



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

PDB ID : 2B3Z / pdb\_00002b3z  
Title : Crystal structure of a bifunctional deaminase and reductase involved in riboflavin biosynthesis  
Authors : Chen, S.J.; Chang, Y.C.; Liaw, S.H.  
Deposited on : 2005-09-22  
Resolution : 2.41 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                                             |
| 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                                                             |

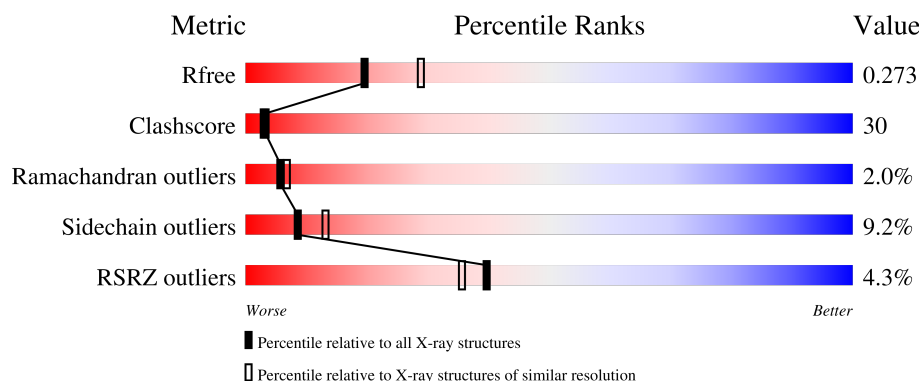
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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                      | 6062 (2.44-2.40)                                      |
| Clashscore            | 190562                      | 6562 (2.44-2.40)                                      |
| Ramachandran outliers | 187476                      | 6481 (2.44-2.40)                                      |
| Sidechain outliers    | 187428                      | 6482 (2.44-2.40)                                      |
| RSRZ outliers         | 180081                      | 6066 (2.44-2.40)                                      |

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     | 373    | <div> <div>2%</div> <div>58% 33% 5% .</div> </div>   |
| 1   | B     | 373    | <div> <div>3%</div> <div>50% 39% 7% . .</div> </div> |
| 1   | C     | 373    | <div> <div>4%</div> <div>52% 35% 9% .</div> </div>   |
| 1   | D     | 373    | <div> <div>8%</div> <div>46% 41% 9% .</div> </div>   |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11267 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 Riboflavin biosynthesis protein ribD.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 359      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2741  | 1740 | 469 | 517 | 15 |         |         |       |
| 1   | B     | 359      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2741  | 1740 | 469 | 517 | 15 |         |         |       |
| 1   | C     | 359      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2741  | 1740 | 469 | 517 | 15 |         |         |       |
| 1   | D     | 360      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1743 | 470 | 519 | 15 |         |         |       |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | -11     | MET      | -      | cloning artifact | UNP P17618 |
| A     | -10     | ARG      | -      | cloning artifact | UNP P17618 |
| A     | -9      | GLY      | -      | cloning artifact | UNP P17618 |
| A     | -8      | SER      | -      | cloning artifact | UNP P17618 |
| A     | -7      | HIS      | -      | cloning artifact | UNP P17618 |
| A     | -6      | HIS      | -      | cloning artifact | UNP P17618 |
| A     | -5      | HIS      | -      | cloning artifact | UNP P17618 |
| A     | -4      | HIS      | -      | cloning artifact | UNP P17618 |
| A     | -3      | HIS      | -      | cloning artifact | UNP P17618 |
| A     | -2      | HIS      | -      | cloning artifact | UNP P17618 |
| A     | -1      | GLY      | -      | cloning artifact | UNP P17618 |
| A     | 0       | SER      | -      | cloning artifact | UNP P17618 |
| B     | -11     | MET      | -      | cloning artifact | UNP P17618 |
| B     | -10     | ARG      | -      | cloning artifact | UNP P17618 |
| B     | -9      | GLY      | -      | cloning artifact | UNP P17618 |
| B     | -8      | SER      | -      | cloning artifact | UNP P17618 |
| B     | -7      | HIS      | -      | cloning artifact | UNP P17618 |
| B     | -6      | HIS      | -      | cloning artifact | UNP P17618 |
| B     | -5      | HIS      | -      | cloning artifact | UNP P17618 |
| B     | -4      | HIS      | -      | cloning artifact | UNP P17618 |
| B     | -3      | HIS      | -      | cloning artifact | UNP P17618 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| B     | -2      | HIS      | -      | cloning artifact | UNP P17618 |
| B     | -1      | GLY      | -      | cloning artifact | UNP P17618 |
| B     | 0       | SER      | -      | cloning artifact | UNP P17618 |
| C     | -11     | MET      | -      | cloning artifact | UNP P17618 |
| C     | -10     | ARG      | -      | cloning artifact | UNP P17618 |
| C     | -9      | GLY      | -      | cloning artifact | UNP P17618 |
| C     | -8      | SER      | -      | cloning artifact | UNP P17618 |
| C     | -7      | HIS      | -      | cloning artifact | UNP P17618 |
| C     | -6      | HIS      | -      | cloning artifact | UNP P17618 |
| C     | -5      | HIS      | -      | cloning artifact | UNP P17618 |
| C     | -4      | HIS      | -      | cloning artifact | UNP P17618 |
| C     | -3      | HIS      | -      | cloning artifact | UNP P17618 |
| C     | -2      | HIS      | -      | cloning artifact | UNP P17618 |
| C     | -1      | GLY      | -      | cloning artifact | UNP P17618 |
| C     | 0       | SER      | -      | cloning artifact | UNP P17618 |
| D     | -11     | MET      | -      | cloning artifact | UNP P17618 |
| D     | -10     | ARG      | -      | cloning artifact | UNP P17618 |
| D     | -9      | GLY      | -      | cloning artifact | UNP P17618 |
| D     | -8      | SER      | -      | cloning artifact | UNP P17618 |
| D     | -7      | HIS      | -      | cloning artifact | UNP P17618 |
| D     | -6      | HIS      | -      | cloning artifact | UNP P17618 |
| D     | -5      | HIS      | -      | cloning artifact | UNP P17618 |
| D     | -4      | HIS      | -      | cloning artifact | UNP P17618 |
| D     | -3      | HIS      | -      | cloning artifact | UNP P17618 |
| D     | -2      | HIS      | -      | cloning artifact | UNP P17618 |
| D     | -1      | GLY      | -      | cloning artifact | UNP P17618 |
| D     | 0       | SER      | -      | cloning artifact | UNP P17618 |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 2   | D     | 1        | Total Zn<br>1 1 | 0       | 0       |

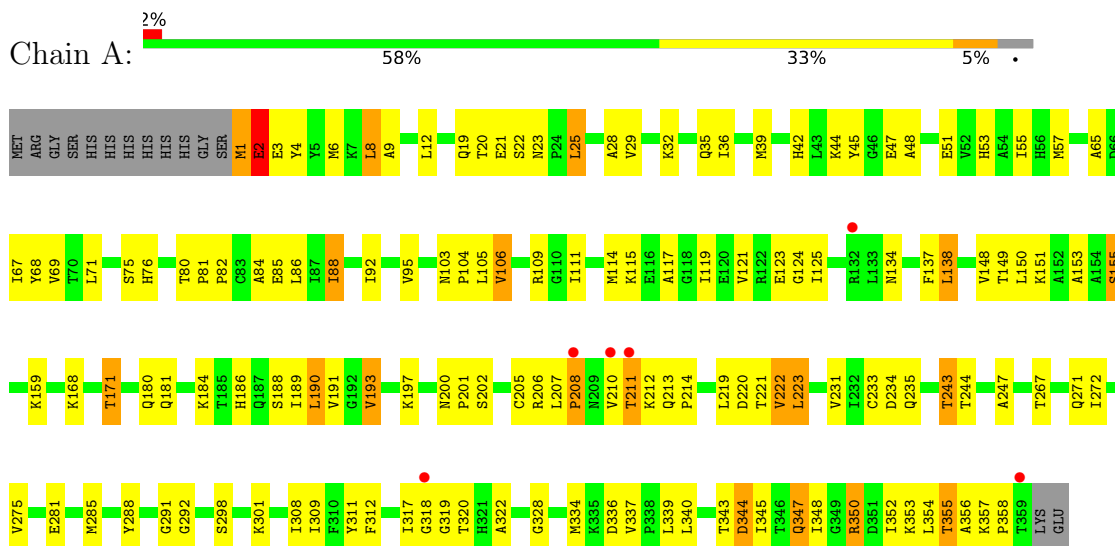
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | A     | 88       | Total<br>88 | O<br>88 | 0       | 0       |
| 3   | B     | 75       | Total<br>75 | O<br>75 | 0       | 0       |
| 3   | C     | 74       | Total<br>74 | O<br>74 | 0       | 0       |
| 3   | D     | 56       | Total<br>56 | O<br>56 | 0       | 0       |

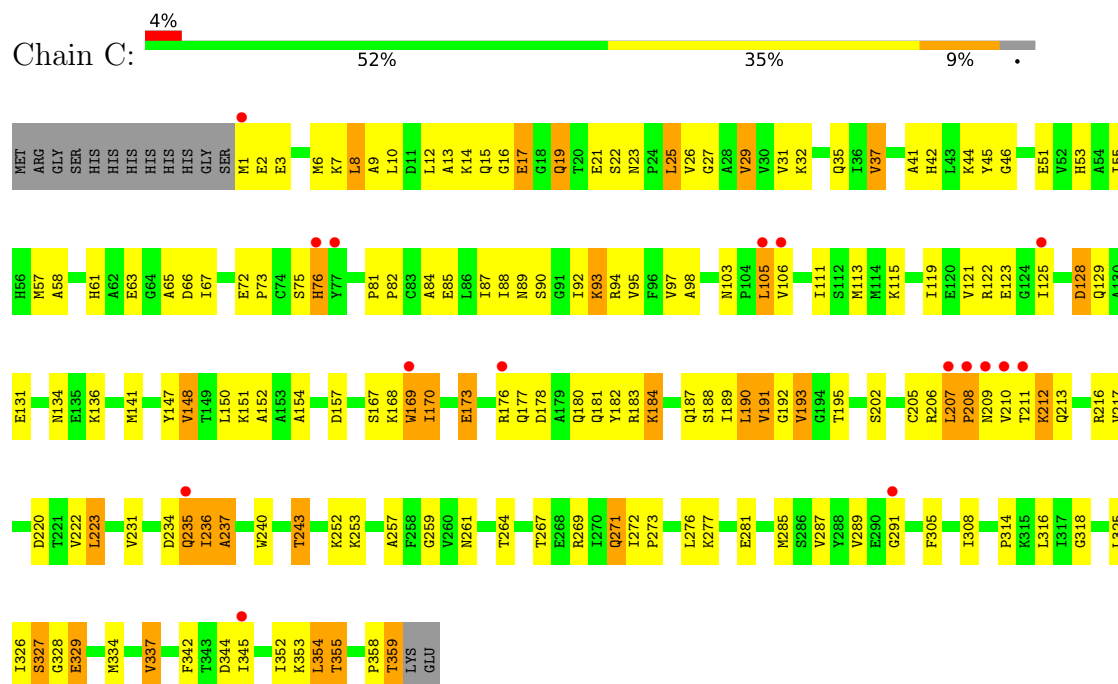
### 3 Residue-property plots

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.

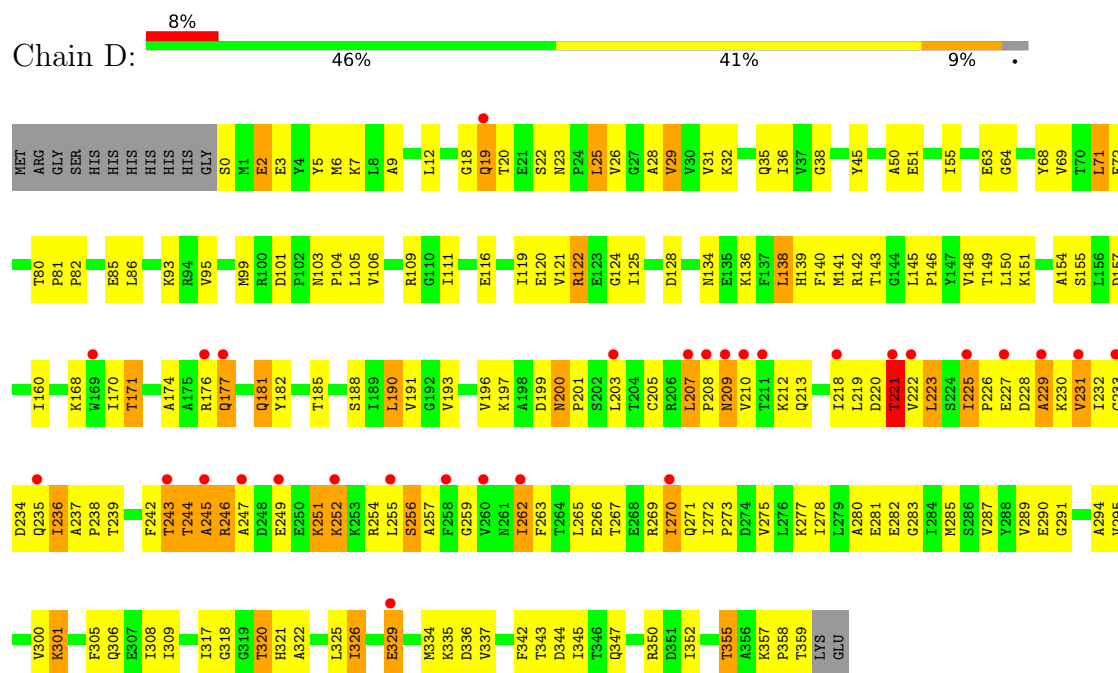
#### • Molecule 1: Riboflavin biosynthesis protein ribD



• Molecule 1: Riboflavin biosynthesis protein ribD



• Molecule 1: Riboflavin biosynthesis protein ribD



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 87.32Å 108.45Å 186.98Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.41<br>50.00 – 2.41                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.4 (50.00-2.41)<br>97.4 (50.00-2.41)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.74 (at 2.39Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.226 , 0.277<br>0.223 , 0.273                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6848 reflections (10.12%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 44.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.197                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 39.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 11267                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
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     | 0.66         | 0/2792      | 1.09        | 22/3778 (0.6%)  |
| 1   | B     | 0.53         | 0/2792      | 1.01        | 11/3778 (0.3%)  |
| 1   | C     | 0.56         | 0/2792      | 1.05        | 12/3778 (0.3%)  |
| 1   | D     | 0.54         | 0/2798      | 1.05        | 15/3786 (0.4%)  |
| All | All   | 0.58         | 0/11174     | 1.05        | 60/15120 (0.4%) |

There are no bond length outliers.

