



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:11 PM UTC

PDB ID : 2RJB / pdb\_00002rjb  
Title : Crystal structure of uncharacterized protein YdcJ (SF1787) from *Shigella flexneri* which includes domain DUF1338. Northeast Structural Genomics Consortium target Sfr276  
Authors : Seetharaman, J.; Chen, Y.; Wang, D.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xia, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2007-10-14  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

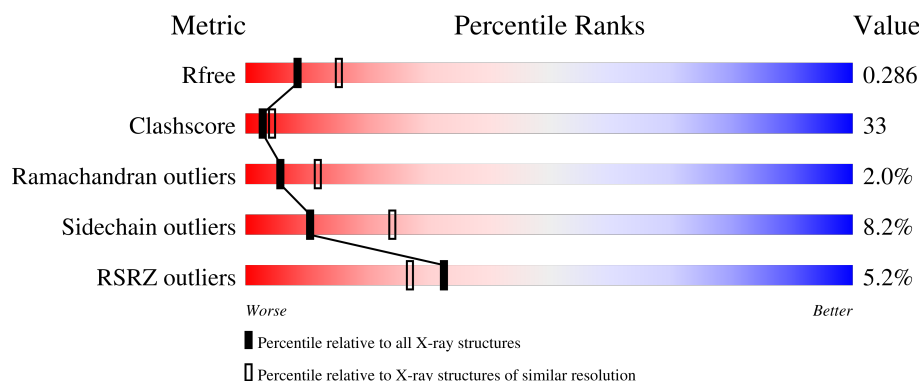
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

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     | 455    | <div> <div>0%</div> <div>51% 34% 6% 8%</div> </div>   |
| 1   | B     | 455    | <div> <div>3%</div> <div>48% 37% 6% 8%</div> </div>   |
| 1   | C     | 455    | <div> <div>3%</div> <div>37% 36% 7% 20%</div> </div>  |
| 1   | D     | 455    | <div> <div>11%</div> <div>38% 38% 5% 18%</div> </div> |

Validation Pipeline (wwPDB-VP) : 2.49

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13227 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 Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 418      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3383  | 2124 | 611 | 632 | 6 | 10 |         |         |       |
| 1   | B     | 418      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3371  | 2118 | 605 | 632 | 6 | 10 |         |         |       |
| 1   | C     | 364      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2961  | 1865 | 529 | 552 | 6 | 9  |         |         |       |
| 1   | D     | 372      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3006  | 1892 | 530 | 569 | 5 | 10 |         |         |       |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 448     | LEU      | -      | expression tag | UNP Q83KU0 |
| A     | 449     | GLU      | -      | expression tag | UNP Q83KU0 |
| A     | 450     | HIS      | -      | expression tag | UNP Q83KU0 |
| A     | 451     | HIS      | -      | expression tag | UNP Q83KU0 |
| A     | 452     | HIS      | -      | expression tag | UNP Q83KU0 |
| A     | 453     | HIS      | -      | expression tag | UNP Q83KU0 |
| A     | 454     | HIS      | -      | expression tag | UNP Q83KU0 |
| A     | 455     | HIS      | -      | expression tag | UNP Q83KU0 |
| B     | 448     | LEU      | -      | expression tag | UNP Q83KU0 |
| B     | 449     | GLU      | -      | expression tag | UNP Q83KU0 |
| B     | 450     | HIS      | -      | expression tag | UNP Q83KU0 |
| B     | 451     | HIS      | -      | expression tag | UNP Q83KU0 |
| B     | 452     | HIS      | -      | expression tag | UNP Q83KU0 |
| B     | 453     | HIS      | -      | expression tag | UNP Q83KU0 |
| B     | 454     | HIS      | -      | expression tag | UNP Q83KU0 |
| B     | 455     | HIS      | -      | expression tag | UNP Q83KU0 |
| C     | 448     | LEU      | -      | expression tag | UNP Q83KU0 |
| C     | 449     | GLU      | -      | expression tag | UNP Q83KU0 |
| C     | 450     | HIS      | -      | expression tag | UNP Q83KU0 |
| C     | 451     | HIS      | -      | expression tag | UNP Q83KU0 |
| C     | 452     | HIS      | -      | expression tag | UNP Q83KU0 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 453     | HIS      | -      | expression tag | UNP Q83KU0 |
| C     | 454     | HIS      | -      | expression tag | UNP Q83KU0 |
| C     | 455     | HIS      | -      | expression tag | UNP Q83KU0 |
| D     | 448     | LEU      | -      | expression tag | UNP Q83KU0 |
| D     | 449     | GLU      | -      | expression tag | UNP Q83KU0 |
| D     | 450     | HIS      | -      | expression tag | UNP Q83KU0 |
| D     | 451     | HIS      | -      | expression tag | UNP Q83KU0 |
| D     | 452     | HIS      | -      | expression tag | UNP Q83KU0 |
| D     | 453     | HIS      | -      | expression tag | UNP Q83KU0 |
| D     | 454     | HIS      | -      | expression tag | UNP Q83KU0 |
| D     | 455     | HIS      | -      | expression tag | UNP Q83KU0 |

