   | 1:B:406:ARG:HB2  | 1.75                     | 0.67              |
| 1:F:333:ILE:CG2  | 1:F:337:MET:HE2  | 2.13                     | 0.67              |
| 1:K:301:LEU:HD11 | 1:K:326:TRP:HB3  | 1.76                     | 0.67              |
| 1:H:149:ASP:O    | 1:H:153:ILE:HG12 | 1.93                     | 0.66              |
| 1:K:70:SER:OG    | 1:K:73:GLU:HG3   | 1.95                     | 0.66              |
| 1:G:392:THR:OG1  | 1:G:395:GLU:HG3  | 1.95                     | 0.66              |
| 1:H:385:LEU:HD11 | 1:H:391:VAL:HG22 | 1.76                     | 0.66              |
| 1:E:323:GLY:HA2  | 1:E:352:GLN:HA   | 1.76                     | 0.66              |
| 1:L:127:GLN:HA   | 1:L:127:GLN:NE2  | 2.11                     | 0.66              |
| 1:C:323:GLY:HA2  | 1:C:352:GLN:HA   | 1.78                     | 0.66              |
| 1:D:254:PRO:HG3  | 1:D:295:LYS:HE3  | 1.77                     | 0.66              |
| 1:F:392:THR:OG1  | 1:F:395:GLU:HG3  | 1.95                     | 0.65              |
| 1:B:25:MET:HG3   | 6:B:434:HOH:O    | 1.95                     | 0.65              |
| 1:A:80:GLU:HG3   | 1:A:85:LYS:NZ    | 2.11                     | 0.65              |
| 1:J:392:THR:OG1  | 1:J:395:GLU:HG3  | 1.96                     | 0.65              |
| 1:A:263:LYS:HB3  | 1:A:264:ARG:HD2  | 1.78                     | 0.65              |
| 1:D:127:GLN:NE2  | 1:D:127:GLN:HA   | 2.12                     | 0.65              |
| 1:G:80:GLU:O     | 1:G:85:LYS:HG2   | 1.97                     | 0.65              |
| 1:E:70:SER:O     | 1:E:74:GLN:HG3   | 1.97                     | 0.65              |
| 1:K:72:ARG:NH2   | 1:K:116:ARG:HD3  | 2.12                     | 0.65              |
| 1:I:127:GLN:HA   | 1:I:127:GLN:NE2  | 2.12                     | 0.64              |
| 1:F:323:GLY:HA2  | 1:F:352:GLN:HA   | 1.79                     | 0.64              |
| 1:D:113:GLN:HA   | 1:D:113:GLN:NE2  | 2.12                     | 0.64              |
| 1:D:339:ARG:O    | 1:D:343:GLU:HG3  | 1.98                     | 0.64              |
| 1:K:323:GLY:HA2  | 1:K:352:GLN:HA   | 1.80                     | 0.64              |
| 1:F:70:SER:O     | 1:F:74:GLN:HG3   | 1.96                     | 0.64              |
| 1:E:180:GLN:NE2  | 1:E:180:GLN:H    | 1.96                     | 0.63              |
| 1:G:198:GLU:O    | 1:G:202:GLN:HG2  | 1.99                     | 0.63              |
| 1:A:323:GLY:HA2  | 1:A:352:GLN:HA   | 1.80                     | 0.62              |
| 1:C:70:SER:OG    | 1:C:73:GLU:HG3   | 2.00                     | 0.62              |
| 1:B:6:ARG:HH11   | 1:B:6:ARG:HG2    | 1.65                     | 0.62              |
| 1:D:323:GLY:HA2  | 1:D:352:GLN:HA   | 1.81                     | 0.62              |
| 1:H:323:GLY:HA2  | 1:H:352:GLN:HA   | 1.82                     | 0.62              |
| 1:C:385:LEU:CD1  | 1:C:391:VAL:HG12 | 2.30                     | 0.61              |
| 1:H:198:GLU:O    | 1:H:202:GLN:HG2  | 2.01                     | 0.61              |
| 1:C:149:ASP:O    | 1:C:153:ILE:HG13 | 1.99                     | 0.61              |
| 1:G:323:GLY:HA2  | 1:G:352:GLN:HA   | 1.81                     | 0.61              |
| 1:K:170:ARG:NH2  | 1:K:223:SER:HB3  | 2.15                     | 0.61              |
| 1:A:72:ARG:HA    | 1:A:72:ARG:HH11  | 1.65                     | 0.61              |
| 1:F:127:GLN:HA   | 1:F:127:GLN:NE2  | 2.14                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:GLU:HG3   | 1:A:85:LYS:HZ1   | 1.65                     | 0.60              |
| 1:J:323:GLY:HA2  | 1:J:352:GLN:HA   | 1.81                     | 0.60              |
| 1:D:402:ASP:HA   | 1:D:406:ARG:HB2  | 1.82                     | 0.60              |
| 1:K:125:GLU:O    | 1:K:128:VAL:HG22 | 2.01                     | 0.60              |
| 1:C:412:VAL:HG23 | 1:C:414:ARG:HB2  | 1.84                     | 0.60              |
| 1:J:70:SER:O     | 1:J:74:GLN:HG3   | 2.02                     | 0.60              |
| 1:F:70:SER:OG    | 1:F:73:GLU:HG3   | 2.02                     | 0.60              |
| 1:H:392:THR:OG1  | 1:H:395:GLU:HG3  | 2.02                     | 0.60              |
| 1:L:124:SER:O    | 1:L:128:VAL:HG22 | 2.02                     | 0.60              |
| 1:A:72:ARG:NH1   | 1:A:72:ARG:HB2   | 2.17                     | 0.59              |
| 1:I:123:THR:OG1  | 1:I:126:GLU:HG3  | 2.01                     | 0.59              |
| 1:E:123:THR:OG1  | 1:E:126:GLU:HG3  | 2.02                     | 0.59              |
| 1:L:113:GLN:NE2  | 1:L:113:GLN:HA   | 2.17                     | 0.59              |
| 1:J:382:ASP:O    | 1:J:386:GLN:HG2  | 2.02                     | 0.59              |
| 1:B:219:TYR:HB3  | 1:B:254:PRO:HG2  | 1.84                     | 0.59              |
| 1:H:139:ASP:OD1  | 1:H:166:HIS:HE1  | 1.86                     | 0.59              |
| 1:J:219:TYR:HB3  | 1:J:254:PRO:HG2  | 1.83                     | 0.59              |
| 1:C:127:GLN:HA   | 1:C:127:GLN:NE2  | 2.16                     | 0.59              |
| 1:K:127:GLN:HA   | 1:K:127:GLN:NE2  | 2.17                     | 0.59              |
| 1:E:402:ASP:HA   | 1:E:406:ARG:HB2  | 1.83                     | 0.59              |
| 1:G:385:LEU:HD23 | 1:G:385:LEU:O    | 2.02                     | 0.59              |
| 1:H:48:TYR:HB3   | 1:H:51:LEU:HD13  | 1.85                     | 0.59              |
| 1:G:402:ASP:HA   | 1:G:406:ARG:HB2  | 1.84                     | 0.59              |
| 1:F:333:ILE:HG22 | 1:F:337:MET:CE   | 2.14                     | 0.59              |
| 1:G:219:TYR:HA   | 1:G:253:ILE:CG2  | 2.32                     | 0.59              |
| 1:A:252:ASN:ND2  | 1:A:295:LYS:HE2  | 2.17                     | 0.59              |
| 1:C:25:MET:HG3   | 6:C:432:HOH:O    | 2.02                     | 0.58              |
| 1:G:371:SER:O    | 1:G:375:GLU:HG3  | 2.03                     | 0.58              |
| 6:H:432:HOH:O    | 1:I:308:GLU:HG2  | 2.03                     | 0.58              |
| 1:A:402:ASP:HA   | 1:A:406:ARG:HB2  | 1.84                     | 0.58              |
| 1:H:385:LEU:HD12 | 1:H:389:TRP:O    | 2.03                     | 0.58              |
| 1:G:382:ASP:O    | 1:G:386:GLN:HG2  | 2.03                     | 0.58              |
| 1:C:70:SER:O     | 1:C:74:GLN:HG3   | 2.04                     | 0.58              |
| 1:K:3:ILE:HG23   | 1:K:8:VAL:HG23   | 1.86                     | 0.58              |
| 1:I:186:ARG:NH1  | 1:I:192:VAL:O    | 2.36                     | 0.58              |
| 1:E:172:ASP:HB2  | 1:E:173:PRO:HD3  | 1.86                     | 0.58              |
| 1:I:323:GLY:HA2  | 1:I:352:GLN:HA   | 1.86                     | 0.58              |
| 1:C:264:ARG:HG2  | 6:C:805:HOH:O    | 2.04                     | 0.58              |
| 1:L:323:GLY:HA2  | 1:L:352:GLN:HA   | 1.85                     | 0.57              |
| 1:L:25:MET:HG3   | 6:L:453:HOH:O    | 2.03                     | 0.57              |
| 1:D:25:MET:HG3   | 6:D:440:HOH:O    | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:112:LEU:HA   | 1:E:115:TYR:CD2  | 2.39                     | 0.57              |
| 1:I:25:MET:HG3   | 6:I:453:HOH:O    | 2.04                     | 0.57              |
| 1:E:149:ASP:O    | 1:E:153:ILE:HG12 | 2.03                     | 0.57              |
| 1:J:166:HIS:HD2  | 6:J:1185:HOH:O   | 1.87                     | 0.57              |
| 1:H:402:ASP:HA   | 1:H:406:ARG:HB2  | 1.85                     | 0.57              |
| 1:B:111:ASP:HB3  | 1:B:114:VAL:HG12 | 1.87                     | 0.57              |
| 1:F:198:GLU:O    | 1:F:202:GLN:HG2  | 2.05                     | 0.57              |
| 1:D:48:TYR:HB3   | 1:D:51:LEU:HD13  | 1.87                     | 0.57              |
| 1:A:152:ARG:HG2  | 1:A:152:ARG:HH11 | 1.69                     | 0.57              |
| 1:K:25:MET:HG3   | 6:K:609:HOH:O    | 2.04                     | 0.57              |
| 1:B:123:THR:OG1  | 1:B:126:GLU:HG3  | 2.05                     | 0.57              |
| 1:B:382:ASP:O    | 1:B:386:GLN:HG2  | 2.06                     | 0.56              |
| 1:L:123:THR:OG1  | 1:L:126:GLU:HG3  | 2.05                     | 0.56              |
| 1:H:146:PRO:O    | 1:H:152:ARG:HD3  | 2.05                     | 0.56              |
| 1:L:276:VAL:HG22 | 1:L:277:GLY:N    | 2.20                     | 0.56              |
| 1:B:112:LEU:HA   | 1:B:115:TYR:CD2  | 2.41                     | 0.56              |
| 1:B:152:ARG:NH1  | 1:B:152:ARG:HB3  | 2.20                     | 0.56              |
| 1:E:252:ASN:ND2  | 1:E:295:LYS:HE2  | 2.21                     | 0.56              |
| 1:B:6:ARG:HG3    | 1:B:382:ASP:OD1  | 2.06                     | 0.56              |
| 1:H:70:SER:OG    | 1:H:73:GLU:HG3   | 2.06                     | 0.56              |
| 1:I:127:GLN:CA   | 1:I:127:GLN:HE21 | 2.14                     | 0.56              |
| 1:K:402:ASP:HA   | 1:K:406:ARG:HB2  | 1.87                     | 0.56              |
| 1:G:56:MET:HE3   | 6:H:599:HOH:O    | 2.05                     | 0.56              |
| 1:I:125:GLU:O    | 1:I:128:VAL:HG22 | 2.06                     | 0.56              |
| 1:G:166:HIS:HD2  | 6:G:1241:HOH:O   | 1.87                     | 0.56              |
| 1:F:219:TYR:HB3  | 1:F:254:PRO:HG2  | 1.88                     | 0.55              |
| 1:J:121:LYS:HB3  | 1:J:121:LYS:NZ   | 2.21                     | 0.55              |
| 1:C:219:TYR:HA   | 1:C:253:ILE:CG2  | 2.36                     | 0.55              |
| 1:J:122:LYS:NZ   | 1:J:127:GLN:NE2  | 2.55                     | 0.55              |
| 1:I:219:TYR:HB3  | 1:I:254:PRO:HG2  | 1.88                     | 0.55              |
| 1:L:106:ASP:OD2  | 1:L:108:ALA:HB3  | 2.06                     | 0.55              |
| 1:K:245:LEU:HB2  | 1:K:246:PRO:HD3  | 1.87                     | 0.55              |
| 1:H:127:GLN:NE2  | 1:H:127:GLN:HA   | 2.20                     | 0.55              |
| 1:G:6:ARG:HG2    | 1:G:6:ARG:HH11   | 1.72                     | 0.55              |
| 2:A:428:REL:O5   | 2:A:428:REL:H2   | 2.07                     | 0.55              |
| 1:E:113:GLN:NE2  | 1:E:113:GLN:HA   | 2.22                     | 0.55              |