All (60) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 320 | THR  | N-CA-C | -9.06 | 99.85       | 112.45   |
| 1   | C     | 291 | GLY  | N-CA-C | 8.77  | 127.69      | 111.12   |
| 1   | D     | 20  | THR  | N-CA-C | -8.76 | 101.32      | 114.64   |
| 1   | D     | 229 | ALA  | N-CA-C | 8.01  | 118.46      | 107.73   |
| 1   | C     | 2   | GLU  | N-CA-C | -7.94 | 102.61      | 111.82   |
| 1   | D     | 320 | THR  | N-CA-C | -7.64 | 99.15       | 110.23   |
| 1   | D     | 101 | ASP  | CA-C-N | 7.37  | 126.63      | 118.97   |
| 1   | D     | 101 | ASP  | C-N-CA | 7.37  | 126.63      | 118.97   |
| 1   | D     | 322 | ALA  | N-CA-C | -7.18 | 100.60      | 109.65   |
| 1   | A     | 65  | ALA  | N-CA-C | 7.08  | 119.12      | 110.41   |
| 1   | A     | 106 | VAL  | N-CA-C | 7.00  | 117.83      | 111.81   |
| 1   | D     | 291 | GLY  | N-CA-C | 6.59  | 122.71      | 111.04   |
| 1   | B     | 251 | LYS  | N-CA-C | -6.49 | 104.13      | 111.14   |
| 1   | D     | 168 | LYS  | N-CA-C | 6.15  | 118.52      | 111.02   |
| 1   | A     | 2   | GLU  | N-CA-C | -6.07 | 104.66      | 111.28   |
| 1   | C     | 148 | VAL  | N-CA-C | 6.07  | 116.67      | 108.17   |
| 1   | C     | 236 | ILE  | N-CA-C | -6.01 | 105.82      | 113.22   |
| 1   | A     | 155 | SER  | N-CA-C | -6.01 | 102.78      | 110.53   |
| 1   | D     | 124 | GLY  | N-CA-C | 5.85  | 122.53      | 114.92   |
| 1   | A     | 8   | LEU  | N-CA-C | -5.83 | 104.83      | 111.07   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 319 | GLY  | N-CA-C  | 5.79  | 126.91      | 113.18   |
| 1   | C     | 213 | GLN  | N-CA-C  | 5.76  | 116.66      | 109.57   |
| 1   | C     | 237 | ALA  | N-CA-C  | 5.73  | 113.17      | 108.07   |
| 1   | D     | 236 | ILE  | N-CA-C  | -5.63 | 108.36      | 113.71   |
| 1   | A     | 358 | PRO  | N-CA-C  | 5.62  | 119.36      | 111.33   |
| 1   | A     | 233 | CYS  | N-CA-C  | 5.61  | 121.15      | 113.97   |
| 1   | B     | 357 | LYS  | CA-C-N  | 5.58  | 125.89      | 119.92   |
| 1   | B     | 357 | LYS  | C-N-CA  | 5.58  | 125.89      | 119.92   |
| 1   | D     | 244 | THR  | N-CA-C  | 5.55  | 115.73      | 108.07   |
| 1   | C     | 202 | SER  | N-CA-C  | -5.51 | 106.72      | 113.50   |
| 1   | C     | 329 | GLU  | N-CA-C  | 5.48  | 117.11      | 111.03   |
| 1   | A     | 344 | ASP  | N-CA-C  | 5.45  | 116.80      | 108.52   |
| 1   | B     | 293 | SER  | N-CA-C  | -5.44 | 105.35      | 111.28   |
| 1   | A     | 336 | ASP  | CA-C-N  | -5.41 | 118.70      | 122.59   |
| 1   | A     | 336 | ASP  | C-N-CA  | -5.41 | 118.70      | 122.59   |
| 1   | B     | 158 | GLY  | N-CA-C  | 5.36  | 123.33      | 115.08   |
| 1   | A     | 81  | PRO  | CA-C-N  | 5.34  | 125.25      | 119.85   |
| 1   | A     | 81  | PRO  | C-N-CA  | 5.34  | 125.25      | 119.85   |
| 1   | A     | 19  | GLN  | N-CA-C  | -5.32 | 105.85      | 114.09   |
| 1   | C     | 207 | LEU  | CA-C-N  | 5.29  | 126.45      | 119.84   |
| 1   | C     | 207 | LEU  | C-N-CA  | 5.29  | 126.45      | 119.84   |
| 1   | A     | 322 | ALA  | N-CA-C  | -5.28 | 103.38      | 109.93   |
| 1   | D     | 200 | ASN  | CA-C-N  | 5.28  | 126.42      | 120.66   |
| 1   | D     | 200 | ASN  | C-N-CA  | 5.28  | 126.42      | 120.66   |
| 1   | A     | 234 | ASP  | N-CA-C  | 5.28  | 118.98      | 112.54   |
| 1   | A     | 148 | VAL  | N-CA-C  | 5.26  | 115.53      | 108.17   |
| 1   | B     | 48  | ALA  | N-CA-C  | 5.25  | 117.07      | 110.24   |
| 1   | B     | 88  | ILE  | N-CA-C  | 5.22  | 115.37      | 110.30   |
| 1   | B     | 148 | VAL  | N-CA-C  | 5.20  | 115.96      | 108.48   |
| 1   | A     | 291 | GLY  | N-CA-C  | 5.19  | 125.49      | 113.18   |
| 1   | B     | 21  | GLU  | CB-CA-C | -5.16 | 110.64      | 116.63   |
| 1   | B     | 183 | ARG  | N-CA-C  | -5.16 | 106.67      | 112.87   |
| 1   | D     | 290 | GLU  | CA-C-N  | -5.13 | 118.58      | 122.33   |
| 1   | D     | 290 | GLU  | C-N-CA  | -5.13 | 118.58      | 122.33   |
| 1   | B     | 154 | ALA  | N-CA-C  | 5.12  | 116.07      | 108.60   |
| 1   | A     | 202 | SER  | N-CA-C  | -5.09 | 106.92      | 113.23   |
| 1   | A     | 124 | GLY  | N-CA-C  | 5.07  | 120.73      | 114.69   |
| 1   | C     | 19  | GLN  | N-CA-C  | -5.05 | 106.27      | 114.09   |
| 1   | A     | 88  | ILE  | CB-CA-C | -5.01 | 105.28      | 111.70   |
| 1   | C     | 169 | TRP  | N-CA-C  | 5.00  | 118.92      | 112.41   |

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     | 2741  | 0        | 2782     | 137     | 0            |
| 1   | B     | 2741  | 0        | 2782     | 193     | 0            |
| 1   | C     | 2741  | 0        | 2782     | 170     | 0            |
| 1   | D     | 2747  | 0        | 2787     | 208     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 88    | 0        | 0        | 25      | 0            |
| 3   | B     | 75    | 0        | 0        | 29      | 0            |
| 3   | C     | 74    | 0        | 0        | 30      | 0            |
| 3   | D     | 56    | 0        | 0        | 31      | 0            |
| All | All   | 11267 | 0        | 11133    | 674     | 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 30.

