



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:15 AM UTC

PDB ID : 3HK7 / pdb\_00003hk7  
Title : Crystal structure of uronate isomerase from *Bacillus halodurans* complexed with zinc and D-Arabinarate, monoclinic crystal form  
Authors : Fedorov, A.A.; Fedorov, E.V.; Nguyen, T.T.; Raushel, F.M.; Almo, S.C.  
Deposited on : 2009-05-22  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

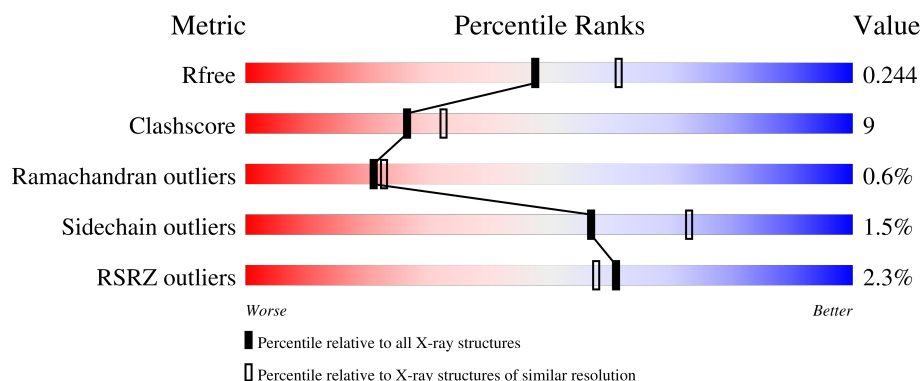
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6164 (2.20-2.20)                                      |
| Clashscore            | 190562                      | 6851 (2.20-2.20)                                      |
| Ramachandran outliers | 187476                      | 6768 (2.20-2.20)                                      |
| Sidechain outliers    | 187428                      | 6769 (2.20-2.20)                                      |
| RSRZ outliers         | 180081                      | 6166 (2.20-2.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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>3%</div> <div>69%</div> <div>26%</div> <div>..</div> </div> |
| 1   | B     | 427    | <div> <div>8%</div> <div>64%</div> <div>31%</div> <div>..</div> </div> |
| 1   | C     | 427    | <div> <div>%</div> <div>79%</div> <div>15%</div> <div>..</div> </div>  |
| 1   | D     | 427    | <div> <div>%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>  |
| 1   | E     | 427    | <div> <div>3%</div> <div>70%</div> <div>24%</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>73%</div><div>21%</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>67%</div><div>28%</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>77%</div><div>18%</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>4%</div><div>72%</div><div>23%</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>74%</div><div>21%</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>%</div><div>75%</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>76%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>   |

## 2 Entry composition

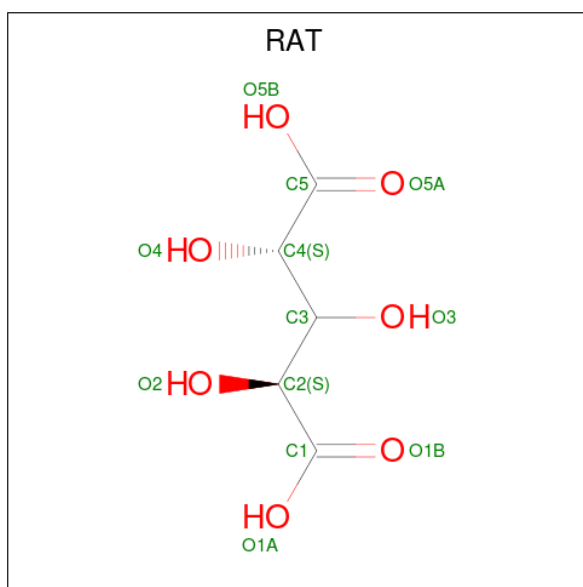
There are 7 unique types of molecules in this entry. The entry contains 42940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

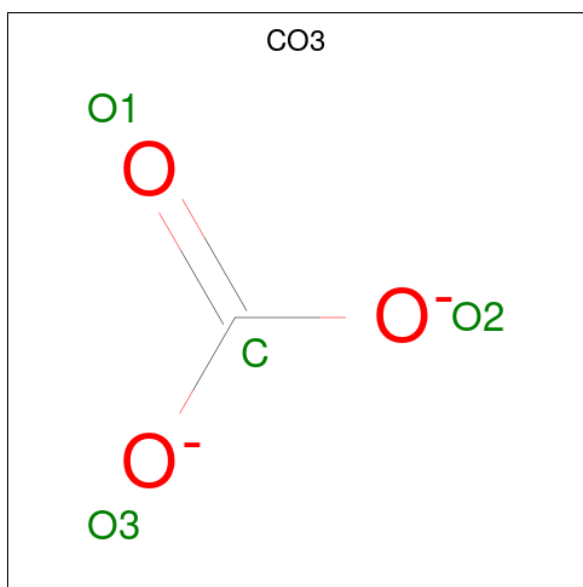
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3404  | 2170 | 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 D-arabinaric acid (CCD ID: RAT) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>7</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |
| 2   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 5 | 7 |         |         |

- Molecule 3 is CARBONATE ION (CCD ID: 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   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 3   | E     | 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   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6   | B     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 6   | E     | 1        | Total Cl<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 6   | G     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |
| 6   | J     | 1        | Total<br>1 | Cl<br>1 | 0       | 0       |

- Molecule 7 is water.

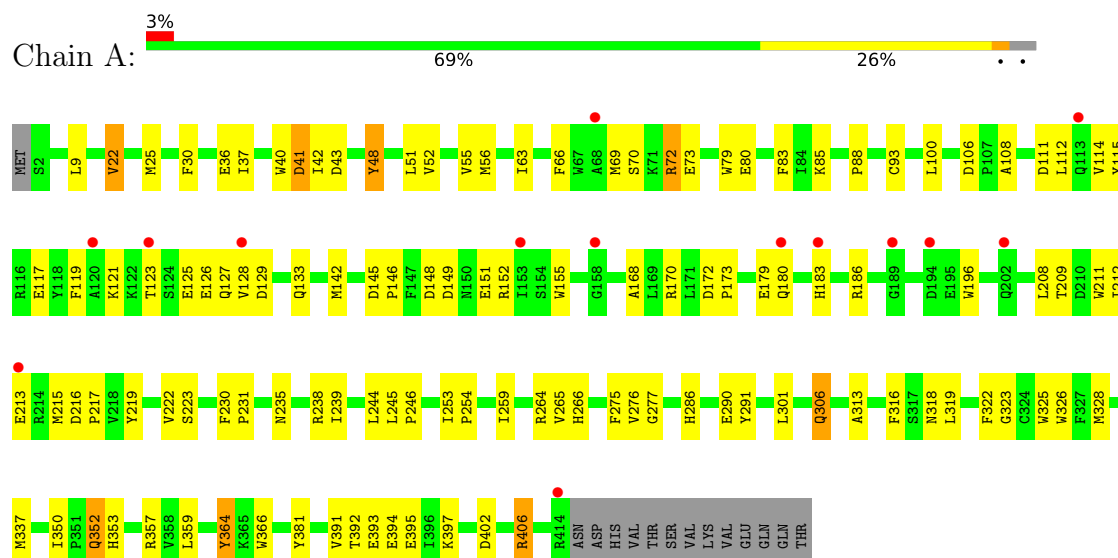
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7   | A     | 111      | Total<br>111 | O<br>111 | 0       | 0       |
| 7   | B     | 89       | Total<br>89  | O<br>89  | 0       | 0       |
| 7   | C     | 182      | Total<br>182 | O<br>182 | 0       | 0       |
| 7   | D     | 204      | Total<br>204 | O<br>204 | 0       | 0       |
| 7   | E     | 160      | Total<br>160 | O<br>160 | 0       | 0       |
| 7   | F     | 166      | Total<br>166 | O<br>166 | 0       | 0       |
| 7   | G     | 110      | Total<br>110 | O<br>110 | 0       | 0       |
| 7   | H     | 178      | Total<br>178 | O<br>178 | 0       | 0       |
| 7   | I     | 122      | Total<br>122 | O<br>122 | 0       | 0       |
| 7   | J     | 165      | Total<br>165 | O<br>165 | 0       | 0       |
| 7   | K     | 194      | Total<br>194 | O<br>194 | 0       | 0       |
| 7   | L     | 199      | Total<br>199 | O<br>199 | 0       | 0       |



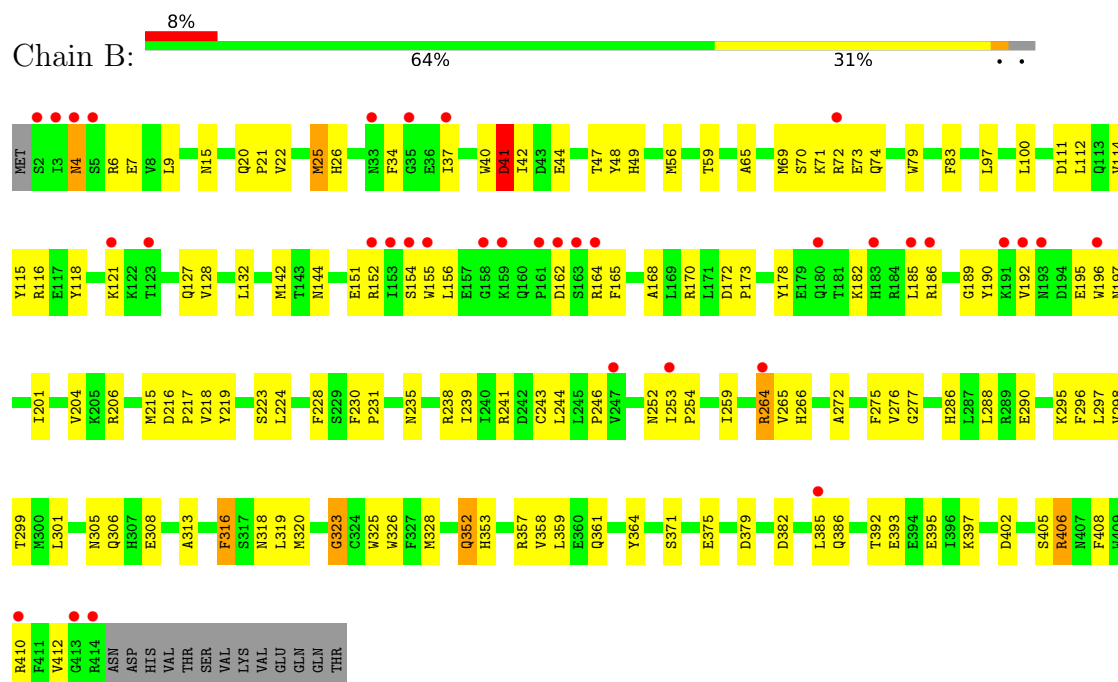
### 3 Residue-property plots

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

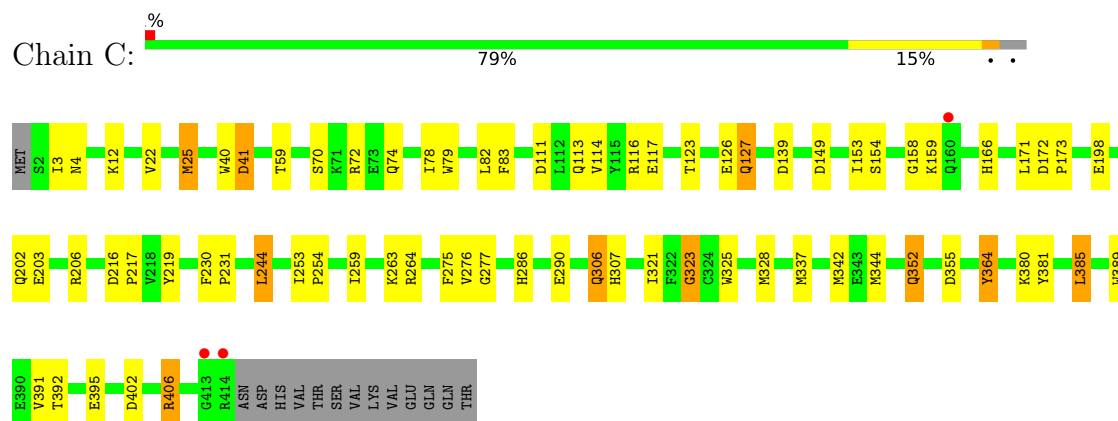
#### • Molecule 1: Uronate isomerase



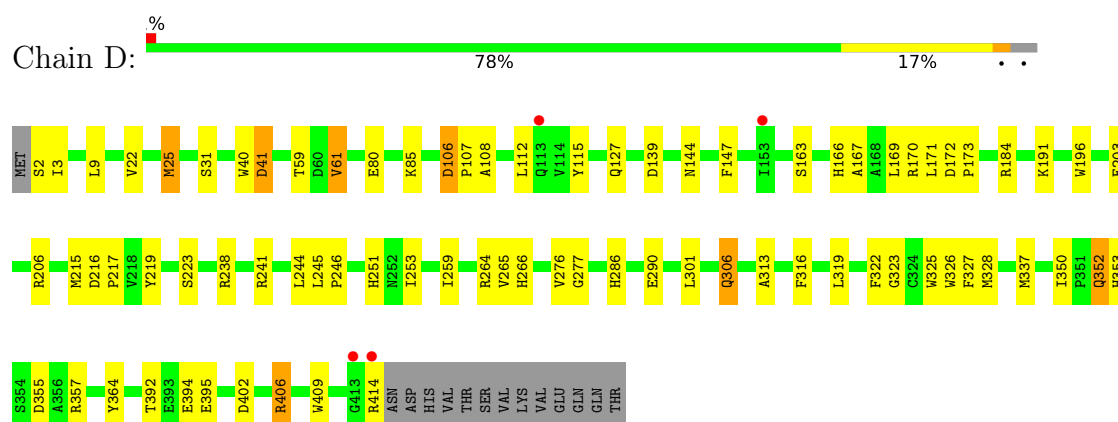
#### • Molecule 1: Uronate isomerase



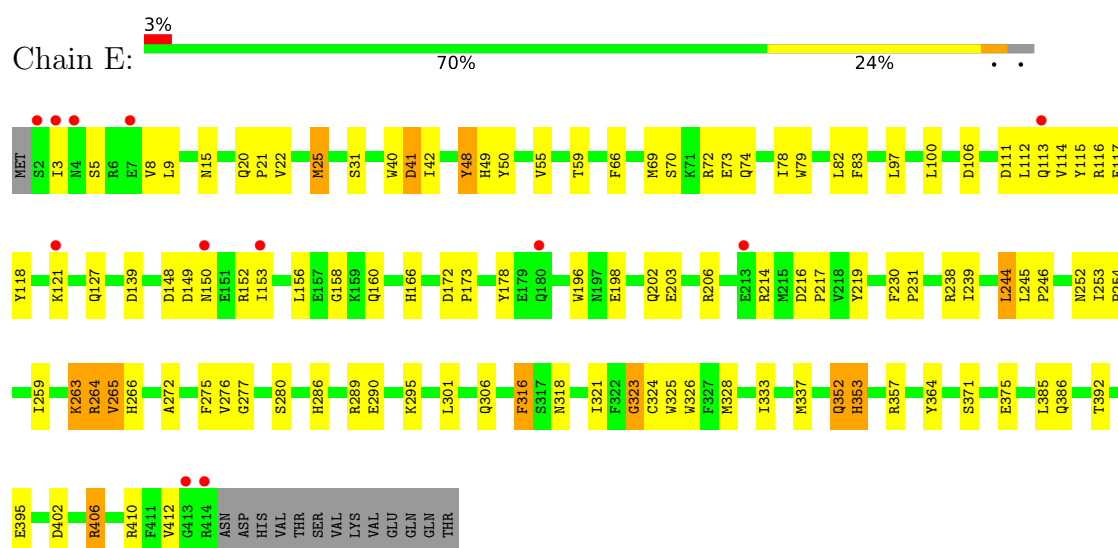
- Molecule 1: Uronate isomerase



- Molecule 1: Uronate isomerase

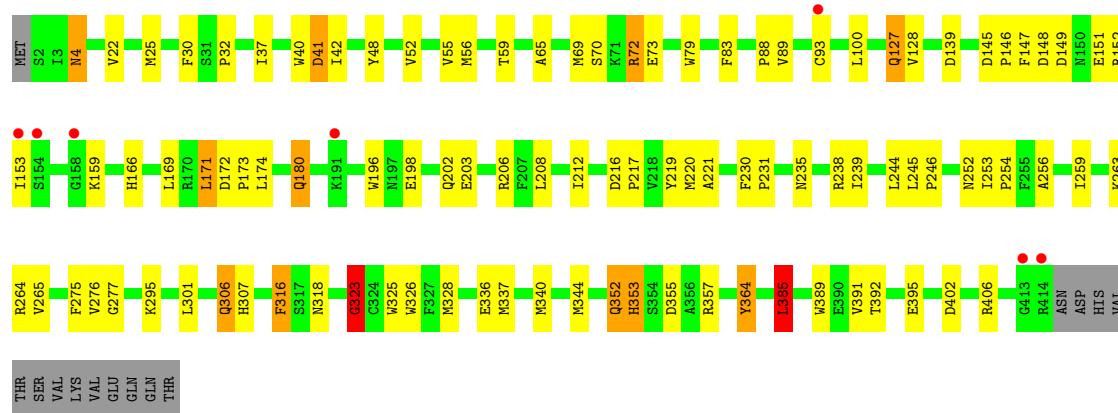


- Molecule 1: Uronate isomerase

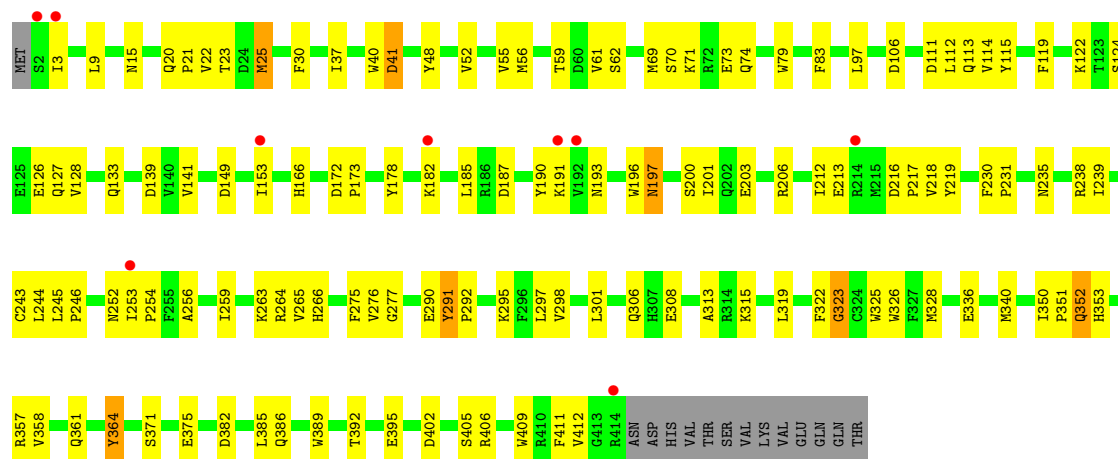


- Molecule 1: Uronate isomerase

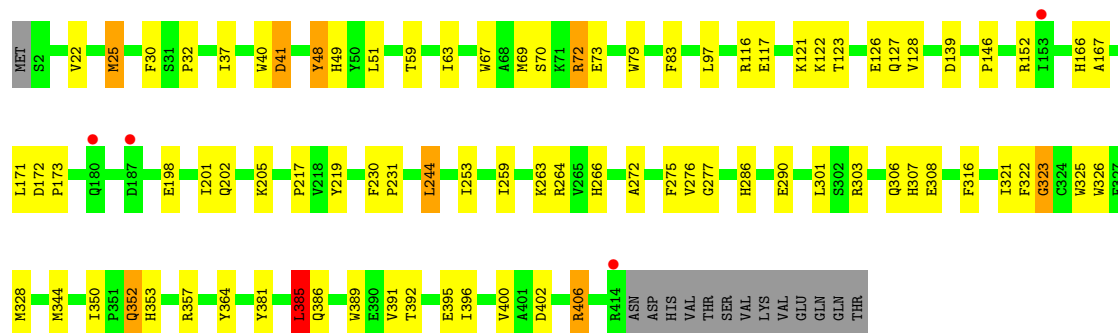
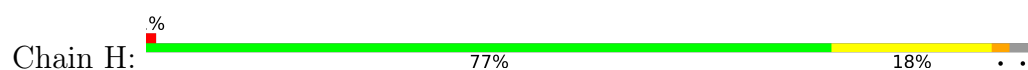