| 1:I:301:LEU:CD1  | 1:I:326:TRP:HB3  | 2.36                     | 0.55              |
| 1:H:263:LYS:CB   | 1:H:264:ARG:HE   | 2.20                     | 0.55              |
| 1:F:113:GLN:HA   | 1:F:113:GLN:NE2  | 2.21                     | 0.55              |
| 1:A:25:MET:HG3   | 6:A:452:HOH:O    | 2.06                     | 0.55              |
| 1:B:230:PHE:HA   | 1:B:231:PRO:C    | 2.26                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:402:ASP:HA   | 1:L:406:ARG:HB2  | 1.88                     | 0.55              |
| 1:B:70:SER:O     | 1:B:74:GLN:HG3   | 2.06                     | 0.55              |
| 1:E:301:LEU:HD11 | 1:E:326:TRP:HB3  | 1.89                     | 0.55              |
| 1:G:254:PRO:HG3  | 1:G:295:LYS:HE3  | 1.88                     | 0.55              |
| 1:F:25:MET:HG3   | 6:F:434:HOH:O    | 2.07                     | 0.54              |
| 1:H:245:LEU:HB2  | 1:H:246:PRO:HD3  | 1.88                     | 0.54              |
| 1:L:328:MET:HE2  | 1:L:328:MET:HA   | 1.89                     | 0.54              |
| 1:G:149:ASP:O    | 1:G:153:ILE:HG13 | 2.07                     | 0.54              |
| 1:J:149:ASP:O    | 1:J:153:ILE:HG13 | 2.08                     | 0.54              |
| 1:A:301:LEU:HD11 | 1:A:326:TRP:HB3  | 1.89                     | 0.54              |
| 6:D:1696:HOH:O   | 1:F:56:MET:HE3   | 2.06                     | 0.54              |
| 1:K:172:ASP:HB2  | 1:K:173:PRO:HD3  | 1.89                     | 0.54              |
| 1:J:128:VAL:CG2  | 6:J:1476:HOH:O   | 2.54                     | 0.54              |
| 1:L:252:ASN:ND2  | 1:L:295:LYS:HE2  | 2.23                     | 0.54              |
| 1:B:263:LYS:HB3  | 1:B:264:ARG:HD3  | 1.88                     | 0.54              |
| 1:L:172:ASP:HB2  | 1:L:173:PRO:HD3  | 1.90                     | 0.54              |
| 1:B:127:GLN:HA   | 1:B:127:GLN:NE2  | 2.22                     | 0.54              |
| 1:G:343:GLU:HG2  | 6:G:432:HOH:O    | 2.08                     | 0.54              |
| 1:E:66:PHE:O     | 1:E:69:MET:HG2   | 2.07                     | 0.54              |
| 1:B:139:ASP:OD1  | 1:B:166:HIS:HE1  | 1.91                     | 0.54              |
| 1:D:152:ARG:HG2  | 1:D:152:ARG:HH11 | 1.73                     | 0.54              |
| 1:J:5:SER:OG     | 1:J:7:GLU:HG2    | 2.07                     | 0.53              |
| 1:B:254:PRO:HG3  | 1:B:412:VAL:HG12 | 1.90                     | 0.53              |
| 1:I:80:GLU:HG3   | 1:I:85:LYS:HE2   | 1.89                     | 0.53              |
| 1:F:385:LEU:HD13 | 1:F:391:VAL:HG13 | 1.91                     | 0.53              |
| 1:E:156:LEU:HD21 | 1:E:214:ARG:NH1  | 2.24                     | 0.53              |
| 1:G:172:ASP:HB2  | 1:G:173:PRO:HD3  | 1.90                     | 0.53              |
| 1:L:202:GLN:HA   | 1:L:202:GLN:HE21 | 1.72                     | 0.53              |
| 1:C:245:LEU:HB2  | 1:C:246:PRO:HD3  | 1.90                     | 0.53              |
| 1:J:276:VAL:HG22 | 1:J:277:GLY:N    | 2.23                     | 0.53              |
| 1:C:128:VAL:CG2  | 6:C:1358:HOH:O   | 2.55                     | 0.53              |
| 1:C:374:ALA:O    | 1:C:378:ILE:HG13 | 2.08                     | 0.53              |
| 1:I:276:VAL:HG22 | 1:I:277:GLY:N    | 2.23                     | 0.53              |
| 1:G:127:GLN:NE2  | 1:G:127:GLN:HA   | 2.14                     | 0.53              |
| 1:D:40:TRP:O     | 1:D:41:ASP:CG    | 2.47                     | 0.53              |
| 1:I:313:ALA:HA   | 1:I:319:LEU:HD23 | 1.91                     | 0.53              |
| 1:L:392:THR:OG1  | 1:L:395:GLU:HG3  | 2.08                     | 0.53              |
| 1:F:219:TYR:HA   | 1:F:253:ILE:CG2  | 2.38                     | 0.53              |
| 1:K:30:PHE:CE2   | 1:K:37:ILE:HG12  | 2.44                     | 0.53              |
| 1:K:216:ASP:OD1  | 1:K:414:ARG:NH2  | 2.42                     | 0.53              |
| 2:K:428:REL:H2   | 2:K:428:REL:O5   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:56:MET:HE2   | 1:J:63:ILE:HB    | 1.90                     | 0.53              |
| 1:E:245:LEU:HB2  | 1:E:246:PRO:HD3  | 1.90                     | 0.53              |
| 1:I:154:SER:O    | 1:I:159:LYS:HB2  | 2.09                     | 0.53              |
| 1:A:111:ASP:OD1  | 1:A:114:VAL:HG23 | 2.09                     | 0.53              |
| 1:A:172:ASP:HB2  | 1:A:173:PRO:HD3  | 1.91                     | 0.52              |
| 1:B:49:HIS:HB2   | 1:B:272:ALA:HB2  | 1.90                     | 0.52              |
| 2:F:428:REL:H2   | 2:F:428:REL:O5   | 2.09                     | 0.52              |
| 1:G:219:TYR:HA   | 1:G:253:ILE:HG22 | 1.90                     | 0.52              |
| 1:H:263:LYS:HB3  | 1:H:264:ARG:HE   | 1.75                     | 0.52              |
| 1:F:385:LEU:HD12 | 1:F:389:TRP:O    | 2.09                     | 0.52              |
| 1:D:70:SER:OG    | 1:D:73:GLU:HG3   | 2.09                     | 0.52              |
| 1:D:78:ILE:HG23  | 1:D:82:LEU:HD12  | 1.91                     | 0.52              |
| 1:I:172:ASP:HB2  | 1:I:173:PRO:HD3  | 1.91                     | 0.52              |
| 1:B:172:ASP:HB2  | 1:B:173:PRO:HD3  | 1.91                     | 0.52              |
| 1:D:301:LEU:HD11 | 1:D:326:TRP:HB3  | 1.92                     | 0.52              |
| 1:K:301:LEU:CD1  | 1:K:326:TRP:HB3  | 2.39                     | 0.52              |
| 1:J:198:GLU:O    | 1:J:202:GLN:HG2  | 2.10                     | 0.52              |
| 1:E:118:TYR:HA   | 1:E:121:LYS:HE3  | 1.92                     | 0.52              |
| 1:E:267:PRO:HG2  | 6:E:1783:HOH:O   | 2.08                     | 0.52              |
| 1:G:124:SER:O    | 1:G:128:VAL:HG13 | 2.10                     | 0.52              |
| 1:B:265:VAL:HG21 | 1:B:275:PHE:HB2  | 1.92                     | 0.52              |
| 1:A:40:TRP:O     | 1:A:41:ASP:CG    | 2.48                     | 0.52              |
| 1:H:352:GLN:HG3  | 1:H:353:HIS:N    | 2.24                     | 0.52              |
| 1:L:202:GLN:HA   | 1:L:202:GLN:NE2  | 2.24                     | 0.52              |
| 1:E:265:VAL:HG21 | 1:E:275:PHE:HB2  | 1.92                     | 0.52              |
| 1:A:391:VAL:O    | 1:A:391:VAL:HG23 | 2.10                     | 0.52              |
| 1:E:197:ASN:HB2  | 6:E:1840:HOH:O   | 2.09                     | 0.52              |
| 1:E:392:THR:OG1  | 1:E:395:GLU:HG3  | 2.09                     | 0.52              |
| 1:H:172:ASP:HB2  | 1:H:173:PRO:HD3  | 1.92                     | 0.52              |
| 1:C:172:ASP:HB2  | 1:C:173:PRO:HD3  | 1.91                     | 0.52              |
| 1:C:123:THR:OG1  | 1:C:126:GLU:HG3  | 2.10                     | 0.52              |
| 1:K:316:PHE:HB3  | 1:K:318:ASN:OD1  | 2.09                     | 0.52              |
| 1:E:219:TYR:HA   | 1:E:253:ILE:CG2  | 2.40                     | 0.52              |
| 1:G:180:GLN:H    | 1:G:180:GLN:NE2  | 2.08                     | 0.52              |
| 1:G:352:GLN:HG3  | 1:G:353:HIS:N    | 2.24                     | 0.52              |
| 1:A:72:ARG:CA    | 1:A:72:ARG:HH11  | 2.23                     | 0.52              |
| 1:B:70:SER:OG    | 1:B:73:GLU:HG3   | 2.10                     | 0.52              |
| 1:F:276:VAL:HG22 | 1:F:277:GLY:N    | 2.25                     | 0.52              |
| 1:E:382:ASP:O    | 1:E:386:GLN:HG2  | 2.10                     | 0.51              |
| 1:D:139:ASP:OD1  | 1:D:166:HIS:HE1  | 1.93                     | 0.51              |
| 1:J:172:ASP:HB2  | 1:J:173:PRO:HD3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:428:REL:O5   | 2:D:428:REL:H2   | 2.10                     | 0.51              |
| 1:A:72:ARG:HH11  | 1:A:72:ARG:CB    | 2.23                     | 0.51              |
| 1:C:209:THR:O    | 1:C:213:GLU:HG3  | 2.10                     | 0.51              |
| 1:E:49:HIS:HB2   | 1:E:272:ALA:HB2  | 1.91                     | 0.51              |
| 1:J:127:GLN:HA   | 1:J:127:GLN:NE2  | 2.14                     | 0.51              |
| 1:H:125:GLU:O    | 1:H:128:VAL:HG22 | 2.10                     | 0.51              |
| 1:C:152:ARG:HH22 | 1:C:184:ARG:NH2  | 2.06                     | 0.51              |
| 1:F:196:TRP:CD1  | 1:F:238:ARG:HD2  | 2.44                     | 0.51              |
| 1:H:181:THR:HG22 | 1:H:185:LEU:CD2  | 2.40                     | 0.51              |
| 1:F:219:TYR:HA   | 1:F:253:ILE:HG22 | 1.91                     | 0.51              |
| 1:G:336:GLU:O    | 1:G:340:MET:HG3  | 2.11                     | 0.51              |
| 1:D:252:ASN:ND2  | 1:D:295:LYS:HE2  | 2.26                     | 0.51              |
| 1:E:212:ILE:HD13 | 1:E:253:ILE:HD12 | 1.91                     | 0.51              |
| 1:J:112:LEU:HA   | 1:J:115:TYR:CD2  | 2.46                     | 0.51              |
| 1:G:276:VAL:HG22 | 1:G:277:GLY:N    | 2.25                     | 0.51              |
| 1:H:25:MET:HG3   | 6:H:479:HOH:O    | 2.10                     | 0.51              |
| 1:C:276:VAL:HG22 | 1:C:277:GLY:N    | 2.25                     | 0.51              |
| 1:H:301:LEU:HD11 | 1:H:326:TRP:HB3  | 1.91                     | 0.51              |
| 1:E:6:ARG:HG2    | 1:E:6:ARG:HH11   | 1.76                     | 0.51              |
| 1:I:218:VAL:HG23 | 1:I:219:TYR:CD2  | 2.46                     | 0.51              |
| 1:J:128:VAL:HA   | 1:J:359:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:388:GLY:HA2  | 1:K:4:ASN:OD1    | 2.11                     | 0.51              |
| 1:B:111:ASP:HB3  | 1:B:114:VAL:CG1  | 2.41                     | 0.50              |
| 1:B:180:GLN:H    | 1:B:180:GLN:HE21 | 1.57                     | 0.50              |
| 1:K:392:THR:OG1  | 1:K:395:GLU:HG3  | 2.11                     | 0.50              |
| 1:I:130:THR:O    | 1:I:134:LEU:HG   | 2.12                     | 0.50              |
| 1:I:149:ASP:O    | 1:I:153:ILE:HG13 | 2.11                     | 0.50              |
| 1:G:245:LEU:HB2  | 1:G:246:PRO:HD3  | 1.93                     | 0.50              |
| 1:H:235:ASN:O    | 1:H:239:ILE:HG13 | 2.11                     | 0.50              |
| 1:I:106:ASP:OD2  | 1:I:108:ALA:HB3  | 2.11                     | 0.50              |