All (674) 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:B:211:THR:HG21 | 3:B:1401:HOH:O  | 1.20                     | 1.31              |
| 1:D:0:SER:HA     | 3:D:1408:HOH:O  | 1.35                     | 1.26              |
| 1:A:211:THR:HG22 | 3:A:1441:HOH:O  | 1.37                     | 1.21              |
| 1:D:245:ALA:HA   | 3:D:1405:HOH:O  | 1.38                     | 1.19              |
| 1:C:271:GLN:HG3  | 3:C:1385:HOH:O  | 1.50                     | 1.10              |
| 1:C:176:ARG:HD3  | 3:C:1381:HOH:O  | 1.51                     | 1.09              |
| 1:D:320:THR:HA   | 3:D:1376:HOH:O  | 1.49                     | 1.09              |
| 1:D:270:ILE:HD13 | 1:D:270:ILE:H   | 1.18                     | 1.08              |
| 1:B:184:LYS:HZ1  | 1:B:207:LEU:HB2 | 1.21                     | 1.03              |
| 1:C:329:GLU:HA   | 3:C:1390:HOH:O  | 1.63                     | 0.99              |
| 1:D:320:THR:CA   | 3:D:1376:HOH:O  | 2.07                     | 0.99              |
| 1:C:85:GLU:HG2   | 1:C:89:ASN:HD21 | 1.24                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:GLY:HA3  | 1:B:330:GLY:CA   | 1.93                     | 0.97              |
| 1:D:223:LEU:HD22 | 1:D:251:LYS:HE3  | 1.45                     | 0.96              |
| 1:D:160:ILE:HD11 | 1:D:325:LEU:HD23 | 1.48                     | 0.95              |
| 3:C:1393:HOH:O   | 1:D:334:MET:HG2  | 1.68                     | 0.93              |
| 1:C:1:MET:N      | 3:C:1369:HOH:O   | 2.01                     | 0.93              |
| 1:D:201:PRO:HG2  | 1:D:203:LEU:HD21 | 1.52                     | 0.91              |
| 1:C:168:LYS:HB2  | 3:C:1393:HOH:O   | 1.70                     | 0.91              |
| 1:A:205:CYS:H    | 1:A:213:GLN:HE22 | 1.19                     | 0.91              |
| 1:D:148:VAL:H    | 1:D:306:GLN:NE2  | 1.68                     | 0.91              |
| 1:B:193:VAL:HG11 | 1:B:220:ASP:CG   | 1.96                     | 0.90              |
| 1:C:37:VAL:HG21  | 1:C:61:HIS:HB2   | 1.55                     | 0.88              |
| 1:D:245:ALA:CA   | 3:D:1405:HOH:O   | 2.07                     | 0.88              |
| 1:B:125:ILE:HD12 | 1:B:125:ILE:H    | 1.39                     | 0.88              |
| 1:D:230:LYS:O    | 1:D:234:ASP:HB3  | 1.74                     | 0.87              |
| 1:D:271:GLN:HG2  | 1:D:273:PRO:HD2  | 1.54                     | 0.87              |
| 1:B:171:THR:HA   | 3:B:1391:HOH:O   | 1.73                     | 0.87              |
| 1:A:25:LEU:H     | 1:A:134:ASN:HD21 | 1.20                     | 0.86              |
| 1:A:350:ARG:CD   | 3:A:1376:HOH:O   | 2.22                     | 0.86              |
| 1:A:318:GLY:HA3  | 1:B:330:GLY:HA3  | 1.56                     | 0.86              |
| 1:B:227:GLU:HG2  | 1:B:255:LEU:HD21 | 1.56                     | 0.85              |
| 1:B:37:VAL:HG11  | 1:B:61:HIS:HB2   | 1.59                     | 0.85              |
| 1:B:148:VAL:H    | 1:B:306:GLN:HE21 | 1.25                     | 0.84              |
| 1:C:169:TRP:N    | 3:C:1393:HOH:O   | 2.05                     | 0.84              |
| 1:A:344:ASP:HB3  | 1:A:355:THR:HG23 | 1.59                     | 0.84              |
| 1:C:344:ASP:HB3  | 1:C:355:THR:CG2  | 2.08                     | 0.83              |
| 1:A:318:GLY:HA3  | 1:B:330:GLY:HA2  | 1.56                     | 0.83              |
| 1:A:221:THR:O    | 1:A:243:THR:HG22 | 1.79                     | 0.83              |
| 1:A:88:ILE:HD11  | 1:A:114:MET:HA   | 1.59                     | 0.83              |
| 1:B:171:THR:CB   | 3:B:1391:HOH:O   | 2.27                     | 0.83              |
| 1:C:37:VAL:HG22  | 1:C:58:ALA:HA    | 1.62                     | 0.82              |
| 1:D:148:VAL:H    | 1:D:306:GLN:HE21 | 1.23                     | 0.82              |
| 1:C:111:ILE:HG23 | 1:C:121:VAL:HG11 | 1.60                     | 0.82              |
| 1:B:243:THR:HG22 | 1:B:244:THR:H    | 1.43                     | 0.81              |
| 1:D:270:ILE:H    | 1:D:270:ILE:CD1  | 1.93                     | 0.81              |
| 1:B:166:ASP:OD1  | 1:B:168:LYS:HB2  | 1.80                     | 0.81              |
| 1:C:31:VAL:HG11  | 3:C:1362:HOH:O   | 1.81                     | 0.80              |
| 1:C:168:LYS:CA   | 3:C:1393:HOH:O   | 2.30                     | 0.79              |
| 1:B:301:LYS:NZ   | 3:B:1377:HOH:O   | 2.14                     | 0.79              |
| 1:B:75:SER:CB    | 1:B:109:ARG:HD2  | 2.14                     | 0.78              |
| 1:C:85:GLU:HG2   | 1:C:89:ASN:ND2   | 1.99                     | 0.78              |
| 1:D:334:MET:O    | 1:D:337:VAL:HG12 | 1.83                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:32:LYS:NZ    | 3:A:1434:HOH:O   | 2.15                     | 0.77              |
| 1:D:150:LEU:HD12 | 1:D:308:ILE:HD11 | 1.67                     | 0.77              |
| 1:A:207:LEU:HB3  | 1:A:208:PRO:HD2  | 1.67                     | 0.77              |
| 1:A:271:GLN:CG   | 3:A:1423:HOH:O   | 2.31                     | 0.76              |
| 1:D:321:HIS:N    | 3:D:1376:HOH:O   | 2.15                     | 0.76              |
| 1:B:269:ARG:NE   | 3:B:1428:HOH:O   | 2.17                     | 0.76              |
| 1:D:270:ILE:HD13 | 1:D:270:ILE:N    | 1.99                     | 0.76              |
| 1:D:320:THR:CG2  | 3:D:1376:HOH:O   | 2.33                     | 0.76              |
| 1:A:22:SER:HA    | 1:A:285:MET:HE2  | 1.67                     | 0.76              |
| 1:B:51:GLU:OE2   | 3:B:1363:HOH:O   | 2.04                     | 0.76              |
| 1:B:177:GLN:HG2  | 3:B:1397:HOH:O   | 1.84                     | 0.76              |
| 1:C:344:ASP:HB3  | 1:C:355:THR:HG23 | 1.67                     | 0.75              |
| 1:A:243:THR:HG21 | 1:A:247:ALA:HB2  | 1.67                     | 0.75              |
| 1:C:271:GLN:HA   | 1:C:271:GLN:HE21 | 1.49                     | 0.75              |
| 1:A:220:ASP:O    | 1:A:243:THR:HG23 | 1.87                     | 0.75              |
| 1:A:12:LEU:HD11  | 1:A:39:MET:HE2   | 1.69                     | 0.75              |
| 1:B:349:GLY:HA3  | 3:B:1383:HOH:O   | 1.86                     | 0.75              |
| 1:B:75:SER:HB3   | 1:B:109:ARG:HD2  | 1.67                     | 0.74              |
| 1:C:168:LYS:CB   | 3:C:1393:HOH:O   | 2.32                     | 0.74              |
| 1:D:301:LYS:HE2  | 1:D:301:LYS:O    | 1.87                     | 0.74              |
| 1:A:271:GLN:HG3  | 3:A:1423:HOH:O   | 1.86                     | 0.74              |
| 1:B:171:THR:CA   | 3:B:1391:HOH:O   | 2.32                     | 0.74              |
| 1:D:266:GLU:H    | 1:D:266:GLU:CD   | 1.96                     | 0.74              |
| 1:D:3:GLU:OE2    | 3:D:1408:HOH:O   | 2.05                     | 0.74              |
| 1:B:111:ILE:HG23 | 1:B:121:VAL:HG11 | 1.70                     | 0.73              |
| 1:B:184:LYS:HB2  | 1:B:184:LYS:NZ   | 2.03                     | 0.73              |
| 1:A:159:LYS:HE2  | 3:A:1366:HOH:O   | 1.88                     | 0.73              |
| 1:B:207:LEU:HB3  | 1:B:208:PRO:CD   | 2.19                     | 0.72              |
| 1:C:76:HIS:O     | 1:C:82:PRO:HG3   | 1.88                     | 0.72              |
| 1:D:221:THR:HG23 | 1:D:270:ILE:HD12 | 1.71                     | 0.72              |
| 1:D:116:GLU:OE1  | 3:D:1384:HOH:O   | 2.08                     | 0.72              |
| 1:C:329:GLU:CA   | 3:C:1390:HOH:O   | 2.28                     | 0.72              |
| 1:D:103:ASN:OD1  | 3:D:1407:HOH:O   | 2.07                     | 0.71              |
| 1:A:68:TYR:OH    | 3:A:1402:HOH:O   | 2.08                     | 0.71              |
| 1:C:329:GLU:O    | 3:C:1390:HOH:O   | 2.08                     | 0.71              |
| 1:D:64:GLY:HA2   | 1:D:93:LYS:HG2   | 1.72                     | 0.71              |
| 1:D:300:VAL:HG21 | 1:D:326:ILE:HD13 | 1.73                     | 0.71              |
| 1:B:125:ILE:HG22 | 1:B:126:LEU:HD13 | 1.73                     | 0.71              |
| 1:D:320:THR:O    | 3:D:1367:HOH:O   | 2.09                     | 0.71              |
| 1:B:37:VAL:HG12  | 1:B:58:ALA:HA    | 1.72                     | 0.71              |
| 1:A:75:SER:OG    | 1:A:109:ARG:HD2  | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:ILE:HD12  | 1:A:117:ALA:CB   | 2.21                     | 0.70              |
| 1:A:207:LEU:HB3  | 1:A:208:PRO:CD   | 2.21                     | 0.70              |
| 1:C:168:LYS:O    | 3:C:1415:HOH:O   | 2.09                     | 0.70              |
| 1:D:308:ILE:C    | 1:D:309:ILE:HD12 | 2.16                     | 0.70              |
| 1:D:249:GLU:O    | 3:D:1383:HOH:O   | 2.10                     | 0.70              |
| 1:D:295:VAL:HG23 | 3:D:1375:HOH:O   | 1.90                     | 0.70              |
| 1:B:37:VAL:HG11  | 1:B:61:HIS:CB    | 2.22                     | 0.69              |
| 1:B:344:ASP:HB3  | 1:B:355:THR:HG23 | 1.74                     | 0.69              |
| 1:C:103:ASN:HA   | 1:C:141:MET:HG3  | 1.73                     | 0.69              |
| 1:D:245:ALA:O    | 3:D:1409:HOH:O   | 2.10                     | 0.69              |
| 1:A:8:LEU:HD21   | 1:A:39:MET:HE3   | 1.73                     | 0.69              |
| 1:C:272:ILE:HB   | 1:C:273:PRO:HD3  | 1.75                     | 0.69              |
| 1:D:32:LYS:HE2   | 1:D:63:GLU:O     | 1.92                     | 0.69              |
| 1:D:99:MET:HE1   | 1:D:138:LEU:HD21 | 1.74                     | 0.69              |
| 1:A:29:VAL:HG22  | 1:A:68:TYR:HB2   | 1.73                     | 0.69              |
| 1:A:123:GLU:OE1  | 3:A:1396:HOH:O   | 2.11                     | 0.68              |
| 1:B:243:THR:HG22 | 1:B:244:THR:N    | 2.08                     | 0.68              |
| 1:C:191:VAL:CG1  | 1:C:195:THR:HB   | 2.23                     | 0.68              |
| 1:D:72:GLU:OE1   | 1:D:111:ILE:HG12 | 1.93                     | 0.68              |
| 1:D:243:THR:HG22 | 1:D:244:THR:H    | 1.59                     | 0.68              |
| 1:A:328:GLY:H    | 1:B:320:THR:HG22 | 1.59                     | 0.68              |
| 1:B:184:LYS:HZ1  | 1:B:207:LEU:CB   | 2.04                     | 0.68              |
| 1:D:146:PRO:HD3  | 1:D:280:ALA:HB2  | 1.75                     | 0.68              |
| 1:C:193:VAL:HG11 | 1:C:220:ASP:CG   | 2.19                     | 0.67              |
| 1:A:80:THR:O     | 3:A:1419:HOH:O   | 2.12                     | 0.67              |
| 1:B:171:THR:HB   | 3:B:1391:HOH:O   | 1.92                     | 0.67              |
| 1:B:51:GLU:O     | 1:B:55:ILE:HG12  | 1.94                     | 0.67              |
| 1:D:247:ALA:HB3  | 3:D:1409:HOH:O   | 1.93                     | 0.67              |
| 1:B:25:LEU:H     | 1:B:134:ASN:HD21 | 1.42                     | 0.67              |
| 1:A:155:SER:HB3  | 1:A:317:ILE:HD12 | 1.75                     | 0.67              |
| 1:B:344:ASP:OD2  | 3:B:1372:HOH:O   | 2.12                     | 0.67              |
| 1:C:216:ARG:HD2  | 1:C:237:ALA:HB3  | 1.76                     | 0.67              |
| 1:C:181:GLN:HG3  | 1:C:182:TYR:N    | 2.09                     | 0.66              |
| 1:D:104:PRO:HG2  | 3:D:1407:HOH:O   | 1.95                     | 0.66              |
| 1:B:167:SER:O    | 1:B:169:TRP:N    | 2.29                     | 0.66              |
| 1:B:184:LYS:HB2  | 1:B:184:LYS:HZ3  | 1.59                     | 0.66              |
| 1:D:6:MET:HG2    | 1:D:125:ILE:HG22 | 1.76                     | 0.66              |
| 1:A:334:MET:HB2  | 1:B:168:LYS:HB3  | 1.78                     | 0.66              |
| 1:B:177:GLN:NE2  | 3:B:1397:HOH:O   | 2.15                     | 0.66              |
| 1:D:200:ASN:HD21 | 1:D:230:LYS:HG2  | 1.59                     | 0.66              |
| 1:B:187:GLN:HE22 | 1:B:285:MET:HE2  | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:23:ASN:ND2   | 1:C:45:TYR:HD2   | 1.94                     | 0.66              |
| 1:D:104:PRO:CD   | 3:D:1407:HOH:O   | 2.43                     | 0.66              |
| 1:D:171:THR:HG21 | 3:D:1391:HOH:O   | 1.94                     | 0.66              |
| 1:A:21:GLU:N     | 3:A:1440:HOH:O   | 2.10                     | 0.66              |
| 1:D:252:LYS:HG2  | 1:D:262:ILE:HD12 | 1.78                     | 0.66              |
| 1:B:151:LYS:HD2  | 1:B:152:ALA:N    | 2.11                     | 0.66              |
| 1:C:187:GLN:OE1  | 1:C:285:MET:HB2  | 1.96                     | 0.65              |
| 1:B:243:THR:HG21 | 1:B:247:ALA:HB2  | 1.77                     | 0.65              |
| 1:C:168:LYS:N    | 3:C:1393:HOH:O   | 2.30                     | 0.65              |
| 1:C:31:VAL:CG1   | 1:C:66:ASP:HB2   | 2.26                     | 0.65              |
| 1:D:140:PHE:CD2  | 1:D:141:MET:HE2  | 2.31                     | 0.65              |
| 1:B:103:ASN:ND2  | 1:B:105:LEU:HD13 | 2.12                     | 0.65              |
| 1:B:57:MET:O     | 3:B:1399:HOH:O   | 2.14                     | 0.65              |
| 1:B:329:GLU:HG3  | 3:B:1377:HOH:O   | 1.96                     | 0.65              |
| 1:B:55:ILE:HG13  | 1:B:86:LEU:CD1   | 2.27                     | 0.65              |
| 1:D:230:LYS:O    | 1:D:232:ILE:N    | 2.31                     | 0.64              |
| 1:C:193:VAL:HG13 | 1:C:220:ASP:HB2  | 1.78                     | 0.64              |
| 1:B:234:ASP:OD2  | 1:B:234:ASP:C    | 2.41                     | 0.64              |
| 1:C:93:LYS:NZ    | 1:C:93:LYS:HB3   | 2.13                     | 0.64              |
| 1:B:207:LEU:HB3  | 1:B:208:PRO:HD2  | 1.78                     | 0.64              |
| 1:D:201:PRO:HG2  | 1:D:203:LEU:CD2  | 2.26                     | 0.64              |
| 1:A:84:ALA:O     | 1:A:88:ILE:HG12  | 1.98                     | 0.64              |
| 1:A:88:ILE:HD13  | 1:A:119:ILE:HD12 | 1.81                     | 0.63              |
| 1:A:151:LYS:HD2  | 1:A:288:TYR:OH   | 1.98                     | 0.63              |
| 1:A:153:ALA:HB1  | 1:A:171:THR:HG23 | 1.80                     | 0.63              |
| 1:D:150:LEU:HD12 | 1:D:308:ILE:CD1  | 2.27                     | 0.63              |
| 1:C:223:LEU:HG   | 1:C:243:THR:HG21 | 1.79                     | 0.63              |
| 1:B:103:ASN:HD21 | 1:B:105:LEU:HD13 | 1.63                     | 0.63              |
| 1:C:37:VAL:HG21  | 1:C:61:HIS:CB    | 2.28                     | 0.63              |
| 1:C:111:ILE:HG22 | 1:C:115:LYS:HD2  | 1.81                     | 0.63              |
| 1:D:99:MET:HE1   | 1:D:138:LEU:HD11 | 1.81                     | 0.62              |
| 1:B:79:LYS:O     | 1:B:80:THR:HG23  | 1.98                     | 0.62              |
| 1:B:269:ARG:CD   | 3:B:1428:HOH:O   | 2.46                     | 0.62              |
| 1:C:105:LEU:HD23 | 1:C:105:LEU:H    | 1.64                     | 0.62              |
| 1:B:312:PHE:HE2  | 1:B:354:LEU:HD12 | 1.65                     | 0.62              |
| 1:D:221:THR:CG2  | 1:D:270:ILE:HD12 | 2.29                     | 0.62              |
| 1:B:151:LYS:HD2  | 1:B:151:LYS:C    | 2.25                     | 0.62              |