• Molecule 1: Uronate isomerase

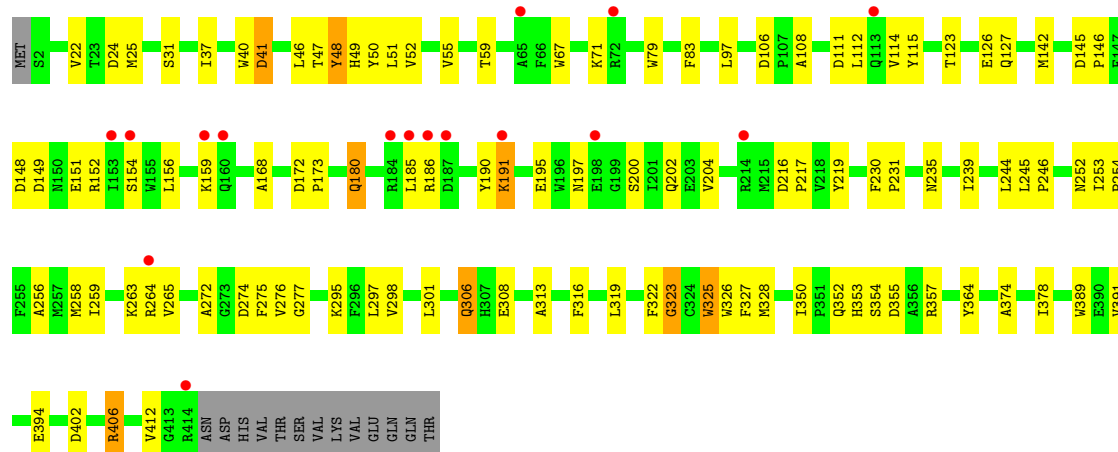


• Molecule 1: Uronate isomerase

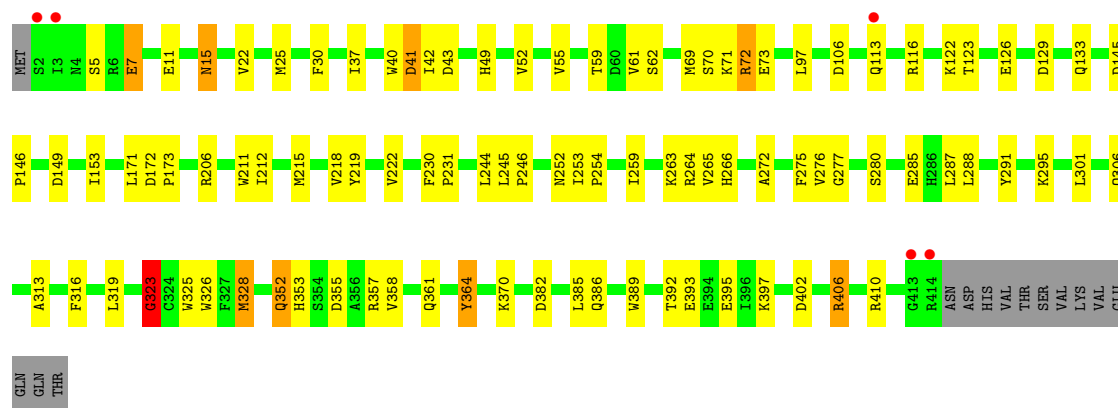


• Molecule 1: Uronate isomerase

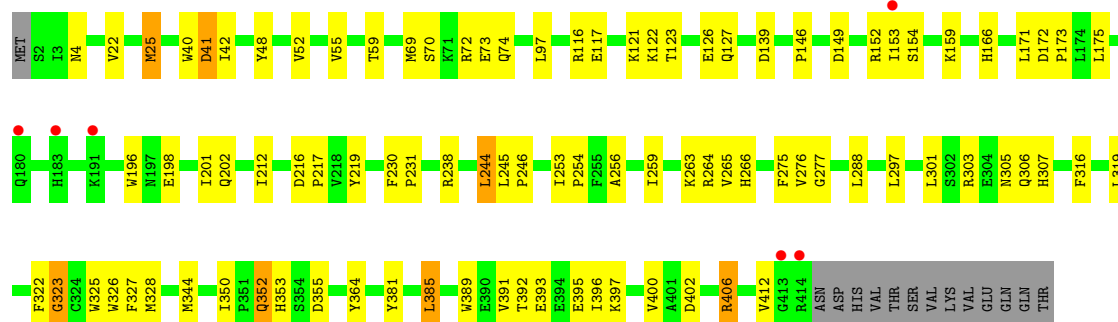
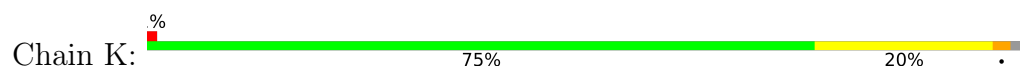




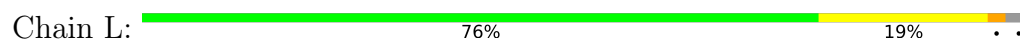
• Molecule 1: Uronate isomerase

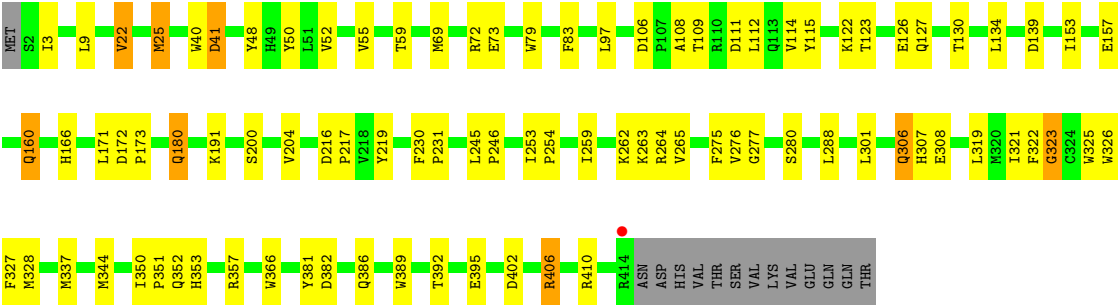


• Molecule 1: Uronate isomerase



• 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, $\alpha$ , $\beta$ , $\gamma$                | 274.82Å 156.52Å 185.96Å<br>90.00° 116.20° 90.00°                                                              | Depositor        |
| Resolution (Å)                                                          | 24.99 – 2.20<br>24.99 – 2.20                                                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.8 (24.99-2.20)<br>98.8 (24.99-2.20)                                                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                                                                          | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                                                               | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 2.10Å)                                                                                               | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                                                                       | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.245<br>0.213 , 0.244                                                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 20190 reflections (5.03%)                                                                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 26.0                                                                                                          | Xtriage          |
| Anisotropy                                                              | 0.309                                                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 35.4                                                                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$                                                   | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h<br>+1/2*k-l<br>0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-<br>1/2*k-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                                                                          | EDS              |
| Total number of atoms                                                   | 42940                                                                                                         | 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 47.80 % 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 9.4235e-05. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.37         | 0/3488  | 0.93        | 13/4726 (0.3%)   |
| 1   | B     | 0.36         | 0/3488  | 0.92        | 13/4726 (0.3%)   |
| 1   | C     | 0.40         | 0/3488  | 0.93        | 12/4726 (0.3%)   |
| 1   | D     | 0.41         | 0/3488  | 0.96        | 18/4726 (0.4%)   |
| 1   | E     | 0.40         | 0/3488  | 0.95        | 21/4726 (0.4%)   |
| 1   | F     | 0.40         | 0/3488  | 0.93        | 17/4726 (0.4%)   |
| 1   | G     | 0.37         | 0/3488  | 0.94        | 19/4726 (0.4%)   |
| 1   | H     | 0.40         | 0/3488  | 0.95        | 17/4726 (0.4%)   |
| 1   | I     | 0.37         | 0/3488  | 0.93        | 16/4726 (0.3%)   |
| 1   | J     | 0.39         | 0/3488  | 0.96        | 21/4726 (0.4%)   |
| 1   | K     | 0.40         | 0/3488  | 0.94        | 18/4726 (0.4%)   |
| 1   | L     | 0.40         | 0/3488  | 0.94        | 17/4726 (0.4%)   |
| All | All   | 0.39         | 0/41856 | 0.94        | 202/56712 (0.4%) |

There are no bond length outliers.