| 1:E:127:GLN:HA   | 1:E:127:GLN:NE2  | 2.24                     | 0.50              |
| 1:I:301:LEU:HD11 | 1:I:326:TRP:HB3  | 1.93                     | 0.50              |
| 1:D:286:HIS:CE1  | 1:D:290:GLU:HG3  | 2.46                     | 0.50              |
| 1:D:51:LEU:HD12  | 1:D:51:LEU:N     | 2.27                     | 0.50              |
| 1:K:112:LEU:HA   | 1:K:115:TYR:CD2  | 2.45                     | 0.50              |
| 1:B:301:LEU:HD11 | 1:B:326:TRP:HB3  | 1.93                     | 0.50              |
| 1:B:252:ASN:ND2  | 1:B:295:LYS:HE2  | 2.26                     | 0.50              |
| 1:H:276:VAL:HG22 | 1:H:277:GLY:N    | 2.26                     | 0.50              |
| 1:A:113:GLN:NE2  | 1:A:116:ARG:HH11 | 2.09                     | 0.50              |
| 1:H:385:LEU:HD13 | 1:H:391:VAL:HG13 | 1.93                     | 0.50              |
| 1:I:70:SER:OG    | 1:I:73:GLU:HG3   | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:409:TRP:HE3  | 1:F:414:ARG:HB2  | 1.77                     | 0.50              |
| 1:D:146:PRO:O    | 1:D:152:ARG:HB2  | 2.12                     | 0.49              |
| 1:E:276:VAL:HG22 | 1:E:277:GLY:N    | 2.27                     | 0.49              |
| 1:A:69:MET:CE    | 1:A:73:GLU:HB3   | 2.42                     | 0.49              |
| 1:H:286:HIS:CE1  | 1:H:290:GLU:HG3  | 2.47                     | 0.49              |
| 1:K:389:TRP:HD1  | 1:K:391:VAL:HG12 | 1.78                     | 0.49              |
| 1:J:352:GLN:HG3  | 1:J:353:HIS:N    | 2.26                     | 0.49              |
| 1:E:286:HIS:CE1  | 1:E:290:GLU:HG3  | 2.47                     | 0.49              |
| 1:J:402:ASP:HA   | 1:J:406:ARG:HB2  | 1.94                     | 0.49              |
| 1:A:179:GLU:HB2  | 1:A:180:GLN:OE1  | 2.11                     | 0.49              |
| 1:J:245:LEU:HB2  | 1:J:246:PRO:HD3  | 1.93                     | 0.49              |
| 1:H:244:LEU:HD13 | 1:H:244:LEU:C    | 2.33                     | 0.49              |
| 1:G:235:ASN:O    | 1:G:239:ILE:HG13 | 2.11                     | 0.49              |
| 1:K:352:GLN:HG3  | 1:K:353:HIS:N    | 2.26                     | 0.49              |
| 1:H:70:SER:O     | 1:H:74:GLN:HG3   | 2.12                     | 0.49              |
| 1:J:409:TRP:HE3  | 1:J:414:ARG:HB2  | 1.77                     | 0.49              |
| 1:F:51:LEU:N     | 1:F:51:LEU:HD12  | 2.27                     | 0.49              |
| 1:E:180:GLN:N    | 1:E:180:GLN:NE2  | 2.60                     | 0.49              |
| 1:A:79:TRP:O     | 1:A:83:PHE:HB2   | 2.12                     | 0.49              |
| 1:L:70:SER:OG    | 1:L:73:GLU:HG3   | 2.11                     | 0.49              |
| 1:A:122:LYS:NZ   | 1:A:127:GLN:NE2  | 2.60                     | 0.49              |
| 1:F:172:ASP:HB2  | 1:F:173:PRO:HD3  | 1.93                     | 0.49              |
| 1:C:14:LYS:NZ    | 1:C:375:GLU:OE2  | 2.45                     | 0.49              |
| 1:A:170:ARG:NH2  | 1:A:223:SER:HB3  | 2.28                     | 0.49              |
| 1:J:230:PHE:HA   | 1:J:231:PRO:C    | 2.33                     | 0.49              |
| 1:K:128:VAL:O    | 1:K:132:LEU:HG   | 2.13                     | 0.49              |
| 1:H:408:PHE:O    | 1:H:412:VAL:HG22 | 2.12                     | 0.49              |
| 1:I:49:HIS:HB2   | 1:I:272:ALA:HB2  | 1.94                     | 0.49              |
| 1:G:230:PHE:HA   | 1:G:231:PRO:C    | 2.31                     | 0.49              |
| 1:H:181:THR:O    | 1:H:185:LEU:HD23 | 2.12                     | 0.49              |
| 1:C:79:TRP:O     | 1:C:83:PHE:HB2   | 2.12                     | 0.49              |
| 1:D:392:THR:OG1  | 1:D:395:GLU:HG3  | 2.11                     | 0.49              |
| 1:E:235:ASN:O    | 1:E:239:ILE:HG13 | 2.12                     | 0.49              |
| 1:K:113:GLN:HE22 | 1:K:116:ARG:HH11 | 1.59                     | 0.49              |
| 1:B:113:GLN:NE2  | 1:B:113:GLN:HA   | 2.28                     | 0.49              |
| 1:F:245:LEU:HB2  | 1:F:246:PRO:HD3  | 1.95                     | 0.49              |
| 1:A:219:TYR:HB3  | 1:A:254:PRO:HG2  | 1.95                     | 0.49              |
| 1:G:40:TRP:O     | 1:G:41:ASP:CG    | 2.51                     | 0.49              |
| 1:L:301:LEU:CD1  | 1:L:326:TRP:HB3  | 2.42                     | 0.49              |
| 1:A:245:LEU:HB2  | 1:A:246:PRO:HD3  | 1.95                     | 0.48              |
| 1:E:128:VAL:O    | 1:E:132:LEU:HG   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:391:VAL:O    | 1:L:391:VAL:HG23 | 2.12                     | 0.48              |
| 1:E:244:LEU:HD13 | 1:E:244:LEU:C    | 2.34                     | 0.48              |
| 1:H:72:ARG:HH12  | 1:H:116:ARG:HD3  | 1.78                     | 0.48              |
| 1:B:158:GLY:O    | 1:B:160:GLN:HG2  | 2.13                     | 0.48              |
| 1:E:352:GLN:HG3  | 1:E:353:HIS:N    | 2.28                     | 0.48              |
| 1:C:198:GLU:O    | 1:C:202:GLN:HG2  | 2.13                     | 0.48              |
| 1:G:5:SER:OG     | 1:G:7:GLU:HG2    | 2.13                     | 0.48              |
| 1:B:40:TRP:O     | 1:B:41:ASP:CG    | 2.51                     | 0.48              |
| 1:H:295:LYS:HE3  | 1:H:411:PHE:O    | 2.13                     | 0.48              |
| 1:F:231:PRO:HD3  | 1:F:286:HIS:CD2  | 2.48                     | 0.48              |
| 1:B:385:LEU:HA   | 1:B:389:TRP:O    | 2.13                     | 0.48              |
| 1:H:40:TRP:O     | 1:H:41:ASP:CB    | 2.57                     | 0.48              |
| 1:L:139:ASP:OD1  | 1:L:166:HIS:HE1  | 1.95                     | 0.48              |
| 1:K:254:PRO:HG3  | 1:K:295:LYS:HE3  | 1.93                     | 0.48              |
| 1:E:51:LEU:N     | 1:E:51:LEU:HD12  | 2.28                     | 0.48              |
| 1:J:122:LYS:NZ   | 1:J:127:GLN:HE22 | 2.11                     | 0.48              |
| 1:K:69:MET:HB3   | 1:K:73:GLU:HB2   | 1.96                     | 0.48              |
| 1:K:276:VAL:HG22 | 1:K:277:GLY:N    | 2.28                     | 0.48              |
| 1:I:402:ASP:HA   | 1:I:406:ARG:HB2  | 1.95                     | 0.48              |
| 1:C:252:ASN:HD21 | 1:C:295:LYS:HE3  | 1.77                     | 0.48              |
| 1:K:152:ARG:HD2  | 1:K:156:LEU:HD11 | 1.94                     | 0.48              |
| 1:D:352:GLN:HG3  | 1:D:353:HIS:N    | 2.28                     | 0.48              |
| 1:B:154:SER:O    | 1:B:159:LYS:HB2  | 2.14                     | 0.48              |
| 1:C:154:SER:O    | 1:C:159:LYS:HB2  | 2.13                     | 0.48              |
| 1:D:172:ASP:HB2  | 1:D:173:PRO:HD3  | 1.96                     | 0.48              |
| 1:D:388:GLY:HA2  | 1:H:4:ASN:OD1    | 2.13                     | 0.48              |
| 1:L:113:GLN:HG2  | 6:L:1347:HOH:O   | 2.13                     | 0.48              |
| 1:J:301:LEU:CD1  | 1:J:326:TRP:HB3  | 2.44                     | 0.48              |
| 1:I:230:PHE:HA   | 1:I:231:PRO:C    | 2.34                     | 0.48              |
| 1:C:8:VAL:O      | 1:C:12:LYS:HG2   | 2.13                     | 0.48              |
| 1:J:49:HIS:HB2   | 1:J:272:ALA:HB2  | 1.94                     | 0.48              |
| 1:F:40:TRP:O     | 1:F:41:ASP:CG    | 2.52                     | 0.48              |
| 1:E:316:PHE:HB3  | 1:E:318:ASN:OD1  | 2.14                     | 0.48              |
| 1:J:30:PHE:CE2   | 1:J:37:ILE:HG13  | 2.49                     | 0.48              |
| 1:A:313:ALA:HA   | 1:A:319:LEU:HD23 | 1.96                     | 0.47              |
| 1:G:385:LEU:HA   | 1:G:389:TRP:O    | 2.14                     | 0.47              |
| 1:D:69:MET:HB3   | 1:D:73:GLU:HB2   | 1.95                     | 0.47              |
| 1:K:209:THR:O    | 1:K:213:GLU:HG3  | 2.13                     | 0.47              |
| 1:A:112:LEU:HA   | 1:A:115:TYR:CD2  | 2.49                     | 0.47              |
| 1:D:276:VAL:HG22 | 1:D:277:GLY:N    | 2.29                     | 0.47              |
| 1:H:32:PRO:HG2   | 1:H:128:VAL:HG21 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:125:GLU:O    | 1:L:128:VAL:HG23 | 2.14                     | 0.47              |
| 1:G:128:VAL:CG2  | 6:G:665:HOH:O    | 2.62                     | 0.47              |
| 1:K:139:ASP:OD1  | 1:K:166:HIS:HE1  | 1.96                     | 0.47              |
| 1:I:219:TYR:HA   | 1:I:253:ILE:CG2  | 2.44                     | 0.47              |
| 1:J:265:VAL:HG21 | 1:J:275:PHE:HB2  | 1.95                     | 0.47              |
| 1:E:275:PHE:CG   | 1:E:276:VAL:N    | 2.82                     | 0.47              |
| 1:J:182:LYS:O    | 1:J:186:ARG:HG2  | 2.14                     | 0.47              |
| 1:G:139:ASP:OD1  | 1:G:166:HIS:HE1  | 1.97                     | 0.47              |
| 1:A:123:THR:OG1  | 1:A:126:GLU:HG3  | 2.13                     | 0.47              |
| 1:I:174:LEU:HD13 | 1:I:175:LEU:HD12 | 1.96                     | 0.47              |
| 1:B:203:GLU:OE1  | 1:B:206:ARG:NH1  | 2.47                     | 0.47              |
| 6:A:445:HOH:O    | 1:B:308:GLU:HG2  | 2.14                     | 0.47              |
| 1:B:316:PHE:HB3  | 1:B:318:ASN:OD1  | 2.14                     | 0.47              |
| 1:K:286:HIS:CE1  | 1:K:290:GLU:HG3  | 2.49                     | 0.47              |
| 1:F:385:LEU:HD11 | 1:F:391:VAL:HG22 | 1.95                     | 0.47              |
| 1:H:322:PHE:HA   | 1:H:350:ILE:O    | 2.14                     | 0.47              |
| 1:G:65:ALA:O     | 1:G:69:MET:HG3   | 2.14                     | 0.47              |
| 1:C:122:LYS:HG3  | 1:C:126:GLU:HB2  | 1.97                     | 0.47              |
| 1:A:286:HIS:CE1  | 1:A:290:GLU:HG3  | 2.49                     | 0.47              |
| 1:F:301:LEU:CD1  | 1:F:326:TRP:HB3  | 2.45                     | 0.47              |
| 2:L:428:REL:O5   | 2:L:428:REL:H2   | 2.14                     | 0.47              |
| 1:C:385:LEU:HD12 | 1:C:389:TRP:O    | 2.15                     | 0.47              |
| 1:F:314:ARG:HD2  | 1:F:344:MET:HB3  | 1.96                     | 0.47              |
| 1:F:244:LEU:HD13 | 1:F:244:LEU:C    | 2.35                     | 0.47              |
| 6:A:1421:HOH:O   | 1:C:56:MET:HE3   | 2.14                     | 0.47              |