| 1:D:120:GLU:OE1  | 3:D:1392:HOH:O   | 2.16                     | 0.61              |
| 1:D:245:ALA:C    | 1:D:247:ALA:H    | 2.07                     | 0.61              |
| 1:D:320:THR:O    | 1:D:321:HIS:HB2  | 2.00                     | 0.61              |
| 1:B:220:ASP:O    | 1:B:243:THR:HG23 | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:95:VAL:CG1   | 1:C:121:VAL:HG22 | 2.29                     | 0.61              |
| 1:D:207:LEU:HD23 | 1:D:208:PRO:HD2  | 1.80                     | 0.61              |
| 1:A:25:LEU:H     | 1:A:134:ASN:ND2  | 1.94                     | 0.61              |
| 1:C:51:GLU:O     | 1:C:55:ILE:HD13  | 2.00                     | 0.61              |
| 1:C:211:THR:O    | 1:C:212:LYS:HB2  | 2.00                     | 0.61              |
| 1:C:21:GLU:HG3   | 1:C:22:SER:H     | 1.64                     | 0.61              |
| 1:C:328:GLY:HA3  | 3:C:1409:HOH:O   | 2.01                     | 0.61              |
| 1:D:170:ILE:HG23 | 1:D:171:THR:N    | 2.16                     | 0.61              |
| 1:A:88:ILE:HD12  | 1:A:117:ALA:HB3  | 1.81                     | 0.61              |
| 1:A:193:VAL:HG22 | 1:A:219:LEU:O    | 2.01                     | 0.61              |
| 1:A:22:SER:HA    | 1:A:285:MET:CE   | 2.30                     | 0.60              |
| 1:C:352:ILE:HG22 | 1:C:354:LEU:CD2  | 2.31                     | 0.60              |
| 1:B:142:ARG:HG3  | 1:B:142:ARG:HH11 | 1.65                     | 0.60              |
| 1:C:42:HIS:N     | 3:C:1378:HOH:O   | 2.32                     | 0.60              |
| 1:C:354:LEU:HD23 | 1:C:354:LEU:N    | 2.16                     | 0.60              |
| 1:C:87:ILE:HG23  | 1:C:92:ILE:HG13  | 1.84                     | 0.60              |
| 1:D:245:ALA:O    | 1:D:247:ALA:N    | 2.33                     | 0.60              |
| 1:C:188:SER:C    | 1:C:189:ILE:HD13 | 2.26                     | 0.60              |
| 1:B:56:HIS:HE1   | 3:B:1382:HOH:O   | 1.84                     | 0.60              |
| 1:C:6:MET:HG3    | 1:C:125:ILE:HB   | 1.83                     | 0.60              |
| 1:D:148:VAL:HB   | 1:D:305:PHE:HA   | 1.84                     | 0.60              |
| 1:C:326:ILE:HB   | 1:D:318:GLY:HA2  | 1.84                     | 0.59              |
| 1:D:181:GLN:HG2  | 1:D:182:TYR:N    | 2.17                     | 0.59              |
| 1:D:208:PRO:O    | 1:D:209:ASN:HB2  | 2.00                     | 0.59              |
| 1:D:223:LEU:HD23 | 1:D:225:ILE:HG22 | 1.83                     | 0.59              |
| 1:D:218:ILE:N    | 1:D:218:ILE:HD12 | 2.18                     | 0.59              |
| 1:B:222:VAL:HG12 | 1:B:222:VAL:O    | 2.02                     | 0.59              |
| 1:D:267:THR:HG22 | 1:D:269:ARG:H    | 1.67                     | 0.58              |
| 1:C:191:VAL:HG13 | 1:C:195:THR:HB   | 1.83                     | 0.58              |
| 1:D:188:SER:OG   | 1:D:287:VAL:HG22 | 2.02                     | 0.58              |
| 1:B:35:GLN:NE2   | 1:D:19:GLN:HB2   | 2.17                     | 0.58              |
| 1:B:75:SER:HB2   | 1:B:109:ARG:HD2  | 1.85                     | 0.58              |
| 1:B:225:ILE:HD13 | 1:B:226:PRO:N    | 2.18                     | 0.58              |
| 1:C:318:GLY:HA2  | 1:D:326:ILE:HG22 | 1.85                     | 0.58              |
| 1:A:318:GLY:CA   | 1:B:330:GLY:HA3  | 2.29                     | 0.58              |
| 1:C:220:ASP:O    | 1:C:243:THR:HG22 | 2.04                     | 0.58              |
| 1:C:271:GLN:CG   | 3:C:1385:HOH:O   | 2.26                     | 0.58              |
| 1:D:222:VAL:HG22 | 1:D:222:VAL:O    | 2.01                     | 0.58              |
| 1:C:176:ARG:CD   | 3:C:1381:HOH:O   | 2.29                     | 0.57              |
| 1:D:295:VAL:N    | 3:D:1375:HOH:O   | 2.16                     | 0.57              |
| 1:D:5:TYR:CE1    | 1:D:36:ILE:HD11  | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:266:GLU:OE2  | 3:B:1408:HOH:O   | 2.17                     | 0.57              |
| 1:A:95:VAL:HG23  | 1:A:119:ILE:HG21 | 1.86                     | 0.57              |
| 1:B:314:PRO:HG3  | 1:B:350:ARG:O    | 2.05                     | 0.57              |
| 1:C:240:TRP:CD1  | 1:C:261:ASN:HB2  | 2.39                     | 0.57              |
| 1:A:21:GLU:HB2   | 1:A:45:TYR:CD1   | 2.40                     | 0.57              |
| 1:B:7:LYS:HA     | 1:B:10:LEU:HD12  | 1.85                     | 0.57              |
| 1:B:55:ILE:HG13  | 1:B:86:LEU:HD11  | 1.87                     | 0.57              |
| 1:D:329:GLU:HB3  | 3:D:1379:HOH:O   | 2.03                     | 0.57              |
| 1:D:25:LEU:HB2   | 1:D:134:ASN:HD21 | 1.69                     | 0.57              |
| 1:D:193:VAL:HG11 | 1:D:220:ASP:CG   | 2.29                     | 0.57              |
| 1:D:344:ASP:O    | 1:D:345:ILE:HD13 | 2.04                     | 0.57              |
| 1:D:111:ILE:HD12 | 1:D:121:VAL:HG11 | 1.87                     | 0.57              |
| 1:A:21:GLU:CA    | 3:A:1440:HOH:O   | 2.52                     | 0.56              |
| 1:B:246:ARG:HG3  | 1:B:246:ARG:HH11 | 1.70                     | 0.56              |
| 1:B:308:ILE:HD11 | 1:B:310:PHE:CZ   | 2.40                     | 0.56              |
| 1:B:184:LYS:HE3  | 1:B:210:VAL:HG12 | 1.86                     | 0.56              |
| 1:A:28:ALA:HA    | 1:A:68:TYR:O     | 2.06                     | 0.56              |
| 1:D:320:THR:HG23 | 3:D:1376:HOH:O   | 2.00                     | 0.56              |
| 1:B:166:ASP:OD1  | 1:B:168:LYS:CB   | 2.53                     | 0.56              |
| 1:B:308:ILE:HD11 | 1:B:310:PHE:CE2  | 2.40                     | 0.56              |
| 1:D:344:ASP:C    | 1:D:345:ILE:HD13 | 2.30                     | 0.56              |
| 1:B:211:THR:O    | 1:B:212:LYS:HB2  | 2.06                     | 0.56              |
| 1:C:267:THR:HG21 | 3:C:1385:HOH:O   | 2.04                     | 0.56              |
| 1:D:104:PRO:HD2  | 3:D:1407:HOH:O   | 2.04                     | 0.56              |
| 1:B:35:GLN:NE2   | 1:D:19:GLN:CB    | 2.69                     | 0.56              |
| 1:D:190:LEU:HB3  | 1:D:289:VAL:HG22 | 1.87                     | 0.56              |
| 1:C:329:GLU:C    | 3:C:1390:HOH:O   | 2.43                     | 0.55              |
| 1:D:99:MET:CE    | 1:D:138:LEU:HD11 | 2.37                     | 0.55              |
| 1:B:254:ARG:HG3  | 1:B:254:ARG:HH11 | 1.71                     | 0.55              |
| 1:C:122:ARG:HD2  | 3:C:1418:HOH:O   | 2.05                     | 0.55              |
| 1:C:353:LYS:C    | 1:C:354:LEU:HD23 | 2.31                     | 0.55              |
| 1:A:44:LYS:HZ2   | 1:C:35:GLN:HE22  | 1.54                     | 0.55              |
| 1:A:51:GLU:O     | 1:A:55:ILE:HG12  | 2.05                     | 0.55              |
| 1:A:271:GLN:CD   | 3:A:1423:HOH:O   | 2.47                     | 0.55              |
| 1:B:44:LYS:NZ    | 1:D:35:GLN:OE1   | 2.35                     | 0.55              |
| 1:C:178:ASP:O    | 1:C:181:GLN:HG2  | 2.05                     | 0.55              |
| 1:D:138:LEU:O    | 1:D:142:ARG:HD2  | 2.06                     | 0.55              |
| 1:D:149:THR:HG23 | 1:D:309:ILE:HD13 | 1.89                     | 0.55              |
| 1:B:53:HIS:HE1   | 3:B:1378:HOH:O   | 1.89                     | 0.55              |
| 1:B:209:ASN:ND2  | 3:B:1401:HOH:O   | 2.40                     | 0.55              |
| 1:B:246:ARG:HG3  | 1:B:246:ARG:NH1  | 2.21                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:344:ASP:HB3  | 1:B:355:THR:CG2  | 2.37                     | 0.55              |
| 1:B:324:SER:OG   | 3:B:1364:HOH:O   | 2.18                     | 0.55              |
| 1:C:6:MET:CE     | 1:C:98:ALA:HB2   | 2.37                     | 0.55              |
| 1:B:67:ILE:HD13  | 1:B:87:ILE:CD1   | 2.37                     | 0.55              |
| 1:C:167:SER:HA   | 1:D:334:MET:CE   | 2.37                     | 0.55              |
| 1:D:344:ASP:HB3  | 1:D:355:THR:HG23 | 1.90                     | 0.55              |
| 1:D:28:ALA:HA    | 1:D:68:TYR:O     | 2.07                     | 0.54              |
| 1:D:255:LEU:C    | 1:D:257:ALA:H    | 2.15                     | 0.54              |
| 1:B:12:LEU:HD21  | 1:B:39:MET:HB3   | 1.89                     | 0.54              |
| 1:B:220:ASP:OD2  | 1:B:225:ILE:HB   | 2.07                     | 0.54              |
| 1:D:80:THR:HB    | 1:D:81:PRO:HD2   | 1.89                     | 0.54              |
| 1:B:355:THR:HG22 | 3:B:1372:HOH:O   | 2.06                     | 0.54              |
| 1:C:55:ILE:HD11  | 1:C:67:ILE:HD12  | 1.88                     | 0.54              |
| 1:D:122:ARG:NH1  | 1:D:122:ARG:HA   | 2.22                     | 0.54              |
| 1:D:139:HIS:O    | 1:D:143:THR:HG23 | 2.08                     | 0.54              |
| 1:D:230:LYS:C    | 1:D:234:ASP:HB3  | 2.33                     | 0.54              |
| 1:B:100:ARG:NH1  | 1:B:123:GLU:OE1  | 2.41                     | 0.54              |
| 1:B:272:ILE:HA   | 1:B:275:VAL:HG22 | 1.90                     | 0.54              |
| 3:C:1393:HOH:O   | 1:D:334:MET:CB   | 2.55                     | 0.54              |
| 1:A:44:LYS:HZ2   | 1:C:35:GLN:NE2   | 2.06                     | 0.54              |
| 1:A:188:SER:C    | 1:A:189:ILE:HD13 | 2.33                     | 0.54              |
| 1:D:200:ASN:ND2  | 1:D:230:LYS:HG2  | 2.22                     | 0.54              |
| 1:C:169:TRP:H    | 1:D:334:MET:HG2  | 1.72                     | 0.54              |
| 1:D:140:PHE:HD2  | 1:D:141:MET:HE2  | 1.72                     | 0.54              |
| 1:C:103:ASN:CA   | 1:C:141:MET:HG3  | 2.38                     | 0.54              |
| 1:D:271:GLN:CG   | 1:D:273:PRO:HD2  | 2.35                     | 0.54              |
| 1:A:193:VAL:HG22 | 1:A:220:ASP:HA   | 1.90                     | 0.53              |
| 1:A:339:LEU:HD11 | 1:B:350:ARG:HE   | 1.73                     | 0.53              |
| 1:A:20:THR:HB    | 1:A:23:ASN:HB2   | 1.91                     | 0.53              |
| 1:B:88:ILE:HD11  | 1:B:114:MET:HA   | 1.90                     | 0.53              |
| 1:A:171:THR:HG23 | 3:A:1372:HOH:O   | 2.08                     | 0.53              |
| 1:A:309:ILE:HG12 | 1:A:355:THR:HB   | 1.89                     | 0.53              |
| 1:B:83:CYS:O     | 1:B:87:ILE:HG12  | 2.08                     | 0.53              |
| 1:A:21:GLU:HA    | 3:A:1440:HOH:O   | 2.09                     | 0.53              |
| 1:A:271:GLN:OE1  | 3:A:1421:HOH:O   | 2.19                     | 0.53              |
| 1:B:234:ASP:O    | 1:B:236:ILE:HG12 | 2.09                     | 0.53              |
| 1:D:106:VAL:HG22 | 1:D:109:ARG:NH2  | 2.24                     | 0.53              |
| 1:C:191:VAL:HG11 | 1:C:195:THR:HB   | 1.91                     | 0.53              |
| 1:C:81:PRO:HB3   | 1:C:85:GLU:OE1   | 2.08                     | 0.53              |
| 1:C:23:ASN:HD21  | 1:C:45:TYR:HD2   | 1.56                     | 0.53              |
| 1:D:225:ILE:HG23 | 1:D:225:ILE:O    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:344:ASP:HB3  | 1:C:355:THR:HG21 | 1.90                     | 0.53              |
| 1:B:269:ARG:HD2  | 3:B:1428:HOH:O   | 2.09                     | 0.53              |
| 1:A:181:GLN:HA   | 1:A:207:LEU:HD11 | 1.91                     | 0.53              |
| 1:B:131:GLU:OE1  | 1:B:142:ARG:NH2  | 2.38                     | 0.52              |
| 1:C:90:SER:OG    | 1:C:92:ILE:HG12  | 2.08                     | 0.52              |
| 1:D:265:LEU:HD12 | 1:D:265:LEU:N    | 2.24                     | 0.52              |
| 1:D:255:LEU:C    | 1:D:257:ALA:N    | 2.65                     | 0.52              |
| 1:B:41:ALA:O     | 1:B:43:LEU:HD22  | 2.08                     | 0.52              |
| 1:B:297:GLY:HA2  | 1:B:326:ILE:HG23 | 1.90                     | 0.52              |
| 1:A:171:THR:HG21 | 3:A:1380:HOH:O   | 2.09                     | 0.52              |
| 1:A:348:ILE:N    | 1:A:348:ILE:HD12 | 2.24                     | 0.52              |
| 1:B:14:LYS:HE3   | 1:B:17:GLU:OE2   | 2.10                     | 0.52              |
| 1:D:205:CYS:H    | 1:D:213:GLN:NE2  | 2.08                     | 0.52              |
| 1:A:272:ILE:O    | 1:A:275:VAL:HG22 | 2.10                     | 0.52              |
| 1:C:66:ASP:OD2   | 1:C:93:LYS:NZ    | 2.42                     | 0.52              |
| 1:D:247:ALA:O    | 3:D:1409:HOH:O   | 2.19                     | 0.52              |
| 1:A:350:ARG:HD3  | 3:A:1376:HOH:O   | 2.01                     | 0.52              |
| 1:D:232:ILE:HG22 | 1:D:233:CYS:N    | 2.25                     | 0.52              |
| 1:D:193:VAL:O    | 1:D:197:LYS:HG2  | 2.10                     | 0.52              |
| 1:D:335:LYS:HG3  | 1:D:336:ASP:OD1  | 2.09                     | 0.52              |
| 1:A:42:HIS:HD2   | 1:A:48:ALA:O     | 1.93                     | 0.51              |
| 1:A:134:ASN:HB2  | 1:A:138:LEU:HD22 | 1.91                     | 0.51              |
| 1:D:104:PRO:CG   | 3:D:1407:HOH:O   | 2.53                     | 0.51              |
| 1:D:143:THR:OG1  | 1:D:145:LEU:HB2  | 2.09                     | 0.51              |
| 1:A:235:GLN:NE2  | 1:A:235:GLN:HA   | 2.25                     | 0.51              |
| 1:B:268:GLU:CD   | 1:B:268:GLU:H    | 2.16                     | 0.51              |
| 1:C:252:LYS:HE2  | 3:C:1388:HOH:O   | 2.09                     | 0.51              |
| 1:C:93:LYS:HB3   | 1:C:93:LYS:HZ3   | 1.75                     | 0.51              |
| 1:A:57:MET:HG3   | 1:C:53:HIS:CD2   | 2.45                     | 0.51              |
| 1:C:23:ASN:ND2   | 1:C:42:HIS:HE1   | 2.09                     | 0.51              |
| 1:C:167:SER:HA   | 1:D:334:MET:HE2  | 1.92                     | 0.51              |
| 1:A:308:ILE:HG22 | 1:A:356:ALA:O    | 2.11                     | 0.51              |
| 1:A:125:ILE:HD12 | 1:A:125:ILE:N    | 2.26                     | 0.51              |
| 1:B:193:VAL:CG1  | 1:B:220:ASP:CG   | 2.78                     | 0.51              |
| 1:B:355:THR:CG2  | 3:B:1372:HOH:O   | 2.58                     | 0.51              |
| 1:B:160:ILE:O    | 1:B:161:ALA:HB2  | 2.09                     | 0.51              |
| 1:C:151:LYS:HD2  | 1:C:151:LYS:C    | 2.36                     | 0.51              |
| 1:D:337:VAL:HG13 | 1:D:337:VAL:O    | 2.11                     | 0.51              |
| 1:A:44:LYS:NZ    | 1:C:35:GLN:NE2   | 2.58                     | 0.51              |
| 1:D:294:ALA:HB3  | 3:D:1375:HOH:O   | 2.11                     | 0.51              |
| 1:A:53:HIS:CG    | 1:C:57:MET:HE2   | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:111:ILE:HG23 | 1:D:121:VAL:HG11 | 1.92                     | 0.50              |
| 1:A:312:PHE:HE2  | 1:A:354:LEU:HD12 | 1.76                     | 0.50              |
| 1:B:272:ILE:HB   | 1:B:273:PRO:HD3  | 1.94                     | 0.50              |
| 1:C:345:ILE:HD13 | 1:D:352:ILE:HD12 | 1.93                     | 0.50              |