All (202) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | H     | 325 | TRP  | N-CA-C | 9.39 | 123.39      | 109.59   |
| 1   | K     | 325 | TRP  | N-CA-C | 8.80 | 122.52      | 109.59   |
| 1   | H     | 306 | GLN  | N-CA-C | 8.59 | 120.26      | 111.07   |
| 1   | K     | 306 | GLN  | N-CA-C | 8.55 | 120.22      | 111.07   |
| 1   | D     | 325 | TRP  | N-CA-C | 8.46 | 122.02      | 109.59   |
| 1   | B     | 325 | TRP  | N-CA-C | 8.44 | 122.17      | 109.25   |
| 1   | C     | 325 | TRP  | N-CA-C | 8.34 | 122.47      | 109.96   |
| 1   | I     | 325 | TRP  | N-CA-C | 8.12 | 122.14      | 109.96   |
| 1   | F     | 325 | TRP  | N-CA-C | 7.98 | 121.93      | 109.96   |
| 1   | F     | 306 | GLN  | N-CA-C | 7.95 | 119.58      | 111.07   |
| 1   | J     | 306 | GLN  | N-CA-C | 7.93 | 119.55      | 111.07   |
| 1   | L     | 306 | GLN  | N-CA-C | 7.92 | 119.55      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 325 | TRP  | N-CA-C | 7.83  | 121.24      | 109.25   |
| 1   | E     | 325 | TRP  | N-CA-C | 7.74  | 121.57      | 109.96   |
| 1   | A     | 259 | ILE  | N-CA-C | 7.70  | 120.18      | 108.71   |
| 1   | B     | 306 | GLN  | N-CA-C | 7.64  | 120.28      | 111.11   |
| 1   | I     | 259 | ILE  | N-CA-C | 7.60  | 120.04      | 108.71   |
| 1   | D     | 406 | ARG  | N-CA-C | 7.45  | 119.40      | 111.28   |
| 1   | L     | 325 | TRP  | N-CA-C | 7.33  | 121.41      | 109.76   |
| 1   | C     | 264 | ARG  | N-CA-C | 7.33  | 121.50      | 111.39   |
| 1   | E     | 266 | HIS  | CA-C-N | 7.20  | 126.73      | 119.24   |
| 1   | E     | 266 | HIS  | C-N-CA | 7.20  | 126.73      | 119.24   |
| 1   | C     | 306 | GLN  | N-CA-C | 7.11  | 119.64      | 111.11   |
| 1   | A     | 325 | TRP  | N-CA-C | 7.10  | 120.61      | 109.96   |
| 1   | F     | 259 | ILE  | N-CA-C | 7.02  | 119.16      | 108.71   |
| 1   | E     | 259 | ILE  | N-CA-C | 6.96  | 119.08      | 108.71   |
| 1   | E     | 306 | GLN  | N-CA-C | 6.93  | 119.42      | 111.11   |
| 1   | L     | 259 | ILE  | N-CA-C | 6.92  | 119.02      | 108.71   |
| 1   | K     | 25  | MET  | N-CA-C | 6.86  | 121.31      | 113.15   |
| 1   | E     | 59  | THR  | N-CA-C | 6.85  | 120.16      | 110.50   |
| 1   | H     | 259 | ILE  | N-CA-C | 6.76  | 118.78      | 108.71   |
| 1   | K     | 266 | HIS  | CA-C-N | 6.75  | 126.27      | 119.24   |
| 1   | K     | 266 | HIS  | C-N-CA | 6.75  | 126.27      | 119.24   |
| 1   | L     | 22  | VAL  | N-CA-C | 6.75  | 118.30      | 108.58   |
| 1   | H     | 25  | MET  | N-CA-C | 6.74  | 121.17      | 113.15   |
| 1   | D     | 264 | ARG  | N-CA-C | 6.74  | 120.69      | 111.39   |
| 1   | F     | 264 | ARG  | N-CA-C | 6.74  | 120.68      | 111.39   |
| 1   | K     | 259 | ILE  | N-CA-C | 6.71  | 118.71      | 108.71   |
| 1   | D     | 25  | MET  | N-CA-C | 6.70  | 121.12      | 113.15   |
| 1   | J     | 325 | TRP  | N-CA-C | 6.69  | 120.40      | 109.76   |
| 1   | A     | 406 | ARG  | N-CA-C | 6.60  | 118.47      | 111.28   |
| 1   | K     | 406 | ARG  | N-CA-C | 6.58  | 118.45      | 111.28   |
| 1   | I     | 25  | MET  | N-CA-C | 6.56  | 120.95      | 113.15   |
| 1   | B     | 259 | ILE  | N-CA-C | 6.54  | 118.46      | 108.71   |
| 1   | B     | 352 | GLN  | N-CA-C | 6.53  | 118.99      | 109.07   |
| 1   | B     | 406 | ARG  | N-CA-C | 6.51  | 118.38      | 111.28   |
| 1   | F     | 171 | LEU  | N-CA-C | 6.48  | 120.49      | 112.59   |
| 1   | H     | 385 | LEU  | N-CA-C | -6.47 | 104.31      | 111.36   |
| 1   | D     | 259 | ILE  | N-CA-C | 6.46  | 118.34      | 108.71   |
| 1   | I     | 22  | VAL  | N-CA-C | 6.45  | 118.31      | 108.71   |
| 1   | H     | 59  | THR  | N-CA-C | 6.44  | 119.58      | 110.50   |
| 1   | A     | 352 | GLN  | N-CA-C | 6.38  | 118.55      | 108.79   |
| 1   | C     | 259 | ILE  | N-CA-C | 6.37  | 118.20      | 108.71   |
| 1   | J     | 259 | ILE  | N-CA-C | 6.35  | 118.17      | 108.71   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 406 | ARG  | N-CA-C | 6.33  | 118.18      | 111.28   |
| 1   | L     | 25  | MET  | N-CA-C | 6.33  | 120.68      | 113.15   |
| 1   | A     | 264 | ARG  | N-CA-C | 6.32  | 120.11      | 111.39   |
| 1   | I     | 264 | ARG  | N-CA-C | 6.31  | 120.10      | 111.39   |
| 1   | K     | 385 | LEU  | N-CA-C | -6.29 | 104.42      | 111.28   |
| 1   | E     | 22  | VAL  | N-CA-C | 6.29  | 118.09      | 108.71   |
| 1   | F     | 59  | THR  | N-CA-C | 6.25  | 119.31      | 110.50   |
| 1   | G     | 306 | GLN  | N-CA-C | 6.24  | 118.60      | 111.11   |
| 1   | A     | 22  | VAL  | N-CA-C | 6.24  | 118.35      | 108.87   |
| 1   | F     | 22  | VAL  | N-CA-C | 6.19  | 117.94      | 108.71   |
| 1   | C     | 406 | ARG  | N-CA-C | 6.16  | 117.99      | 111.28   |
| 1   | G     | 357 | ARG  | N-CA-C | -6.15 | 106.09      | 113.97   |
| 1   | H     | 352 | GLN  | N-CA-C | 6.15  | 118.41      | 109.07   |
| 1   | J     | 59  | THR  | N-CA-C | 6.13  | 118.68      | 110.35   |
| 1   | K     | 352 | GLN  | N-CA-C | 6.12  | 118.37      | 109.07   |
| 1   | B     | 266 | HIS  | CA-C-N | 6.10  | 127.46      | 119.84   |
| 1   | B     | 266 | HIS  | C-N-CA | 6.10  | 127.46      | 119.84   |
| 1   | H     | 22  | VAL  | N-CA-C | 6.09  | 117.07      | 108.36   |
| 1   | J     | 266 | HIS  | CA-C-N | 6.07  | 126.24      | 119.32   |
| 1   | J     | 266 | HIS  | C-N-CA | 6.07  | 126.24      | 119.32   |
| 1   | C     | 158 | GLY  | N-CA-C | 6.03  | 123.39      | 115.36   |
| 1   | J     | 263 | LYS  | N-CA-C | 6.00  | 118.97      | 110.50   |
| 1   | E     | 406 | ARG  | N-CA-C | 6.00  | 117.82      | 111.28   |
| 1   | D     | 306 | GLN  | N-CA-C | 5.98  | 118.29      | 111.11   |
| 1   | A     | 306 | GLN  | N-CA-C | 5.98  | 118.28      | 111.11   |
| 1   | G     | 259 | ILE  | N-CA-C | 5.97  | 117.61      | 108.71   |
| 1   | K     | 59  | THR  | N-CA-C | 5.95  | 118.44      | 110.35   |
| 1   | J     | 357 | ARG  | N-CA-C | -5.93 | 106.21      | 113.50   |
| 1   | L     | 264 | ARG  | N-CA-C | 5.91  | 119.50      | 111.17   |
| 1   | E     | 264 | ARG  | N-CA-C | 5.88  | 119.47      | 111.17   |
| 1   | E     | 25  | MET  | N-CA-C | 5.87  | 121.46      | 113.37   |
| 1   | A     | 48  | TYR  | N-CA-C | -5.85 | 101.99      | 110.24   |
| 1   | B     | 357 | ARG  | N-CA-C | -5.84 | 106.49      | 113.97   |
| 1   | K     | 22  | VAL  | N-CA-C | 5.84  | 117.41      | 108.71   |
| 1   | I     | 406 | ARG  | N-CA-C | 5.84  | 117.64      | 111.28   |
| 1   | I     | 357 | ARG  | N-CA-C | -5.82 | 106.31      | 113.41   |
| 1   | L     | 59  | THR  | N-CA-C | 5.82  | 118.70      | 110.50   |
| 1   | H     | 171 | LEU  | N-CA-C | 5.80  | 119.95      | 112.41   |
| 1   | F     | 48  | TYR  | N-CA-C | -5.78 | 102.08      | 110.24   |
| 1   | C     | 171 | LEU  | N-CA-C | 5.76  | 119.62      | 112.59   |
| 1   | J     | 22  | VAL  | N-CA-C | 5.75  | 117.28      | 108.71   |
| 1   | H     | 263 | LYS  | N-CA-C | 5.75  | 118.79      | 110.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | L     | 406 | ARG  | N-CA-C | 5.75  | 118.32      | 111.71   |
| 1   | J     | 106 | ASP  | CA-C-N | 5.74  | 125.36      | 119.56   |
| 1   | J     | 106 | ASP  | C-N-CA | 5.74  | 125.36      | 119.56   |
| 1   | J     | 122 | LYS  | N-CA-C | 5.74  | 118.58      | 109.81   |
| 1   | G     | 263 | LYS  | N-CA-C | 5.73  | 118.75      | 110.28   |
| 1   | G     | 291 | TYR  | CA-C-N | 5.72  | 125.85      | 119.32   |
| 1   | G     | 291 | TYR  | C-N-CA | 5.72  | 125.85      | 119.32   |
| 1   | L     | 171 | LEU  | N-CA-C | 5.72  | 119.84      | 112.41   |
| 1   | D     | 106 | ASP  | CA-C-N | 5.71  | 125.33      | 119.56   |
| 1   | D     | 106 | ASP  | C-N-CA | 5.71  | 125.33      | 119.56   |
| 1   | I     | 306 | GLN  | N-CA-C | 5.71  | 117.96      | 111.11   |
| 1   | B     | 22  | VAL  | N-CA-C | 5.69  | 117.52      | 108.87   |
| 1   | G     | 352 | GLN  | N-CA-C | 5.69  | 117.72      | 109.07   |
| 1   | E     | 353 | HIS  | N-CA-C | -5.65 | 100.48      | 109.07   |
| 1   | G     | 59  | THR  | N-CA-C | 5.63  | 118.39      | 110.23   |
| 1   | D     | 31  | SER  | N-CA-C | -5.61 | 103.15      | 109.60   |
| 1   | F     | 316 | PHE  | N-CA-C | 5.61  | 117.53      | 108.34   |
| 1   | C     | 263 | LYS  | N-CA-C | 5.59  | 118.56      | 110.28   |
| 1   | J     | 264 | ARG  | N-CA-C | 5.57  | 119.07      | 111.39   |
| 1   | K     | 48  | TYR  | N-CA-C | -5.56 | 102.41      | 110.24   |
| 1   | D     | 357 | ARG  | N-CA-C | -5.56 | 106.86      | 113.97   |
| 1   | G     | 265 | VAL  | N-CA-C | -5.55 | 105.52      | 113.07   |
| 1   | L     | 357 | ARG  | N-CA-C | -5.55 | 106.68      | 113.50   |
| 1   | A     | 357 | ARG  | N-CA-C | -5.53 | 106.67      | 113.41   |
| 1   | H     | 122 | LYS  | N-CA-C | 5.52  | 117.36      | 109.14   |
| 1   | D     | 316 | PHE  | N-CA-C | 5.51  | 117.39      | 108.34   |
| 1   | H     | 316 | PHE  | N-CA-C | 5.50  | 117.38      | 108.41   |
| 1   | I     | 298 | VAL  | N-CA-C | 5.50  | 116.65      | 108.46   |
| 1   | D     | 266 | HIS  | CA-C-N | 5.50  | 125.59      | 119.32   |
| 1   | D     | 266 | HIS  | C-N-CA | 5.50  | 125.59      | 119.32   |
| 1   | G     | 266 | HIS  | CA-C-N | 5.49  | 125.58      | 119.32   |
| 1   | G     | 266 | HIS  | C-N-CA | 5.49  | 125.58      | 119.32   |
| 1   | D     | 22  | VAL  | N-CA-C | 5.47  | 116.87      | 108.71   |
| 1   | K     | 263 | LYS  | N-CA-C | 5.47  | 118.38      | 110.28   |
| 1   | G     | 298 | VAL  | N-CA-C | 5.47  | 116.61      | 108.46   |
| 1   | C     | 22  | VAL  | N-CA-C | 5.47  | 116.85      | 108.71   |
| 1   | J     | 406 | ARG  | N-CA-C | 5.46  | 116.91      | 111.07   |
| 1   | E     | 352 | GLN  | N-CA-C | 5.45  | 117.36      | 109.07   |
| 1   | E     | 316 | PHE  | N-CA-C | 5.42  | 117.24      | 108.41   |
| 1   | L     | 351 | PRO  | N-CA-C | 5.42  | 121.06      | 113.53   |
| 1   | F     | 352 | GLN  | N-CA-C | 5.42  | 117.30      | 109.07   |
| 1   | K     | 42  | ILE  | N-CA-C | 5.41  | 116.14      | 110.62   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 263 | LYS  | N-CA-C | 5.41  | 118.08      | 110.23   |
| 1   | I     | 316 | PHE  | N-CA-C | 5.41  | 117.23      | 108.41   |
| 1   | F     | 357 | ARG  | N-CA-C | -5.41 | 106.85      | 113.50   |
| 1   | K     | 175 | LEU  | N-CA-C | 5.41  | 117.25      | 111.36   |
| 1   | J     | 171 | LEU  | N-CA-C | 5.39  | 120.55      | 112.94   |
| 1   | J     | 316 | PHE  | N-CA-C | 5.39  | 117.18      | 108.34   |
| 1   | L     | 48  | TYR  | N-CA-C | -5.39 | 102.32      | 110.24   |
| 1   | G     | 351 | PRO  | N-CA-C | 5.38  | 121.17      | 113.47   |
| 1   | K     | 264 | ARG  | N-CA-C | 5.38  | 118.82      | 111.39   |
| 1   | E     | 106 | ASP  | CA-C-N | 5.38  | 125.05      | 119.56   |
| 1   | E     | 106 | ASP  | C-N-CA | 5.38  | 125.05      | 119.56   |
| 1   | I     | 59  | THR  | N-CA-C | 5.37  | 118.23      | 110.28   |
| 1   | I     | 263 | LYS  | N-CA-C | 5.36  | 118.21      | 110.28   |
| 1   | B     | 264 | ARG  | N-CA-C | 5.35  | 118.82      | 111.54   |
| 1   | C     | 352 | GLN  | N-CA-C | 5.34  | 117.19      | 109.07   |
| 1   | I     | 31  | SER  | N-CA-C | -5.33 | 103.47      | 109.60   |
| 1   | J     | 352 | GLN  | N-CA-C | 5.33  | 117.17      | 109.07   |
| 1   | D     | 191 | LYS  | N-CA-C | 5.29  | 117.81      | 109.39   |
| 1   | L     | 280 | SER  | N-CA-C | -5.28 | 102.67      | 110.48   |
| 1   | G     | 22  | VAL  | N-CA-C | 5.27  | 116.56      | 108.71   |
| 1   | D     | 352 | GLN  | N-CA-C | 5.27  | 116.85      | 108.79   |
| 1   | I     | 353 | HIS  | N-CA-C | -5.26 | 101.07      | 109.07   |
| 1   | E     | 48  | TYR  | N-CA-C | -5.25 | 102.84      | 110.24   |
| 1   | L     | 353 | HIS  | N-CA-C | -5.25 | 101.10      | 109.23   |
| 1   | H     | 357 | ARG  | N-CA-C | -5.25 | 107.05      | 113.50   |
| 1   | C     | 59  | THR  | N-CA-C | 5.24  | 117.89      | 110.50   |
| 1   | G     | 25  | MET  | N-CA-C | 5.24  | 119.39      | 113.15   |
| 1   | E     | 31  | SER  | N-CA-C | -5.24 | 103.57      | 109.60   |
| 1   | F     | 4   | ASN  | N-CA-C | 5.24  | 119.38      | 112.89   |
| 1   | E     | 280 | SER  | N-CA-C | -5.22 | 102.75      | 110.48   |
| 1   | H     | 266 | HIS  | CA-C-N | 5.22  | 126.36      | 119.84   |
| 1   | H     | 266 | HIS  | C-N-CA | 5.22  | 126.36      | 119.84   |
| 1   | B     | 48  | TYR  | N-CA-C | -5.21 | 102.89      | 110.24   |
| 1   | I     | 48  | TYR  | N-CA-C | -5.20 | 102.68      | 110.23   |
| 1   | F     | 353 | HIS  | N-CA-C | -5.19 | 101.19      | 109.07   |
| 1   | E     | 265 | VAL  | N-CA-C | -5.17 | 106.03      | 113.07   |
| 1   | F     | 323 | GLY  | N-CA-C | 5.17  | 125.42      | 113.18   |
| 1   | D     | 171 | LEU  | N-CA-C | 5.16  | 119.11      | 112.41   |
| 1   | D     | 163 | SER  | N-CA-C | 5.16  | 118.35      | 111.75   |
| 1   | A     | 266 | HIS  | CA-C-N | 5.15  | 125.44      | 119.47   |
| 1   | A     | 266 | HIS  | C-N-CA | 5.15  | 125.44      | 119.47   |
| 1   | C     | 25  | MET  | N-CA-C | 5.15  | 120.48      | 113.37   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 323 | GLY  | N-CA-C | 5.15  | 125.38      | 113.18   |
| 1   | B     | 316 | PHE  | N-CA-C | 5.13  | 116.77      | 108.41   |
| 1   | K     | 171 | LEU  | N-CA-C | 5.12  | 119.07      | 112.41   |
| 1   | J     | 42  | ILE  | N-CA-C | 5.12  | 115.84      | 110.62   |
| 1   | J     | 328 | MET  | N-CA-C | -5.11 | 107.09      | 113.38   |
| 1   | G     | 106 | ASP  | CA-C-N | 5.11  | 124.90      | 119.28   |
| 1   | G     | 106 | ASP  | C-N-CA | 5.11  | 124.90      | 119.28   |
| 1   | B     | 59  | THR  | N-CA-C | 5.11  | 117.70      | 110.50   |
| 1   | G     | 48  | TYR  | N-CA-C | -5.10 | 102.84      | 110.23   |
| 1   | L     | 265 | VAL  | N-CA-C | -5.09 | 105.42      | 112.50   |
| 1   | F     | 263 | LYS  | N-CA-C | 5.08  | 117.80      | 110.28   |
| 1   | E     | 357 | ARG  | N-CA-C | -5.08 | 107.25      | 113.50   |
| 1   | H     | 48  | TYR  | N-CA-C | -5.08 | 103.07      | 110.24   |
| 1   | L     | 50  | TYR  | N-CA-C | -5.08 | 105.74      | 111.28   |
| 1   | A     | 291 | TYR  | CA-C-N | 5.08  | 124.74      | 119.56   |
| 1   | A     | 291 | TYR  | C-N-CA | 5.08  | 124.74      | 119.56   |
| 1   | J     | 280 | SER  | N-CA-C | -5.07 | 102.97      | 110.48   |
| 1   | L     | 263 | LYS  | N-CA-C | 5.05  | 117.75      | 110.28   |
| 1   | I     | 50  | TYR  | N-CA-C | -5.04 | 105.78      | 111.28   |
| 1   | F     | 89  | VAL  | N-CA-C | 5.04  | 119.51      | 112.50   |
| 1   | K     | 316 | PHE  | N-CA-C | 5.04  | 116.60      | 108.34   |
| 1   | F     | 385 | LEU  | N-CA-C | -5.01 | 105.82      | 111.28   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3404  | 0        | 3328     | 80      | 0            |
| 1   | B     | 3404  | 0        | 3328     | 91      | 0            |
| 1   | C     | 3404  | 0        | 3328     | 48      | 0            |
| 1   | D     | 3404  | 0        | 3328     | 45      | 0            |
| 1   | E     | 3404  | 0        | 3328     | 75      | 0            |
| 1   | F     | 3404  | 0        | 3328     | 67      | 0            |
| 1   | G     | 3404  | 0        | 3328     | 77      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | H     | 3404  | 0        | 3328     | 51      | 0            |
| 1   | I     | 3404  | 0        | 3328     | 67      | 0            |
| 1   | J     | 3404  | 0        | 3328     | 52      | 0            |
| 1   | K     | 3404  | 0        | 3328     | 58      | 0            |
| 1   | L     | 3404  | 0        | 3328     | 58      | 0            |
| 2   | A     | 12    | 0        | 5        | 0       | 0            |
| 2   | B     | 12    | 0        | 5        | 0       | 0            |
| 2   | C     | 12    | 0        | 5        | 0       | 0            |
| 2   | D     | 12    | 0        | 5        | 0       | 0            |
| 2   | E     | 12    | 0        | 5        | 0       | 0            |
| 2   | F     | 12    | 0        | 5        | 0       | 0            |
| 2   | G     | 12    | 0        | 5        | 0       | 0            |
| 2   | H     | 12    | 0        | 5        | 0       | 0            |
| 2   | I     | 12    | 0        | 5        | 0       | 0            |
| 2   | J     | 12    | 0        | 5        | 0       | 0            |
| 2   | K     | 12    | 0        | 5        | 0       | 0            |
| 2   | L     | 12    | 0        | 5        | 0       | 0            |
| 3   | A     | 8     | 0        | 0        | 0       | 0            |
| 3   | C     | 4     | 0        | 0        | 0       | 0            |
| 3   | D     | 4     | 0        | 0        | 0       | 0            |
| 3   | E     | 8     | 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     | 8     | 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            |
| 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   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 1     | 0        | 0        | 0       | 0            |
| 5   | L     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 1     | 0        | 0        | 0       | 0            |
| 6   | J     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 111   | 0        | 0        | 2       | 0            |
| 7   | B     | 89    | 0        | 0        | 2       | 0            |
| 7   | C     | 182   | 0        | 0        | 5       | 0            |
| 7   | D     | 204   | 0        | 0        | 4       | 0            |
| 7   | E     | 160   | 0        | 0        | 2       | 0            |
| 7   | F     | 166   | 0        | 0        | 2       | 0            |
| 7   | G     | 110   | 0        | 0        | 3       | 0            |
| 7   | H     | 178   | 0        | 0        | 3       | 0            |
| 7   | I     | 122   | 0        | 0        | 4       | 0            |
| 7   | J     | 165   | 0        | 0        | 3       | 0            |
| 7   | K     | 194   | 0        | 0        | 3       | 0            |
| 7   | L     | 199   | 0        | 0        | 4       | 0            |
| All | All   | 42940 | 0        | 39996    | 757     | 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 (757) 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:E:333:ILE:HG22 | 1:E:337:MET:HE2  | 1.15                     | 1.12              |
| 1:A:72:ARG:HB2   | 1:A:72:ARG:HH11  | 1.14                     | 1.10              |
| 1:E:55:VAL:HG11  | 1:E:78:ILE:HG12  | 1.43                     | 0.99              |
| 1:C:127:GLN:HA   | 1:C:127:GLN:HE21 | 1.30                     | 0.95              |
| 1:E:333:ILE:CG2  | 1:E:337:MET:HE2  | 1.97                     | 0.93              |
| 1:H:32:PRO:HG3   | 1:H:128:VAL:HG21 | 1.49                     | 0.93              |
| 1:F:32:PRO:HG3   | 1:F:128:VAL:HG21 | 1.49                     | 0.92              |
| 1:B:34:PHE:HB3   | 1:B:37:ILE:HD11  | 1.51                     | 0.92              |
| 1:K:385:LEU:HD11 | 1:K:391:VAL:HG12 | 1.54                     | 0.90              |
| 1:A:72:ARG:HB2   | 1:A:72:ARG:NH1   | 1.88                     | 0.88              |
| 1:E:72:ARG:HH11  | 1:E:72:ARG:HB2   | 1.40                     | 0.85              |
| 1:E:328:MET:HB3  | 1:E:337:MET:HE1  | 1.57                     | 0.85              |
| 1:A:127:GLN:HE21 | 1:A:127:GLN:HA   | 1.44                     | 0.83              |
| 1:B:162:ASP:OD1  | 1:B:164:ARG:HG2  | 1.79                     | 0.82              |
| 1:L:109:THR:HG22 | 1:L:111:ASP:HB2  | 1.60                     | 0.82              |
| 1:F:171:LEU:HD11 | 1:F:220:MET:HE2  | 1.61                     | 0.81              |
| 1:F:127:GLN:HE21 | 1:F:127:GLN:HA   | 1.45                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:69:MET:HE2   | 1:E:73:GLU:HB3   | 1.62                     | 0.79              |
| 1:E:3:ILE:HG23   | 1:E:8:VAL:HG13   | 1.66                     | 0.76              |
| 1:F:72:ARG:HH11  | 1:F:72:ARG:HB2   | 1.49                     | 0.76              |
| 1:L:127:GLN:HE21 | 1:L:127:GLN:HA   | 1.51                     | 0.75              |
| 1:B:9:LEU:HD22   | 1:B:385:LEU:HD22 | 1.69                     | 0.73              |
| 1:B:402:ASP:HA   | 1:B:406:ARG:HB2  | 1.70                     | 0.73              |
| 1:E:72:ARG:HB2   | 1:E:72:ARG:NH1   | 2.03                     | 0.72              |
| 1:C:149:ASP:O    | 1:C:153:ILE:HG12 | 1.90                     | 0.72              |
| 1:E:371:SER:O    | 1:E:375:GLU:HG3  | 1.89                     | 0.71              |
| 1:E:9:LEU:HD22   | 1:E:385:LEU:HD22 | 1.73                     | 0.71              |
| 1:K:385:LEU:HD11 | 1:K:391:VAL:CG1  | 2.21                     | 0.71              |
| 1:L:109:THR:CG2  | 1:L:111:ASP:HB2  | 2.21                     | 0.70              |
| 1:E:410:ARG:HD3  | 7:E:462:HOH:O    | 1.91                     | 0.70              |
| 1:A:328:MET:HE2  | 1:A:328:MET:HA   | 1.73                     | 0.69              |
| 1:I:191:LYS:HE3  | 1:I:191:LYS:HA   | 1.75                     | 0.69              |
| 1:A:48:TYR:HB3   | 1:A:51:LEU:HD13  | 1.74                     | 0.68              |
| 1:C:402:ASP:HA   | 1:C:406:ARG:HB2  | 1.75                     | 0.68              |
| 1:I:149:ASP:HA   | 1:I:152:ARG:HH12 | 1.60                     | 0.67              |
| 1:K:72:ARG:NH2   | 1:K:116:ARG:HD3  | 2.10                     | 0.67              |
| 1:A:127:GLN:HA   | 1:A:127:GLN:NE2  | 2.09                     | 0.67              |
| 1:E:333:ILE:HG22 | 1:E:337:MET:CE   | 2.09                     | 0.67              |
| 1:I:328:MET:HE2  | 1:I:328:MET:HA   | 1.77                     | 0.66              |
| 1:C:127:GLN:HA   | 1:C:127:GLN:NE2  | 2.08                     | 0.66              |
| 1:E:55:VAL:HG12  | 1:E:82:LEU:HG    | 1.78                     | 0.66              |
| 1:B:219:TYR:HB3  | 1:B:254:PRO:HG2  | 1.78                     | 0.66              |
| 1:I:180:GLN:H    | 1:I:180:GLN:NE2  | 1.94                     | 0.66              |
| 1:I:154:SER:OG   | 1:I:159:LYS:HD2  | 1.95                     | 0.66              |
| 1:G:402:ASP:HA   | 1:G:406:ARG:HB2  | 1.78                     | 0.65              |
| 1:A:402:ASP:HA   | 1:A:406:ARG:HB2  | 1.79                     | 0.65              |
| 1:I:308:GLU:HG2  | 7:I:431:HOH:O    | 1.96                     | 0.65              |
| 1:B:162:ASP:HB3  | 1:B:165:PHE:HD2  | 1.59                     | 0.65              |
| 1:B:40:TRP:O     | 1:B:41:ASP:HB3   | 1.97                     | 0.65              |
| 7:G:1677:HOH:O   | 1:H:321:ILE:HG12 | 1.96                     | 0.65              |
| 1:K:381:TYR:O    | 1:K:385:LEU:HD13 | 1.97                     | 0.65              |
| 1:B:371:SER:O    | 1:B:375:GLU:HG3  | 1.97                     | 0.64              |
| 1:L:127:GLN:HA   | 1:L:127:GLN:NE2  | 2.11                     | 0.64              |
| 1:E:392:THR:OG1  | 1:E:395:GLU:HG3  | 1.96                     | 0.64              |
| 1:I:323:GLY:HA2  | 1:I:352:GLN:HA   | 1.78                     | 0.64              |
| 1:H:323:GLY:HA2  | 1:H:352:GLN:HA   | 1.80                     | 0.64              |
| 1:A:80:GLU:O     | 1:A:85:LYS:HG2   | 1.97                     | 0.63              |
| 1:A:211:TRP:CE3  | 1:A:215:MET:HE3  | 2.32                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:342:MET:SD   | 1:C:380:LYS:HG3  | 2.38                     | 0.63              |
| 1:K:323:GLY:HA2  | 1:K:352:GLN:HA   | 1.81                     | 0.63              |
| 1:B:254:PRO:HG3  | 1:B:412:VAL:HG12 | 1.80                     | 0.63              |
| 1:F:208:LEU:HD22 | 1:F:220:MET:CE   | 2.28                     | 0.63              |
| 1:F:25:MET:HG3   | 7:F:443:HOH:O    | 1.99                     | 0.62              |
| 1:K:245:LEU:HB2  | 1:K:246:PRO:HD3  | 1.81                     | 0.62              |
| 1:E:149:ASP:O    | 1:E:153:ILE:HG12 | 1.99                     | 0.62              |
| 1:I:180:GLN:H    | 1:I:180:GLN:HE21 | 1.48                     | 0.62              |
| 1:G:25:MET:HG3   | 7:G:441:HOH:O    | 1.98                     | 0.62              |
| 1:J:392:THR:OG1  | 1:J:395:GLU:HG3  | 1.99                     | 0.62              |
| 1:L:323:GLY:HA2  | 1:L:352:GLN:HA   | 1.80                     | 0.62              |
| 1:E:5:SER:OG     | 1:E:8:VAL:HG12   | 2.00                     | 0.61              |
| 1:B:41:ASP:OD1   | 1:B:44:GLU:HG2   | 2.00                     | 0.61              |
| 1:B:392:THR:OG1  | 1:B:395:GLU:HG3  | 2.00                     | 0.61              |
| 1:G:178:TYR:CE2  | 1:G:182:LYS:HE2  | 2.34                     | 0.61              |
| 1:H:25:MET:HG3   | 7:H:438:HOH:O    | 1.99                     | 0.61              |
| 1:I:265:VAL:HG21 | 1:I:275:PHE:HB2  | 1.83                     | 0.61              |
| 1:A:72:ARG:HH11  | 1:A:72:ARG:CB    | 2.04                     | 0.61              |
| 1:H:72:ARG:NH2   | 1:H:116:ARG:HD3  | 2.17                     | 0.60              |
| 1:A:112:LEU:HA   | 1:A:115:TYR:CD2  | 2.36                     | 0.60              |
| 1:C:203:GLU:OE2  | 1:C:206:ARG:HD3  | 2.02                     | 0.60              |
| 1:B:70:SER:O     | 1:B:74:GLN:HG3   | 2.01                     | 0.60              |
| 1:F:4:ASN:HB2    | 7:I:750:HOH:O    | 2.02                     | 0.60              |
| 1:B:352:GLN:HG3  | 1:B:353:HIS:N    | 2.16                     | 0.59              |
| 1:D:144:ASN:HB2  | 1:D:215:MET:CE   | 2.32                     | 0.59              |
| 1:G:69:MET:HE2   | 1:G:73:GLU:HB3   | 1.84                     | 0.59              |
| 1:B:144:ASN:HA   | 1:B:151:GLU:OE2  | 2.01                     | 0.59              |
| 1:C:323:GLY:HA2  | 1:C:352:GLN:HA   | 1.84                     | 0.59              |
| 1:E:214:ARG:HG2  | 1:E:214:ARG:HH11 | 1.67                     | 0.59              |
| 1:A:25:MET:HG3   | 7:A:487:HOH:O    | 2.02                     | 0.59              |
| 1:F:127:GLN:HA   | 1:F:127:GLN:NE2  | 2.16                     | 0.59              |
| 1:G:197:ASN:ND2  | 1:G:200:SER:H    | 1.99                     | 0.59              |
| 1:J:254:PRO:HG3  | 1:J:295:LYS:HE3  | 1.83                     | 0.59              |
| 1:D:402:ASP:HA   | 1:D:406:ARG:HB2  | 1.85                     | 0.59              |
| 1:A:323:GLY:HA2  | 1:A:352:GLN:HA   | 1.83                     | 0.59              |
| 1:L:328:MET:HA   | 1:L:328:MET:HE2  | 1.85                     | 0.58              |
| 1:B:20:GLN:NE2   | 1:B:21:PRO:HD2   | 2.18                     | 0.58              |
| 1:H:392:THR:OG1  | 1:H:395:GLU:HG3  | 2.03                     | 0.58              |
| 1:I:202:GLN:HA   | 1:I:202:GLN:NE2  | 2.18                     | 0.58              |
| 1:G:392:THR:OG1  | 1:G:395:GLU:HG3  | 2.02                     | 0.58              |
| 1:A:394:GLU:HB2  | 7:A:446:HOH:O    | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:392:THR:OG1  | 1:C:395:GLU:HG3  | 2.02                     | 0.58              |
| 1:D:328:MET:HE2  | 1:D:328:MET:HA   | 1.86                     | 0.58              |
| 1:G:3:ILE:HG21   | 1:G:9:LEU:HB2    | 1.85                     | 0.58              |
| 1:J:402:ASP:HA   | 1:J:406:ARG:HB2  | 1.85                     | 0.58              |
| 1:E:245:LEU:HB2  | 1:E:246:PRO:HD3  | 1.84                     | 0.58              |
| 1:B:323:GLY:HA2  | 1:B:352:GLN:HA   | 1.86                     | 0.57              |
| 1:D:170:ARG:NH2  | 1:D:223:SER:HB3  | 2.20                     | 0.57              |
| 1:G:9:LEU:HD22   | 1:G:385:LEU:HD22 | 1.86                     | 0.57              |
| 1:D:2:SER:N      | 1:H:386:GLN:NE2  | 2.52                     | 0.57              |
| 1:K:254:PRO:HG3  | 1:K:412:VAL:HG12 | 1.84                     | 0.57              |
| 1:A:40:TRP:O     | 1:A:41:ASP:CG    | 2.47                     | 0.57              |
| 1:G:193:ASN:HD22 | 1:G:197:ASN:HD21 | 1.51                     | 0.57              |
| 1:G:197:ASN:C    | 1:G:197:ASN:HD22 | 2.12                     | 0.57              |
| 1:L:3:ILE:HG21   | 1:L:9:LEU:HD13   | 1.87                     | 0.57              |
| 1:A:393:GLU:HG2  | 1:A:397:LYS:HE3  | 1.86                     | 0.57              |
| 1:D:323:GLY:HA2  | 1:D:352:GLN:HA   | 1.86                     | 0.57              |
| 1:I:127:GLN:OE1  | 1:I:127:GLN:HA   | 2.04                     | 0.57              |
| 1:D:392:THR:OG1  | 1:D:395:GLU:HG3  | 2.04                     | 0.57              |
| 1:B:172:ASP:HB2  | 1:B:173:PRO:HD3  | 1.87                     | 0.57              |
| 1:E:323:GLY:HA2  | 1:E:352:GLN:HA   | 1.86                     | 0.57              |
| 1:E:328:MET:HB3  | 1:E:337:MET:CE   | 2.30                     | 0.57              |
| 1:K:123:THR:OG1  | 1:K:126:GLU:HG3  | 2.05                     | 0.57              |
| 1:I:180:GLN:NE2  | 1:I:180:GLN:N    | 2.52                     | 0.56              |
| 1:L:180:GLN:H    | 1:L:180:GLN:NE2  | 2.03                     | 0.56              |
| 1:G:382:ASP:O    | 1:G:386:GLN:HG2  | 2.04                     | 0.56              |
| 1:A:52:VAL:O     | 1:A:55:VAL:HG12  | 2.06                     | 0.56              |