| 1:G:198:GLU:HA   | 1:G:198:GLU:OE1  | 2.15                     | 0.47              |
| 1:A:72:ARG:HB2   | 1:A:72:ARG:HH11  | 1.80                     | 0.47              |
| 1:B:274:ASP:O    | 1:C:315:LYS:HD2  | 2.15                     | 0.47              |
| 1:J:308:GLU:HG2  | 6:J:450:HOH:O    | 2.14                     | 0.47              |
| 1:G:25:MET:HG3   | 6:G:445:HOH:O    | 2.13                     | 0.47              |
| 1:A:9:LEU:HD21   | 1:A:381:TYR:HB2  | 1.96                     | 0.47              |
| 1:A:127:GLN:CA   | 1:A:127:GLN:HE21 | 2.11                     | 0.46              |
| 1:I:41:ASP:OD2   | 1:I:41:ASP:C     | 2.54                     | 0.46              |
| 1:K:195:GLU:HG3  | 1:K:197:ASN:HD22 | 1.81                     | 0.46              |
| 1:J:322:PHE:HA   | 1:J:350:ILE:O    | 2.15                     | 0.46              |
| 1:F:149:ASP:O    | 1:F:153:ILE:HG13 | 2.15                     | 0.46              |
| 1:B:216:ASP:N    | 1:B:217:PRO:CD   | 2.78                     | 0.46              |
| 1:A:352:GLN:HG3  | 1:A:353:HIS:N    | 2.30                     | 0.46              |
| 1:L:9:LEU:HD21   | 1:L:381:TYR:CB   | 2.46                     | 0.46              |
| 1:A:66:PHE:CZ    | 1:A:74:GLN:HB3   | 2.50                     | 0.46              |
| 1:C:30:PHE:CE2   | 1:C:37:ILE:HG13  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:385:LEU:HD23 | 1:G:385:LEU:C    | 2.36                     | 0.46              |
| 1:B:286:HIS:CE1  | 1:B:290:GLU:HG3  | 2.50                     | 0.46              |
| 1:D:394:GLU:HB2  | 6:D:1235:HOH:O   | 2.14                     | 0.46              |
| 1:L:219:TYR:HA   | 1:L:253:ILE:CG2  | 2.45                     | 0.46              |
| 1:H:122:LYS:HD3  | 6:H:1304:HOH:O   | 2.16                     | 0.46              |
| 1:B:218:VAL:HG23 | 1:B:219:TYR:CD2  | 2.51                     | 0.46              |
| 1:L:265:VAL:HG11 | 1:L:275:PHE:HB3  | 1.97                     | 0.46              |
| 1:F:230:PHE:HA   | 1:F:231:PRO:C    | 2.35                     | 0.46              |
| 1:B:306:GLN:O    | 1:B:310:VAL:HG23 | 2.15                     | 0.46              |
| 1:J:203:GLU:OE2  | 1:J:206:ARG:NH1  | 2.49                     | 0.46              |
| 1:E:139:ASP:OD1  | 1:E:166:HIS:HE1  | 1.98                     | 0.46              |
| 1:G:70:SER:O     | 1:G:74:GLN:HG3   | 2.15                     | 0.46              |
| 1:B:125:GLU:O    | 1:B:128:VAL:HG13 | 2.15                     | 0.46              |
| 1:B:276:VAL:HG22 | 1:B:277:GLY:N    | 2.31                     | 0.46              |
| 1:A:322:PHE:HA   | 1:A:350:ILE:O    | 2.16                     | 0.46              |
| 1:F:191:LYS:HB3  | 1:F:191:LYS:NZ   | 2.31                     | 0.46              |
| 1:L:154:SER:O    | 1:L:159:LYS:HB2  | 2.15                     | 0.46              |
| 1:D:127:GLN:HE21 | 1:D:127:GLN:CA   | 2.15                     | 0.46              |
| 1:G:180:GLN:NE2  | 1:G:180:GLN:N    | 2.63                     | 0.46              |
| 1:J:113:GLN:HA   | 1:J:113:GLN:NE2  | 2.30                     | 0.46              |
| 1:A:51:LEU:N     | 1:A:51:LEU:HD12  | 2.31                     | 0.46              |
| 1:B:51:LEU:N     | 1:B:51:LEU:HD12  | 2.31                     | 0.46              |
| 1:B:352:GLN:HG3  | 1:B:353:HIS:N    | 2.30                     | 0.46              |
| 1:H:264:ARG:HH11 | 1:H:264:ARG:HG2  | 1.80                     | 0.46              |
| 1:L:198:GLU:O    | 1:L:202:GLN:HG2  | 2.16                     | 0.46              |
| 1:J:198:GLU:OE1  | 1:J:198:GLU:HA   | 2.16                     | 0.46              |
| 1:L:69:MET:HB3   | 1:L:73:GLU:HB2   | 1.98                     | 0.46              |
| 1:K:393:GLU:O    | 1:K:397:LYS:HG2  | 2.15                     | 0.46              |
| 1:B:322:PHE:HA   | 1:B:350:ILE:O    | 2.16                     | 0.46              |
| 1:J:122:LYS:HZ1  | 1:J:127:GLN:NE2  | 2.13                     | 0.46              |
| 1:J:254:PRO:HG3  | 1:J:412:VAL:HG12 | 1.97                     | 0.46              |
| 1:C:122:LYS:CG   | 1:C:126:GLU:HB2  | 2.46                     | 0.46              |
| 1:H:254:PRO:HG3  | 1:H:295:LYS:HE2  | 1.97                     | 0.46              |
| 1:A:230:PHE:HA   | 1:A:231:PRO:C    | 2.35                     | 0.46              |
| 1:B:235:ASN:O    | 1:B:239:ILE:HG13 | 2.16                     | 0.46              |
| 1:H:216:ASP:N    | 1:H:217:PRO:CD   | 2.79                     | 0.46              |
| 1:G:122:LYS:HZ1  | 1:G:127:GLN:HA   | 1.80                     | 0.45              |
| 1:C:127:GLN:HG3  | 1:C:359:LEU:HD23 | 1.97                     | 0.45              |
| 1:J:107:PRO:HA   | 1:J:115:TYR:OH   | 2.15                     | 0.45              |
| 1:C:40:TRP:O     | 1:C:41:ASP:CG    | 2.54                     | 0.45              |
| 1:G:286:HIS:CE1  | 1:G:290:GLU:HG3  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:306:GLN:O    | 1:E:310:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:328:MET:HB3  | 1:F:337:MET:HE1  | 1.98                     | 0.45              |
| 1:L:142:MET:O    | 1:L:168:ALA:HB3  | 2.16                     | 0.45              |
| 1:E:385:LEU:HA   | 1:E:389:TRP:O    | 2.16                     | 0.45              |
| 1:I:152:ARG:O    | 1:I:156:LEU:HG   | 2.17                     | 0.45              |
| 1:E:230:PHE:HA   | 1:E:231:PRO:C    | 2.35                     | 0.45              |
| 1:L:322:PHE:HA   | 1:L:350:ILE:O    | 2.16                     | 0.45              |
| 1:G:409:TRP:HA   | 1:G:412:VAL:HG22 | 1.97                     | 0.45              |
| 1:A:392:THR:OG1  | 1:A:395:GLU:HG3  | 2.16                     | 0.45              |
| 1:H:128:VAL:O    | 1:H:132:LEU:HG   | 2.15                     | 0.45              |
| 1:H:139:ASP:OD1  | 1:H:166:HIS:CE1  | 2.69                     | 0.45              |
| 1:K:182:LYS:HA   | 1:K:185:LEU:HD12 | 1.98                     | 0.45              |
| 1:G:169:LEU:HG   | 1:G:171:LEU:HD21 | 1.98                     | 0.45              |
| 1:E:152:ARG:HH11 | 1:E:152:ARG:HG2  | 1.81                     | 0.45              |
| 1:H:275:PHE:CG   | 1:H:276:VAL:N    | 2.82                     | 0.45              |
| 1:E:286:HIS:NE2  | 1:E:290:GLU:HG3  | 2.32                     | 0.45              |
| 1:A:219:TYR:HA   | 1:A:253:ILE:CG2  | 2.47                     | 0.45              |
| 1:L:301:LEU:HD11 | 1:L:326:TRP:HB3  | 1.99                     | 0.45              |
| 1:K:52:VAL:O     | 1:K:55:VAL:HG12  | 2.16                     | 0.45              |
| 1:A:265:VAL:HG21 | 1:A:275:PHE:HB2  | 1.99                     | 0.45              |
| 1:E:79:TRP:O     | 1:E:83:PHE:HB2   | 2.17                     | 0.45              |
| 6:D:435:HOH:O    | 1:E:308:GLU:HG2  | 2.17                     | 0.45              |
| 1:I:264:ARG:HG2  | 6:I:1147:HOH:O   | 2.17                     | 0.45              |
| 1:I:391:VAL:HG23 | 1:I:391:VAL:O    | 2.16                     | 0.45              |
| 1:G:128:VAL:HA   | 1:G:359:LEU:HD21 | 1.97                     | 0.45              |
| 1:J:113:GLN:O    | 1:J:117:GLU:HG3  | 2.16                     | 0.45              |
| 1:D:382:ASP:O    | 1:D:386:GLN:HG2  | 2.17                     | 0.45              |
| 1:D:391:VAL:O    | 1:D:391:VAL:HG23 | 2.17                     | 0.45              |
| 1:F:125:GLU:O    | 1:F:128:VAL:HG13 | 2.17                     | 0.45              |
| 1:A:30:PHE:CE2   | 1:A:37:ILE:HG12  | 2.52                     | 0.45              |
| 1:A:106:ASP:OD2  | 1:A:108:ALA:HB3  | 2.16                     | 0.45              |
| 1:L:149:ASP:O    | 1:L:153:ILE:HG13 | 2.16                     | 0.45              |
| 1:L:230:PHE:HA   | 1:L:231:PRO:C    | 2.37                     | 0.45              |
| 1:D:113:GLN:CA   | 1:D:113:GLN:NE2  | 2.78                     | 0.45              |
| 1:E:122:LYS:NZ   | 1:E:127:GLN:NE2  | 2.64                     | 0.45              |
| 1:I:70:SER:O     | 1:I:74:GLN:HG3   | 2.17                     | 0.45              |
| 1:C:244:LEU:C    | 1:C:244:LEU:HD13 | 2.37                     | 0.45              |
| 1:C:124:SER:O    | 1:C:128:VAL:HG13 | 2.17                     | 0.45              |
| 1:L:30:PHE:CE2   | 1:L:37:ILE:HG12  | 2.52                     | 0.45              |
| 1:B:29:LEU:O     | 1:B:142:MET:HG2  | 2.17                     | 0.45              |
| 1:F:72:ARG:HH11  | 1:F:72:ARG:CB    | 2.09                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:122:LYS:NZ   | 1:I:127:GLN:NE2  | 2.64                     | 0.45              |
| 1:L:40:TRP:CE3   | 1:L:127:GLN:HG2  | 2.52                     | 0.45              |
| 1:F:352:GLN:HG3  | 1:F:353:HIS:N    | 2.32                     | 0.45              |
| 1:J:276:VAL:CG2  | 1:J:277:GLY:N    | 2.80                     | 0.44              |
| 1:E:6:ARG:HG3    | 1:E:382:ASP:OD1  | 2.17                     | 0.44              |
| 1:A:113:GLN:HE22 | 1:A:116:ARG:HH11 | 1.64                     | 0.44              |
| 1:F:301:LEU:HD11 | 1:F:326:TRP:HB3  | 1.99                     | 0.44              |
| 1:D:9:LEU:HD21   | 1:D:381:TYR:HB2  | 1.98                     | 0.44              |
| 1:D:409:TRP:HA   | 1:D:412:VAL:HG22 | 1.98                     | 0.44              |
| 1:F:145:ASP:HA   | 1:F:146:PRO:HD2  | 1.91                     | 0.44              |
| 1:D:245:LEU:HB2  | 1:D:246:PRO:HD3  | 1.98                     | 0.44              |
| 1:K:40:TRP:O     | 1:K:41:ASP:CG    | 2.55                     | 0.44              |
| 1:K:170:ARG:HH21 | 1:K:223:SER:HB3  | 1.82                     | 0.44              |
| 1:H:301:LEU:CD1  | 1:H:326:TRP:HB3  | 2.46                     | 0.44              |
| 1:H:220:MET:CE   | 1:H:253:ILE:HD11 | 2.48                     | 0.44              |
| 1:G:308:GLU:HG2  | 6:G:443:HOH:O    | 2.16                     | 0.44              |
| 1:D:106:ASP:OD2  | 1:D:108:ALA:HB3  | 2.17                     | 0.44              |
| 1:E:40:TRP:O     | 1:E:41:ASP:CG    | 2.55                     | 0.44              |
| 1:J:25:MET:HG3   | 6:J:439:HOH:O    | 2.17                     | 0.44              |