| 1:D:320:THR:O    | 1:D:321:HIS:CB   | 2.59                     | 0.50              |
| 1:A:350:ARG:HD2  | 3:A:1376:HOH:O   | 1.97                     | 0.50              |
| 1:D:122:ARG:HA   | 1:D:122:ARG:HH11 | 1.75                     | 0.50              |
| 1:A:205:CYS:SG   | 1:A:210:VAL:HG12 | 2.52                     | 0.50              |
| 1:A:345:ILE:HG23 | 1:A:354:LEU:CD2  | 2.42                     | 0.50              |
| 1:B:220:ASP:CG   | 1:B:223:LEU:HA   | 2.36                     | 0.50              |
| 1:C:191:VAL:HG12 | 1:C:192:GLY:O    | 2.11                     | 0.50              |
| 1:B:272:ILE:O    | 1:B:275:VAL:HG22 | 2.11                     | 0.50              |
| 1:C:234:ASP:OD2  | 1:C:235:GLN:N    | 2.45                     | 0.50              |
| 1:B:42:HIS:HD2   | 1:B:48:ALA:O     | 1.94                     | 0.50              |
| 1:C:6:MET:HE2    | 1:C:98:ALA:HB2   | 1.93                     | 0.50              |
| 1:D:358:PRO:O    | 1:D:359:THR:C    | 2.55                     | 0.50              |
| 1:B:125:ILE:H    | 1:B:125:ILE:CD1  | 2.15                     | 0.50              |
| 1:D:145:LEU:HD21 | 1:D:277:LYS:HE3  | 1.93                     | 0.50              |
| 1:D:105:LEU:N    | 3:D:1407:HOH:O   | 2.45                     | 0.50              |
| 1:C:32:LYS:NZ    | 3:C:1384:HOH:O   | 2.45                     | 0.49              |
| 1:D:246:ARG:HG3  | 1:D:246:ARG:HH11 | 1.77                     | 0.49              |
| 1:D:278:ILE:O    | 1:D:281:GLU:HB2  | 2.11                     | 0.49              |
| 1:A:2:GLU:OE2    | 1:A:2:GLU:N      | 2.46                     | 0.49              |
| 1:A:21:GLU:HG3   | 1:A:45:TYR:CG    | 2.47                     | 0.49              |
| 1:D:26:VAL:HG23  | 1:D:50:ALA:HB2   | 1.94                     | 0.49              |
| 1:D:226:PRO:C    | 1:D:228:ASP:H    | 2.19                     | 0.49              |
| 1:B:93:LYS:HG3   | 1:B:94:ARG:N     | 2.26                     | 0.49              |
| 1:C:352:ILE:HG22 | 1:C:354:LEU:HD21 | 1.94                     | 0.49              |
| 1:D:242:PHE:CE2  | 1:D:275:VAL:HG13 | 2.48                     | 0.49              |
| 1:B:315:LYS:NZ   | 3:B:1417:HOH:O   | 2.23                     | 0.49              |
| 1:A:105:LEU:HD12 | 1:A:105:LEU:O    | 2.13                     | 0.49              |
| 1:C:111:ILE:HD12 | 1:C:121:VAL:HG11 | 1.94                     | 0.49              |
| 1:C:358:PRO:C    | 1:C:359:THR:HG23 | 2.37                     | 0.49              |
| 1:A:243:THR:HG22 | 1:A:244:THR:H    | 1.78                     | 0.49              |
| 1:D:128:ASP:HB2  | 3:D:1401:HOH:O   | 2.13                     | 0.49              |
| 1:D:226:PRO:C    | 1:D:228:ASP:N    | 2.70                     | 0.49              |
| 1:C:31:VAL:HG13  | 1:C:66:ASP:HB2   | 1.93                     | 0.49              |
| 1:C:211:THR:O    | 1:C:211:THR:HG22 | 2.12                     | 0.49              |
| 1:A:125:ILE:HD12 | 1:A:125:ILE:H    | 1.77                     | 0.49              |
| 1:A:190:LEU:HD12 | 1:A:190:LEU:C    | 2.38                     | 0.49              |
| 1:B:71:LEU:HD22  | 1:B:72:GLU:H     | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:184:LYS:HZ3  | 1:B:207:LEU:HD12 | 1.78                     | 0.49              |
| 1:B:77:TYR:O     | 1:B:78:GLY:O     | 2.31                     | 0.48              |
| 1:C:173:GLU:O    | 1:C:177:GLN:HB2  | 2.13                     | 0.48              |
| 1:D:149:THR:CG2  | 1:D:309:ILE:HD13 | 2.43                     | 0.48              |
| 1:D:229:ALA:HA   | 1:D:233:CYS:SG   | 2.53                     | 0.48              |
| 1:D:234:ASP:O    | 1:D:234:ASP:OD1  | 2.31                     | 0.48              |
| 1:A:184:LYS:NZ   | 3:A:1448:HOH:O   | 2.36                     | 0.48              |
| 1:C:66:ASP:OD2   | 1:C:94:ARG:HG2   | 2.12                     | 0.48              |
| 1:D:251:LYS:HA   | 1:D:254:ARG:HB3  | 1.94                     | 0.48              |
| 1:B:210:VAL:HG21 | 1:B:213:GLN:HE21 | 1.77                     | 0.48              |
| 1:A:150:LEU:HB2  | 1:A:308:ILE:HD12 | 1.96                     | 0.48              |
| 1:B:258:PHE:N    | 1:B:258:PHE:CD1  | 2.81                     | 0.48              |
| 1:C:180:GLN:NE2  | 1:C:183:ARG:HD2  | 2.29                     | 0.48              |
| 1:D:223:LEU:HD22 | 1:D:251:LYS:CE   | 2.32                     | 0.48              |
| 1:A:82:PRO:HG2   | 1:A:85:GLU:HB2   | 1.94                     | 0.48              |
| 1:B:182:TYR:C    | 1:B:184:LYS:N    | 2.69                     | 0.48              |
| 1:B:268:GLU:CD   | 1:B:268:GLU:N    | 2.72                     | 0.48              |
| 1:D:140:PHE:HA   | 1:D:145:LEU:O    | 2.14                     | 0.48              |
| 1:B:184:LYS:NZ   | 1:B:207:LEU:HD12 | 2.28                     | 0.48              |
| 1:B:199:ASP:O    | 1:B:200:ASN:C    | 2.56                     | 0.48              |
| 1:C:173:GLU:HA   | 3:C:1381:HOH:O   | 2.12                     | 0.48              |
| 1:C:190:LEU:HD22 | 1:C:217:VAL:CG1  | 2.43                     | 0.48              |
| 1:C:352:ILE:HD13 | 1:D:345:ILE:HD12 | 1.94                     | 0.48              |
| 1:D:19:GLN:OE1   | 1:D:19:GLN:O     | 2.31                     | 0.48              |
| 1:D:82:PRO:HG2   | 1:D:85:GLU:HB2   | 1.96                     | 0.48              |
| 1:A:111:ILE:HG23 | 1:A:121:VAL:HG11 | 1.96                     | 0.48              |
| 1:A:197:LYS:NZ   | 3:A:1368:HOH:O   | 2.36                     | 0.48              |
| 1:C:119:ILE:HD12 | 1:C:119:ILE:N    | 2.28                     | 0.48              |
| 1:C:37:VAL:HG22  | 1:C:58:ALA:CA    | 2.38                     | 0.48              |
| 1:A:88:ILE:HD13  | 1:A:119:ILE:CD1  | 2.43                     | 0.48              |
| 1:A:222:VAL:HG13 | 1:A:222:VAL:O    | 2.13                     | 0.48              |
| 1:B:125:ILE:HD12 | 1:B:125:ILE:N    | 2.20                     | 0.48              |
| 1:B:309:ILE:HG12 | 1:B:355:THR:HB   | 1.95                     | 0.48              |
| 1:D:255:LEU:O    | 1:D:257:ALA:N    | 2.47                     | 0.48              |
| 1:B:73:PRO:HA    | 3:B:1363:HOH:O   | 2.12                     | 0.47              |
| 1:C:31:VAL:CG1   | 3:C:1362:HOH:O   | 2.52                     | 0.47              |
| 1:C:154:ALA:HB2  | 1:C:325:LEU:HD21 | 1.95                     | 0.47              |
| 1:A:1:MET:HE2    | 1:A:4:TYR:HB3    | 1.96                     | 0.47              |
| 1:B:148:VAL:H    | 1:B:306:GLN:NE2  | 2.03                     | 0.47              |
| 1:B:240:TRP:CD1  | 1:B:261:ASN:HB2  | 2.49                     | 0.47              |
| 1:B:312:PHE:CE2  | 1:B:354:LEU:HD12 | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:236:ILE:HG22 | 1:C:236:ILE:O    | 2.13                     | 0.47              |
| 1:A:190:LEU:HD12 | 1:A:191:VAL:N    | 2.28                     | 0.47              |
| 1:C:26:VAL:O     | 1:C:41:ALA:HA    | 2.15                     | 0.47              |
| 1:D:140:PHE:CE2  | 1:D:141:MET:HE2  | 2.49                     | 0.47              |
| 1:D:234:ASP:O    | 1:D:236:ILE:N    | 2.46                     | 0.47              |
| 1:D:272:ILE:HB   | 1:D:273:PRO:HD3  | 1.96                     | 0.47              |
| 1:B:187:GLN:NE2  | 1:B:285:MET:HE2  | 2.27                     | 0.47              |
| 1:D:200:ASN:ND2  | 1:D:230:LYS:CG   | 2.78                     | 0.47              |
| 1:D:230:LYS:C    | 1:D:232:ILE:N    | 2.72                     | 0.47              |
| 1:D:23:ASN:OD1   | 1:D:45:TYR:CD1   | 2.67                     | 0.47              |
| 1:D:193:VAL:CG1  | 1:D:220:ASP:HA   | 2.45                     | 0.47              |
| 1:A:272:ILE:HD13 | 1:A:298:SER:HB3  | 1.97                     | 0.47              |
| 1:B:93:LYS:HG3   | 1:B:94:ARG:HG3   | 1.97                     | 0.47              |
| 1:B:103:ASN:C    | 1:B:105:LEU:H    | 2.23                     | 0.47              |
| 1:B:106:VAL:HG22 | 1:B:109:ARG:HH21 | 1.79                     | 0.47              |
| 1:B:162:THR:C    | 1:B:164:THR:H    | 2.22                     | 0.47              |
| 1:B:182:TYR:C    | 1:B:184:LYS:H    | 2.21                     | 0.47              |
| 1:C:150:LEU:HD23 | 1:C:289:VAL:HB   | 1.97                     | 0.47              |
| 3:C:1393:HOH:O   | 1:D:334:MET:CG   | 2.41                     | 0.47              |
| 1:D:105:LEU:HD13 | 1:D:105:LEU:O    | 2.15                     | 0.47              |
| 1:D:151:LYS:HA   | 1:D:309:ILE:O    | 2.14                     | 0.47              |
| 1:D:170:ILE:HG23 | 1:D:171:THR:H    | 1.80                     | 0.47              |
| 1:D:190:LEU:CB   | 1:D:289:VAL:HG22 | 2.44                     | 0.47              |
| 1:D:245:ALA:C    | 3:D:1405:HOH:O   | 2.49                     | 0.47              |
| 1:D:300:VAL:HG21 | 1:D:326:ILE:CD1  | 2.42                     | 0.47              |
| 1:B:277:LYS:HE2  | 1:B:277:LYS:HB3  | 1.76                     | 0.47              |
| 1:C:97:VAL:O     | 1:C:123:GLU:HA   | 2.15                     | 0.47              |
| 1:B:8:LEU:O      | 1:B:12:LEU:HD13  | 2.15                     | 0.47              |
| 1:B:71:LEU:HD22  | 1:B:72:GLU:N     | 2.30                     | 0.47              |
| 1:C:31:VAL:HG12  | 1:C:66:ASP:HB2   | 1.95                     | 0.47              |
| 1:C:37:VAL:HG22  | 1:C:37:VAL:O     | 2.15                     | 0.47              |
| 1:D:193:VAL:HG13 | 1:D:219:LEU:O    | 2.15                     | 0.47              |
| 1:A:149:THR:OG1  | 1:A:186:HIS:HE1  | 1.98                     | 0.46              |
| 1:A:193:VAL:CG2  | 1:A:220:ASP:HA   | 2.44                     | 0.46              |
| 1:C:9:ALA:O      | 1:C:27:GLY:HA3   | 2.15                     | 0.46              |
| 1:C:277:LYS:NZ   | 1:C:281:GLU:OE2  | 2.41                     | 0.46              |
| 1:B:258:PHE:N    | 1:B:258:PHE:HD1  | 2.13                     | 0.46              |
| 1:C:105:LEU:H    | 1:C:105:LEU:CD2  | 2.23                     | 0.46              |
| 1:D:225:ILE:HD13 | 1:D:225:ILE:C    | 2.40                     | 0.46              |
| 1:A:308:ILE:HG23 | 1:A:308:ILE:O    | 2.15                     | 0.46              |
| 1:B:97:VAL:O     | 1:B:123:GLU:HA   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:126:LEU:HD12 | 1:B:126:LEU:N    | 2.31                     | 0.46              |
| 1:B:142:ARG:HG3  | 1:B:142:ARG:NH1  | 2.29                     | 0.46              |
| 1:C:84:ALA:HB3   | 1:C:113:MET:HE2  | 1.97                     | 0.46              |
| 1:D:222:VAL:O    | 1:D:223:LEU:C    | 2.59                     | 0.46              |
| 1:B:137:PHE:HD1  | 1:B:138:LEU:HD12 | 1.79                     | 0.46              |
| 1:A:67:ILE:HG22  | 1:A:92:ILE:HG21  | 1.98                     | 0.46              |
| 1:A:344:ASP:HB3  | 1:A:355:THR:CG2  | 2.39                     | 0.46              |
| 1:C:42:HIS:HB3   | 3:C:1378:HOH:O   | 2.13                     | 0.46              |
| 1:C:191:VAL:CG1  | 1:C:192:GLY:O    | 2.64                     | 0.46              |
| 1:B:101:ASP:OD2  | 1:B:102:PRO:HD2  | 2.16                     | 0.46              |
| 1:D:252:LYS:O    | 1:D:262:ILE:HD13 | 2.16                     | 0.46              |
| 1:B:105:LEU:HD12 | 1:B:105:LEU:N    | 2.30                     | 0.46              |
| 1:B:222:VAL:O    | 1:B:222:VAL:CG1  | 2.62                     | 0.46              |
| 1:B:329:GLU:CB   | 3:B:1377:HOH:O   | 2.63                     | 0.46              |
| 1:B:102:PRO:O    | 1:B:104:PRO:HD3  | 2.16                     | 0.46              |
| 1:C:188:SER:O    | 1:C:189:ILE:HD13 | 2.16                     | 0.46              |
| 1:A:212:LYS:N    | 3:A:1441:HOH:O   | 2.49                     | 0.45              |
| 1:D:270:ILE:HG12 | 1:D:270:ILE:O    | 2.15                     | 0.45              |
| 1:A:155:SER:HB3  | 1:A:317:ILE:CD1  | 2.45                     | 0.45              |
| 1:C:37:VAL:CG2   | 1:C:58:ALA:HA    | 2.41                     | 0.45              |
| 1:C:76:HIS:C     | 1:C:82:PRO:HG3   | 2.41                     | 0.45              |
| 1:C:252:LYS:NZ   | 1:C:264:THR:OG1  | 2.46                     | 0.45              |
| 1:B:31:VAL:O     | 1:B:65:ALA:HB1   | 2.17                     | 0.45              |
| 1:D:196:VAL:HG11 | 1:D:225:ILE:HG12 | 1.99                     | 0.45              |
| 1:C:207:LEU:HA   | 1:C:208:PRO:HD3  | 1.82                     | 0.45              |
| 1:C:342:PHE:CE2  | 1:D:352:ILE:HG12 | 2.51                     | 0.45              |
| 1:D:236:ILE:O    | 1:D:237:ALA:HB2  | 2.16                     | 0.45              |
| 1:A:207:LEU:N    | 1:A:210:VAL:HG11 | 2.32                     | 0.45              |
| 1:B:196:VAL:HG21 | 1:B:218:ILE:HD13 | 1.97                     | 0.45              |
| 1:C:150:LEU:CD2  | 1:C:289:VAL:HB   | 2.47                     | 0.45              |
| 1:C:157:ASP:OD1  | 1:C:316:LEU:HA   | 2.17                     | 0.45              |
| 1:D:201:PRO:C    | 1:D:203:LEU:HD22 | 2.42                     | 0.45              |
| 1:D:230:LYS:C    | 1:D:232:ILE:H    | 2.24                     | 0.45              |
| 1:A:211:THR:HG22 | 1:A:212:LYS:N    | 2.32                     | 0.45              |
| 1:B:125:ILE:CG2  | 1:B:126:LEU:HD13 | 2.43                     | 0.45              |
| 1:B:177:GLN:CG   | 3:B:1397:HOH:O   | 2.54                     | 0.45              |
| 1:D:99:MET:HE1   | 1:D:138:LEU:CD2  | 2.43                     | 0.45              |
| 1:D:343:THR:HG21 | 1:D:357:LYS:HD2  | 1.99                     | 0.45              |
| 1:D:347:GLN:HG3  | 1:D:352:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:223:LEU:HD22 | 1:B:247:ALA:HB1  | 1.98                     | 0.45              |
| 1:C:16:GLY:O     | 1:C:17:GLU:C     | 2.60                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:181:GLN:HA   | 1:D:207:LEU:HD12 | 1.99                     | 0.45              |
| 1:B:272:ILE:O    | 1:B:275:VAL:CG2  | 2.64                     | 0.45              |
| 1:A:88:ILE:CD1   | 1:A:114:MET:HA   | 2.38                     | 0.45              |
| 1:A:115:LYS:NZ   | 3:A:1415:HOH:O   | 2.48                     | 0.45              |
| 1:A:207:LEU:H    | 1:A:210:VAL:HG11 | 1.82                     | 0.45              |
| 1:B:164:THR:O    | 1:B:164:THR:CG2  | 2.64                     | 0.45              |
| 1:D:193:VAL:HG13 | 1:D:220:ASP:HA   | 1.98                     | 0.45              |
| 1:C:105:LEU:HG   | 1:C:106:VAL:H    | 1.82                     | 0.45              |
| 1:C:32:LYS:HD3   | 1:C:65:ALA:HB2   | 1.99                     | 0.44              |
| 1:C:181:GLN:CG   | 1:C:182:TYR:N    | 2.78                     | 0.44              |
| 1:D:256:SER:HB2  | 1:D:262:ILE:HD13 | 1.98                     | 0.44              |
| 1:D:301:LYS:HE2  | 1:D:301:LYS:C    | 2.41                     | 0.44              |
| 1:C:334:MET:HA   | 1:C:337:VAL:HG13 | 1.99                     | 0.44              |