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

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

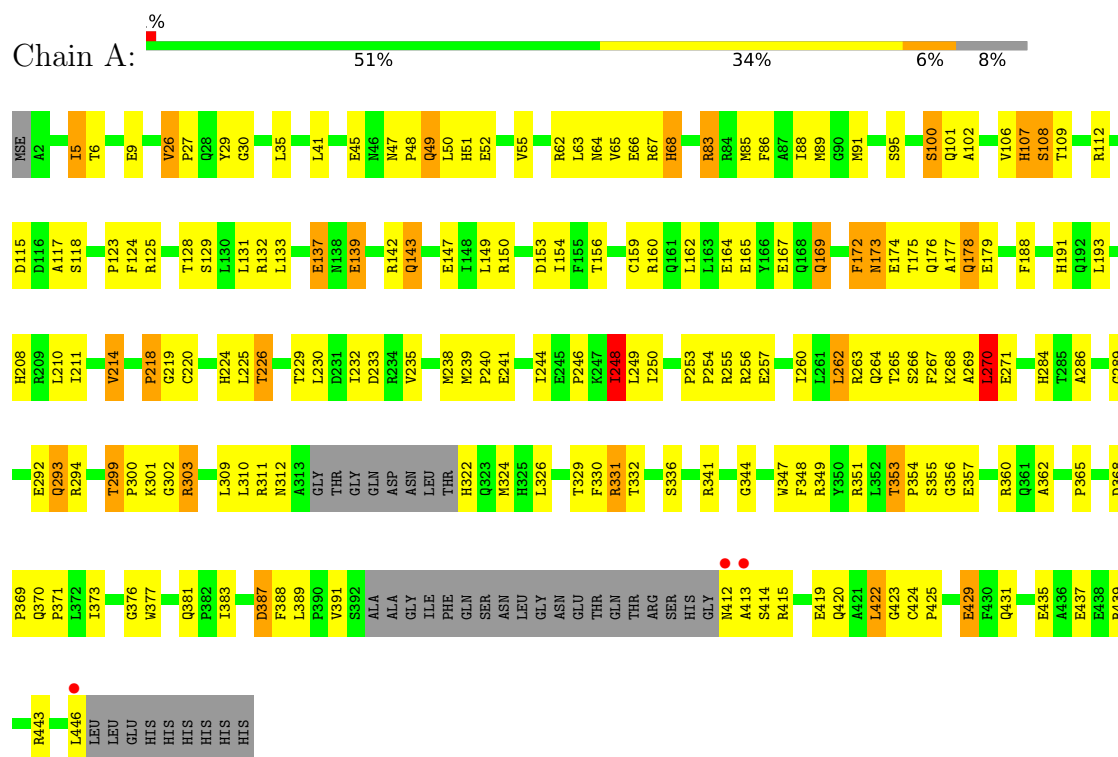
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | A     | 198      | Total<br>198 | O<br>198 | 0       | 0       |
| 3   | B     | 148      | Total<br>148 | O<br>148 | 0       | 0       |
| 3   | C     | 93       | Total<br>93  | O<br>93  | 0       | 0       |
| 3   | D     | 63       | Total<br>63  | O<br>63  | 0       | 0       |