| 1:E:128:VAL:CG2  | 6:E:1666:HOH:O   | 2.65                     | 0.44              |
| 1:K:2:SER:HA     | 6:K:1242:HOH:O   | 2.17                     | 0.44              |
| 1:E:313:ALA:HA   | 1:E:319:LEU:HD23 | 1.99                     | 0.44              |
| 1:D:170:ARG:NH2  | 1:D:223:SER:HB3  | 2.33                     | 0.44              |
| 1:I:414:ARG:HH11 | 1:I:414:ARG:HG3  | 1.82                     | 0.44              |
| 1:L:67:TRP:CE3   | 1:L:67:TRP:HA    | 2.52                     | 0.44              |
| 1:G:313:ALA:HA   | 1:G:319:LEU:HD23 | 1.98                     | 0.44              |
| 1:B:113:GLN:HE21 | 1:B:113:GLN:HA   | 1.83                     | 0.44              |
| 1:J:203:GLU:CD   | 1:J:206:ARG:NH1  | 2.70                     | 0.44              |
| 1:A:276:VAL:HG22 | 1:A:277:GLY:N    | 2.32                     | 0.44              |
| 1:I:112:LEU:HA   | 1:I:115:TYR:CD2  | 2.53                     | 0.44              |
| 1:G:185:LEU:HB3  | 1:G:190:TYR:HB2  | 1.99                     | 0.44              |
| 1:H:197:ASN:ND2  | 1:H:199:GLY:H    | 2.15                     | 0.44              |
| 1:L:40:TRP:O     | 1:L:41:ASP:CG    | 2.55                     | 0.44              |
| 1:D:231:PRO:HD3  | 1:D:286:HIS:CG   | 2.52                     | 0.44              |
| 1:G:358:VAL:HB   | 1:G:361:GLN:HG3  | 1.99                     | 0.44              |
| 1:A:42:ILE:HD13  | 1:A:100:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:219:TYR:HA   | 1:D:253:ILE:CG2  | 2.47                     | 0.44              |
| 1:C:275:PHE:CG   | 1:C:276:VAL:N    | 2.86                     | 0.44              |
| 1:D:112:LEU:HA   | 1:D:115:TYR:CD2  | 2.53                     | 0.44              |
| 1:K:250:LYS:HD3  | 1:K:251:HIS:CE1  | 2.53                     | 0.44              |
| 1:F:112:LEU:HA   | 1:F:115:TYR:CD2  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:67:TRP:CE3   | 1:I:67:TRP:HA    | 2.52                     | 0.44              |
| 1:L:182:LYS:HB2  | 1:L:182:LYS:NZ   | 2.33                     | 0.44              |
| 1:C:69:MET:HB3   | 1:C:73:GLU:HB2   | 1.98                     | 0.44              |
| 1:L:276:VAL:CG2  | 1:L:277:GLY:N    | 2.80                     | 0.44              |
| 1:D:326:TRP:HB3  | 1:D:327:PHE:H    | 1.52                     | 0.44              |
| 1:C:313:ALA:HA   | 1:C:319:LEU:HD23 | 1.99                     | 0.44              |
| 1:J:208:LEU:O    | 1:J:212:ILE:HG13 | 2.18                     | 0.44              |
| 1:J:225:PRO:HA   | 1:J:261:VAL:O    | 2.17                     | 0.44              |
| 1:F:139:ASP:OD1  | 1:F:166:HIS:HE1  | 2.01                     | 0.44              |
| 1:H:113:GLN:NE2  | 1:H:113:GLN:HA   | 2.33                     | 0.44              |
| 1:F:322:PHE:HA   | 1:F:350:ILE:O    | 2.17                     | 0.44              |
| 1:H:385:LEU:HA   | 1:H:385:LEU:HD12 | 1.92                     | 0.43              |
| 1:L:352:GLN:HG3  | 1:L:353:HIS:N    | 2.33                     | 0.43              |
| 1:J:275:PHE:CG   | 1:J:276:VAL:N    | 2.86                     | 0.43              |
| 1:G:275:PHE:CG   | 1:G:276:VAL:N    | 2.86                     | 0.43              |
| 1:A:286:HIS:NE2  | 1:A:290:GLU:HG3  | 2.33                     | 0.43              |
| 1:G:322:PHE:HA   | 1:G:350:ILE:O    | 2.18                     | 0.43              |
| 1:F:374:ALA:O    | 1:F:378:ILE:HG13 | 2.17                     | 0.43              |
| 1:L:313:ALA:HA   | 1:L:319:LEU:HD23 | 2.00                     | 0.43              |
| 1:H:123:THR:OG1  | 1:H:126:GLU:HG3  | 2.18                     | 0.43              |
| 1:H:40:TRP:CE3   | 1:H:127:GLN:HG2  | 2.53                     | 0.43              |
| 1:I:275:PHE:CG   | 1:I:276:VAL:N    | 2.86                     | 0.43              |
| 1:E:30:PHE:CE2   | 1:E:37:ILE:HG13  | 2.53                     | 0.43              |
| 1:L:52:VAL:O     | 1:L:55:VAL:HG12  | 2.18                     | 0.43              |
| 1:F:4:ASN:HB2    | 6:I:1261:HOH:O   | 2.18                     | 0.43              |
| 1:F:235:ASN:O    | 1:F:239:ILE:HG13 | 2.19                     | 0.43              |
| 1:I:276:VAL:CG2  | 1:I:277:GLY:N    | 2.81                     | 0.43              |
| 1:A:70:SER:O     | 1:A:74:GLN:HG3   | 2.18                     | 0.43              |
| 1:D:80:GLU:O     | 1:D:85:LYS:HG3   | 2.18                     | 0.43              |
| 1:J:235:ASN:O    | 1:J:239:ILE:HG13 | 2.18                     | 0.43              |
| 1:I:139:ASP:OD1  | 1:I:166:HIS:HE1  | 2.01                     | 0.43              |
| 1:C:182:LYS:HB2  | 1:C:182:LYS:NZ   | 2.33                     | 0.43              |
| 1:H:265:VAL:HG21 | 1:H:275:PHE:HB2  | 1.99                     | 0.43              |
| 1:F:326:TRP:HB3  | 1:F:327:PHE:H    | 1.58                     | 0.43              |
| 1:C:196:TRP:CZ2  | 1:C:201:ILE:HG12 | 2.54                     | 0.43              |
| 1:D:178:TYR:CD1  | 1:D:239:ILE:HD11 | 2.54                     | 0.43              |
| 1:K:186:ARG:NH2  | 1:K:192:VAL:O    | 2.44                     | 0.43              |
| 1:J:336:GLU:O    | 1:J:340:MET:HG3  | 2.19                     | 0.43              |
| 1:E:191:LYS:HB2  | 1:E:191:LYS:NZ   | 2.33                     | 0.43              |
| 1:J:122:LYS:HZ3  | 1:J:127:GLN:HE22 | 1.66                     | 0.43              |
| 1:L:128:VAL:CG2  | 6:L:986:HOH:O    | 2.67                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:231:PRO:HD3  | 1:B:286:HIS:CG   | 2.53                     | 0.43              |
| 1:J:69:MET:HB2   | 1:J:73:GLU:HB2   | 2.00                     | 0.43              |
| 1:F:152:ARG:HH22 | 1:F:184:ARG:HH22 | 1.67                     | 0.43              |
| 1:C:139:ASP:OD1  | 1:C:166:HIS:HE1  | 2.00                     | 0.43              |
| 1:G:112:LEU:HA   | 1:G:115:TYR:CD2  | 2.53                     | 0.43              |
| 1:E:154:SER:O    | 1:E:159:LYS:HB2  | 2.18                     | 0.43              |
| 1:A:139:ASP:OD1  | 1:A:166:HIS:HE1  | 2.00                     | 0.43              |
| 1:A:149:ASP:OD1  | 1:A:152:ARG:NH2  | 2.51                     | 0.43              |
| 1:I:128:VAL:HG23 | 1:I:129:ASP:N    | 2.33                     | 0.43              |
| 1:A:409:TRP:HA   | 1:A:412:VAL:HG22 | 1.99                     | 0.43              |
| 1:J:128:VAL:HG12 | 1:J:359:LEU:HD22 | 2.00                     | 0.43              |
| 1:I:40:TRP:O     | 1:I:41:ASP:CB    | 2.67                     | 0.43              |
| 1:L:264:ARG:HG2  | 6:L:610:HOH:O    | 2.18                     | 0.43              |
| 1:J:321:ILE:HG12 | 6:L:1830:HOH:O   | 2.17                     | 0.43              |
| 2:H:428:REL:H2   | 2:H:428:REL:O5   | 2.18                     | 0.43              |
| 1:F:275:PHE:CG   | 1:F:276:VAL:N    | 2.87                     | 0.43              |
| 1:E:224:LEU:HD13 | 1:E:228:PHE:CD1  | 2.53                     | 0.43              |
| 1:D:150:ASN:O    | 1:D:153:ILE:HG22 | 2.19                     | 0.43              |
| 1:A:244:LEU:C    | 1:A:244:LEU:HD13 | 2.38                     | 0.43              |
| 1:B:244:LEU:C    | 1:B:244:LEU:HD13 | 2.39                     | 0.43              |
| 1:H:128:VAL:CG2  | 6:H:1281:HOH:O   | 2.67                     | 0.43              |
| 1:A:295:LYS:HB3  | 1:A:411:PHE:CZ   | 2.54                     | 0.43              |
| 1:J:389:TRP:HB2  | 1:L:97:LEU:HD13  | 2.01                     | 0.43              |
| 1:L:112:LEU:HA   | 1:L:115:TYR:CD2  | 2.53                     | 0.43              |
| 1:G:201:ILE:O    | 1:G:205:LYS:HG3  | 2.18                     | 0.43              |
| 1:E:180:GLN:HE21 | 1:E:180:GLN:H    | 1.62                     | 0.42              |
| 1:G:409:TRP:HE3  | 1:G:414:ARG:HB2  | 1.83                     | 0.42              |
| 1:F:216:ASP:N    | 1:F:217:PRO:CD   | 2.82                     | 0.42              |
| 1:E:301:LEU:CD1  | 1:E:326:TRP:HB3  | 2.49                     | 0.42              |
| 1:H:79:TRP:O     | 1:H:83:PHE:HB2   | 2.19                     | 0.42              |
| 1:D:105:LEU:O    | 1:D:107:PRO:HD3  | 2.18                     | 0.42              |
| 1:H:230:PHE:HA   | 1:H:231:PRO:C    | 2.40                     | 0.42              |
| 1:E:42:ILE:HD13  | 1:E:100:LEU:HD21 | 1.99                     | 0.42              |
| 1:C:256:ALA:HA   | 1:C:297:LEU:O    | 2.19                     | 0.42              |
| 1:D:286:HIS:NE2  | 1:D:290:GLU:HG3  | 2.33                     | 0.42              |
| 1:L:245:LEU:HB2  | 1:L:246:PRO:HD3  | 2.01                     | 0.42              |
| 1:C:385:LEU:HD12 | 1:C:385:LEU:HA   | 1.86                     | 0.42              |
| 1:C:128:VAL:HA   | 1:C:359:LEU:HD21 | 2.01                     | 0.42              |
| 1:D:149:ASP:OD1  | 1:D:152:ARG:NH2  | 2.52                     | 0.42              |
| 1:I:316:PHE:HB3  | 1:I:318:ASN:OD1  | 2.18                     | 0.42              |
| 1:D:123:THR:OG1  | 1:D:126:GLU:HG3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:154:SER:HB3  | 1:D:159:LYS:HG3  | 2.00                     | 0.42              |
| 1:K:244:LEU:C    | 1:K:244:LEU:HD13 | 2.40                     | 0.42              |
| 1:B:6:ARG:NH1    | 1:B:6:ARG:HG2    | 2.32                     | 0.42              |
| 1:J:128:VAL:HG12 | 1:J:359:LEU:CD2  | 2.49                     | 0.42              |
| 1:H:170:ARG:NH2  | 1:H:223:SER:HB3  | 2.34                     | 0.42              |
| 1:E:69:MET:HG3   | 1:E:74:GLN:HG2   | 2.02                     | 0.42              |
| 1:E:326:TRP:HB3  | 1:E:327:PHE:H    | 1.61                     | 0.42              |
| 1:I:40:TRP:O     | 1:I:41:ASP:CG    | 2.58                     | 0.42              |
| 1:C:216:ASP:N    | 1:C:217:PRO:CD   | 2.83                     | 0.42              |
| 1:J:387:ALA:O    | 1:L:107:PRO:HG2  | 2.20                     | 0.42              |
| 1:H:414:ARG:HG3  | 1:H:414:ARG:HH11 | 1.85                     | 0.42              |
| 1:C:180:GLN:N    | 1:C:180:GLN:NE2  | 2.68                     | 0.42              |
| 1:H:66:PHE:O     | 1:H:69:MET:HG2   | 2.19                     | 0.42              |