| 1:D:99:MET:HE1   | 1:D:138:LEU:CG   | 2.48                     | 0.44              |
| 1:D:177:GLN:HE21 | 1:D:177:GLN:HB3  | 1.61                     | 0.44              |
| 1:D:281:GLU:C    | 1:D:283:GLY:H    | 2.24                     | 0.44              |
| 1:A:350:ARG:NE   | 3:A:1376:HOH:O   | 2.47                     | 0.44              |
| 1:B:103:ASN:C    | 1:B:103:ASN:HD22 | 2.25                     | 0.44              |
| 1:B:181:GLN:O    | 1:B:184:LYS:HB3  | 2.17                     | 0.44              |
| 1:B:243:THR:CG2  | 1:B:244:THR:H    | 2.21                     | 0.44              |
| 1:D:71:LEU:HD22  | 1:D:72:GLU:H     | 1.83                     | 0.44              |
| 1:A:8:LEU:HD11   | 1:A:39:MET:CE    | 2.47                     | 0.44              |
| 1:A:222:VAL:O    | 1:A:222:VAL:CG1  | 2.65                     | 0.44              |
| 1:A:347:GLN:HG2  | 1:A:352:ILE:HG12 | 2.00                     | 0.44              |
| 1:B:298:SER:O    | 1:B:302:GLU:HG2  | 2.18                     | 0.44              |
| 1:C:17:GLU:O     | 1:C:19:GLN:HG3   | 2.18                     | 0.44              |
| 1:C:223:LEU:CG   | 1:C:243:THR:HG21 | 2.47                     | 0.44              |
| 1:A:47:GLU:OE2   | 1:C:61:HIS:HE1   | 2.01                     | 0.44              |
| 1:B:9:ALA:O      | 1:B:27:GLY:HA3   | 2.17                     | 0.44              |
| 1:B:134:ASN:O    | 1:B:138:LEU:HD13 | 2.18                     | 0.44              |
| 1:B:206:ARG:HB2  | 1:B:206:ARG:NH1  | 2.32                     | 0.44              |
| 1:B:209:ASN:CG   | 1:B:209:ASN:O    | 2.60                     | 0.44              |
| 1:B:311:TYR:CE1  | 1:B:353:LYS:HD2  | 2.53                     | 0.44              |
| 1:D:26:VAL:HG23  | 1:D:50:ALA:CB    | 2.48                     | 0.44              |
| 1:C:25:LEU:H     | 1:C:134:ASN:HD21 | 1.66                     | 0.44              |
| 1:C:136:LYS:HG2  | 1:C:147:TYR:CG   | 2.53                     | 0.44              |
| 1:D:22:SER:HA    | 1:D:285:MET:HE1  | 1.98                     | 0.44              |
| 1:D:231:VAL:HB   | 1:D:239:THR:HG21 | 2.00                     | 0.44              |
| 1:D:252:LYS:NZ   | 1:D:252:LYS:HB2  | 2.32                     | 0.44              |
| 1:A:188:SER:O    | 1:A:189:ILE:HD13 | 2.18                     | 0.44              |
| 1:A:243:THR:CG2  | 1:A:247:ALA:HB2  | 2.43                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:67:ILE:HB    | 1:B:92:ILE:HD13  | 1.99                     | 0.44              |
| 1:C:14:LYS:O     | 1:C:17:GLU:HB2   | 2.17                     | 0.44              |
| 1:C:23:ASN:HD21  | 1:C:46:GLY:H     | 1.65                     | 0.44              |
| 1:C:88:ILE:HG13  | 1:C:89:ASN:N     | 2.32                     | 0.44              |
| 1:C:180:GLN:HE22 | 1:C:183:ARG:HD2  | 1.83                     | 0.44              |
| 1:D:223:LEU:CD2  | 1:D:225:ILE:HG22 | 2.47                     | 0.44              |
| 1:A:25:LEU:N     | 1:A:134:ASN:HD21 | 2.01                     | 0.43              |
| 1:B:105:LEU:N    | 1:B:105:LEU:CD1  | 2.81                     | 0.43              |
| 1:B:148:VAL:HG22 | 1:B:287:VAL:HG13 | 1.99                     | 0.43              |
| 1:B:184:LYS:NZ   | 1:B:207:LEU:HB2  | 2.09                     | 0.43              |
| 1:B:233:CYS:O    | 1:B:235:GLN:N    | 2.51                     | 0.43              |
| 1:D:155:SER:HB3  | 1:D:317:ILE:HG13 | 2.00                     | 0.43              |
| 1:B:115:LYS:C    | 1:B:117:ALA:H    | 2.25                     | 0.43              |
| 1:D:95:VAL:HG23  | 1:D:119:ILE:HG21 | 1.99                     | 0.43              |
| 1:D:22:SER:HA    | 1:D:285:MET:CE   | 2.48                     | 0.43              |
| 1:A:180:GLN:OE1  | 1:A:206:ARG:N    | 2.43                     | 0.43              |
| 1:B:184:LYS:O    | 1:B:184:LYS:HG3  | 2.19                     | 0.43              |
| 1:B:206:ARG:HB2  | 1:B:206:ARG:CZ   | 2.48                     | 0.43              |
| 1:C:8:LEU:O      | 1:C:12:LEU:HD13  | 2.19                     | 0.43              |
| 1:D:45:TYR:CD2   | 1:D:45:TYR:C     | 2.96                     | 0.43              |
| 1:A:53:HIS:HB3   | 1:C:57:MET:CE    | 2.48                     | 0.43              |
| 1:A:137:PHE:HD1  | 1:A:138:LEU:HD13 | 1.83                     | 0.43              |
| 1:A:357:LYS:NZ   | 3:A:1405:HOH:O   | 2.51                     | 0.43              |
| 1:B:329:GLU:OE1  | 1:B:329:GLU:HA   | 2.18                     | 0.43              |
| 1:D:256:SER:HB2  | 1:D:262:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:213:GLN:NE2  | 1:A:214:PRO:HD2  | 2.33                     | 0.43              |
| 1:D:350:ARG:NH1  | 3:D:1411:HOH:O   | 2.48                     | 0.43              |
| 1:D:231:VAL:O    | 1:D:239:THR:HG21 | 2.19                     | 0.43              |
| 1:B:43:LEU:HD22  | 1:B:43:LEU:N     | 2.34                     | 0.43              |
| 1:B:205:CYS:HB3  | 1:B:213:GLN:HE22 | 1.83                     | 0.43              |
| 1:C:95:VAL:HG12  | 1:C:121:VAL:HG22 | 1.99                     | 0.43              |
| 1:D:190:LEU:HD11 | 1:D:219:LEU:HG   | 2.00                     | 0.43              |
| 1:A:223:LEU:HB2  | 1:A:243:THR:HG21 | 2.00                     | 0.43              |
| 1:D:174:ALA:O    | 1:D:177:GLN:HB3  | 2.18                     | 0.43              |
| 1:A:6:MET:O      | 1:A:9:ALA:HB3    | 2.19                     | 0.42              |
| 1:A:76:HIS:O     | 1:A:82:PRO:HB3   | 2.19                     | 0.42              |
| 1:A:292:GLY:CA   | 3:A:1377:HOH:O   | 2.67                     | 0.42              |
| 1:B:200:ASN:O    | 1:B:200:ASN:CG   | 2.62                     | 0.42              |
| 1:C:7:LYS:HA     | 1:C:7:LYS:HD2    | 1.84                     | 0.42              |
| 1:C:148:VAL:HB   | 1:C:305:PHE:HA   | 2.00                     | 0.42              |
| 1:D:9:ALA:HA     | 1:D:12:LEU:HD12  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:311:TYR:OH   | 1:A:353:LYS:HE2  | 2.19                     | 0.42              |
| 1:B:250:GLU:O    | 1:B:254:ARG:HB2  | 2.20                     | 0.42              |
| 1:C:10:LEU:O     | 1:C:13:ALA:HB3   | 2.19                     | 0.42              |
| 1:D:99:MET:HE1   | 1:D:138:LEU:CD1  | 2.48                     | 0.42              |
| 1:D:170:ILE:CG2  | 1:D:171:THR:N    | 2.80                     | 0.42              |
| 1:A:53:HIS:HB3   | 1:C:57:MET:HE2   | 2.01                     | 0.42              |
| 1:B:232:ILE:HD12 | 1:B:255:LEU:HD22 | 2.01                     | 0.42              |
| 1:C:190:LEU:CD1  | 1:C:190:LEU:C    | 2.92                     | 0.42              |
| 1:C:206:ARG:O    | 1:C:207:LEU:C    | 2.62                     | 0.42              |
| 1:C:257:ALA:C    | 1:C:259:GLY:H    | 2.27                     | 0.42              |
| 1:D:230:LYS:O    | 1:D:231:VAL:C    | 2.61                     | 0.42              |
| 1:D:237:ALA:HB1  | 1:D:238:PRO:CD   | 2.49                     | 0.42              |
| 1:A:138:LEU:HD12 | 1:A:138:LEU:HA   | 1.79                     | 0.42              |
| 1:C:151:LYS:HD2  | 1:C:152:ALA:N    | 2.33                     | 0.42              |
| 1:C:193:VAL:CG1  | 1:C:220:ASP:CG   | 2.91                     | 0.42              |
| 1:D:51:GLU:O     | 1:D:55:ILE:HG13  | 2.20                     | 0.42              |
| 1:D:181:GLN:CG   | 1:D:182:TYR:N    | 2.82                     | 0.42              |
| 1:A:106:VAL:O    | 1:A:109:ARG:HB2  | 2.19                     | 0.42              |
| 1:B:296:HIS:HB3  | 1:B:326:ILE:CD1  | 2.50                     | 0.42              |
| 1:D:309:ILE:HD12 | 1:D:309:ILE:N    | 2.35                     | 0.42              |
| 1:A:36:ILE:CD1   | 1:C:15:GLN:HG3   | 2.50                     | 0.42              |
| 1:A:95:VAL:HG23  | 1:A:119:ILE:CG2  | 2.50                     | 0.42              |
| 1:A:168:LYS:O    | 1:B:334:MET:HG3  | 2.20                     | 0.42              |
| 1:B:178:ASP:O    | 1:B:181:GLN:HG2  | 2.20                     | 0.42              |
| 1:C:72:GLU:HA    | 1:C:73:PRO:HD3   | 1.92                     | 0.42              |
| 1:D:103:ASN:C    | 1:D:105:LEU:H    | 2.28                     | 0.42              |
| 1:A:334:MET:HE2  | 1:B:170:ILE:HA   | 2.01                     | 0.42              |
| 1:C:169:TRP:O    | 1:C:170:ILE:C    | 2.63                     | 0.42              |
| 1:B:28:ALA:HA    | 1:B:68:TYR:O     | 2.20                     | 0.41              |
| 1:B:111:ILE:HD12 | 1:B:123:GLU:OE1  | 2.20                     | 0.41              |
| 1:B:164:THR:O    | 1:B:164:THR:HG23 | 2.18                     | 0.41              |
| 1:B:329:GLU:HB3  | 3:B:1377:HOH:O   | 2.20                     | 0.41              |
| 1:C:253:LYS:HE3  | 1:C:253:LYS:HB2  | 1.91                     | 0.41              |
| 1:C:205:CYS:HB3  | 1:C:210:VAL:HG11 | 2.01                     | 0.41              |
| 1:B:205:CYS:O    | 1:B:210:VAL:HG11 | 2.21                     | 0.41              |
| 1:B:223:LEU:HB2  | 1:B:243:THR:HG21 | 2.03                     | 0.41              |
| 1:D:143:THR:C    | 1:D:145:LEU:N    | 2.74                     | 0.41              |
| 1:B:200:ASN:N    | 1:B:201:PRO:CD   | 2.84                     | 0.41              |
| 1:C:75:SER:HA    | 1:C:82:PRO:HB3   | 2.02                     | 0.41              |
| 1:A:35:GLN:OE1   | 1:C:44:LYS:NZ    | 2.43                     | 0.41              |
| 1:A:317:ILE:HG22 | 1:A:318:GLY:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:327:SER:HB3  | 1:C:328:GLY:H    | 1.63                     | 0.41              |
| 1:D:154:ALA:HB2  | 1:D:160:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:39:MET:CE    | 1:C:15:GLN:HG2   | 2.49                     | 0.41              |
| 1:A:103:ASN:HA   | 1:A:104:PRO:HD3  | 1.91                     | 0.41              |
| 1:B:171:THR:OG1  | 1:B:175:ALA:HB3  | 2.21                     | 0.41              |
| 1:D:29:VAL:HA    | 1:D:38:GLY:O     | 2.20                     | 0.41              |
| 1:D:208:PRO:O    | 1:D:209:ASN:CB   | 2.67                     | 0.41              |
| 1:A:1:MET:HE2    | 1:A:4:TYR:CB     | 2.51                     | 0.41              |
| 1:D:136:LYS:HE3  | 1:D:185:THR:O    | 2.20                     | 0.41              |
| 1:B:190:LEU:HA   | 1:B:217:VAL:O    | 2.20                     | 0.41              |
| 1:B:233:CYS:C    | 1:B:235:GLN:H    | 2.29                     | 0.41              |
| 1:C:37:VAL:O     | 1:C:37:VAL:CG2   | 2.69                     | 0.41              |
| 1:C:190:LEU:C    | 1:C:190:LEU:HD12 | 2.45                     | 0.41              |
| 1:B:12:LEU:CD2   | 1:B:39:MET:HB3   | 2.51                     | 0.41              |
| 1:B:65:ALA:O     | 1:B:92:ILE:HG23  | 2.20                     | 0.41              |
| 1:B:103:ASN:O    | 1:B:105:LEU:N    | 2.53                     | 0.41              |
| 1:B:253:LYS:HB3  | 1:B:253:LYS:HE2  | 1.90                     | 0.41              |
| 1:C:128:ASP:O    | 1:C:131:GLU:HB3  | 2.21                     | 0.41              |
| 1:C:234:ASP:OD2  | 1:C:234:ASP:C    | 2.64                     | 0.41              |
| 1:C:276:LEU:HD23 | 1:C:276:LEU:HA   | 1.91                     | 0.41              |
| 1:D:263:PHE:CD1  | 1:D:263:PHE:N    | 2.88                     | 0.41              |
| 1:D:266:GLU:CD   | 1:D:266:GLU:N    | 2.71                     | 0.41              |
| 1:B:103:ASN:C    | 1:B:105:LEU:N    | 2.76                     | 0.41              |
| 1:C:42:HIS:CA    | 3:C:1378:HOH:O   | 2.69                     | 0.41              |
| 1:D:2:GLU:H      | 1:D:2:GLU:HG2    | 1.53                     | 0.41              |
| 1:D:122:ARG:NH1  | 3:D:1365:HOH:O   | 2.53                     | 0.41              |
| 1:D:210:VAL:HG23 | 1:D:210:VAL:O    | 2.20                     | 0.41              |
| 1:A:312:PHE:CE2  | 1:A:354:LEU:HD12 | 2.54                     | 0.40              |
| 1:C:90:SER:HG    | 1:C:92:ILE:HG12  | 1.87                     | 0.40              |
| 1:C:169:TRP:HZ3  | 1:D:335:LYS:N    | 2.19                     | 0.40              |
| 1:C:326:ILE:HG12 | 1:D:157:ASP:HB2  | 2.03                     | 0.40              |
| 1:A:1:MET:HA     | 1:A:1:MET:CE     | 2.51                     | 0.40              |
| 1:A:29:VAL:O     | 1:A:29:VAL:HG23  | 2.20                     | 0.40              |
| 1:B:161:ALA:HB3  | 1:B:323:PRO:HG3  | 2.02                     | 0.40              |
| 1:D:143:THR:C    | 1:D:145:LEU:H    | 2.29                     | 0.40              |
| 1:D:176:ARG:HE   | 1:D:176:ARG:HB3  | 1.63                     | 0.40              |
| 1:A:125:ILE:H    | 1:A:125:ILE:CD1  | 2.34                     | 0.40              |
| 1:A:345:ILE:HG23 | 1:A:354:LEU:HD23 | 2.02                     | 0.40              |
| 1:B:103:ASN:ND2  | 1:B:103:ASN:C    | 2.79                     | 0.40              |
| 1:C:29:VAL:O     | 1:C:29:VAL:HG22  | 2.20                     | 0.40              |
| 1:C:37:VAL:HG23  | 3:C:1372:HOH:O   | 2.20                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:200:ASN:N    | 1:A:201:PRO:CD  | 2.84                     | 0.40              |
| 1:B:314:PRO:HD3  | 1:B:351:ASP:OD2 | 2.22                     | 0.40              |
| 1:B:244:THR:HB   | 3:B:1404:HOH:O  | 2.20                     | 0.40              |
| 1:C:184:LYS:CB   | 1:C:184:LYS:NZ  | 2.85                     | 0.40              |
| 1:C:223:LEU:HD23 | 1:C:223:LEU:HA  | 1.89                     | 0.40              |
| 1:C:314:PRO:HG3  | 1:D:342:PHE:CD2 | 2.57                     | 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     | 357/373 (96%)   | 336 (94%)  | 19 (5%)  | 2 (1%)   | 21          | 30 |
| 1   | B     | 357/373 (96%)   | 320 (90%)  | 28 (8%)  | 9 (2%)   | 4           | 4  |
| 1   | C     | 357/373 (96%)   | 332 (93%)  | 21 (6%)  | 4 (1%)   | 11          | 16 |
| 1   | D     | 358/373 (96%)   | 310 (87%)  | 35 (10%) | 13 (4%)  | 2           | 2  |
| All | All   | 1429/1492 (96%) | 1298 (91%) | 103 (7%) | 28 (2%)  | 6           | 7  |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 208 | PRO  |
| 1   | B     | 78  | GLY  |
| 1   | B     | 168 | LYS  |
| 1   | B     | 234 | ASP  |
| 1   | B     | 235 | GLN  |
| 1   | C     | 212 | LYS  |
| 1   | D     | 235 | GLN  |
| 1   | D     | 246 | ARG  |
| 1   | B     | 208 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 212 | LYS  |
| 1   | C     | 170 | ILE  |
| 1   | D     | 231 | VAL  |
| 1   | D     | 329 | GLU  |
| 1   | A     | 211 | THR  |
| 1   | B     | 209 | ASN  |
| 1   | C     | 17  | GLU  |
| 1   | D     | 259 | GLY  |
| 1   | D     | 282 | GLU  |
| 1   | B     | 107 | ALA  |
| 1   | D     | 209 | ASN  |
| 1   | D     | 212 | LYS  |
| 1   | D     | 256 | SER  |
| 1   | C     | 208 | PRO  |
| 1   | D     | 221 | THR  |
| 1   | D     | 245 | ALA  |
| 1   | D     | 18  | GLY  |
| 1   | D     | 262 | ILE  |
| 1   | B     | 104 | PRO  |