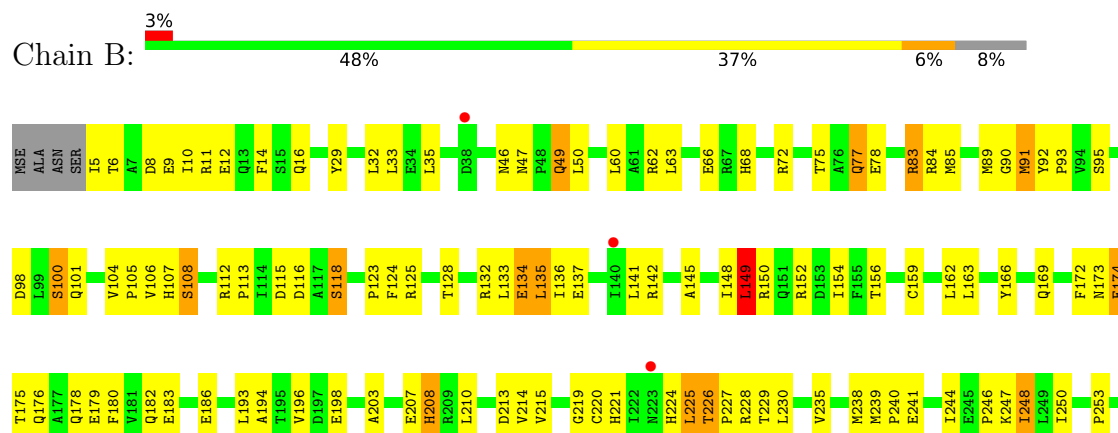
### 3 Residue-property plots [i](#)

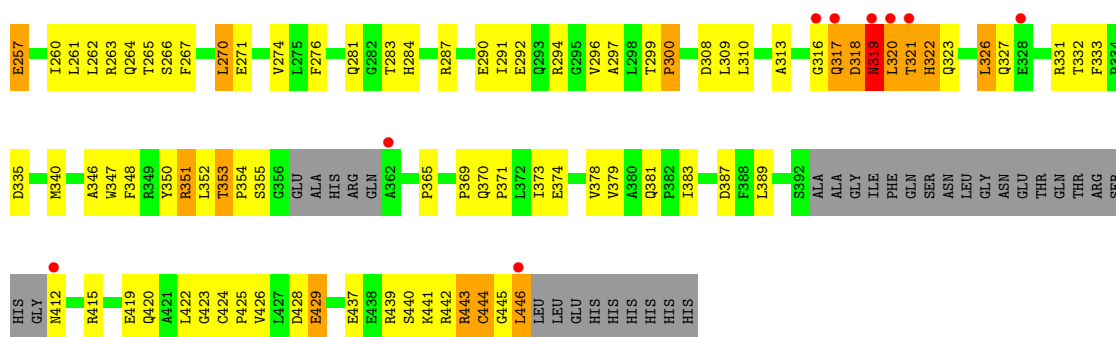
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein

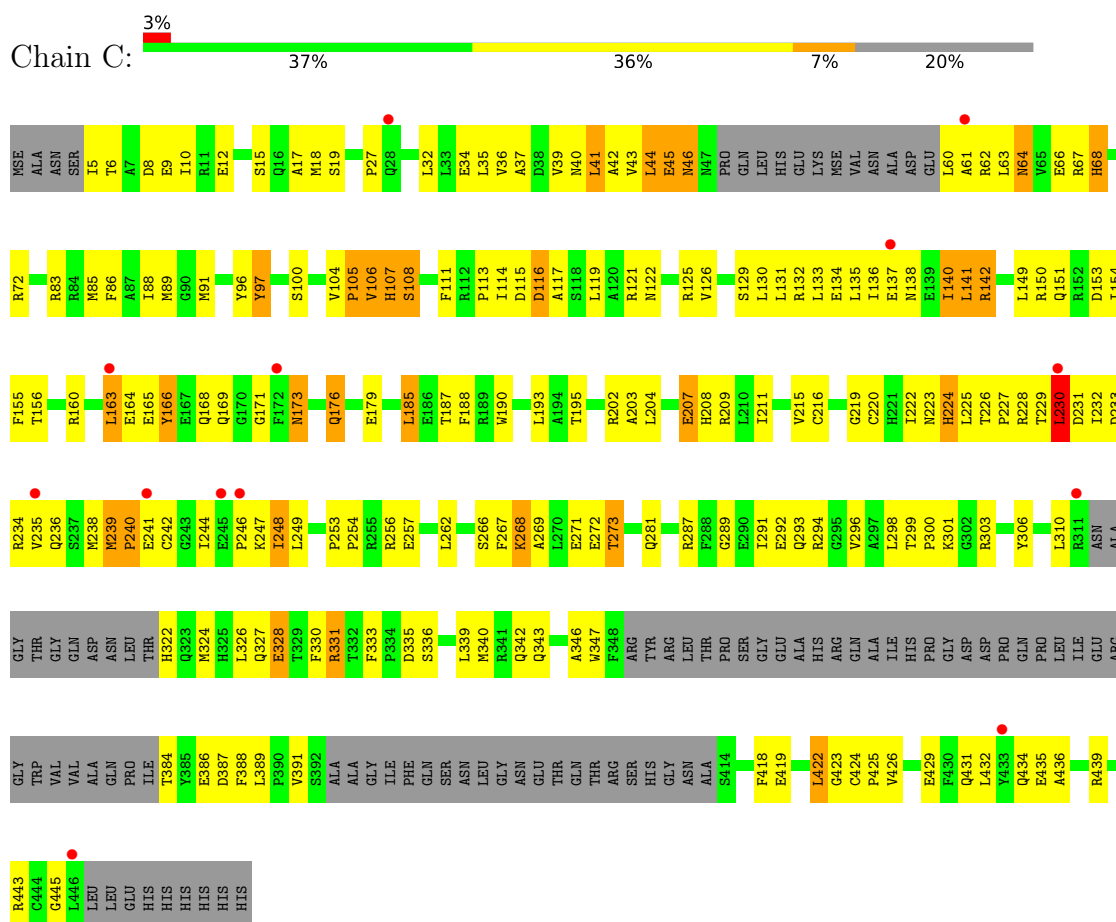


- Molecule 1: Uncharacterized protein

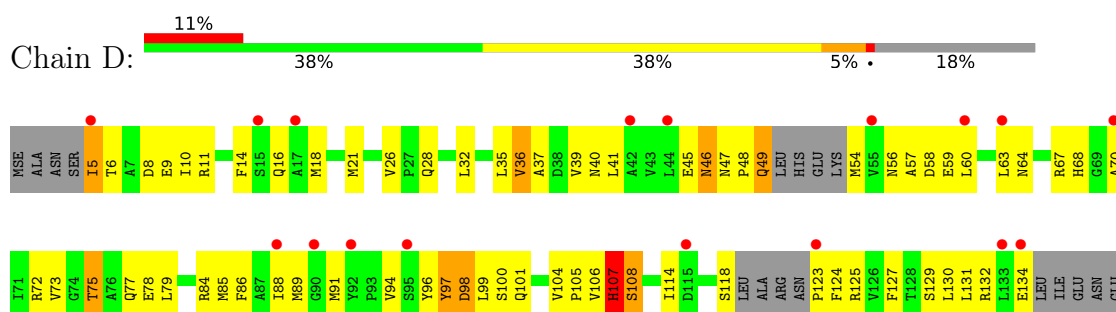


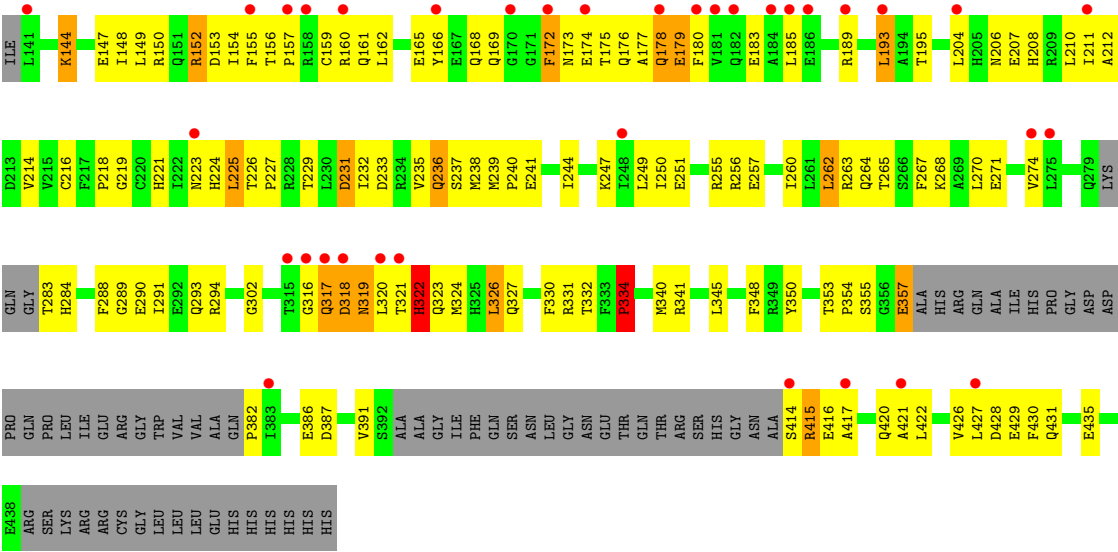


• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 192.21Å 76.39Å 159.05Å<br>90.00° 116.55° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 41.12 – 2.60<br>41.12 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 87.0 (41.12-2.60)<br>94.4 (41.12-2.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.27 (at 2.58Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.281<br>0.242 , 0.286                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3238 reflections (2.60%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 36.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.162                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 48.8                                                 | 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                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 13227                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 45.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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     | 0.51         | 0/3443      | 0.98        | 14/4645 (0.3%)  |
| 1   | B     | 0.49         | 0/3430      | 1.02        | 15/4629 (0.3%)  |
| 1   | C     | 0.40         | 0/3008      | 0.94        | 9/4048 (0.2%)   |
| 1   | D     | 0.37         | 0/3055      | 0.92        | 12/4116 (0.3%)  |
| All | All   | 0.45         | 0/12936     | 0.97        | 50/17438 (0.3%) |

There are no bond length outliers.