| 1:D:172:ASP:HB2  | 1:D:173:PRO:HD3  | 1.87                     | 0.56              |
| 1:E:70:SER:O     | 1:E:74:GLN:HG3   | 2.04                     | 0.56              |
| 1:F:208:LEU:HD22 | 1:F:220:MET:HE1  | 1.87                     | 0.56              |
| 1:F:392:THR:OG1  | 1:F:395:GLU:HG3  | 2.04                     | 0.56              |
| 1:B:230:PHE:HA   | 1:B:231:PRO:C    | 2.30                     | 0.56              |
| 1:L:191:LYS:NZ   | 1:L:191:LYS:HB3  | 2.20                     | 0.56              |
| 1:D:106:ASP:OD2  | 1:D:108:ALA:HB3  | 2.06                     | 0.56              |
| 1:D:394:GLU:HG2  | 7:D:570:HOH:O    | 2.05                     | 0.56              |
| 1:G:230:PHE:HA   | 1:G:231:PRO:C    | 2.30                     | 0.56              |
| 1:K:117:GLU:O    | 1:K:121:LYS:HD2  | 2.06                     | 0.56              |
| 1:L:122:LYS:HZ1  | 1:L:127:GLN:NE2  | 2.04                     | 0.56              |
| 1:A:106:ASP:OD2  | 1:A:108:ALA:HB3  | 2.06                     | 0.56              |
| 1:B:218:VAL:HG23 | 1:B:219:TYR:CD2  | 2.40                     | 0.56              |
| 1:E:352:GLN:HG3  | 1:E:353:HIS:N    | 2.21                     | 0.56              |
| 1:G:70:SER:O     | 1:G:74:GLN:HG3   | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:40:TRP:O     | 1:I:41:ASP:CG    | 2.49                     | 0.56              |
| 1:I:106:ASP:OD2  | 1:I:108:ALA:HB3  | 2.06                     | 0.55              |
| 1:K:392:THR:OG1  | 1:K:395:GLU:HG3  | 2.06                     | 0.55              |
| 1:F:254:PRO:HG3  | 1:F:295:LYS:HE3  | 1.89                     | 0.55              |
| 1:F:402:ASP:HA   | 1:F:406:ARG:HB2  | 1.89                     | 0.55              |
| 1:E:402:ASP:HA   | 1:E:406:ARG:HB2  | 1.88                     | 0.55              |
| 1:I:245:LEU:HB2  | 1:I:246:PRO:HD3  | 1.89                     | 0.55              |
| 1:F:70:SER:OG    | 1:F:73:GLU:HG3   | 2.07                     | 0.55              |
| 1:H:286:HIS:CE1  | 1:H:290:GLU:HG3  | 2.42                     | 0.55              |
| 1:B:40:TRP:O     | 1:B:41:ASP:CB    | 2.55                     | 0.55              |
| 1:B:265:VAL:HG21 | 1:B:275:PHE:HB2  | 1.88                     | 0.55              |
| 1:G:219:TYR:HB3  | 1:G:254:PRO:HG2  | 1.88                     | 0.55              |
| 1:G:371:SER:O    | 1:G:375:GLU:HG3  | 2.07                     | 0.55              |
| 1:H:30:PHE:CE2   | 1:H:37:ILE:HG13  | 2.42                     | 0.55              |
| 1:H:381:TYR:O    | 1:H:385:LEU:HD23 | 2.07                     | 0.55              |
| 1:A:127:GLN:HE21 | 1:A:127:GLN:CA   | 2.13                     | 0.55              |
| 1:B:410:ARG:HB3  | 1:B:410:ARG:NH1  | 2.22                     | 0.55              |
| 1:A:301:LEU:HD11 | 1:A:326:TRP:HB3  | 1.89                     | 0.54              |
| 1:B:47:THR:OG1   | 1:B:71:LYS:HE3   | 2.07                     | 0.54              |
| 1:B:189:GLY:O    | 1:B:206:ARG:NH2  | 2.40                     | 0.54              |
| 1:C:219:TYR:HA   | 1:C:253:ILE:CG2  | 2.38                     | 0.54              |
| 1:F:208:LEU:O    | 1:F:212:ILE:HG13 | 2.08                     | 0.54              |
| 1:G:290:GLU:C    | 1:G:292:PRO:HD3  | 2.33                     | 0.54              |
| 1:A:183:HIS:HA   | 1:A:186:ARG:HD2  | 1.89                     | 0.54              |
| 1:B:410:ARG:CB   | 1:B:410:ARG:HH11 | 2.21                     | 0.54              |
| 1:A:149:ASP:OD1  | 1:A:152:ARG:NH2  | 2.40                     | 0.54              |
| 1:A:245:LEU:HB2  | 1:A:246:PRO:HD3  | 1.89                     | 0.54              |
| 1:G:40:TRP:O     | 1:G:41:ASP:CG    | 2.51                     | 0.54              |
| 1:G:122:LYS:HG3  | 1:G:126:GLU:HB2  | 1.89                     | 0.54              |
| 1:D:40:TRP:O     | 1:D:41:ASP:CG    | 2.50                     | 0.54              |
| 1:G:245:LEU:HB2  | 1:G:246:PRO:HD3  | 1.89                     | 0.54              |
| 1:I:258:MET:HE2  | 1:I:325:TRP:CE2  | 2.42                     | 0.54              |
| 1:J:370:LYS:NZ   | 7:J:826:HOH:O    | 2.38                     | 0.54              |
| 1:E:265:VAL:HG21 | 1:E:275:PHE:HB2  | 1.90                     | 0.54              |
| 1:G:3:ILE:N      | 1:G:3:ILE:HD12   | 2.22                     | 0.54              |
| 1:G:328:MET:HA   | 1:G:328:MET:HE2  | 1.89                     | 0.54              |
| 1:E:49:HIS:HB2   | 1:E:272:ALA:HB2  | 1.90                     | 0.54              |
| 1:I:313:ALA:HA   | 1:I:319:LEU:HD23 | 1.89                     | 0.54              |
| 1:B:111:ASP:OD1  | 1:B:114:VAL:HG23 | 2.08                     | 0.54              |
| 1:B:128:VAL:O    | 1:B:132:LEU:HG   | 2.08                     | 0.54              |
| 1:B:316:PHE:HB3  | 1:B:318:ASN:OD1  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:144:ASN:HB2  | 1:D:215:MET:HE3  | 1.90                     | 0.54              |
| 1:E:117:GLU:O    | 1:E:121:LYS:HG3  | 2.07                     | 0.54              |
| 1:F:323:GLY:HA2  | 1:F:352:GLN:HA   | 1.89                     | 0.54              |
| 1:D:245:LEU:HB2  | 1:D:246:PRO:HD3  | 1.90                     | 0.53              |
| 1:G:323:GLY:HA2  | 1:G:352:GLN:HA   | 1.88                     | 0.53              |
| 1:H:301:LEU:HD11 | 1:H:326:TRP:HB3  | 1.89                     | 0.53              |
| 1:I:123:THR:OG1  | 1:I:126:GLU:HG3  | 2.08                     | 0.53              |
| 1:I:202:GLN:HA   | 1:I:202:GLN:HE21 | 1.72                     | 0.53              |
| 1:J:230:PHE:HA   | 1:J:231:PRO:C    | 2.33                     | 0.53              |
| 1:J:385:LEU:HA   | 1:J:389:TRP:O    | 2.08                     | 0.53              |
| 1:K:198:GLU:O    | 1:K:202:GLN:HG2  | 2.08                     | 0.53              |
| 1:C:276:VAL:HG22 | 1:C:277:GLY:N    | 2.23                     | 0.53              |
| 1:G:185:LEU:HB3  | 1:G:190:TYR:HB2  | 1.91                     | 0.53              |
| 1:G:308:GLU:HG2  | 7:G:434:HOH:O    | 2.07                     | 0.53              |
| 1:C:219:TYR:HB3  | 1:C:254:PRO:HG2  | 1.90                     | 0.53              |
| 1:E:55:VAL:CG1   | 1:E:78:ILE:HG12  | 2.29                     | 0.53              |
| 1:J:323:GLY:HA2  | 1:J:352:GLN:HA   | 1.90                     | 0.53              |
| 1:B:72:ARG:HH21  | 1:B:116:ARG:HD3  | 1.74                     | 0.53              |
| 1:L:122:LYS:NZ   | 1:L:127:GLN:NE2  | 2.57                     | 0.53              |
| 1:H:127:GLN:OE1  | 1:H:127:GLN:HA   | 2.09                     | 0.52              |
| 1:J:30:PHE:CE2   | 1:J:37:ILE:HG13  | 2.44                     | 0.52              |
| 1:L:306:GLN:OE1  | 1:L:337:MET:HE3  | 2.09                     | 0.52              |
| 1:A:172:ASP:HB2  | 1:A:173:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:265:VAL:HG21 | 1:A:275:PHE:HB2  | 1.89                     | 0.52              |
| 1:J:393:GLU:HG2  | 1:J:397:LYS:HE3  | 1.92                     | 0.52              |
| 1:K:402:ASP:HA   | 1:K:406:ARG:HB2  | 1.91                     | 0.52              |
| 1:B:44:GLU:OE2   | 1:B:71:LYS:HE2   | 2.09                     | 0.52              |
| 1:B:65:ALA:O     | 1:B:69:MET:HG3   | 2.08                     | 0.52              |
| 1:B:155:TRP:CZ3  | 1:B:215:MET:HA   | 2.44                     | 0.52              |
| 1:G:276:VAL:HG22 | 1:G:277:GLY:N    | 2.24                     | 0.52              |
| 1:I:186:ARG:HA   | 1:I:190:TYR:O    | 2.10                     | 0.52              |
| 1:B:195:GLU:HG3  | 1:B:197:ASN:ND2  | 2.25                     | 0.52              |
| 1:C:3:ILE:HD12   | 1:C:12:LYS:HD2   | 1.91                     | 0.52              |
| 1:E:148:ASP:OD2  | 1:E:150:ASN:HB3  | 2.09                     | 0.52              |
| 1:K:393:GLU:HG2  | 1:K:397:LYS:NZ   | 2.24                     | 0.52              |
| 1:A:111:ASP:OD1  | 1:A:114:VAL:HG23 | 2.10                     | 0.52              |
| 1:H:48:TYR:HB3   | 1:H:51:LEU:HD23  | 1.92                     | 0.52              |
| 1:F:180:GLN:H    | 1:F:180:GLN:NE2  | 2.07                     | 0.52              |
| 1:F:180:GLN:NE2  | 1:F:180:GLN:N    | 2.58                     | 0.52              |
| 1:F:219:TYR:HA   | 1:F:253:ILE:CG2  | 2.40                     | 0.52              |
| 1:L:392:THR:OG1  | 1:L:395:GLU:HG3  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:182:LYS:HA   | 1:B:185:LEU:HD12 | 1.90                     | 0.52              |
| 1:B:186:ARG:NH1  | 1:B:192:VAL:O    | 2.41                     | 0.52              |
| 1:H:276:VAL:HG22 | 1:H:277:GLY:N    | 2.24                     | 0.52              |
| 1:J:276:VAL:HG22 | 1:J:277:GLY:N    | 2.24                     | 0.52              |
| 1:C:381:TYR:O    | 1:C:385:LEU:HD22 | 2.10                     | 0.52              |
| 1:F:196:TRP:CD1  | 1:F:238:ARG:HD2  | 2.45                     | 0.52              |
| 1:F:276:VAL:HG22 | 1:F:277:GLY:N    | 2.25                     | 0.52              |
| 1:G:235:ASN:O    | 1:G:239:ILE:HG13 | 2.09                     | 0.52              |
| 1:D:139:ASP:OD1  | 1:D:166:HIS:HE1  | 1.93                     | 0.52              |
| 1:J:313:ALA:HA   | 1:J:319:LEU:HD23 | 1.92                     | 0.52              |
| 1:H:70:SER:OG    | 1:H:73:GLU:HG3   | 2.10                     | 0.51              |
| 1:H:123:THR:OG1  | 1:H:126:GLU:HG3  | 2.11                     | 0.51              |
| 1:I:149:ASP:HA   | 1:I:152:ARG:NH1  | 2.23                     | 0.51              |
| 1:I:230:PHE:HA   | 1:I:231:PRO:C    | 2.35                     | 0.51              |
| 1:D:3:ILE:HG21   | 1:D:9:LEU:HD13   | 1.92                     | 0.51              |
| 1:F:245:LEU:HB2  | 1:F:246:PRO:HD3  | 1.92                     | 0.51              |
| 1:H:117:GLU:O    | 1:H:121:LYS:HG3  | 2.10                     | 0.51              |
| 1:J:70:SER:OG    | 1:J:73:GLU:HG3   | 2.10                     | 0.51              |
| 1:K:172:ASP:HB2  | 1:K:173:PRO:HD3  | 1.92                     | 0.51              |
| 1:K:219:TYR:HB3  | 1:K:254:PRO:HG2  | 1.92                     | 0.51              |
| 1:A:286:HIS:CE1  | 1:A:290:GLU:HG3  | 2.46                     | 0.51              |
| 1:B:410:ARG:NH1  | 1:B:410:ARG:CB   | 2.73                     | 0.51              |
| 1:E:301:LEU:O    | 1:E:328:MET:HE3  | 2.11                     | 0.51              |
| 1:F:139:ASP:OD1  | 1:F:166:HIS:HE1  | 1.93                     | 0.51              |
| 1:A:170:ARG:NH2  | 1:A:223:SER:HB3  | 2.26                     | 0.51              |
| 1:E:254:PRO:HG3  | 1:E:412:VAL:HG12 | 1.93                     | 0.51              |
| 1:L:245:LEU:HB2  | 1:L:246:PRO:HD3  | 1.93                     | 0.51              |
| 1:E:79:TRP:O     | 1:E:83:PHE:HB2   | 2.11                     | 0.51              |
| 1:H:402:ASP:HA   | 1:H:406:ARG:HB2  | 1.93                     | 0.51              |
| 1:A:306:GLN:OE1  | 1:A:337:MET:HE3  | 2.11                     | 0.51              |
| 1:A:66:PHE:HA    | 1:A:69:MET:HE3   | 1.92                     | 0.51              |
| 1:A:392:THR:OG1  | 1:A:395:GLU:HG3  | 2.10                     | 0.51              |
| 1:B:252:ASN:ND2  | 1:B:295:LYS:HE2  | 2.26                     | 0.51              |
| 1:F:172:ASP:HB2  | 1:F:173:PRO:HD3  | 1.91                     | 0.51              |
| 1:H:396:ILE:O    | 1:H:400:VAL:HG23 | 2.11                     | 0.51              |
| 1:L:172:ASP:HB2  | 1:L:173:PRO:HD3  | 1.93                     | 0.51              |
| 1:B:112:LEU:HA   | 1:B:115:TYR:CD2  | 2.46                     | 0.51              |
| 1:C:286:HIS:CE1  | 1:C:290:GLU:HG3  | 2.46                     | 0.51              |
| 1:F:252:ASN:ND2  | 1:F:295:LYS:HE2  | 2.26                     | 0.51              |
| 1:G:122:LYS:HD3  | 1:G:127:GLN:CA   | 2.41                     | 0.51              |
| 1:A:393:GLU:CG   | 1:A:397:LYS:HE3  | 2.40                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:47:THR:OG1   | 1:I:71:LYS:HE2   | 2.10                     | 0.50              |
| 1:A:56:MET:HE2   | 1:A:63:ILE:HB    | 1.92                     | 0.50              |
| 1:C:321:ILE:HG12 | 7:C:1266:HOH:O   | 2.12                     | 0.50              |
| 1:L:139:ASP:OD1  | 1:L:166:HIS:HE1  | 1.93                     | 0.50              |
| 1:B:410:ARG:HH11 | 1:B:410:ARG:HB2  | 1.76                     | 0.50              |
| 1:F:56:MET:HE3   | 7:F:707:HOH:O    | 2.12                     | 0.50              |
| 1:C:70:SER:O     | 1:C:74:GLN:HG3   | 2.11                     | 0.50              |
| 1:C:79:TRP:O     | 1:C:83:PHE:HB2   | 2.11                     | 0.50              |
| 1:E:198:GLU:OE2  | 1:E:202:GLN:HG2  | 2.11                     | 0.50              |
| 1:E:219:TYR:HA   | 1:E:253:ILE:HG23 | 1.93                     | 0.50              |
| 1:F:230:PHE:HA   | 1:F:231:PRO:C    | 2.37                     | 0.50              |
| 1:G:196:TRP:CD1  | 1:G:238:ARG:HD2  | 2.46                     | 0.50              |
| 1:H:219:TYR:HA   | 1:H:253:ILE:CG2  | 2.41                     | 0.50              |
| 1:I:172:ASP:HB2  | 1:I:173:PRO:HD3  | 1.93                     | 0.50              |
| 1:B:264:ARG:NH1  | 1:B:264:ARG:HB2  | 2.26                     | 0.50              |
| 1:F:88:PRO:C     | 1:F:93:CYS:SG    | 2.95                     | 0.50              |
| 1:F:235:ASN:O    | 1:F:239:ILE:HG13 | 2.12                     | 0.50              |
| 1:I:112:LEU:HA   | 1:I:115:TYR:CD2  | 2.46                     | 0.50              |
| 1:F:301:LEU:O    | 1:F:328:MET:HE3  | 2.12                     | 0.50              |
| 1:I:191:LYS:HE3  | 1:I:191:LYS:CA   | 2.40                     | 0.50              |
| 1:I:374:ALA:O    | 1:I:378:ILE:HG13 | 2.12                     | 0.50              |
| 1:L:40:TRP:O     | 1:L:41:ASP:CG    | 2.54                     | 0.50              |
| 1:E:172:ASP:HB2  | 1:E:173:PRO:HD3  | 1.94                     | 0.50              |
| 1:F:306:GLN:OE1  | 1:F:337:MET:HE3  | 2.11                     | 0.50              |
| 1:F:169:LEU:HD23 | 1:F:220:MET:HE3  | 1.92                     | 0.50              |
| 1:K:265:VAL:HG21 | 1:K:275:PHE:HB2  | 1.93                     | 0.50              |
| 1:L:230:PHE:HA   | 1:L:231:PRO:C    | 2.37                     | 0.50              |
| 1:B:301:LEU:HD11 | 1:B:326:TRP:HB3  | 1.94                     | 0.50              |
| 1:B:308:GLU:HG2  | 7:B:439:HOH:O    | 2.12                     | 0.50              |
| 1:J:328:MET:HA   | 1:J:328:MET:HE2  | 1.92                     | 0.50              |
| 1:G:97:LEU:HD13  | 1:H:389:TRP:HB2  | 1.94                     | 0.49              |
| 1:L:130:THR:O    | 1:L:134:LEU:HG   | 2.12                     | 0.49              |
| 1:A:70:SER:OG    | 1:A:73:GLU:HG3   | 2.12                     | 0.49              |
| 1:B:79:TRP:O     | 1:B:83:PHE:HB2   | 2.12                     | 0.49              |
| 1:C:306:GLN:OE1  | 1:C:337:MET:HE3  | 2.12                     | 0.49              |
| 1:E:263:LYS:C    | 1:E:264:ARG:HG2  | 2.36                     | 0.49              |
| 1:K:70:SER:OG    | 1:K:73:GLU:HG3   | 2.12                     | 0.49              |
| 1:C:25:MET:HG3   | 7:C:431:HOH:O    | 2.12                     | 0.49              |
| 1:D:196:TRP:CD1  | 1:D:238:ARG:HD2  | 2.47                     | 0.49              |
| 1:F:40:TRP:O     | 1:F:41:ASP:CG    | 2.55                     | 0.49              |
| 1:A:212:ILE:HD13 | 1:A:253:ILE:HD12 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:391:VAL:HG23 | 1:A:391:VAL:O    | 2.12                     | 0.49              |
| 1:C:4:ASN:HB2    | 7:K:1425:HOH:O   | 2.10                     | 0.49              |
| 1:G:30:PHE:CD2   | 1:G:37:ILE:HG13  | 2.46                     | 0.49              |
| 1:F:79:TRP:O     | 1:F:83:PHE:HB2   | 2.13                     | 0.49              |
| 1:G:172:ASP:HB2  | 1:G:173:PRO:HD3  | 1.94                     | 0.49              |
| 1:H:385:LEU:HD21 | 1:H:391:VAL:CG1  | 2.42                     | 0.49              |
| 1:K:276:VAL:HG22 | 1:K:277:GLY:N    | 2.26                     | 0.49              |
| 1:A:313:ALA:HA   | 1:A:319:LEU:HD23 | 1.94                     | 0.49              |
| 1:D:219:TYR:HA   | 1:D:253:ILE:HG22 | 1.95                     | 0.49              |
| 1:G:30:PHE:CE2   | 1:G:37:ILE:HG13  | 2.48                     | 0.49              |
| 7:C:1313:HOH:O   | 1:K:4:ASN:HB2    | 2.11                     | 0.49              |
| 1:F:52:VAL:O     | 1:F:55:VAL:HG12  | 2.13                     | 0.49              |
| 1:G:139:ASP:OD1  | 1:G:166:HIS:HE1  | 1.96                     | 0.49              |
| 1:G:389:TRP:HB2  | 1:I:97:LEU:HD13  | 1.95                     | 0.49              |
| 1:L:402:ASP:HA   | 1:L:406:ARG:HB2  | 1.95                     | 0.49              |
| 1:A:79:TRP:O     | 1:A:83:PHE:HB2   | 2.13                     | 0.49              |
| 1:E:276:VAL:HG22 | 1:E:277:GLY:N    | 2.27                     | 0.49              |
| 1:F:171:LEU:CD1  | 1:F:220:MET:HE2  | 2.38                     | 0.49              |
| 1:G:124:SER:O    | 1:G:128:VAL:HG23 | 2.12                     | 0.49              |
| 1:G:301:LEU:HD11 | 1:G:326:TRP:HB3  | 1.95                     | 0.49              |
| 1:K:127:GLN:OE1  | 1:K:127:GLN:HA   | 2.13                     | 0.49              |
| 1:L:276:VAL:HG22 | 1:L:277:GLY:N    | 2.28                     | 0.49              |
| 1:F:198:GLU:OE2  | 1:F:202:GLN:NE2  | 2.45                     | 0.48              |
| 1:I:301:LEU:CD1  | 1:I:326:TRP:HB3  | 2.43                     | 0.48              |
| 1:J:40:TRP:O     | 1:J:41:ASP:CG    | 2.56                     | 0.48              |
| 1:K:139:ASP:OD1  | 1:K:166:HIS:HE1  | 1.96                     | 0.48              |
| 1:L:9:LEU:HD21   | 1:L:381:TYR:HB3  | 1.93                     | 0.48              |
| 1:A:209:THR:O    | 1:A:213:GLU:HG3  | 2.13                     | 0.48              |
| 1:B:42:ILE:HD13  | 1:B:100:LEU:HD21 | 1.95                     | 0.48              |
| 1:E:244:LEU:C    | 1:E:244:LEU:HD13 | 2.38                     | 0.48              |
| 1:J:5:SER:HB2    | 1:J:7:GLU:HG2    | 1.94                     | 0.48              |
| 1:J:149:ASP:O    | 1:J:153:ILE:HG13 | 2.12                     | 0.48              |
| 1:A:235:ASN:O    | 1:A:239:ILE:HG13 | 2.13                     | 0.48              |
| 1:F:41:ASP:C     | 1:F:41:ASP:OD1   | 2.56                     | 0.48              |
| 1:G:149:ASP:O    | 1:G:153:ILE:HG13 | 2.13                     | 0.48              |
| 1:H:381:TYR:O    | 1:H:385:LEU:CD2  | 2.61                     | 0.48              |
| 1:A:66:PHE:O     | 1:A:69:MET:HG2   | 2.14                     | 0.48              |
| 1:B:219:TYR:HA   | 1:B:253:ILE:CG2  | 2.42                     | 0.48              |
| 1:E:219:TYR:HB3  | 1:E:254:PRO:HG2  | 1.94                     | 0.48              |
| 1:J:69:MET:HB3   | 1:J:73:GLU:HB2   | 1.96                     | 0.48              |
| 1:I:276:VAL:HG22 | 1:I:277:GLY:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:3:ILE:HG23   | 1:E:8:VAL:CG1    | 2.39                     | 0.48              |
| 1:G:336:GLU:O    | 1:G:340:MET:HG3  | 2.14                     | 0.48              |
| 1:A:117:GLU:O    | 1:A:121:LYS:HG2  | 2.14                     | 0.48              |
| 1:A:230:PHE:HA   | 1:A:231:PRO:C    | 2.38                     | 0.48              |
| 1:B:216:ASP:N    | 1:B:217:PRO:CD   | 2.77                     | 0.48              |
| 1:B:276:VAL:HG22 | 1:B:277:GLY:N    | 2.28                     | 0.48              |
| 1:E:40:TRP:O     | 1:E:41:ASP:CG    | 2.56                     | 0.48              |
| 1:E:97:LEU:HD13  | 1:F:389:TRP:HB2  | 1.96                     | 0.48              |
| 1:F:42:ILE:HD13  | 1:F:100:LEU:HD21 | 1.95                     | 0.48              |
| 1:I:67:TRP:HA    | 1:I:67:TRP:CE3   | 2.48                     | 0.48              |
| 1:J:172:ASP:HB2  | 1:J:173:PRO:HD3  | 1.95                     | 0.48              |
| 1:A:219:TYR:HB3  | 1:A:254:PRO:HG2  | 1.96                     | 0.48              |
| 1:A:322:PHE:HA   | 1:A:350:ILE:O    | 2.14                     | 0.48              |
| 1:B:195:GLU:HG3  | 1:B:197:ASN:HD22 | 1.78                     | 0.48              |
| 1:K:230:PHE:HA   | 1:K:231:PRO:C    | 2.38                     | 0.48              |
| 1:C:172:ASP:HB2  | 1:C:173:PRO:HD3  | 1.95                     | 0.48              |
| 1:C:219:TYR:HA   | 1:C:253:ILE:HG22 | 1.95                     | 0.48              |
| 1:E:70:SER:OG    | 1:E:73:GLU:HG3   | 2.14                     | 0.48              |
| 1:A:208:LEU:O    | 1:A:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:B:152:ARG:NH1  | 1:B:156:LEU:HD11 | 2.29                     | 0.48              |
| 1:G:352:GLN:HG3  | 1:G:353:HIS:N    | 2.28                     | 0.48              |
| 1:J:288:LEU:CD2  | 1:J:319:LEU:HB2  | 2.44                     | 0.48              |
| 1:L:322:PHE:HA   | 1:L:350:ILE:O    | 2.13                     | 0.48              |
| 1:A:128:VAL:HA   | 1:A:359:LEU:HD21 | 1.95                     | 0.47              |
| 1:E:112:LEU:HA   | 1:E:115:TYR:CD2  | 2.49                     | 0.47              |
| 1:J:352:GLN:HG3  | 1:J:353:HIS:N    | 2.28                     | 0.47              |
| 1:K:25:MET:HG3   | 7:K:445:HOH:O    | 2.13                     | 0.47              |
| 1:L:122:LYS:NZ   | 1:L:127:GLN:HE22 | 2.12                     | 0.47              |
| 1:G:295:LYS:HD3  | 1:G:411:PHE:O    | 2.13                     | 0.47              |
| 1:G:313:ALA:HA   | 1:G:319:LEU:HD23 | 1.96                     | 0.47              |
| 1:H:385:LEU:HD21 | 1:H:391:VAL:HG11 | 1.97                     | 0.47              |
| 1:D:301:LEU:HD11 | 1:D:326:TRP:HB3  | 1.96                     | 0.47              |
| 1:G:243:CYS:C    | 1:G:246:PRO:HD2  | 2.38                     | 0.47              |
| 1:G:291:TYR:N    | 1:G:292:PRO:HD3  | 2.29                     | 0.47              |
| 1:J:410:ARG:HD3  | 7:J:466:HOH:O    | 2.13                     | 0.47              |
| 1:A:172:ASP:OD1  | 1:A:222:VAL:HA   | 2.15                     | 0.47              |
| 1:C:328:MET:HE2  | 1:C:328:MET:HA   | 1.96                     | 0.47              |
| 1:D:170:ARG:HH21 | 1:D:223:SER:HB3  | 1.79                     | 0.47              |
| 1:D:286:HIS:CE1  | 1:D:290:GLU:HG3  | 2.49                     | 0.47              |
| 1:J:382:ASP:O    | 1:J:386:GLN:HG2  | 2.14                     | 0.47              |
| 1:F:148:ASP:OD2  | 1:F:151:GLU:HG3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:69:MET:HB3   | 1:L:73:GLU:HB2   | 1.97                     | 0.47              |
| 1:A:301:LEU:CD1  | 1:A:326:TRP:HB3  | 2.44                     | 0.47              |
| 1:I:111:ASP:OD1  | 1:I:114:VAL:HG23 | 2.14                     | 0.47              |
| 1:I:394:GLU:HG2  | 7:I:461:HOH:O    | 2.13                     | 0.47              |
| 1:I:402:ASP:HA   | 1:I:406:ARG:HB2  | 1.96                     | 0.47              |
| 1:K:72:ARG:HH22  | 1:K:116:ARG:HD3  | 1.79                     | 0.47              |
| 1:K:352:GLN:HG3  | 1:K:353:HIS:N    | 2.29                     | 0.47              |
| 1:L:180:GLN:NE2  | 1:L:180:GLN:N    | 2.62                     | 0.47              |
| 1:L:308:GLU:HG2  | 7:L:462:HOH:O    | 2.13                     | 0.47              |
| 1:B:264:ARG:HB2  | 1:B:264:ARG:HH11 | 1.80                     | 0.47              |
| 1:F:352:GLN:HG3  | 1:F:353:HIS:N    | 2.29                     | 0.47              |
| 1:G:112:LEU:HA   | 1:G:115:TYR:CD2  | 2.50                     | 0.47              |
| 1:J:129:ASP:O    | 1:J:133:GLN:HB2  | 2.14                     | 0.47              |
| 1:J:389:TRP:HB2  | 1:L:97:LEU:HD13  | 1.97                     | 0.47              |
| 1:A:22:VAL:HG11  | 1:A:366:TRP:CE2  | 2.49                     | 0.47              |
| 1:B:25:MET:HG3   | 7:B:446:HOH:O    | 2.15                     | 0.47              |
| 1:G:20:GLN:NE2   | 1:G:21:PRO:HD2   | 2.30                     | 0.47              |
| 1:K:196:TRP:CZ2  | 1:K:201:ILE:HG12 | 2.49                     | 0.47              |
| 1:K:202:GLN:HA   | 1:K:202:GLN:NE2  | 2.30                     | 0.47              |
| 1:B:275:PHE:CG   | 1:B:276:VAL:N    | 2.83                     | 0.47              |
| 1:I:146:PRO:O    | 1:I:152:ARG:HD3  | 2.14                     | 0.47              |
| 1:I:254:PRO:HG2  | 1:I:412:VAL:HA   | 1.97                     | 0.47              |
| 1:J:49:HIS:HB2   | 1:J:272:ALA:HB2  | 1.97                     | 0.47              |
| 1:A:9:LEU:HD21   | 1:A:381:TYR:HB3  | 1.97                     | 0.46              |
| 1:G:216:ASP:N    | 1:G:217:PRO:CD   | 2.79                     | 0.46              |
| 1:I:111:ASP:CG   | 1:I:114:VAL:HG23 | 2.40                     | 0.46              |
| 1:K:244:LEU:HD13 | 1:K:244:LEU:C    | 2.41                     | 0.46              |
| 1:E:230:PHE:HA   | 1:E:231:PRO:C    | 2.39                     | 0.46              |
| 1:L:127:GLN:HE21 | 1:L:127:GLN:CA   | 2.18                     | 0.46              |
| 1:B:286:HIS:CE1  | 1:B:290:GLU:HG3  | 2.50                     | 0.46              |
| 1:D:276:VAL:HG22 | 1:D:277:GLY:N    | 2.30                     | 0.46              |
| 1:F:198:GLU:O    | 1:F:202:GLN:HG2  | 2.15                     | 0.46              |
| 1:H:40:TRP:O     | 1:H:41:ASP:CG    | 2.59                     | 0.46              |
| 1:J:11:GLU:O     | 1:J:15:ASN:HB2   | 2.16                     | 0.46              |
| 1:C:41:ASP:OD1   | 1:C:41:ASP:C     | 2.59                     | 0.46              |
| 1:E:113:GLN:HE22 | 1:E:116:ARG:HH11 | 1.63                     | 0.46              |
| 1:I:301:LEU:HD11 | 1:I:326:TRP:HB3  | 1.97                     | 0.46              |
| 1:A:142:MET:O    | 1:A:168:ALA:HB3  | 2.16                     | 0.46              |
| 1:B:56:MET:HE3   | 7:C:1242:HOH:O   | 2.15                     | 0.46              |
| 1:F:203:GLU:OE2  | 1:F:206:ARG:NH1  | 2.49                     | 0.46              |
| 1:H:303:ARG:HB2  | 1:H:328:MET:HE1  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:149:ASP:HA   | 1:K:152:ARG:NH1  | 2.30                     | 0.46              |
| 1:D:112:LEU:HA   | 1:D:115:TYR:CD2  | 2.50                     | 0.46              |
| 1:I:252:ASN:HD21 | 1:I:295:LYS:CE   | 2.29                     | 0.46              |
| 1:A:41:ASP:HA    | 1:A:119:PHE:CD1  | 2.51                     | 0.46              |
| 1:A:244:LEU:HD13 | 1:A:244:LEU:C    | 2.40                     | 0.46              |
| 1:A:393:GLU:O    | 1:A:397:LYS:HG3  | 2.16                     | 0.46              |
| 1:B:301:LEU:CD1  | 1:B:326:TRP:HB3  | 2.46                     | 0.46              |
| 1:C:230:PHE:HA   | 1:C:231:PRO:C    | 2.41                     | 0.46              |
| 1:E:41:ASP:OD1   | 1:E:41:ASP:C     | 2.58                     | 0.46              |
| 1:I:200:SER:O    | 1:I:204:VAL:HG23 | 2.15                     | 0.46              |
| 1:K:40:TRP:O     | 1:K:41:ASP:CG    | 2.58                     | 0.46              |
| 1:K:122:LYS:NZ   | 1:K:122:LYS:HB3  | 2.31                     | 0.46              |
| 1:C:244:LEU:HD13 | 1:C:244:LEU:C    | 2.40                     | 0.46              |
| 1:F:147:PHE:CZ   | 1:F:174:LEU:HB2  | 2.51                     | 0.46              |
| 1:B:301:LEU:O    | 1:B:328:MET:HE3  | 2.16                     | 0.45              |
| 1:D:322:PHE:HA   | 1:D:350:ILE:O    | 2.16                     | 0.45              |
| 1:E:20:GLN:NE2   | 1:E:21:PRO:HD2   | 2.31                     | 0.45              |
| 1:E:111:ASP:CG   | 1:E:114:VAL:HG23 | 2.42                     | 0.45              |
| 1:B:49:HIS:HB2   | 1:B:272:ALA:HB2  | 1.97                     | 0.45              |
| 1:F:149:ASP:OD1  | 1:F:152:ARG:NH2  | 2.50                     | 0.45              |
| 1:F:180:GLN:H    | 1:F:180:GLN:HE21 | 1.63                     | 0.45              |
| 1:G:193:ASN:HD22 | 1:G:197:ASN:ND2  | 2.13                     | 0.45              |
| 1:H:139:ASP:OD1  | 1:H:166:HIS:HE1  | 1.99                     | 0.45              |
| 1:B:219:TYR:CB   | 1:B:254:PRO:HG2  | 2.46                     | 0.45              |
| 1:H:79:TRP:O     | 1:H:83:PHE:HB2   | 2.16                     | 0.45              |
| 1:H:201:ILE:O    | 1:H:205:LYS:HG3  | 2.16                     | 0.45              |
| 1:H:264:ARG:HH11 | 1:H:264:ARG:HB2  | 1.80                     | 0.45              |
| 1:I:252:ASN:HD21 | 1:I:295:LYS:HE3  | 1.80                     | 0.45              |
| 1:D:25:MET:HG3   | 7:D:438:HOH:O    | 2.14                     | 0.45              |
| 1:K:122:LYS:HB3  | 1:K:122:LYS:HZ3  | 1.81                     | 0.45              |
| 1:K:154:SER:O    | 1:K:159:LYS:HB2  | 2.16                     | 0.45              |
| 1:A:219:TYR:HA   | 1:A:253:ILE:CG2  | 2.46                     | 0.45              |