| 1:H:69:MET:HB2   | 1:H:73:GLU:HB2   | 2.01                     | 0.42              |
| 1:E:56:MET:HE1   | 1:E:63:ILE:N     | 2.34                     | 0.42              |
| 1:K:232:GLU:O    | 1:K:237:GLY:HA3  | 2.20                     | 0.42              |
| 1:A:252:ASN:HD21 | 1:A:295:LYS:HE2  | 1.83                     | 0.42              |
| 1:B:152:ARG:HD2  | 1:B:156:LEU:HD11 | 2.01                     | 0.42              |
| 1:K:216:ASP:N    | 1:K:217:PRO:CD   | 2.83                     | 0.42              |
| 1:G:180:GLN:H    | 1:G:180:GLN:HE21 | 1.66                     | 0.42              |
| 1:E:361:GLN:O    | 1:E:365:LYS:HG2  | 2.20                     | 0.42              |
| 1:A:167:ALA:O    | 1:A:217:PRO:HA   | 2.19                     | 0.42              |
| 1:D:322:PHE:HA   | 1:D:350:ILE:O    | 2.20                     | 0.42              |
| 1:L:79:TRP:O     | 1:L:83:PHE:HB2   | 2.20                     | 0.42              |
| 1:C:358:VAL:HB   | 1:C:361:GLN:HG3  | 2.02                     | 0.42              |
| 1:C:219:TYR:HA   | 1:C:253:ILE:HG22 | 2.01                     | 0.42              |
| 1:H:181:THR:HG22 | 1:H:185:LEU:HD21 | 2.02                     | 0.42              |
| 1:K:97:LEU:HD13  | 1:L:389:TRP:HB2  | 2.01                     | 0.42              |
| 1:D:139:ASP:OD1  | 1:D:166:HIS:CE1  | 2.73                     | 0.42              |
| 1:J:8:VAL:O      | 1:J:12:LYS:HG2   | 2.19                     | 0.42              |
| 1:H:297:LEU:HD23 | 1:H:320:MET:HB3  | 2.02                     | 0.42              |
| 1:K:32:PRO:HG2   | 1:K:128:VAL:HG21 | 2.00                     | 0.41              |
| 1:A:301:LEU:CD1  | 1:A:326:TRP:HB3  | 2.49                     | 0.41              |
| 1:F:389:TRP:HD1  | 1:F:391:VAL:HG12 | 1.84                     | 0.41              |
| 1:G:152:ARG:HG2  | 1:G:156:LEU:HG   | 2.01                     | 0.41              |
| 1:E:9:LEU:O      | 1:E:13:VAL:HG23  | 2.20                     | 0.41              |
| 1:D:42:ILE:HD13  | 1:D:100:LEU:HD21 | 2.01                     | 0.41              |
| 1:J:408:PHE:O    | 1:J:412:VAL:HG22 | 2.20                     | 0.41              |
| 1:B:275:PHE:CG   | 1:B:276:VAL:N    | 2.84                     | 0.41              |
| 1:D:230:PHE:HA   | 1:D:231:PRO:C    | 2.39                     | 0.41              |
| 1:K:219:TYR:HA   | 1:K:253:ILE:CG2  | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:216:ASP:N    | 1:E:217:PRO:CD   | 2.83                     | 0.41              |
| 2:C:428:REL:H2   | 2:C:428:REL:O5   | 2.20                     | 0.41              |
| 1:E:244:LEU:CD1  | 1:E:244:LEU:C    | 2.88                     | 0.41              |
| 1:J:301:LEU:HD11 | 1:J:326:TRP:HB3  | 2.03                     | 0.41              |
| 1:A:409:TRP:HE3  | 1:A:414:ARG:HB2  | 1.84                     | 0.41              |
| 1:E:196:TRP:CD1  | 1:E:238:ARG:HD2  | 2.54                     | 0.41              |
| 1:K:308:GLU:HG2  | 6:K:433:HOH:O    | 2.19                     | 0.41              |
| 1:G:196:TRP:CD1  | 1:G:238:ARG:HD2  | 2.55                     | 0.41              |
| 1:B:98:THR:HB    | 1:B:364:TYR:HB2  | 2.02                     | 0.41              |
| 1:J:40:TRP:O     | 1:J:41:ASP:CG    | 2.58                     | 0.41              |
| 1:K:275:PHE:CG   | 1:K:276:VAL:N    | 2.87                     | 0.41              |
| 1:E:63:ILE:HG23  | 1:E:64:GLU:N     | 2.36                     | 0.41              |
| 1:I:392:THR:OG1  | 1:I:395:GLU:HG3  | 2.20                     | 0.41              |
| 1:D:40:TRP:CE3   | 1:D:127:GLN:HG2  | 2.56                     | 0.41              |
| 1:K:40:TRP:CE3   | 1:K:127:GLN:HG2  | 2.55                     | 0.41              |
| 1:G:276:VAL:CG2  | 1:G:277:GLY:N    | 2.84                     | 0.41              |
| 1:G:190:TYR:CD1  | 1:G:206:ARG:NH1  | 2.89                     | 0.41              |
| 1:F:18:ASN:ND2   | 6:F:1397:HOH:O   | 2.53                     | 0.41              |
| 1:B:200:SER:O    | 1:B:204:VAL:HG23 | 2.21                     | 0.41              |
| 1:I:374:ALA:O    | 1:I:378:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:149:ASP:OD1  | 1:B:152:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:326:TRP:HB3  | 1:B:327:PHE:H    | 1.57                     | 0.41              |
| 1:I:231:PRO:HD3  | 1:I:286:HIS:CD2  | 2.55                     | 0.41              |
| 1:C:196:TRP:CD1  | 1:C:238:ARG:HD2  | 2.55                     | 0.41              |
| 1:I:322:PHE:HA   | 1:I:350:ILE:O    | 2.20                     | 0.41              |
| 1:K:235:ASN:O    | 1:K:239:ILE:HG13 | 2.21                     | 0.41              |
| 1:E:169:LEU:HG   | 1:E:171:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:122:LYS:NZ   | 1:A:127:GLN:HE22 | 2.18                     | 0.41              |
| 1:I:192:VAL:HG23 | 1:I:192:VAL:O    | 2.21                     | 0.41              |
| 1:L:159:LYS:HA   | 1:L:159:LYS:HD3  | 1.91                     | 0.41              |
| 1:A:275:PHE:CG   | 1:A:276:VAL:N    | 2.88                     | 0.41              |
| 1:E:100:LEU:O    | 1:E:105:LEU:HB2  | 2.20                     | 0.41              |
| 1:G:152:ARG:NH2  | 1:G:184:ARG:HH22 | 2.19                     | 0.41              |
| 1:C:112:LEU:HA   | 1:C:115:TYR:CD2  | 2.56                     | 0.41              |
| 1:C:322:PHE:HA   | 1:C:350:ILE:O    | 2.20                     | 0.41              |
| 1:G:49:HIS:HB2   | 1:G:272:ALA:HB2  | 2.02                     | 0.41              |
| 1:F:386:GLN:NE2  | 1:I:4:ASN:OD1    | 2.54                     | 0.41              |
| 1:H:326:TRP:HB3  | 1:H:327:PHE:H    | 1.65                     | 0.41              |
| 1:F:316:PHE:HB3  | 1:F:318:ASN:OD1  | 2.20                     | 0.41              |
| 2:G:428:REL:H2   | 2:G:428:REL:O5   | 2.21                     | 0.41              |
| 1:I:186:ARG:HH11 | 1:I:186:ARG:HG2  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:254:PRO:HG3  | 1:F:412:VAL:HG12 | 2.02                     | 0.41              |
| 1:G:254:PRO:HG2  | 1:G:412:VAL:HA   | 2.03                     | 0.41              |
| 1:F:265:VAL:HG21 | 1:F:275:PHE:HB2  | 2.03                     | 0.41              |
| 1:A:69:MET:HE1   | 1:A:73:GLU:HB3   | 2.02                     | 0.41              |
| 1:K:139:ASP:OD1  | 1:K:166:HIS:CE1  | 2.73                     | 0.41              |
| 1:D:391:VAL:O    | 1:D:391:VAL:CG2  | 2.69                     | 0.41              |
| 1:I:235:ASN:O    | 1:I:239:ILE:HG13 | 2.20                     | 0.41              |
| 1:E:322:PHE:HA   | 1:E:350:ILE:O    | 2.20                     | 0.41              |
| 1:F:313:ALA:HA   | 1:F:319:LEU:HD23 | 2.02                     | 0.41              |
| 1:C:301:LEU:CD1  | 1:C:326:TRP:HB3  | 2.51                     | 0.41              |
| 1:I:51:LEU:HD12  | 1:I:51:LEU:N     | 2.36                     | 0.41              |
| 1:D:301:LEU:CD1  | 1:D:326:TRP:HB3  | 2.50                     | 0.41              |
| 1:J:106:ASP:HA   | 1:J:107:PRO:HD2  | 1.94                     | 0.41              |
| 1:B:244:LEU:CD1  | 1:B:244:LEU:C    | 2.90                     | 0.41              |
| 1:K:212:ILE:HD13 | 1:K:253:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:224:LEU:HD13 | 1:B:228:PHE:CD1  | 2.55                     | 0.41              |
| 1:K:169:LEU:HG   | 1:K:171:LEU:HD21 | 2.02                     | 0.41              |
| 1:E:113:GLN:HE21 | 1:E:113:GLN:HA   | 1.84                     | 0.40              |
| 1:J:52:VAL:O     | 1:J:55:VAL:HG12  | 2.21                     | 0.40              |
| 1:B:313:ALA:HA   | 1:B:319:LEU:HD23 | 2.03                     | 0.40              |
| 1:G:30:PHE:CE2   | 1:G:37:ILE:HG13  | 2.56                     | 0.40              |
| 1:K:322:PHE:HA   | 1:K:350:ILE:O    | 2.21                     | 0.40              |
| 1:K:385:LEU:HD21 | 1:K:391:VAL:HG22 | 2.04                     | 0.40              |
| 1:J:123:THR:OG1  | 1:J:126:GLU:HG3  | 2.21                     | 0.40              |
| 1:G:265:VAL:HG21 | 1:G:275:PHE:HB2  | 2.04                     | 0.40              |
| 1:G:288:LEU:CD2  | 1:G:319:LEU:HB2  | 2.51                     | 0.40              |
| 1:D:111:ASP:OD1  | 1:D:114:VAL:HG23 | 2.21                     | 0.40              |
| 1:L:49:HIS:HB2   | 1:L:272:ALA:HB2  | 2.02                     | 0.40              |
| 1:J:313:ALA:HA   | 1:J:319:LEU:HD23 | 2.03                     | 0.40              |
| 1:I:245:LEU:HB2  | 1:I:246:PRO:HD3  | 2.04                     | 0.40              |
| 1:L:394:GLU:HB2  | 6:L:674:HOH:O    | 2.20                     | 0.40              |
| 1:D:265:VAL:HG21 | 1:D:275:PHE:HB2  | 2.02                     | 0.40              |
| 1:G:6:ARG:HG3    | 1:G:382:ASP:OD1  | 2.22                     | 0.40              |
| 1:G:6:ARG:HG2    | 1:G:6:ARG:NH1    | 2.37                     | 0.40              |
| 1:E:149:ASP:OD1  | 1:E:152:ARG:NH2  | 2.54                     | 0.40              |
| 1:F:276:VAL:CG2  | 1:F:277:GLY:N    | 2.83                     | 0.40              |
| 1:E:203:GLU:OE1  | 1:E:206:ARG:NH1  | 2.54                     | 0.40              |
| 1:C:386:GLN:NE2  | 1:L:4:ASN:OD1    | 2.55                     | 0.40              |
| 1:F:208:LEU:O    | 1:F:212:ILE:HG13 | 2.21                     | 0.40              |
| 1:J:148:ASP:OD2  | 1:J:151:GLU:HG3  | 2.22                     | 0.40              |
| 1:I:52:VAL:O     | 1:I:55:VAL:HG12  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:301:LEU:HD11 | 1:G:326:TRP:HB3  | 2.04                     | 0.40              |
| 1:H:409:TRP:HA   | 1:H:412:VAL:HG22 | 2.03                     | 0.40              |
| 1:F:40:TRP:O     | 1:F:41:ASP:CB    | 2.70                     | 0.40              |
| 1:C:170:ARG:NH2  | 1:C:223:SER:HB3  | 2.36                     | 0.40              |
| 1:E:145:ASP:HA   | 1:E:146:PRO:HD2  | 1.92                     | 0.40              |
| 1:H:204:VAL:O    | 1:H:207:PHE:HB3  | 2.22                     | 0.40              |
| 1:F:154:SER:O    | 1:F:159:LYS:HB2  | 2.22                     | 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     | 411/427 (96%)   | 398 (97%)  | 10 (2%)  | 3 (1%)   | 26          | 21 |