### 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     | 293/305 (96%)   | 269 (92%)  | 24 (8%)  | 10          | 17 |
| 1   | B     | 293/305 (96%)   | 269 (92%)  | 24 (8%)  | 10          | 17 |
| 1   | C     | 293/305 (96%)   | 262 (89%)  | 31 (11%) | 6           | 9  |
| 1   | D     | 294/305 (96%)   | 265 (90%)  | 29 (10%) | 7           | 11 |
| All | All   | 1173/1220 (96%) | 1065 (91%) | 108 (9%) | 8           | 13 |

All (108) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 2   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | GLU  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 69  | VAL  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 86  | LEU  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 171 | THR  |
| 1   | A     | 190 | LEU  |
| 1   | A     | 193 | VAL  |
| 1   | A     | 222 | VAL  |
| 1   | A     | 223 | LEU  |
| 1   | A     | 231 | VAL  |
| 1   | A     | 243 | THR  |
| 1   | A     | 267 | THR  |
| 1   | A     | 281 | GLU  |
| 1   | A     | 301 | LYS  |
| 1   | A     | 337 | VAL  |
| 1   | A     | 340 | LEU  |
| 1   | A     | 343 | THR  |
| 1   | A     | 347 | GLN  |
| 1   | A     | 350 | ARG  |
| 1   | A     | 355 | THR  |
| 1   | B     | 12  | LEU  |
| 1   | B     | 25  | LEU  |
| 1   | B     | 71  | LEU  |
| 1   | B     | 80  | THR  |
| 1   | B     | 116 | GLU  |
| 1   | B     | 123 | GLU  |
| 1   | B     | 128 | ASP  |
| 1   | B     | 138 | LEU  |
| 1   | B     | 164 | THR  |
| 1   | B     | 184 | LYS  |
| 1   | B     | 212 | LYS  |
| 1   | B     | 225 | ILE  |
| 1   | B     | 228 | ASP  |
| 1   | B     | 234 | ASP  |
| 1   | B     | 248 | ASP  |
| 1   | B     | 254 | ARG  |
| 1   | B     | 258 | PHE  |
| 1   | B     | 268 | GLU  |
| 1   | B     | 287 | VAL  |
| 1   | B     | 308 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 320 | THR  |
| 1   | B     | 324 | SER  |
| 1   | B     | 343 | THR  |
| 1   | B     | 355 | THR  |
| 1   | C     | 3   | GLU  |
| 1   | C     | 8   | LEU  |
| 1   | C     | 25  | LEU  |
| 1   | C     | 29  | VAL  |
| 1   | C     | 37  | VAL  |
| 1   | C     | 63  | GLU  |
| 1   | C     | 76  | HIS  |
| 1   | C     | 93  | LYS  |
| 1   | C     | 105 | LEU  |
| 1   | C     | 128 | ASP  |
| 1   | C     | 129 | GLN  |
| 1   | C     | 173 | GLU  |
| 1   | C     | 184 | LYS  |
| 1   | C     | 190 | LEU  |
| 1   | C     | 191 | VAL  |
| 1   | C     | 193 | VAL  |
| 1   | C     | 209 | ASN  |
| 1   | C     | 222 | VAL  |
| 1   | C     | 223 | LEU  |
| 1   | C     | 231 | VAL  |
| 1   | C     | 235 | GLN  |
| 1   | C     | 243 | THR  |
| 1   | C     | 269 | ARG  |
| 1   | C     | 271 | GLN  |
| 1   | C     | 287 | VAL  |
| 1   | C     | 308 | ILE  |
| 1   | C     | 327 | SER  |
| 1   | C     | 337 | VAL  |
| 1   | C     | 354 | LEU  |
| 1   | C     | 355 | THR  |
| 1   | C     | 359 | THR  |
| 1   | D     | 2   | GLU  |
| 1   | D     | 7   | LYS  |
| 1   | D     | 19  | GLN  |
| 1   | D     | 25  | LEU  |
| 1   | D     | 29  | VAL  |
| 1   | D     | 31  | VAL  |
| 1   | D     | 69  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 71  | LEU  |
| 1   | D     | 86  | LEU  |
| 1   | D     | 122 | ARG  |
| 1   | D     | 138 | LEU  |
| 1   | D     | 171 | THR  |
| 1   | D     | 177 | GLN  |
| 1   | D     | 181 | GLN  |
| 1   | D     | 190 | LEU  |
| 1   | D     | 191 | VAL  |
| 1   | D     | 199 | ASP  |
| 1   | D     | 207 | LEU  |
| 1   | D     | 221 | THR  |
| 1   | D     | 223 | LEU  |
| 1   | D     | 225 | ILE  |
| 1   | D     | 227 | GLU  |
| 1   | D     | 243 | THR  |
| 1   | D     | 251 | LYS  |
| 1   | D     | 252 | LYS  |
| 1   | D     | 270 | ILE  |
| 1   | D     | 301 | LYS  |
| 1   | D     | 326 | ILE  |
| 1   | D     | 355 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 19  | GLN  |
| 1   | A     | 23  | ASN  |
| 1   | A     | 42  | HIS  |
| 1   | A     | 53  | HIS  |
| 1   | A     | 134 | ASN  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 186 | HIS  |
| 1   | A     | 209 | ASN  |
| 1   | A     | 213 | GLN  |
| 1   | A     | 235 | GLN  |
| 1   | A     | 296 | HIS  |
| 1   | A     | 321 | HIS  |
| 1   | A     | 341 | GLN  |
| 1   | B     | 23  | ASN  |
| 1   | B     | 42  | HIS  |
| 1   | B     | 103 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 134 | ASN  |
| 1   | B     | 181 | GLN  |
| 1   | B     | 186 | HIS  |
| 1   | B     | 306 | GLN  |
| 1   | B     | 341 | GLN  |
| 1   | B     | 347 | GLN  |
| 1   | C     | 15  | GLN  |
| 1   | C     | 23  | ASN  |
| 1   | C     | 35  | GLN  |
| 1   | C     | 42  | HIS  |
| 1   | C     | 53  | HIS  |
| 1   | C     | 56  | HIS  |
| 1   | C     | 61  | HIS  |
| 1   | C     | 89  | ASN  |
| 1   | C     | 180 | GLN  |
| 1   | C     | 209 | ASN  |
| 1   | C     | 271 | GLN  |
| 1   | C     | 341 | GLN  |
| 1   | D     | 53  | HIS  |
| 1   | D     | 89  | ASN  |
| 1   | D     | 134 | ASN  |
| 1   | D     | 177 | GLN  |
| 1   | D     | 180 | GLN  |
| 1   | D     | 181 | GLN  |
| 1   | D     | 186 | HIS  |
| 1   | D     | 306 | GLN  |
| 1   | D     | 321 | HIS  |
| 1   | D     | 347 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 359/373 (96%)   | -0.14  | 6 (1%) 69 66  | 18, 36, 57, 71        | 0     |
| 1   | B     | 359/373 (96%)   | 0.21   | 10 (2%) 55 51 | 22, 45, 72, 95        | 0     |
| 1   | C     | 359/373 (96%)   | 0.24   | 16 (4%) 38 34 | 25, 45, 69, 93        | 0     |
| 1   | D     | 360/373 (96%)   | 0.48   | 30 (8%) 17 14 | 25, 50, 92, 99        | 0     |
| All | All   | 1437/1492 (96%) | 0.20   | 62 (4%) 40 35 | 18, 43, 80, 99        | 0     |