| 1:B:196:TRP:CD1  | 1:B:238:ARG:HD2  | 2.52                     | 0.45              |
| 1:B:408:PHE:O    | 1:B:412:VAL:HG22 | 2.17                     | 0.45              |
| 1:G:244:LEU:C    | 1:G:244:LEU:HD13 | 2.42                     | 0.45              |
| 1:H:172:ASP:HB2  | 1:H:173:PRO:HD3  | 1.98                     | 0.45              |
| 1:J:252:ASN:ND2  | 1:J:295:LYS:HE2  | 2.31                     | 0.45              |
| 1:J:301:LEU:CD1  | 1:J:326:TRP:HB3  | 2.46                     | 0.45              |
| 1:K:146:PRO:O    | 1:K:152:ARG:HD3  | 2.16                     | 0.45              |
| 1:B:244:LEU:C    | 1:B:244:LEU:HD13 | 2.41                     | 0.45              |
| 1:D:169:LEU:HA   | 1:D:215:MET:HE1  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:203:GLU:OE2  | 1:D:206:ARG:HD3  | 2.16                     | 0.45              |
| 1:F:221:ALA:HB2  | 1:F:256:ALA:HB3  | 1.99                     | 0.45              |
| 1:B:197:ASN:O    | 1:B:201:ILE:HG13 | 2.16                     | 0.45              |
| 1:C:72:ARG:HG3   | 1:C:72:ARG:HH11  | 1.81                     | 0.45              |
| 1:C:166:HIS:HD2  | 7:C:1096:HOH:O   | 1.99                     | 0.45              |
| 1:E:113:GLN:NE2  | 1:E:116:ARG:HH11 | 2.15                     | 0.45              |
| 1:L:382:ASP:O    | 1:L:386:GLN:HG2  | 2.17                     | 0.45              |
| 1:A:128:VAL:HG23 | 1:A:129:ASP:N    | 2.32                     | 0.45              |
| 1:D:352:GLN:HG3  | 1:D:353:HIS:N    | 2.31                     | 0.45              |
| 1:J:244:LEU:HD13 | 1:J:244:LEU:C    | 2.42                     | 0.45              |
| 1:L:153:ILE:O    | 1:L:157:GLU:HG3  | 2.16                     | 0.45              |
| 1:E:252:ASN:ND2  | 1:E:295:LYS:HE2  | 2.32                     | 0.45              |
| 1:H:308:GLU:HG2  | 7:H:471:HOH:O    | 2.16                     | 0.45              |
| 1:I:37:ILE:CD1   | 1:I:151:GLU:HG2  | 2.47                     | 0.45              |
| 1:I:152:ARG:O    | 1:I:156:LEU:HG   | 2.17                     | 0.45              |
| 1:K:149:ASP:HA   | 1:K:152:ARG:HH12 | 1.82                     | 0.45              |
| 1:H:30:PHE:CD2   | 1:H:37:ILE:HG13  | 2.52                     | 0.45              |
| 1:J:287:LEU:O    | 1:J:291:TYR:HB2  | 2.17                     | 0.45              |
| 1:K:216:ASP:N    | 1:K:217:PRO:CD   | 2.80                     | 0.45              |
| 1:L:112:LEU:HA   | 1:L:115:TYR:CD2  | 2.51                     | 0.45              |
| 1:B:215:MET:HB2  | 1:B:217:PRO:HD3  | 1.99                     | 0.44              |
| 1:E:196:TRP:CD1  | 1:E:238:ARG:HD2  | 2.52                     | 0.44              |
| 1:I:195:GLU:HG3  | 1:I:197:ASN:ND2  | 2.33                     | 0.44              |
| 1:I:219:TYR:HA   | 1:I:253:ILE:CG2  | 2.47                     | 0.44              |
| 1:A:88:PRO:HB2   | 1:A:93:CYS:HB3   | 1.98                     | 0.44              |
| 1:B:118:TYR:HA   | 1:B:121:LYS:NZ   | 2.33                     | 0.44              |
| 1:B:190:TYR:HE1  | 1:B:206:ARG:HG2  | 1.82                     | 0.44              |
| 1:B:235:ASN:O    | 1:B:239:ILE:HG13 | 2.17                     | 0.44              |
| 1:E:139:ASP:OD1  | 1:E:166:HIS:HE1  | 2.00                     | 0.44              |
| 1:G:191:LYS:O    | 1:G:203:GLU:HG3  | 2.17                     | 0.44              |
| 1:J:212:ILE:HD13 | 1:J:253:ILE:HD12 | 1.98                     | 0.44              |
| 1:K:322:PHE:HA   | 1:K:350:ILE:O    | 2.17                     | 0.44              |
| 1:B:297:LEU:HD23 | 1:B:320:MET:HB3  | 1.99                     | 0.44              |
| 1:D:80:GLU:HG3   | 1:D:85:LYS:HE3   | 1.98                     | 0.44              |
| 1:E:219:TYR:HA   | 1:E:253:ILE:CG2  | 2.47                     | 0.44              |
| 1:F:276:VAL:CG2  | 1:F:277:GLY:N    | 2.80                     | 0.44              |
| 1:G:56:MET:HE3   | 7:H:498:HOH:O    | 2.17                     | 0.44              |
| 1:G:252:ASN:HD21 | 1:G:295:LYS:HE3  | 1.82                     | 0.44              |
| 1:H:230:PHE:HA   | 1:H:231:PRO:C    | 2.42                     | 0.44              |
| 1:J:123:THR:OG1  | 1:J:126:GLU:HG3  | 2.18                     | 0.44              |
| 1:B:243:CYS:O    | 1:B:246:PRO:HG2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:322:PHE:HA   | 1:G:350:ILE:O    | 2.18                     | 0.44              |
| 1:H:275:PHE:CG   | 1:H:276:VAL:N    | 2.85                     | 0.44              |
| 1:H:72:ARG:NH1   | 1:H:72:ARG:HG3   | 2.32                     | 0.44              |
| 1:I:48:TYR:HB3   | 1:I:51:LEU:HD23  | 2.00                     | 0.44              |
| 1:A:276:VAL:HG22 | 1:A:277:GLY:N    | 2.32                     | 0.44              |
| 1:E:72:ARG:HH21  | 1:E:116:ARG:HD3  | 1.82                     | 0.44              |
| 1:G:203:GLU:OE1  | 1:G:206:ARG:NH1  | 2.49                     | 0.44              |
| 1:B:182:LYS:O    | 1:B:186:ARG:HG3  | 2.18                     | 0.44              |
| 1:C:127:GLN:HE21 | 1:C:127:GLN:CA   | 2.08                     | 0.44              |
| 1:H:307:HIS:CD2  | 1:H:344:MET:HE1  | 2.52                     | 0.44              |
| 1:K:212:ILE:HD13 | 1:K:253:ILE:HD12 | 1.99                     | 0.44              |
| 1:L:79:TRP:O     | 1:L:83:PHE:HB2   | 2.18                     | 0.44              |
| 1:B:313:ALA:HA   | 1:B:319:LEU:HD23 | 1.99                     | 0.44              |
| 1:D:326:TRP:HB3  | 1:D:327:PHE:H    | 1.64                     | 0.44              |
| 1:H:69:MET:HB3   | 1:H:73:GLU:HB2   | 2.00                     | 0.44              |
| 1:A:41:ASP:OD1   | 1:A:43:ASP:N     | 2.51                     | 0.44              |
| 1:A:170:ARG:HH21 | 1:A:223:SER:HB3  | 1.83                     | 0.44              |
| 1:C:139:ASP:OD1  | 1:C:166:HIS:HE1  | 2.01                     | 0.44              |
| 1:F:219:TYR:HA   | 1:F:253:ILE:HG22 | 2.00                     | 0.44              |
| 1:F:265:VAL:HG21 | 1:F:275:PHE:HB2  | 2.00                     | 0.44              |
| 1:H:63:ILE:HD11  | 1:H:67:TRP:NE1   | 2.33                     | 0.44              |
| 1:I:235:ASN:O    | 1:I:239:ILE:HG13 | 2.18                     | 0.44              |
| 1:J:265:VAL:HG21 | 1:J:275:PHE:HB2  | 2.00                     | 0.44              |
| 1:K:41:ASP:C     | 1:K:41:ASP:OD1   | 2.61                     | 0.44              |
| 1:L:106:ASP:OD2  | 1:L:108:ALA:HB3  | 2.18                     | 0.44              |
| 1:L:219:TYR:HB3  | 1:L:254:PRO:HG2  | 2.00                     | 0.44              |
| 1:E:316:PHE:HB3  | 1:E:318:ASN:OD1  | 2.18                     | 0.43              |
| 1:J:211:TRP:CE3  | 1:J:215:MET:HE3  | 2.53                     | 0.43              |
| 1:J:245:LEU:HB2  | 1:J:246:PRO:HD3  | 1.99                     | 0.43              |
| 1:L:180:GLN:H    | 1:L:180:GLN:HE21 | 1.66                     | 0.43              |
| 1:A:9:LEU:HD21   | 1:A:381:TYR:CB   | 2.48                     | 0.43              |
| 1:E:203:GLU:OE1  | 1:E:206:ARG:NH1  | 2.51                     | 0.43              |
| 1:G:409:TRP:HA   | 1:G:412:VAL:HG22 | 2.00                     | 0.43              |
| 1:H:67:TRP:HA    | 1:H:67:TRP:CE3   | 2.53                     | 0.43              |
| 1:F:30:PHE:CE2   | 1:F:37:ILE:HG13  | 2.52                     | 0.43              |
| 1:J:358:VAL:HB   | 1:J:361:GLN:HG3  | 1.99                     | 0.43              |
| 1:A:352:GLN:HG3  | 1:A:353:HIS:N    | 2.33                     | 0.43              |
| 1:E:214:ARG:HG2  | 1:E:214:ARG:NH1  | 2.34                     | 0.43              |
| 1:H:352:GLN:HG3  | 1:H:353:HIS:N    | 2.33                     | 0.43              |
| 1:I:275:PHE:CG   | 1:I:276:VAL:N    | 2.86                     | 0.43              |
| 1:K:303:ARG:HB2  | 1:K:328:MET:HE1  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:4:ASN:C      | 1:B:4:ASN:HD22   | 2.24                     | 0.43              |
| 1:D:127:GLN:OE1  | 1:D:127:GLN:HA   | 2.18                     | 0.43              |
| 1:F:30:PHE:CD2   | 1:F:37:ILE:HG13  | 2.53                     | 0.43              |
| 1:G:218:VAL:HG23 | 1:G:219:TYR:CD2  | 2.54                     | 0.43              |
| 1:J:275:PHE:CG   | 1:J:276:VAL:N    | 2.87                     | 0.43              |
| 1:B:97:LEU:HD13  | 1:C:389:TRP:HB2  | 2.00                     | 0.43              |
| 1:C:111:ASP:OD1  | 1:C:114:VAL:HG23 | 2.18                     | 0.43              |
| 1:C:198:GLU:O    | 1:C:202:GLN:HG2  | 2.19                     | 0.43              |
| 1:E:275:PHE:CG   | 1:E:276:VAL:N    | 2.87                     | 0.43              |
| 1:G:358:VAL:HB   | 1:G:361:GLN:HG3  | 2.00                     | 0.43              |
| 1:H:41:ASP:OD1   | 1:H:41:ASP:C     | 2.61                     | 0.43              |
| 7:K:961:HOH:O    | 1:L:321:ILE:HG12 | 2.17                     | 0.43              |
| 1:C:40:TRP:O     | 1:C:41:ASP:CG    | 2.62                     | 0.43              |
| 1:D:251:HIS:HB2  | 1:D:253:ILE:HG12 | 2.00                     | 0.43              |
| 1:G:122:LYS:HD3  | 1:G:127:GLN:N    | 2.33                     | 0.43              |
| 1:L:123:THR:OG1  | 1:L:126:GLU:HG3  | 2.19                     | 0.43              |
| 1:L:301:LEU:HD11 | 1:L:326:TRP:HB3  | 2.01                     | 0.43              |
| 1:F:149:ASP:O    | 1:F:153:ILE:HG13 | 2.19                     | 0.43              |
| 1:F:336:GLU:O    | 1:F:340:MET:HG3  | 2.19                     | 0.43              |
| 1:G:127:GLN:HA   | 1:G:127:GLN:OE1  | 2.17                     | 0.43              |
| 1:K:396:ILE:O    | 1:K:400:VAL:HG23 | 2.18                     | 0.43              |
| 1:E:158:GLY:O    | 1:E:160:GLN:HG2  | 2.19                     | 0.43              |
| 1:A:196:TRP:CD1  | 1:A:238:ARG:HD2  | 2.53                     | 0.43              |
| 1:B:6:ARG:NH2    | 1:B:379:ASP:OD1  | 2.51                     | 0.43              |
| 1:G:256:ALA:HA   | 1:G:297:LEU:O    | 2.19                     | 0.43              |
| 1:H:97:LEU:HD13  | 1:I:389:TRP:HB2  | 1.99                     | 0.43              |
| 1:I:67:TRP:HA    | 1:I:67:TRP:HE3   | 1.83                     | 0.43              |
| 1:J:30:PHE:CD2   | 1:J:37:ILE:HG13  | 2.53                     | 0.43              |
| 1:J:219:TYR:HA   | 1:J:253:ILE:CG2  | 2.49                     | 0.43              |
| 1:K:97:LEU:HD13  | 1:L:389:TRP:HB2  | 2.00                     | 0.43              |
| 1:L:288:LEU:CD2  | 1:L:319:LEU:HB2  | 2.49                     | 0.43              |
| 1:L:410:ARG:HD3  | 7:L:539:HOH:O    | 2.19                     | 0.43              |
| 1:A:148:ASP:OD2  | 1:A:151:GLU:HG3  | 2.20                     | 0.42              |
| 1:C:40:TRP:CE3   | 1:C:127:GLN:HG2  | 2.54                     | 0.42              |
| 1:D:166:HIS:HD2  | 7:D:815:HOH:O    | 2.01                     | 0.42              |
| 1:E:276:VAL:CG2  | 1:E:277:GLY:N    | 2.81                     | 0.42              |
| 1:F:72:ARG:HH11  | 1:F:72:ARG:CB    | 2.23                     | 0.42              |
| 1:K:288:LEU:HD11 | 1:K:319:LEU:HD22 | 2.02                     | 0.42              |
| 1:L:111:ASP:OD1  | 1:L:114:VAL:HG23 | 2.20                     | 0.42              |
| 1:C:72:ARG:HG3   | 1:C:72:ARG:NH1   | 2.34                     | 0.42              |
| 1:C:154:SER:O    | 1:C:159:LYS:HB2  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:307:HIS:CD2  | 1:C:344:MET:HE1  | 2.54                     | 0.42              |
| 1:E:216:ASP:N    | 1:E:217:PRO:CD   | 2.83                     | 0.42              |
| 1:F:307:HIS:CD2  | 1:F:344:MET:HE1  | 2.54                     | 0.42              |
| 1:F:385:LEU:CD1  | 1:F:391:VAL:HG23 | 2.49                     | 0.42              |
| 1:G:69:MET:HB3   | 1:G:73:GLU:HB2   | 2.01                     | 0.42              |
| 1:H:322:PHE:HA   | 1:H:350:ILE:O    | 2.19                     | 0.42              |
| 1:I:40:TRP:O     | 1:I:41:ASP:CB    | 2.67                     | 0.42              |
| 1:I:148:ASP:OD2  | 1:I:151:GLU:HG3  | 2.19                     | 0.42              |
| 1:I:326:TRP:HB3  | 1:I:327:PHE:H    | 1.68                     | 0.42              |
| 1:K:219:TYR:HA   | 1:K:253:ILE:CG2  | 2.49                     | 0.42              |
| 1:L:160:GLN:HE21 | 1:L:160:GLN:HA   | 1.84                     | 0.42              |
| 1:L:200:SER:O    | 1:L:204:VAL:HG23 | 2.19                     | 0.42              |
| 1:C:216:ASP:N    | 1:C:217:PRO:CD   | 2.83                     | 0.42              |
| 1:F:316:PHE:HB3  | 1:F:318:ASN:OD1  | 2.19                     | 0.42              |
| 1:I:41:ASP:OD2   | 1:I:41:ASP:C     | 2.62                     | 0.42              |
| 1:I:52:VAL:O     | 1:I:55:VAL:HG12  | 2.19                     | 0.42              |
| 1:I:195:GLU:HG3  | 1:I:197:ASN:HD22 | 1.85                     | 0.42              |
| 1:K:69:MET:HB3   | 1:K:73:GLU:HB2   | 2.01                     | 0.42              |
| 1:L:166:HIS:HD2  | 7:L:1341:HOH:O   | 2.01                     | 0.42              |
| 1:A:40:TRP:O     | 1:A:41:ASP:CB    | 2.68                     | 0.42              |
| 1:B:70:SER:OG    | 1:B:73:GLU:HG3   | 2.20                     | 0.42              |
| 1:D:41:ASP:OD1   | 1:D:41:ASP:C     | 2.62                     | 0.42              |
| 1:E:48:TYR:CD2   | 1:E:50:TYR:HB2   | 2.54                     | 0.42              |
| 1:G:191:LYS:C    | 1:G:203:GLU:HG3  | 2.44                     | 0.42              |
| 1:G:197:ASN:ND2  | 1:G:197:ASN:H    | 2.16                     | 0.42              |
| 1:I:142:MET:O    | 1:I:168:ALA:HB3  | 2.19                     | 0.42              |
| 1:J:25:MET:HG3   | 7:J:450:HOH:O    | 2.19                     | 0.42              |
| 1:A:179:GLU:HB2  | 1:A:180:GLN:OE1  | 2.20                     | 0.42              |
| 1:E:127:GLN:HA   | 1:E:127:GLN:OE1  | 2.20                     | 0.42              |
| 1:G:25:MET:HA    | 1:G:141:VAL:CG2  | 2.50                     | 0.42              |
| 1:H:244:LEU:HD13 | 1:H:244:LEU:C    | 2.44                     | 0.42              |
| 1:K:196:TRP:CD1  | 1:K:238:ARG:HD2  | 2.54                     | 0.42              |
| 1:L:52:VAL:O     | 1:L:55:VAL:HG12  | 2.19                     | 0.42              |
| 1:B:111:ASP:CG   | 1:B:114:VAL:HG23 | 2.45                     | 0.42              |
| 1:D:40:TRP:O     | 1:D:41:ASP:CB    | 2.67                     | 0.42              |
| 1:G:275:PHE:CG   | 1:G:276:VAL:N    | 2.87                     | 0.42              |
| 1:H:49:HIS:HB2   | 1:H:272:ALA:HB2  | 2.01                     | 0.42              |
| 1:K:70:SER:O     | 1:K:74:GLN:HG3   | 2.19                     | 0.42              |
| 1:L:326:TRP:HB3  | 1:L:327:PHE:H    | 1.67                     | 0.42              |
| 1:D:59:THR:OG1   | 1:D:61:VAL:HG13  | 2.19                     | 0.42              |
| 1:F:216:ASP:N    | 1:F:217:PRO:CD   | 2.83                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:216:ASP:N    | 1:I:217:PRO:CD   | 2.83                     | 0.42              |
| 1:J:97:LEU:HD13  | 1:K:389:TRP:HB2  | 2.01                     | 0.42              |
| 1:A:123:THR:OG1  | 1:A:126:GLU:HG3  | 2.19                     | 0.42              |
| 1:A:216:ASP:N    | 1:A:217:PRO:CD   | 2.83                     | 0.42              |
| 1:B:162:ASP:HB3  | 1:B:165:PHE:CD2  | 2.48                     | 0.42              |
| 1:B:382:ASP:O    | 1:B:386:GLN:HG2  | 2.19                     | 0.42              |
| 1:H:198:GLU:OE2  | 1:H:202:GLN:HG2  | 2.19                     | 0.42              |
| 1:J:41:ASP:OD1   | 1:J:41:ASP:C     | 2.63                     | 0.42              |
| 1:K:149:ASP:O    | 1:K:153:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:40:TRP:O     | 1:A:41:ASP:OD2   | 2.38                     | 0.41              |
| 1:F:65:ALA:O     | 1:F:69:MET:HG3   | 2.20                     | 0.41              |
| 1:F:146:PRO:O    | 1:F:152:ARG:HB2  | 2.19                     | 0.41              |
| 1:G:212:ILE:HD13 | 1:G:253:ILE:HD11 | 2.02                     | 0.41              |
| 1:I:40:TRP:CE3   | 1:I:127:GLN:HG2  | 2.55                     | 0.41              |
| 1:I:256:ALA:HA   | 1:I:297:LEU:O    | 2.20                     | 0.41              |
| 1:J:172:ASP:OD1  | 1:J:222:VAL:HA   | 2.20                     | 0.41              |
| 1:L:25:MET:HG3   | 7:L:438:HOH:O    | 2.20                     | 0.41              |
| 1:L:41:ASP:OD1   | 1:L:41:ASP:C     | 2.64                     | 0.41              |
| 1:D:238:ARG:HG2  | 1:D:241:ARG:NH2  | 2.35                     | 0.41              |
| 1:E:286:HIS:CE1  | 1:E:290:GLU:HG3  | 2.55                     | 0.41              |
| 1:G:111:ASP:CG   | 1:G:114:VAL:HG23 | 2.46                     | 0.41              |
| 1:J:285:GLU:OE1  | 1:L:262:LYS:HE2  | 2.20                     | 0.41              |
| 1:B:142:MET:O    | 1:B:168:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:238:ARG:HG2  | 1:B:241:ARG:NH2  | 2.35                     | 0.41              |
| 1:B:358:VAL:HB   | 1:B:361:GLN:HG3  | 2.01                     | 0.41              |
| 1:C:72:ARG:NH2   | 1:C:116:ARG:HD3  | 2.35                     | 0.41              |
| 1:D:106:ASP:HA   | 1:D:107:PRO:HD3  | 1.83                     | 0.41              |
| 1:D:306:GLN:OE1  | 1:D:337:MET:HE3  | 2.20                     | 0.41              |
| 1:E:42:ILE:HD13  | 1:E:100:LEU:HD21 | 2.02                     | 0.41              |
| 1:G:264:ARG:HG3  | 1:G:264:ARG:HH11 | 1.84                     | 0.41              |
| 1:H:167:ALA:O    | 1:H:217:PRO:HA   | 2.20                     | 0.41              |
| 1:K:301:LEU:HD11 | 1:K:326:TRP:HB3  | 2.02                     | 0.41              |
| 1:A:30:PHE:CE2   | 1:A:37:ILE:HG12  | 2.55                     | 0.41              |
| 1:D:139:ASP:OD1  | 1:D:166:HIS:CE1  | 2.74                     | 0.41              |
| 1:E:178:TYR:CD1  | 1:E:239:ILE:HD11 | 2.55                     | 0.41              |
| 1:G:70:SER:OG    | 1:G:73:GLU:HG3   | 2.20                     | 0.41              |
| 1:G:79:TRP:O     | 1:G:83:PHE:HB2   | 2.20                     | 0.41              |
| 1:J:393:GLU:CG   | 1:J:397:LYS:HE3  | 2.51                     | 0.41              |
| 1:A:42:ILE:HD13  | 1:A:100:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:151:GLU:O    | 1:B:154:SER:HB3  | 2.20                     | 0.41              |
| 1:B:298:VAL:HG12 | 1:B:299:THR:N    | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:40:TRP:O     | 1:C:41:ASP:CB    | 2.69                     | 0.41              |
| 1:C:123:THR:OG1  | 1:C:126:GLU:HG3  | 2.20                     | 0.41              |
| 1:L:219:TYR:HA   | 1:L:253:ILE:CG2  | 2.50                     | 0.41              |
| 1:B:127:GLN:HA   | 1:B:127:GLN:OE1  | 2.20                     | 0.41              |
| 1:C:78:ILE:HG23  | 1:C:82:LEU:HD12  | 2.03                     | 0.41              |
| 1:C:113:GLN:O    | 1:C:117:GLU:HG3  | 2.21                     | 0.41              |
| 1:E:3:ILE:CG2    | 1:E:8:VAL:HG13   | 2.45                     | 0.41              |
| 1:E:66:PHE:CZ    | 1:E:74:GLN:HB3   | 2.55                     | 0.41              |
| 1:E:301:LEU:CD1  | 1:E:326:TRP:HB3  | 2.50                     | 0.41              |
| 1:I:145:ASP:HA   | 1:I:146:PRO:HD2  | 1.99                     | 0.41              |
| 1:I:322:PHE:HA   | 1:I:350:ILE:O    | 2.19                     | 0.41              |
| 1:J:52:VAL:O     | 1:J:55:VAL:HG12  | 2.21                     | 0.41              |
| 1:F:203:GLU:CD   | 1:F:206:ARG:NH1  | 2.78                     | 0.41              |
| 1:G:301:LEU:CD1  | 1:G:326:TRP:HB3  | 2.50                     | 0.41              |
| 1:G:364:TYR:CD1  | 1:G:364:TYR:C    | 2.99                     | 0.41              |
| 1:J:218:VAL:HG23 | 1:J:219:TYR:CD2  | 2.56                     | 0.41              |
| 1:B:224:LEU:HD13 | 1:B:228:PHE:CD1  | 2.55                     | 0.41              |
| 1:E:324:CYS:HB3  | 1:E:337:MET:HE1  | 2.01                     | 0.41              |
| 1:F:385:LEU:HD12 | 1:F:389:TRP:O    | 2.20                     | 0.41              |
| 1:G:315:LYS:HD2  | 1:I:274:ASP:O    | 2.20                     | 0.41              |
| 1:J:72:ARG:NH2   | 1:J:116:ARG:HD3  | 2.36                     | 0.41              |
| 1:J:364:TYR:CD1  | 1:J:364:TYR:C    | 2.98                     | 0.41              |
| 1:L:111:ASP:CG   | 1:L:114:VAL:HG23 | 2.46                     | 0.41              |
| 1:A:40:TRP:CE3   | 1:A:127:GLN:HG2  | 2.56                     | 0.41              |
| 1:A:41:ASP:OD1   | 1:A:41:ASP:C     | 2.63                     | 0.41              |
| 1:B:128:VAL:HA   | 1:B:359:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:170:ARG:HH21 | 1:B:223:SER:HB3  | 1.86                     | 0.41              |
| 1:B:288:LEU:HD23 | 1:B:296:PHE:CD2  | 2.56                     | 0.41              |
| 1:D:313:ALA:HA   | 1:D:319:LEU:HD23 | 2.03                     | 0.41              |
| 1:D:409:TRP:HE3  | 1:D:414:ARG:HB2  | 1.86                     | 0.41              |
| 7:D:1369:HOH:O   | 1:E:321:ILE:HG12 | 2.19                     | 0.41              |
| 1:E:118:TYR:HA   | 1:E:121:LYS:NZ   | 2.36                     | 0.41              |
| 1:F:301:LEU:CD1  | 1:F:326:TRP:HB3  | 2.51                     | 0.41              |
| 1:F:364:TYR:CD1  | 1:F:364:TYR:C    | 2.99                     | 0.41              |
| 1:G:41:ASP:HA    | 1:G:119:PHE:CD1  | 2.56                     | 0.41              |
| 1:G:61:VAL:HG12  | 1:G:62:SER:O     | 2.20                     | 0.41              |
| 1:H:146:PRO:O    | 1:H:152:ARG:HD3  | 2.21                     | 0.41              |
| 1:J:43:ASP:OD2   | 1:J:72:ARG:NH1   | 2.54                     | 0.41              |
| 1:K:275:PHE:CG   | 1:K:276:VAL:N    | 2.89                     | 0.41              |
| 1:K:326:TRP:HB3  | 1:K:327:PHE:H    | 1.66                     | 0.41              |
| 1:L:216:ASP:N    | 1:L:217:PRO:CD   | 2.83                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:307:HIS:CD2 | 1:L:344:MET:HE1  | 2.55                     | 0.41              |
| 1:A:145:ASP:HA  | 1:A:146:PRO:HD2  | 1.94                     | 0.41              |
| 1:D:147:PHE:O   | 1:D:184:ARG:NH2  | 2.42                     | 0.41              |
| 1:G:52:VAL:O    | 1:G:55:VAL:HG12  | 2.21                     | 0.41              |
| 1:J:145:ASP:HA  | 1:J:146:PRO:HD2  | 1.96                     | 0.41              |
| 1:K:69:MET:HE2  | 1:K:73:GLU:HB3   | 2.02                     | 0.41              |
| 1:K:276:VAL:CG2 | 1:K:277:GLY:N    | 2.84                     | 0.41              |
| 1:A:275:PHE:CG  | 1:A:276:VAL:N    | 2.89                     | 0.40              |
| 1:A:316:PHE:HB3 | 1:A:318:ASN:OD1  | 2.22                     | 0.40              |
| 1:C:244:LEU:C   | 1:C:244:LEU:CD1  | 2.94                     | 0.40              |
| 1:C:275:PHE:CG  | 1:C:276:VAL:N    | 2.90                     | 0.40              |
| 1:D:265:VAL:O   | 1:E:289:ARG:HD3  | 2.20                     | 0.40              |
| 1:E:25:MET:HG3  | 7:E:452:HOH:O    | 2.21                     | 0.40              |
| 1:G:196:TRP:CZ2 | 1:G:201:ILE:HG12 | 2.56                     | 0.40              |
| 1:B:204:VAL:HB  | 1:B:243:CYS:SG   | 2.62                     | 0.40              |
| 1:H:276:VAL:CG2 | 1:H:277:GLY:N    | 2.84                     | 0.40              |
| 1:I:24:ASP:OD2  | 1:I:354:SER:OG   | 2.36                     | 0.40              |
| 1:I:306:GLN:HB2 | 7:I:471:HOH:O    | 2.22                     | 0.40              |
| 1:K:301:LEU:CD1 | 1:K:326:TRP:HB3  | 2.52                     | 0.40              |
| 1:K:307:HIS:CD2 | 1:K:344:MET:HE1  | 2.57                     | 0.40              |
| 1:A:125:GLU:O   | 1:A:128:VAL:HG22 | 2.21                     | 0.40              |
| 1:A:364:TYR:CD1 | 1:A:364:TYR:C    | 2.99                     | 0.40              |
| 1:B:72:ARG:NH2  | 1:B:116:ARG:HD3  | 2.35                     | 0.40              |
| 1:D:216:ASP:N   | 1:D:217:PRO:CD   | 2.84                     | 0.40              |
| 1:E:152:ARG:O   | 1:E:156:LEU:HG   | 2.21                     | 0.40              |
| 1:I:79:TRP:O    | 1:I:83:PHE:HB2   | 2.21                     | 0.40              |
| 1:L:40:TRP:CE3  | 1:L:127:GLN:HG2  | 2.56                     | 0.40              |
| 1:B:393:GLU:HG2 | 1:B:397:LYS:NZ   | 2.35                     | 0.40              |
| 1:F:275:PHE:CG  | 1:F:276:VAL:N    | 2.90                     | 0.40              |
| 1:G:40:TRP:O    | 1:G:41:ASP:CB    | 2.70                     | 0.40              |
| 1:I:49:HIS:HB2  | 1:I:272:ALA:HB2  | 2.02                     | 0.40              |
| 1:K:52:VAL:O    | 1:K:55:VAL:HG12  | 2.22                     | 0.40              |
| 1:L:275:PHE:CG  | 1:L:276:VAL:N    | 2.89                     | 0.40              |
| 1:A:155:TRP:CZ3 | 1:A:215:MET:HA   | 2.56                     | 0.40              |
| 1:B:178:TYR:CD1 | 1:B:239:ILE:HD11 | 2.56                     | 0.40              |
| 1:C:276:VAL:CG2 | 1:C:277:GLY:N    | 2.84                     | 0.40              |
| 1:C:364:TYR:CD1 | 1:C:364:TYR:C    | 2.99                     | 0.40              |
| 1:D:167:ALA:HB1 | 1:D:215:MET:HE3  | 2.03                     | 0.40              |
| 1:F:145:ASP:HA  | 1:F:146:PRO:HD2  | 1.93                     | 0.40              |
| 1:H:72:ARG:HG3  | 1:H:72:ARG:HH11  | 1.87                     | 0.40              |
| 1:J:61:VAL:HG12 | 1:J:62:SER:O     | 2.22                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:K:256:ALA:HA  | 1:K:297:LEU:O   | 2.21                     | 0.40              |
| 1:L:22:VAL:HG11 | 1:L:366:TRP:CE2 | 2.56                     | 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%)   | 396 (96%)  | 13 (3%)  | 2 (0%)   | 24          | 27 |
| 1   | B     | 411/427 (96%)   | 391 (95%)  | 15 (4%)  | 5 (1%)   | 10          | 8  |
| 1   | C     | 411/427 (96%)   | 397 (97%)  | 12 (3%)  | 2 (0%)   | 24          | 27 |
| 1   | D     | 411/427 (96%)   | 403 (98%)  | 7 (2%)   | 1 (0%)   | 43          | 51 |
| 1   | E     | 411/427 (96%)   | 395 (96%)  | 14 (3%)  | 2 (0%)   | 24          | 27 |
| 1   | F     | 411/427 (96%)   | 397 (97%)  | 11 (3%)  | 3 (1%)   | 18          | 19 |
| 1   | G     | 411/427 (96%)   | 397 (97%)  | 11 (3%)  | 3 (1%)   | 18          | 19 |
| 1   | H     | 411/427 (96%)   | 399 (97%)  | 10 (2%)  | 2 (0%)   | 24          | 27 |
| 1   | I     | 411/427 (96%)   | 396 (96%)  | 13 (3%)  | 2 (0%)   | 24          | 27 |
| 1   | J     | 411/427 (96%)   | 399 (97%)  | 10 (2%)  | 2 (0%)   | 24          | 27 |
| 1   | K     | 411/427 (96%)   | 403 (98%)  | 6 (2%)   | 2 (0%)   | 24          | 27 |
| 1   | L     | 411/427 (96%)   | 397 (97%)  | 12 (3%)  | 2 (0%)   | 24          | 27 |
| All | All   | 4932/5124 (96%) | 4770 (97%) | 134 (3%) | 28 (1%)  | 21          | 23 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 41  | ASP  |
| 1   | C     | 41  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 41  | ASP  |
| 1   | E     | 41  | ASP  |
| 1   | F     | 159 | LYS  |
| 1   | G     | 41  | ASP  |
| 1   | H     | 41  | ASP  |
| 1   | I     | 41  | ASP  |
| 1   | J     | 41  | ASP  |
| 1   | A     | 41  | ASP  |
| 1   | F     | 41  | ASP  |
| 1   | I     | 323 | GLY  |
| 1   | K     | 41  | ASP  |
| 1   | L     | 41  | ASP  |
| 1   | G     | 323 | GLY  |
| 1   | A     | 36  | GLU  |
| 1   | B     | 405 | SER  |
| 1   | G     | 405 | SER  |
| 1   | J     | 323 | GLY  |
| 1   | B     | 26  | HIS  |
| 1   | H     | 323 | GLY  |
| 1   | B     | 25  | MET  |
| 1   | L     | 323 | GLY  |
| 1   | E     | 323 | GLY  |
| 1   | B     | 323 | GLY  |
| 1   | C     | 323 | GLY  |
| 1   | F     | 323 | GLY  |
| 1   | K     | 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%) | 370 (99%) | 3 (1%)   | 73          | 85 |
| 1   | B     | 373/387 (96%) | 367 (98%) | 6 (2%)   | 55          | 71 |
| 1   | C     | 373/387 (96%) | 367 (98%) | 6 (2%)   | 55          | 71 |
| 1   | D     | 373/387 (96%) | 369 (99%) | 4 (1%)   | 65          | 79 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | E     | 373/387 (96%)   | 369 (99%)  | 4 (1%)   | 65          | 79 |
| 1   | F     | 373/387 (96%)   | 366 (98%)  | 7 (2%)   | 50          | 66 |
| 1   | G     | 373/387 (96%)   | 364 (98%)  | 9 (2%)   | 43          | 58 |
| 1   | H     | 373/387 (96%)   | 369 (99%)  | 4 (1%)   | 65          | 79 |
| 1   | I     | 373/387 (96%)   | 365 (98%)  | 8 (2%)   | 47          | 63 |
| 1   | J     | 373/387 (96%)   | 365 (98%)  | 8 (2%)   | 47          | 63 |
| 1   | K     | 373/387 (96%)   | 369 (99%)  | 4 (1%)   | 65          | 79 |
| 1   | L     | 373/387 (96%)   | 370 (99%)  | 3 (1%)   | 73          | 85 |
| All | All   | 4476/4644 (96%) | 4410 (98%) | 66 (2%)  | 57          | 73 |