| 1   | B     | 411/427 (96%)   | 398 (97%)  | 10 (2%)  | 3 (1%)   | 26          | 21 |
| 1   | C     | 411/427 (96%)   | 399 (97%)  | 10 (2%)  | 2 (0%)   | 34          | 30 |
| 1   | D     | 411/427 (96%)   | 399 (97%)  | 10 (2%)  | 2 (0%)   | 34          | 30 |
| 1   | E     | 411/427 (96%)   | 396 (96%)  | 12 (3%)  | 3 (1%)   | 26          | 21 |
| 1   | F     | 411/427 (96%)   | 396 (96%)  | 14 (3%)  | 1 (0%)   | 52          | 53 |
| 1   | G     | 411/427 (96%)   | 401 (98%)  | 8 (2%)   | 2 (0%)   | 34          | 30 |
| 1   | H     | 411/427 (96%)   | 394 (96%)  | 15 (4%)  | 2 (0%)   | 34          | 30 |
| 1   | I     | 411/427 (96%)   | 396 (96%)  | 13 (3%)  | 2 (0%)   | 34          | 30 |
| 1   | J     | 411/427 (96%)   | 401 (98%)  | 8 (2%)   | 2 (0%)   | 34          | 30 |
| 1   | K     | 411/427 (96%)   | 399 (97%)  | 10 (2%)  | 2 (0%)   | 34          | 30 |
| 1   | L     | 411/427 (96%)   | 399 (97%)  | 10 (2%)  | 2 (0%)   | 34          | 30 |
| All | All   | 4932/5124 (96%) | 4776 (97%) | 130 (3%) | 26 (0%)  | 34          | 30 |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 41  | ASP  |
| 1   | H     | 41  | ASP  |
| 1   | I     | 41  | ASP  |
| 1   | J     | 41  | ASP  |
| 1   | K     | 41  | ASP  |
| 1   | L     | 41  | ASP  |
| 1   | A     | 41  | ASP  |
| 1   | C     | 41  | ASP  |
| 1   | D     | 41  | ASP  |
| 1   | E     | 41  | ASP  |
| 1   | F     | 41  | ASP  |
| 1   | G     | 41  | ASP  |
| 1   | G     | 323 | GLY  |
| 1   | H     | 323 | GLY  |
| 1   | J     | 323 | GLY  |
| 1   | K     | 323 | GLY  |
| 1   | B     | 323 | GLY  |
| 1   | E     | 159 | LYS  |
| 1   | E     | 323 | GLY  |
| 1   | A     | 36  | GLU  |
| 1   | I     | 323 | GLY  |
| 1   | L     | 323 | GLY  |
| 1   | A     | 323 | GLY  |
| 1   | B     | 405 | SER  |
| 1   | C     | 323 | GLY  |
| 1   | D     | 323 | GLY  |

### 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     | 373/387 (96%) | 366 (98%) | 7 (2%)   | 65          | 70 |
| 1   | B     | 373/387 (96%) | 364 (98%) | 9 (2%)   | 57          | 61 |
| 1   | C     | 373/387 (96%) | 368 (99%) | 5 (1%)   | 76          | 82 |
| 1   | D     | 373/387 (96%) | 368 (99%) | 5 (1%)   | 76          | 82 |
| 1   | E     | 373/387 (96%) | 365 (98%) | 8 (2%)   | 61          | 66 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | F     | 373/387 (96%)   | 366 (98%)  | 7 (2%)   | 65          | 70 |
| 1   | G     | 373/387 (96%)   | 366 (98%)  | 7 (2%)   | 65          | 70 |
| 1   | H     | 373/387 (96%)   | 368 (99%)  | 5 (1%)   | 76          | 82 |
| 1   | I     | 373/387 (96%)   | 368 (99%)  | 5 (1%)   | 76          | 82 |
| 1   | J     | 373/387 (96%)   | 368 (99%)  | 5 (1%)   | 76          | 82 |
| 1   | K     | 373/387 (96%)   | 366 (98%)  | 7 (2%)   | 65          | 70 |
| 1   | L     | 373/387 (96%)   | 368 (99%)  | 5 (1%)   | 76          | 82 |
| All | All   | 4476/4644 (96%) | 4401 (98%) | 75 (2%)  | 68          | 74 |

All (75) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 72  | ARG  |
| 1   | A     | 127 | GLN  |
| 1   | A     | 129 | ASP  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 264 | ARG  |
| 1   | A     | 364 | TYR  |
| 1   | B     | 127 | GLN  |
| 1   | B     | 128 | VAL  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 187 | ASP  |
| 1   | B     | 194 | ASP  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 252 | ASN  |
| 1   | B     | 264 | ARG  |
| 1   | B     | 364 | TYR  |
| 1   | C     | 127 | GLN  |
| 1   | C     | 182 | LYS  |
| 1   | C     | 364 | TYR  |
| 1   | C     | 385 | LEU  |
| 1   | C     | 414 | ARG  |
| 1   | D     | 127 | GLN  |
| 1   | D     | 133 | GLN  |
| 1   | D     | 194 | ASP  |
| 1   | D     | 252 | ASN  |
| 1   | D     | 364 | TYR  |
| 1   | E     | 15  | ASN  |
| 1   | E     | 127 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 175 | LEU  |
| 1   | E     | 180 | GLN  |
| 1   | E     | 191 | LYS  |
| 1   | E     | 244 | LEU  |
| 1   | E     | 355 | ASP  |
| 1   | E     | 364 | TYR  |
| 1   | F     | 72  | ARG  |
| 1   | F     | 127 | GLN  |
| 1   | F     | 128 | VAL  |
| 1   | F     | 191 | LYS  |
| 1   | F     | 305 | ASN  |
| 1   | F     | 364 | TYR  |
| 1   | F     | 385 | LEU  |
| 1   | G     | 15  | ASN  |
| 1   | G     | 72  | ARG  |
| 1   | G     | 127 | GLN  |
| 1   | G     | 180 | GLN  |
| 1   | G     | 187 | ASP  |
| 1   | G     | 194 | ASP  |
| 1   | G     | 364 | TYR  |
| 1   | H     | 41  | ASP  |
| 1   | H     | 127 | GLN  |
| 1   | H     | 264 | ARG  |
| 1   | H     | 364 | TYR  |
| 1   | H     | 385 | LEU  |
| 1   | I     | 86  | ARG  |
| 1   | I     | 127 | GLN  |
| 1   | I     | 133 | GLN  |
| 1   | I     | 355 | ASP  |
| 1   | I     | 364 | TYR  |
| 1   | J     | 15  | ASN  |
| 1   | J     | 121 | LYS  |
| 1   | J     | 127 | GLN  |
| 1   | J     | 364 | TYR  |
| 1   | J     | 390 | GLU  |
| 1   | K     | 113 | GLN  |
| 1   | K     | 127 | GLN  |
| 1   | K     | 194 | ASP  |
| 1   | K     | 252 | ASN  |
| 1   | K     | 264 | ARG  |
| 1   | K     | 364 | TYR  |
| 1   | K     | 386 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 127 | GLN  |
| 1   | L     | 133 | GLN  |
| 1   | L     | 182 | LYS  |
| 1   | L     | 244 | LEU  |
| 1   | L     | 364 | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ASN  |
| 1   | A     | 113 | GLN  |
| 1   | A     | 127 | GLN  |
| 1   | A     | 166 | HIS  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 293 | ASN  |
| 1   | B     | 18  | ASN  |
| 1   | B     | 113 | GLN  |
| 1   | B     | 127 | GLN  |
| 1   | B     | 166 | HIS  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 202 | GLN  |
| 1   | B     | 252 | ASN  |
| 1   | B     | 293 | ASN  |
| 1   | C     | 18  | ASN  |
| 1   | C     | 127 | GLN  |
| 1   | C     | 166 | HIS  |
| 1   | C     | 180 | GLN  |
| 1   | C     | 202 | GLN  |
| 1   | C     | 252 | ASN  |
| 1   | C     | 293 | ASN  |
| 1   | C     | 386 | GLN  |
| 1   | D     | 18  | ASN  |
| 1   | D     | 74  | GLN  |
| 1   | D     | 113 | GLN  |
| 1   | D     | 127 | GLN  |
| 1   | D     | 166 | HIS  |
| 1   | D     | 202 | GLN  |
| 1   | D     | 252 | ASN  |
| 1   | D     | 293 | ASN  |
| 1   | E     | 18  | ASN  |
| 1   | E     | 113 | GLN  |
| 1   | E     | 127 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 160 | GLN  |
| 1   | E     | 166 | HIS  |
| 1   | E     | 180 | GLN  |
| 1   | E     | 202 | GLN  |
| 1   | E     | 235 | ASN  |
| 1   | E     | 252 | ASN  |
| 1   | E     | 293 | ASN  |
| 1   | F     | 18  | ASN  |
| 1   | F     | 101 | GLN  |
| 1   | F     | 113 | GLN  |
| 1   | F     | 127 | GLN  |
| 1   | F     | 166 | HIS  |
| 1   | F     | 180 | GLN  |
| 1   | F     | 202 | GLN  |
| 1   | F     | 252 | ASN  |
| 1   | F     | 293 | ASN  |
| 1   | F     | 386 | GLN  |
| 1   | G     | 18  | ASN  |
| 1   | G     | 127 | GLN  |
| 1   | G     | 160 | GLN  |
| 1   | G     | 166 | HIS  |
| 1   | G     | 180 | GLN  |
| 1   | G     | 193 | ASN  |
| 1   | H     | 18  | ASN  |
| 1   | H     | 127 | GLN  |
| 1   | H     | 166 | HIS  |
| 1   | H     | 180 | GLN  |
| 1   | H     | 193 | ASN  |
| 1   | H     | 197 | ASN  |
| 1   | H     | 286 | HIS  |
| 1   | H     | 386 | GLN  |
| 1   | I     | 18  | ASN  |
| 1   | I     | 127 | GLN  |
| 1   | I     | 166 | HIS  |
| 1   | I     | 293 | ASN  |
| 1   | J     | 18  | ASN  |
| 1   | J     | 113 | GLN  |
| 1   | J     | 127 | GLN  |
| 1   | J     | 166 | HIS  |
| 1   | J     | 252 | ASN  |
| 1   | K     | 18  | ASN  |
| 1   | K     | 113 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 127 | GLN  |
| 1   | K     | 160 | GLN  |
| 1   | K     | 166 | HIS  |
| 1   | K     | 252 | ASN  |
| 1   | K     | 286 | HIS  |
| 1   | K     | 386 | GLN  |
| 1   | L     | 18  | ASN  |
| 1   | L     | 113 | GLN  |
| 1   | L     | 127 | GLN  |
| 1   | L     | 166 | HIS  |
| 1   | L     | 202 | GLN  |
| 1   | L     | 252 | ASN  |
| 1   | L     | 293 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 16 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 | $\# Z  > 2$ |
| 2   | REL  | A     | 428 | 4    | 8,12,12      | 1.12 | 1 (12%)     | 10,16,16    | 0.98 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CO3  | A     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 3   | CO3  | A     | 430 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | B     | 428 | 4    | 8,12,12      | 1.05 | 0        | 10,16,16    | 0.78 | 0        |
| 2   | REL  | C     | 428 | 4    | 8,12,12      | 1.10 | 1 (12%)  | 10,16,16    | 1.03 | 0        |
| 3   | CO3  | C     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | D     | 428 | 4    | 8,12,12      | 0.95 | 0        | 10,16,16    | 0.98 | 0        |
| 3   | CO3  | D     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 3   | CO3  | D     | 430 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | E     | 428 | 4    | 8,12,12      | 1.26 | 1 (12%)  | 10,16,16    | 0.88 | 0        |
| 2   | REL  | F     | 428 | 4    | 8,12,12      | 1.00 | 0        | 10,16,16    | 1.10 | 0        |
| 3   | CO3  | F     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | G     | 428 | 4    | 8,12,12      | 0.98 | 0        | 10,16,16    | 1.01 | 0        |
| 3   | CO3  | G     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | H     | 428 | 4    | 8,12,12      | 1.03 | 1 (12%)  | 10,16,16    | 0.93 | 0        |
| 3   | CO3  | H     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | I     | 428 | 4    | 8,12,12      | 0.96 | 0        | 10,16,16    | 0.90 | 0        |
| 3   | CO3  | I     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | J     | 428 | 4    | 8,12,12      | 1.10 | 0        | 10,16,16    | 0.95 | 0        |
| 3   | CO3  | J     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | K     | 428 | 4    | 8,12,12      | 0.91 | 0        | 10,16,16    | 0.93 | 0        |
| 3   | CO3  | K     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 2   | REL  | L     | 428 | 4    | 8,12,12      | 0.94 | 0        | 10,16,16    | 0.91 | 0        |