All (62) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 207 | LEU  | 4.9  |
| 1   | B     | 208 | PRO  | 4.3  |
| 1   | D     | 262 | ILE  | 4.1  |
| 1   | D     | 208 | PRO  | 3.7  |
| 1   | B     | 207 | LEU  | 3.7  |
| 1   | B     | 77  | TYR  | 3.7  |
| 1   | C     | 291 | GLY  | 3.6  |
| 1   | D     | 270 | ILE  | 3.5  |
| 1   | C     | 76  | HIS  | 3.4  |
| 1   | C     | 210 | VAL  | 3.3  |
| 1   | B     | 210 | VAL  | 3.3  |
| 1   | B     | 291 | GLY  | 3.2  |
| 1   | C     | 169 | TRP  | 3.2  |
| 1   | C     | 208 | PRO  | 3.2  |
| 1   | D     | 222 | VAL  | 3.1  |
| 1   | C     | 211 | THR  | 3.0  |
| 1   | D     | 245 | ALA  | 3.0  |
| 1   | D     | 255 | LEU  | 2.9  |
| 1   | A     | 208 | PRO  | 2.7  |
| 1   | A     | 211 | THR  | 2.7  |
| 1   | D     | 210 | VAL  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 229 | ALA  | 2.7  |
| 1   | B     | 211 | THR  | 2.7  |
| 1   | C     | 1   | MET  | 2.7  |
| 1   | A     | 210 | VAL  | 2.6  |
| 1   | A     | 132 | ARG  | 2.6  |
| 1   | B     | 78  | GLY  | 2.6  |
| 1   | D     | 225 | ILE  | 2.6  |
| 1   | C     | 207 | LEU  | 2.6  |
| 1   | D     | 209 | ASN  | 2.5  |
| 1   | B     | 169 | TRP  | 2.4  |
| 1   | D     | 211 | THR  | 2.4  |
| 1   | D     | 203 | LEU  | 2.4  |
| 1   | C     | 209 | ASN  | 2.4  |
| 1   | D     | 169 | TRP  | 2.3  |
| 1   | C     | 235 | GLN  | 2.3  |
| 1   | D     | 221 | THR  | 2.3  |
| 1   | D     | 243 | THR  | 2.3  |
| 1   | A     | 359 | THR  | 2.3  |
| 1   | D     | 252 | LYS  | 2.3  |
| 1   | D     | 19  | GLN  | 2.2  |
| 1   | B     | 209 | ASN  | 2.2  |
| 1   | C     | 345 | ILE  | 2.2  |
| 1   | C     | 106 | VAL  | 2.2  |
| 1   | C     | 105 | LEU  | 2.2  |
| 1   | D     | 233 | CYS  | 2.2  |
| 1   | D     | 177 | GLN  | 2.1  |
| 1   | D     | 249 | GLU  | 2.1  |
| 1   | D     | 260 | VAL  | 2.1  |
| 1   | C     | 125 | ILE  | 2.1  |
| 1   | C     | 176 | ARG  | 2.1  |
| 1   | D     | 176 | ARG  | 2.1  |
| 1   | D     | 218 | ILE  | 2.1  |
| 1   | C     | 77  | TYR  | 2.1  |
| 1   | D     | 231 | VAL  | 2.1  |
| 1   | A     | 318 | GLY  | 2.1  |
| 1   | D     | 227 | GLU  | 2.1  |
| 1   | D     | 235 | GLN  | 2.0  |
| 1   | B     | 80  | THR  | 2.0  |
| 1   | D     | 258 | PHE  | 2.0  |
| 1   | D     | 247 | ALA  | 2.0  |
| 1   | D     | 329 | GLU  | 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   | ZN   | C     | 1360 | 1/1   | 0.98 | 0.04 | 51,51,51,51                 | 0     |
| 2   | ZN   | B     | 1360 | 1/1   | 0.99 | 0.02 | 44,44,44,44                 | 0     |
| 2   | ZN   | A     | 1360 | 1/1   | 0.99 | 0.02 | 31,31,31,31                 | 0     |
| 2   | ZN   | D     | 1360 | 1/1   | 0.99 | 0.06 | 41,41,41,41                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.