All (66) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 72  | ARG  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 364 | TYR  |
| 1   | B     | 4   | ASN  |
| 1   | B     | 7   | GLU  |
| 1   | B     | 15  | ASN  |
| 1   | B     | 41  | ASP  |
| 1   | B     | 305 | ASN  |
| 1   | B     | 364 | TYR  |
| 1   | C     | 127 | GLN  |
| 1   | C     | 244 | LEU  |
| 1   | C     | 355 | ASP  |
| 1   | C     | 364 | TYR  |
| 1   | C     | 385 | LEU  |
| 1   | C     | 391 | VAL  |
| 1   | D     | 61  | VAL  |
| 1   | D     | 244 | LEU  |
| 1   | D     | 355 | ASP  |
| 1   | D     | 364 | TYR  |
| 1   | E     | 15  | ASN  |
| 1   | E     | 244 | LEU  |
| 1   | E     | 364 | TYR  |
| 1   | E     | 386 | GLN  |
| 1   | F     | 72  | ARG  |
| 1   | F     | 127 | GLN  |
| 1   | F     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 244 | LEU  |
| 1   | F     | 355 | ASP  |
| 1   | F     | 364 | TYR  |
| 1   | F     | 385 | LEU  |
| 1   | G     | 15  | ASN  |
| 1   | G     | 23  | THR  |
| 1   | G     | 71  | LYS  |
| 1   | G     | 113 | GLN  |
| 1   | G     | 133 | GLN  |
| 1   | G     | 187 | ASP  |
| 1   | G     | 197 | ASN  |
| 1   | G     | 213 | GLU  |
| 1   | G     | 364 | TYR  |
| 1   | H     | 72  | ARG  |
| 1   | H     | 244 | LEU  |
| 1   | H     | 364 | TYR  |
| 1   | H     | 385 | LEU  |
| 1   | I     | 46  | LEU  |
| 1   | I     | 180 | GLN  |
| 1   | I     | 185 | LEU  |
| 1   | I     | 191 | LYS  |
| 1   | I     | 244 | LEU  |
| 1   | I     | 355 | ASP  |
| 1   | I     | 364 | TYR  |
| 1   | I     | 391 | VAL  |
| 1   | J     | 7   | GLU  |
| 1   | J     | 15  | ASN  |
| 1   | J     | 71  | LYS  |
| 1   | J     | 72  | ARG  |
| 1   | J     | 113 | GLN  |
| 1   | J     | 206 | ARG  |
| 1   | J     | 355 | ASP  |
| 1   | J     | 364 | TYR  |
| 1   | K     | 244 | LEU  |
| 1   | K     | 305 | ASN  |
| 1   | K     | 355 | ASP  |
| 1   | K     | 364 | TYR  |
| 1   | L     | 72  | ARG  |
| 1   | L     | 160 | GLN  |
| 1   | L     | 180 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ASN  |
| 1   | A     | 20  | GLN  |
| 1   | A     | 113 | GLN  |
| 1   | A     | 127 | GLN  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 166 | HIS  |
| 1   | A     | 202 | GLN  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 293 | ASN  |
| 1   | B     | 4   | ASN  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 113 | GLN  |
| 1   | B     | 166 | HIS  |
| 1   | B     | 202 | GLN  |
| 1   | B     | 251 | HIS  |
| 1   | B     | 252 | ASN  |
| 1   | C     | 4   | ASN  |
| 1   | C     | 18  | ASN  |
| 1   | C     | 20  | GLN  |
| 1   | C     | 101 | GLN  |
| 1   | C     | 127 | GLN  |
| 1   | C     | 150 | ASN  |
| 1   | C     | 160 | GLN  |
| 1   | C     | 166 | HIS  |
| 1   | C     | 180 | GLN  |
| 1   | C     | 193 | ASN  |
| 1   | C     | 202 | GLN  |
| 1   | C     | 252 | ASN  |
| 1   | D     | 18  | ASN  |
| 1   | D     | 150 | ASN  |
| 1   | D     | 166 | HIS  |
| 1   | D     | 180 | GLN  |
| 1   | D     | 183 | HIS  |
| 1   | D     | 193 | ASN  |
| 1   | D     | 252 | ASN  |
| 1   | D     | 293 | ASN  |
| 1   | D     | 367 | HIS  |
| 1   | E     | 18  | ASN  |
| 1   | E     | 20  | GLN  |
| 1   | E     | 113 | GLN  |
| 1   | E     | 166 | HIS  |
| 1   | E     | 252 | ASN  |
| 1   | E     | 293 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 4   | ASN  |
| 1   | F     | 18  | ASN  |
| 1   | F     | 101 | GLN  |
| 1   | F     | 127 | GLN  |
| 1   | F     | 166 | HIS  |
| 1   | F     | 180 | GLN  |
| 1   | F     | 252 | ASN  |
| 1   | F     | 293 | ASN  |
| 1   | F     | 386 | GLN  |
| 1   | G     | 133 | GLN  |
| 1   | G     | 166 | HIS  |
| 1   | G     | 193 | ASN  |
| 1   | G     | 197 | ASN  |
| 1   | G     | 252 | ASN  |
| 1   | H     | 18  | ASN  |
| 1   | H     | 20  | GLN  |
| 1   | H     | 101 | GLN  |
| 1   | H     | 133 | GLN  |
| 1   | H     | 150 | ASN  |
| 1   | H     | 166 | HIS  |
| 1   | H     | 193 | ASN  |
| 1   | H     | 235 | ASN  |
| 1   | H     | 367 | HIS  |
| 1   | H     | 386 | GLN  |
| 1   | I     | 18  | ASN  |
| 1   | I     | 166 | HIS  |
| 1   | I     | 180 | GLN  |
| 1   | I     | 183 | HIS  |
| 1   | I     | 202 | GLN  |
| 1   | I     | 252 | ASN  |
| 1   | I     | 293 | ASN  |
| 1   | I     | 367 | HIS  |
| 1   | J     | 4   | ASN  |
| 1   | J     | 18  | ASN  |
| 1   | J     | 20  | GLN  |
| 1   | J     | 150 | ASN  |
| 1   | J     | 166 | HIS  |
| 1   | J     | 252 | ASN  |
| 1   | K     | 4   | ASN  |
| 1   | K     | 18  | ASN  |
| 1   | K     | 101 | GLN  |
| 1   | K     | 113 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 150 | ASN  |
| 1   | K     | 160 | GLN  |
| 1   | K     | 166 | HIS  |
| 1   | K     | 202 | GLN  |
| 1   | K     | 252 | ASN  |
| 1   | K     | 330 | ASN  |
| 1   | K     | 367 | HIS  |
| 1   | K     | 386 | GLN  |
| 1   | L     | 20  | GLN  |
| 1   | L     | 101 | GLN  |
| 1   | L     | 113 | GLN  |
| 1   | L     | 127 | GLN  |
| 1   | L     | 160 | GLN  |
| 1   | L     | 166 | HIS  |
| 1   | L     | 180 | GLN  |
| 1   | L     | 193 | ASN  |
| 1   | L     | 252 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 20 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   | RAT  | G     | 428 | 4    | 11,11,11     | 1.20 | 0        | 13,15,15    | 0.97 | 0        |
| 3   | CO3  | E     | 429 | -    | 3,3,3        | 0.89 | 0        | 2,3,3       | 0.06 | 0        |
| 2   | RAT  | B     | 428 | 4    | 11,11,11     | 1.22 | 1 (9%)   | 13,15,15    | 0.95 | 0        |
| 3   | CO3  | K     | 430 | -    | 3,3,3        | 0.70 | 0        | 2,3,3       | 0.04 | 0        |
| 2   | RAT  | A     | 428 | 4    | 11,11,11     | 1.23 | 0        | 13,15,15    | 1.01 | 0        |
| 3   | CO3  | K     | 429 | -    | 3,3,3        | 0.83 | 0        | 2,3,3       | 0.06 | 0        |
| 2   | RAT  | I     | 428 | 4    | 11,11,11     | 1.23 | 0        | 13,15,15    | 1.08 | 0        |
| 3   | CO3  | J     | 429 | -    | 3,3,3        | 0.85 | 0        | 2,3,3       | 0.05 | 0        |
| 2   | RAT  | K     | 428 | 4    | 11,11,11     | 1.12 | 0        | 13,15,15    | 0.91 | 0        |
| 2   | RAT  | F     | 428 | 4    | 11,11,11     | 1.26 | 1 (9%)   | 13,15,15    | 0.99 | 0        |
| 2   | RAT  | D     | 428 | 4    | 11,11,11     | 1.15 | 0        | 13,15,15    | 0.95 | 0        |
| 3   | CO3  | A     | 429 | -    | 3,3,3        | 0.99 | 0        | 2,3,3       | 0.18 | 0        |
| 3   | CO3  | C     | 429 | -    | 3,3,3        | 0.85 | 0        | 2,3,3       | 0.14 | 0        |
| 2   | RAT  | H     | 428 | 4    | 11,11,11     | 1.09 | 0        | 13,15,15    | 0.96 | 0        |
| 2   | RAT  | E     | 428 | 4    | 11,11,11     | 1.22 | 1 (9%)   | 13,15,15    | 0.90 | 0        |
| 3   | CO3  | I     | 429 | -    | 3,3,3        | 0.69 | 0        | 2,3,3       | 0.26 | 0        |
| 3   | CO3  | E     | 430 | -    | 3,3,3        | 0.81 | 0        | 2,3,3       | 0.13 | 0        |
| 3   | CO3  | G     | 429 | -    | 3,3,3        | 0.87 | 0        | 2,3,3       | 0.09 | 0        |
| 2   | RAT  | J     | 428 | 4    | 11,11,11     | 1.19 | 0        | 13,15,15    | 0.92 | 0        |
| 3   | CO3  | H     | 429 | -    | 3,3,3        | 0.72 | 0        | 2,3,3       | 0.08 | 0        |
| 3   | CO3  | A     | 430 | -    | 3,3,3        | 0.84 | 0        | 2,3,3       | 0.06 | 0        |
| 2   | RAT  | C     | 428 | 4    | 11,11,11     | 1.16 | 1 (9%)   | 13,15,15    | 0.96 | 0        |
| 3   | CO3  | D     | 429 | -    | 3,3,3        | 0.80 | 0        | 2,3,3       | 0.13 | 0        |
| 2   | RAT  | L     | 428 | 4    | 11,11,11     | 1.17 | 0        | 13,15,15    | 1.08 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | RAT  | K     | 428 | 4    | -       | 1/16/16/16 | -     |
| 2   | RAT  | F     | 428 | 4    | -       | 1/16/16/16 | -     |
| 2   | RAT  | G     | 428 | 4    | -       | 5/16/16/16 | -     |
| 2   | RAT  | D     | 428 | 4    | -       | 0/16/16/16 | -     |
| 2   | RAT  | A     | 428 | 4    | -       | 0/16/16/16 | -     |
| 2   | RAT  | J     | 428 | 4    | -       | 7/16/16/16 | -     |
| 2   | RAT  | I     | 428 | 4    | -       | 0/16/16/16 | -     |
| 2   | RAT  | C     | 428 | 4    | -       | 0/16/16/16 | -     |
| 2   | RAT  | E     | 428 | 4    | -       | 5/16/16/16 | -     |
| 2   | RAT  | H     | 428 | 4    | -       | 0/16/16/16 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | RAT  | L     | 428 | 4    | -       | 2/16/16/16 | -     |
| 2   | RAT  | B     | 428 | 4    | -       | 5/16/16/16 | -     |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | E     | 428 | RAT  | C4-C5 | 2.46 | 1.56        | 1.52     |
| 2   | B     | 428 | RAT  | C4-C5 | 2.45 | 1.56        | 1.52     |
| 2   | F     | 428 | RAT  | C4-C5 | 2.44 | 1.56        | 1.52     |
| 2   | C     | 428 | RAT  | C4-C5 | 2.25 | 1.55        | 1.52     |