| 3   | CO3  | L     | 429 | -    | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | REL  | A     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | A     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 3   | CO3  | A     | 430 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | B     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 2   | REL  | C     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | C     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | D     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | D     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 3   | CO3  | D     | 430 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | E     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 2   | REL  | F     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | F     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | REL  | G     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | G     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | H     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | H     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | I     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | I     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | J     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | J     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | K     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | K     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | REL  | L     | 428 | 4    | -       | 0/12/18/18 | 0/0/0/0 |
| 3   | CO3  | L     | 429 | -    | -       | 0/0/0/0    | 0/0/0/0 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | C     | 428 | REL  | C2-C1 | 2.02 | 1.53        | 1.50     |
| 2   | A     | 428 | REL  | C2-C1 | 2.04 | 1.53        | 1.50     |
| 2   | H     | 428 | REL  | C2-C1 | 2.18 | 1.54        | 1.50     |
| 2   | E     | 428 | REL  | C2-C1 | 2.36 | 1.54        | 1.50     |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 428 | REL  | 1       | 0            |
| 2   | C     | 428 | REL  | 1       | 0            |
| 2   | D     | 428 | REL  | 1       | 0            |
| 2   | F     | 428 | REL  | 1       | 0            |
| 2   | G     | 428 | REL  | 1       | 0            |
| 2   | H     | 428 | REL  | 1       | 0            |
| 2   | K     | 428 | REL  | 1       | 0            |
| 2   | L     | 428 | REL  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 413/427 (96%)   | -0.13  | 6 (1%) 76 81  | 18, 28, 47, 64        | 0     |
| 1   | B     | 413/427 (96%)   | 0.10   | 16 (3%) 43 52 | 19, 30, 50, 65        | 0     |
| 1   | C     | 413/427 (96%)   | -0.15  | 3 (0%) 89 91  | 17, 27, 43, 63        | 0     |
| 1   | D     | 413/427 (96%)   | -0.26  | 3 (0%) 89 91  | 15, 25, 42, 62        | 0     |
| 1   | E     | 413/427 (96%)   | -0.05  | 7 (1%) 73 78  | 18, 29, 47, 65        | 0     |
| 1   | F     | 413/427 (96%)   | -0.06  | 9 (2%) 65 71  | 18, 28, 46, 65        | 0     |
| 1   | G     | 413/427 (96%)   | -0.05  | 7 (1%) 73 78  | 18, 28, 46, 64        | 0     |
| 1   | H     | 413/427 (96%)   | -0.13  | 3 (0%) 89 91  | 17, 28, 47, 65        | 0     |
| 1   | I     | 413/427 (96%)   | -0.12  | 6 (1%) 76 81  | 18, 28, 48, 64        | 0     |
| 1   | J     | 413/427 (96%)   | -0.17  | 3 (0%) 89 91  | 16, 27, 43, 64        | 0     |
| 1   | K     | 413/427 (96%)   | -0.14  | 7 (1%) 73 78  | 17, 27, 47, 62        | 0     |
| 1   | L     | 413/427 (96%)   | -0.26  | 4 (0%) 84 87  | 16, 25, 44, 62        | 0     |
| All | All   | 4956/5124 (96%) | -0.12  | 74 (1%) 76 81 | 15, 28, 46, 65        | 0     |

All (74) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 414 | ARG  | 5.9  |
| 1   | H     | 414 | ARG  | 4.7  |
| 1   | B     | 414 | ARG  | 4.7  |
| 1   | D     | 414 | ARG  | 4.5  |
| 1   | L     | 414 | ARG  | 4.4  |
| 1   | K     | 414 | ARG  | 4.0  |
| 1   | J     | 414 | ARG  | 3.7  |
| 1   | E     | 414 | ARG  | 3.7  |
| 1   | I     | 414 | ARG  | 3.6  |
| 1   | E     | 121 | LYS  | 3.6  |
| 1   | G     | 414 | ARG  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 414 | ARG  | 3.4  |
| 1   | B     | 113 | GLN  | 3.3  |
| 1   | I     | 183 | HIS  | 3.2  |
| 1   | B     | 153 | ILE  | 3.1  |
| 1   | B     | 204 | VAL  | 3.1  |
| 1   | A     | 414 | ARG  | 3.0  |
| 1   | E     | 68  | ALA  | 3.0  |
| 1   | A     | 194 | ASP  | 2.9  |
| 1   | G     | 199 | GLY  | 2.9  |
| 1   | D     | 68  | ALA  | 2.9  |
| 1   | E     | 413 | GLY  | 2.8  |
| 1   | B     | 247 | VAL  | 2.8  |
| 1   | A     | 68  | ALA  | 2.8  |
| 1   | B     | 191 | LYS  | 2.7  |
| 1   | D     | 60  | ASP  | 2.7  |
| 1   | K     | 183 | HIS  | 2.7  |
| 1   | F     | 413 | GLY  | 2.7  |
| 1   | C     | 121 | LYS  | 2.6  |
| 1   | G     | 194 | ASP  | 2.6  |
| 1   | G     | 250 | LYS  | 2.6  |
| 1   | B     | 186 | ARG  | 2.6  |
| 1   | B     | 194 | ASP  | 2.6  |
| 1   | I     | 194 | ASP  | 2.6  |
| 1   | F     | 194 | ASP  | 2.5  |
| 1   | A     | 195 | GLU  | 2.5  |
| 1   | K     | 197 | ASN  | 2.5  |
| 1   | B     | 2   | SER  | 2.5  |
| 1   | A     | 183 | HIS  | 2.5  |
| 1   | J     | 2   | SER  | 2.5  |
| 1   | K     | 194 | ASP  | 2.5  |
| 1   | B     | 65  | ALA  | 2.4  |
| 1   | G     | 198 | GLU  | 2.4  |
| 1   | E     | 2   | SER  | 2.4  |
| 1   | H     | 195 | GLU  | 2.4  |
| 1   | C     | 413 | GLY  | 2.4  |
| 1   | B     | 200 | SER  | 2.3  |
| 1   | B     | 183 | HIS  | 2.3  |
| 1   | F     | 180 | GLN  | 2.3  |
| 1   | I     | 186 | ARG  | 2.3  |
| 1   | K     | 180 | GLN  | 2.3  |
| 1   | B     | 250 | LYS  | 2.2  |
| 1   | F     | 68  | ALA  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 195 | GLU  | 2.2  |
| 1   | B     | 251 | HIS  | 2.2  |
| 1   | H     | 128 | VAL  | 2.2  |
| 1   | B     | 180 | GLN  | 2.2  |
| 1   | F     | 192 | VAL  | 2.2  |
| 1   | F     | 113 | GLN  | 2.2  |
| 1   | I     | 264 | ARG  | 2.2  |
| 1   | L     | 183 | HIS  | 2.2  |
| 1   | E     | 60  | ASP  | 2.2  |
| 1   | L     | 113 | GLN  | 2.1  |
| 1   | A     | 60  | ASP  | 2.1  |
| 1   | J     | 121 | LYS  | 2.1  |
| 1   | K     | 191 | LYS  | 2.1  |
| 1   | L     | 121 | LYS  | 2.1  |
| 1   | E     | 113 | GLN  | 2.1  |
| 1   | K     | 195 | GLU  | 2.1  |
| 1   | F     | 183 | HIS  | 2.1  |
| 1   | B     | 413 | GLY  | 2.0  |
| 1   | I     | 121 | LYS  | 2.0  |
| 1   | G     | 264 | ARG  | 2.0  |
| 1   | F     | 153 | ILE  | 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 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 4   | ZN   | H     | 430 | 1/1   | 1.00 | 0.14 | 1.86 | 33,33,33,33                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 2   | REL  | B     | 428 | 13/13 | 0.93 | 0.15 | 1.11  | 29,31,34,34                | 0     |
| 3   | CO3  | F     | 429 | 4/4   | 0.95 | 0.14 | 1.10  | 24,25,26,29                | 0     |
| 2   | REL  | G     | 428 | 13/13 | 0.95 | 0.14 | 0.94  | 25,27,29,29                | 0     |
| 3   | CO3  | K     | 429 | 4/4   | 0.98 | 0.13 | 0.87  | 20,22,22,23                | 0     |
| 2   | REL  | A     | 428 | 13/13 | 0.93 | 0.12 | 0.84  | 28,31,32,32                | 0     |
| 2   | REL  | L     | 428 | 13/13 | 0.91 | 0.13 | 0.84  | 24,27,29,29                | 0     |
| 3   | CO3  | I     | 429 | 4/4   | 0.97 | 0.14 | 0.80  | 23,24,26,26                | 0     |
| 5   | CL   | H     | 431 | 1/1   | 1.00 | 0.14 | 0.75  | 21,21,21,21                | 0     |
| 3   | CO3  | D     | 429 | 4/4   | 0.98 | 0.13 | 0.65  | 18,20,21,21                | 0     |
| 3   | CO3  | C     | 429 | 4/4   | 0.96 | 0.13 | 0.58  | 22,22,23,24                | 0     |
| 3   | CO3  | H     | 429 | 4/4   | 0.98 | 0.13 | 0.57  | 24,25,25,25                | 0     |
| 5   | CL   | A     | 432 | 1/1   | 1.00 | 0.13 | 0.55  | 23,23,23,23                | 0     |
| 3   | CO3  | A     | 429 | 4/4   | 0.95 | 0.11 | 0.51  | 23,24,25,27                | 0     |
| 2   | REL  | K     | 428 | 13/13 | 0.92 | 0.12 | 0.48  | 26,30,31,31                | 0     |
| 3   | CO3  | L     | 429 | 4/4   | 0.99 | 0.12 | 0.41  | 19,20,23,25                | 0     |
| 3   | CO3  | A     | 430 | 4/4   | 0.98 | 0.12 | 0.25  | 21,22,23,25                | 0     |
| 2   | REL  | J     | 428 | 13/13 | 0.96 | 0.12 | 0.24  | 25,28,31,31                | 0     |
| 5   | CL   | K     | 431 | 1/1   | 1.00 | 0.12 | 0.24  | 21,21,21,21                | 0     |
| 2   | REL  | I     | 428 | 13/13 | 0.92 | 0.12 | 0.16  | 27,31,32,32                | 0     |
| 2   | REL  | E     | 428 | 13/13 | 0.94 | 0.12 | 0.14  | 27,30,34,34                | 0     |
| 2   | REL  | D     | 428 | 13/13 | 0.94 | 0.12 | 0.09  | 25,27,28,29                | 0     |
| 2   | REL  | F     | 428 | 13/13 | 0.94 | 0.12 | 0.09  | 25,28,31,31                | 0     |
| 4   | ZN   | F     | 430 | 1/1   | 0.99 | 0.13 | 0.04  | 30,30,30,30                | 0     |
| 2   | REL  | H     | 428 | 13/13 | 0.94 | 0.10 | -0.11 | 25,31,33,33                | 0     |
| 4   | ZN   | B     | 429 | 1/1   | 0.99 | 0.12 | -0.25 | 36,36,36,36                | 0     |
| 3   | CO3  | D     | 430 | 4/4   | 0.99 | 0.11 | -0.34 | 20,20,21,24                | 0     |
| 2   | REL  | C     | 428 | 13/13 | 0.94 | 0.10 | -0.42 | 26,29,30,30                | 0     |
| 3   | CO3  | J     | 429 | 4/4   | 0.99 | 0.10 | -0.48 | 18,18,20,22                | 0     |
| 4   | ZN   | I     | 430 | 1/1   | 0.98 | 0.12 | -0.63 | 32,32,32,32                | 0     |
| 4   | ZN   | L     | 430 | 1/1   | 0.99 | 0.10 | -0.91 | 24,24,24,24                | 0     |
| 4   | ZN   | C     | 430 | 1/1   | 1.00 | 0.09 | -1.63 | 26,26,26,26                | 0     |
| 4   | ZN   | E     | 429 | 1/1   | 0.98 | 0.08 | -1.69 | 27,27,27,27                | 0     |
| 4   | ZN   | J     | 430 | 1/1   | 1.00 | 0.10 | -2.07 | 25,25,25,25                | 0     |
| 3   | CO3  | G     | 429 | 4/4   | 0.99 | 0.06 | -2.19 | 19,21,22,22                | 0     |
| 4   | ZN   | G     | 430 | 1/1   | 1.00 | 0.09 | -2.28 | 27,27,27,27                | 0     |
| 4   | ZN   | A     | 431 | 1/1   | 0.99 | 0.08 | -2.36 | 27,27,27,27                | 0     |
| 5   | CL   | F     | 431 | 1/1   | 1.00 | 0.08 | -2.51 | 20,20,20,20                | 0     |
| 4   | ZN   | D     | 431 | 1/1   | 0.99 | 0.06 | -4.39 | 21,21,21,21                | 0     |
| 4   | ZN   | K     | 430 | 1/1   | 1.00 | 0.09 | -     | 29,29,29,29                | 0     |



## 6.5 Other polymers ⓘ

There are no such residues in this entry.