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | G     | 428 | RAT  | O1A-C1-C2-O2 |
| 2   | G     | 428 | RAT  | O1B-C1-C2-O2 |
| 2   | G     | 428 | RAT  | O1B-C1-C2-C3 |
| 2   | B     | 428 | RAT  | O1A-C1-C2-O2 |
| 2   | B     | 428 | RAT  | O1A-C1-C2-C3 |
| 2   | B     | 428 | RAT  | O1B-C1-C2-C3 |
| 2   | J     | 428 | RAT  | O1B-C1-C2-C3 |
| 2   | B     | 428 | RAT  | O1B-C1-C2-O2 |
| 2   | J     | 428 | RAT  | O1A-C1-C2-C3 |
| 2   | J     | 428 | RAT  | O1A-C1-C2-O2 |
| 2   | E     | 428 | RAT  | O1A-C1-C2-C3 |
| 2   | B     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | E     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | F     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | G     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | J     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | K     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | E     | 428 | RAT  | O1B-C1-C2-C3 |
| 2   | E     | 428 | RAT  | O1A-C1-C2-O2 |
| 2   | J     | 428 | RAT  | O1B-C1-C2-O2 |
| 2   | J     | 428 | RAT  | C3-C4-C5-O5B |
| 2   | J     | 428 | RAT  | O4-C4-C5-O5B |
| 2   | G     | 428 | RAT  | O1A-C1-C2-C3 |
| 2   | L     | 428 | RAT  | C2-C3-C4-O4  |
| 2   | E     | 428 | RAT  | O1B-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | L     | 428 | RAT  | O1A-C1-C2-C3 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 413/427 (96%)   | 0.24   | 14 (3%) 48 45  | 17, 33, 53, 67        | 0     |
| 1   | B     | 413/427 (96%)   | 0.55   | 35 (8%) 16 14  | 19, 37, 61, 83        | 0     |
| 1   | C     | 413/427 (96%)   | -0.23  | 3 (0%) 84 82   | 16, 25, 41, 61        | 0     |
| 1   | D     | 413/427 (96%)   | -0.27  | 4 (0%) 79 77   | 14, 24, 39, 63        | 0     |
| 1   | E     | 413/427 (96%)   | -0.04  | 12 (2%) 53 50  | 15, 27, 44, 72        | 0     |
| 1   | F     | 413/427 (96%)   | -0.07  | 7 (1%) 69 66   | 15, 27, 49, 67        | 0     |
| 1   | G     | 413/427 (96%)   | 0.14   | 9 (2%) 62 59   | 18, 31, 51, 71        | 0     |
| 1   | H     | 413/427 (96%)   | -0.29  | 4 (0%) 79 77   | 15, 25, 42, 61        | 0     |
| 1   | I     | 413/427 (96%)   | 0.11   | 16 (3%) 43 40  | 16, 30, 51, 67        | 0     |
| 1   | J     | 413/427 (96%)   | -0.29  | 5 (1%) 76 74   | 15, 25, 41, 73        | 0     |
| 1   | K     | 413/427 (96%)   | -0.28  | 6 (1%) 72 69   | 14, 24, 43, 63        | 0     |
| 1   | L     | 413/427 (96%)   | -0.33  | 1 (0%) 91 90   | 15, 23, 39, 62        | 0     |
| All | All   | 4956/5124 (96%) | -0.06  | 116 (2%) 61 58 | 14, 27, 49, 83        | 0     |

All (116) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 3   | ILE  | 5.8  |
| 1   | F     | 158 | GLY  | 4.7  |
| 1   | H     | 414 | ARG  | 4.6  |
| 1   | F     | 93  | CYS  | 4.5  |
| 1   | F     | 413 | GLY  | 4.4  |
| 1   | B     | 2   | SER  | 4.4  |
| 1   | K     | 414 | ARG  | 4.2  |
| 1   | J     | 2   | SER  | 4.1  |
| 1   | L     | 414 | ARG  | 4.0  |
| 1   | I     | 414 | ARG  | 4.0  |
| 1   | E     | 3   | ILE  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 162 | ASP  | 3.7  |
| 1   | E     | 414 | ARG  | 3.7  |
| 1   | F     | 153 | ILE  | 3.7  |
| 1   | B     | 37  | ILE  | 3.6  |
| 1   | D     | 414 | ARG  | 3.6  |
| 1   | E     | 2   | SER  | 3.6  |
| 1   | B     | 414 | ARG  | 3.6  |
| 1   | F     | 414 | ARG  | 3.6  |
| 1   | A     | 414 | ARG  | 3.5  |
| 1   | J     | 414 | ARG  | 3.4  |
| 1   | I     | 191 | LYS  | 3.4  |
| 1   | B     | 154 | SER  | 3.4  |
| 1   | E     | 150 | ASN  | 3.2  |
| 1   | B     | 153 | ILE  | 3.1  |
| 1   | B     | 253 | ILE  | 3.0  |
| 1   | B     | 191 | LYS  | 3.0  |
| 1   | B     | 180 | GLN  | 3.0  |
| 1   | G     | 2   | SER  | 2.9  |
| 1   | B     | 152 | ARG  | 2.9  |
| 1   | E     | 180 | GLN  | 2.9  |
| 1   | A     | 120 | ALA  | 2.8  |
| 1   | B     | 193 | ASN  | 2.7  |
| 1   | D     | 153 | ILE  | 2.7  |
| 1   | I     | 153 | ILE  | 2.7  |
| 1   | B     | 155 | TRP  | 2.7  |
| 1   | H     | 180 | GLN  | 2.7  |
| 1   | I     | 185 | LEU  | 2.7  |
| 1   | G     | 414 | ARG  | 2.6  |
| 1   | J     | 3   | ILE  | 2.6  |
| 1   | B     | 4   | ASN  | 2.6  |
| 1   | E     | 413 | GLY  | 2.6  |
| 1   | I     | 72  | ARG  | 2.5  |
| 1   | I     | 186 | ARG  | 2.5  |
| 1   | J     | 413 | GLY  | 2.5  |
| 1   | B     | 161 | PRO  | 2.5  |
| 1   | B     | 123 | THR  | 2.5  |
| 1   | A     | 128 | VAL  | 2.5  |
| 1   | G     | 153 | ILE  | 2.5  |
| 1   | B     | 158 | GLY  | 2.5  |
| 1   | K     | 180 | GLN  | 2.5  |
| 1   | B     | 410 | ARG  | 2.5  |
| 1   | C     | 414 | ARG  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 3   | ILE  | 2.5  |
| 1   | G     | 253 | ILE  | 2.5  |
| 1   | I     | 65  | ALA  | 2.5  |
| 1   | B     | 72  | ARG  | 2.4  |
| 1   | H     | 153 | ILE  | 2.4  |
| 1   | I     | 159 | LYS  | 2.4  |
| 1   | B     | 186 | ARG  | 2.4  |
| 1   | B     | 164 | ARG  | 2.4  |
| 1   | I     | 113 | GLN  | 2.4  |
| 1   | B     | 192 | VAL  | 2.4  |
| 1   | K     | 183 | HIS  | 2.4  |
| 1   | D     | 113 | GLN  | 2.4  |
| 1   | E     | 4   | ASN  | 2.4  |
| 1   | A     | 113 | GLN  | 2.4  |
| 1   | D     | 413 | GLY  | 2.3  |
| 1   | A     | 213 | GLU  | 2.3  |
| 1   | B     | 196 | TRP  | 2.3  |
| 1   | B     | 185 | LEU  | 2.3  |
| 1   | F     | 191 | LYS  | 2.3  |
| 1   | G     | 192 | VAL  | 2.3  |
| 1   | B     | 5   | SER  | 2.3  |
| 1   | E     | 153 | ILE  | 2.3  |
| 1   | K     | 191 | LYS  | 2.3  |
| 1   | B     | 385 | LEU  | 2.2  |
| 1   | A     | 158 | GLY  | 2.2  |
| 1   | K     | 413 | GLY  | 2.2  |
| 1   | E     | 113 | GLN  | 2.2  |
| 1   | I     | 187 | ASP  | 2.2  |
| 1   | A     | 189 | GLY  | 2.2  |
| 1   | B     | 413 | GLY  | 2.2  |
| 1   | B     | 183 | HIS  | 2.2  |
| 1   | E     | 7   | GLU  | 2.2  |
| 1   | C     | 160 | GLN  | 2.2  |
| 1   | G     | 191 | LYS  | 2.2  |
| 1   | F     | 154 | SER  | 2.2  |
| 1   | A     | 153 | ILE  | 2.2  |
| 1   | A     | 194 | ASP  | 2.2  |
| 1   | B     | 163 | SER  | 2.2  |
| 1   | B     | 33  | ASN  | 2.1  |
| 1   | I     | 160 | GLN  | 2.1  |
| 1   | A     | 68  | ALA  | 2.1  |
| 1   | G     | 214 | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 213 | GLU  | 2.1  |
| 1   | I     | 198 | GLU  | 2.1  |
| 1   | J     | 113 | GLN  | 2.1  |
| 1   | C     | 413 | GLY  | 2.1  |
| 1   | I     | 214 | ARG  | 2.1  |
| 1   | A     | 180 | GLN  | 2.1  |
| 1   | I     | 264 | ARG  | 2.1  |
| 1   | A     | 123 | THR  | 2.1  |
| 1   | I     | 154 | SER  | 2.1  |
| 1   | B     | 121 | LYS  | 2.1  |
| 1   | B     | 159 | LYS  | 2.1  |
| 1   | H     | 187 | ASP  | 2.1  |
| 1   | K     | 153 | ILE  | 2.1  |
| 1   | B     | 247 | VAL  | 2.1  |
| 1   | B     | 35  | GLY  | 2.1  |
| 1   | I     | 184 | ARG  | 2.1  |
| 1   | E     | 121 | LYS  | 2.0  |
| 1   | G     | 182 | LYS  | 2.0  |
| 1   | A     | 183 | HIS  | 2.0  |
| 1   | A     | 202 | GLN  | 2.0  |
| 1   | B     | 264 | ARG  | 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 oligosaccharides 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. 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  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | RAT  | B     | 428 | 12/12 | 0.93 | 0.08 | 31,33,34,34                 | 0     |
| 2   | RAT  | A     | 428 | 12/12 | 0.94 | 0.07 | 31,32,35,36                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | RAT  | E     | 428 | 12/12 | 0.94 | 0.08 | 23,26,28,30                 | 0     |
| 2   | RAT  | F     | 428 | 12/12 | 0.94 | 0.08 | 25,26,29,30                 | 0     |
| 2   | RAT  | G     | 428 | 12/12 | 0.94 | 0.07 | 27,30,31,32                 | 0     |
| 2   | RAT  | J     | 428 | 12/12 | 0.94 | 0.07 | 21,25,29,30                 | 0     |
| 2   | RAT  | I     | 428 | 12/12 | 0.95 | 0.07 | 31,33,33,34                 | 0     |
| 3   | CO3  | A     | 429 | 4/4   | 0.95 | 0.07 | 27,27,28,31                 | 0     |
| 2   | RAT  | D     | 428 | 12/12 | 0.96 | 0.06 | 25,26,28,28                 | 0     |
| 2   | RAT  | C     | 428 | 12/12 | 0.96 | 0.06 | 17,23,25,25                 | 0     |
| 2   | RAT  | L     | 428 | 12/12 | 0.96 | 0.06 | 23,26,29,30                 | 0     |
| 2   | RAT  | H     | 428 | 12/12 | 0.96 | 0.06 | 23,25,27,28                 | 0     |
| 3   | CO3  | G     | 429 | 4/4   | 0.96 | 0.07 | 20,22,22,24                 | 0     |
| 5   | NA   | H     | 431 | 1/1   | 0.96 | 0.03 | 23,23,23,23                 | 0     |
| 2   | RAT  | K     | 428 | 12/12 | 0.97 | 0.06 | 22,25,27,27                 | 0     |
| 3   | CO3  | I     | 429 | 4/4   | 0.97 | 0.06 | 25,27,28,30                 | 0     |
| 3   | CO3  | E     | 429 | 4/4   | 0.97 | 0.05 | 16,16,18,20                 | 0     |
| 3   | CO3  | H     | 429 | 4/4   | 0.98 | 0.04 | 20,21,21,21                 | 0     |
| 3   | CO3  | A     | 430 | 4/4   | 0.98 | 0.05 | 21,21,22,26                 | 0     |
| 3   | CO3  | J     | 429 | 4/4   | 0.98 | 0.04 | 18,19,20,22                 | 0     |
| 3   | CO3  | K     | 429 | 4/4   | 0.98 | 0.04 | 19,19,21,22                 | 0     |
| 3   | CO3  | K     | 430 | 4/4   | 0.98 | 0.04 | 20,21,23,23                 | 0     |
| 4   | ZN   | A     | 431 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 4   | ZN   | B     | 429 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 5   | NA   | A     | 432 | 1/1   | 0.98 | 0.03 | 25,25,25,25                 | 0     |
| 3   | CO3  | C     | 429 | 4/4   | 0.98 | 0.05 | 25,25,26,26                 | 0     |
| 4   | ZN   | D     | 430 | 1/1   | 0.99 | 0.06 | 23,23,23,23                 | 0     |
| 4   | ZN   | E     | 431 | 1/1   | 0.99 | 0.04 | 30,30,30,30                 | 0     |
| 4   | ZN   | F     | 429 | 1/1   | 0.99 | 0.03 | 30,30,30,30                 | 0     |
| 4   | ZN   | G     | 430 | 1/1   | 0.99 | 0.04 | 36,36,36,36                 | 0     |
| 4   | ZN   | H     | 430 | 1/1   | 0.99 | 0.02 | 32,32,32,32                 | 0     |
| 4   | ZN   | I     | 430 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 4   | ZN   | L     | 429 | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |
| 3   | CO3  | D     | 429 | 4/4   | 0.99 | 0.03 | 20,21,21,26                 | 0     |
| 5   | NA   | D     | 431 | 1/1   | 0.99 | 0.03 | 18,18,18,18                 | 0     |
| 3   | CO3  | E     | 430 | 4/4   | 0.99 | 0.04 | 24,24,25,29                 | 0     |
| 5   | NA   | L     | 430 | 1/1   | 0.99 | 0.02 | 22,22,22,22                 | 0     |
| 6   | CL   | G     | 431 | 1/1   | 0.99 | 0.02 | 21,21,21,21                 | 0     |
| 4   | ZN   | C     | 430 | 1/1   | 1.00 | 0.03 | 26,26,26,26                 | 0     |
| 4   | ZN   | J     | 430 | 1/1   | 1.00 | 0.02 | 32,32,32,32                 | 0     |
| 6   | CL   | B     | 430 | 1/1   | 1.00 | 0.02 | 21,21,21,21                 | 0     |
| 6   | CL   | E     | 432 | 1/1   | 1.00 | 0.06 | 13,13,13,13                 | 0     |
| 4   | ZN   | K     | 431 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 6   | CL   | J     | 431 | 1/1   | 1.00 | 0.04 | 14,14,14,14                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.