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 321 | THR  | N-CA-C | -11.39 | 96.89       | 112.94   |
| 1   | A     | 108 | SER  | N-CA-C | 10.23  | 122.20      | 108.38   |
| 1   | B     | 248 | ILE  | N-CA-C | 10.10  | 120.97      | 110.36   |
| 1   | D     | 322 | HIS  | N-CA-C | -9.03  | 100.06      | 113.61   |
| 1   | B     | 415 | ARG  | N-CA-C | -8.45  | 102.01      | 111.14   |
| 1   | B     | 313 | ALA  | N-CA-C | -8.41  | 98.65       | 110.50   |
| 1   | C     | 216 | CYS  | N-CA-C | 8.39   | 123.17      | 113.19   |
| 1   | B     | 226 | THR  | N-CA-C | 7.17   | 119.94      | 109.04   |
| 1   | C     | 108 | SER  | N-CA-C | 6.73   | 118.34      | 108.86   |
| 1   | D     | 237 | SER  | N-CA-C | -6.56  | 103.96      | 112.23   |
| 1   | B     | 331 | ARG  | N-CA-C | -6.55  | 104.18      | 111.71   |
| 1   | D     | 323 | GLN  | N-CA-C | -6.53  | 104.57      | 112.54   |
| 1   | B     | 444 | CYS  | N-CA-C | -6.53  | 106.27      | 114.56   |
| 1   | A     | 112 | ARG  | N-CA-C | 6.50   | 114.07      | 108.22   |
| 1   | A     | 387 | ASP  | N-CA-C | 6.39   | 118.30      | 109.29   |
| 1   | C     | 179 | GLU  | N-CA-C | -6.34  | 104.06      | 110.97   |
| 1   | A     | 331 | ARG  | N-CA-C | -6.22  | 104.79      | 112.38   |
| 1   | C     | 331 | ARG  | N-CA-C | -6.14  | 105.28      | 112.89   |
| 1   | C     | 257 | GLU  | N-CA-C | -6.05  | 104.76      | 111.36   |
| 1   | D     | 172 | PHE  | N-CA-C | 6.03   | 118.48      | 110.53   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 108 | SER  | N-CA-C  | 6.01  | 117.33      | 108.86   |
| 1   | D     | 98  | ASP  | N-CA-CB | -5.92 | 103.72      | 110.35   |
| 1   | C     | 46  | ASN  | N-CA-C  | -5.86 | 104.52      | 112.26   |
| 1   | D     | 331 | ARG  | N-CA-C  | -5.64 | 105.22      | 111.71   |
| 1   | B     | 264 | GLN  | N-CA-C  | 5.57  | 117.87      | 109.23   |
| 1   | D     | 330 | PHE  | N-CA-C  | 5.57  | 119.94      | 113.20   |
| 1   | C     | 230 | LEU  | N-CA-C  | -5.52 | 100.30      | 109.46   |
| 1   | A     | 26  | VAL  | CA-C-N  | 5.42  | 124.87      | 119.24   |
| 1   | A     | 26  | VAL  | C-N-CA  | 5.42  | 124.87      | 119.24   |
| 1   | A     | 226 | THR  | N-CA-C  | 5.40  | 119.41      | 109.10   |
| 1   | D     | 223 | ASN  | N-CA-C  | -5.39 | 105.49      | 111.36   |
| 1   | D     | 326 | LEU  | N-CA-C  | -5.38 | 105.49      | 111.36   |
| 1   | B     | 113 | PRO  | N-CA-C  | -5.37 | 103.70      | 111.22   |
| 1   | B     | 281 | GLN  | N-CA-C  | 5.36  | 117.48      | 108.96   |
| 1   | A     | 47  | ASN  | CA-C-N  | 5.36  | 124.69      | 118.85   |
| 1   | A     | 47  | ASN  | C-N-CA  | 5.36  | 124.69      | 118.85   |
| 1   | B     | 423 | GLY  | N-CA-C  | -5.35 | 108.11      | 114.48   |
| 1   | D     | 107 | HIS  | N-CA-C  | -5.33 | 101.87      | 110.14   |
| 1   | C     | 166 | TYR  | N-CA-C  | -5.33 | 105.37      | 111.07   |
| 1   | C     | 106 | VAL  | N-CA-C  | 5.30  | 115.19      | 107.88   |
| 1   | D     | 26  | VAL  | CA-C-N  | 5.27  | 124.89      | 119.05   |
| 1   | D     | 26  | VAL  | C-N-CA  | 5.27  | 124.89      | 119.05   |
| 1   | A     | 100 | SER  | N-CA-C  | -5.25 | 105.61      | 112.23   |
| 1   | A     | 214 | VAL  | N-CA-C  | 5.25  | 118.48      | 111.44   |
| 1   | B     | 322 | HIS  | N-CA-C  | -5.20 | 105.68      | 112.23   |
| 1   | A     | 388 | PHE  | N-CA-C  | 5.18  | 116.54      | 109.18   |
| 1   | B     | 149 | LEU  | N-CA-C  | 5.12  | 116.56      | 110.97   |
| 1   | A     | 293 | GLN  | N-CA-C  | -5.10 | 99.66       | 108.69   |
| 1   | B     | 319 | ASN  | N-CA-C  | 5.04  | 118.17      | 110.20   |
| 1   | A     | 154 | ILE  | N-CA-C  | 5.04  | 119.50      | 112.50   |

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     | 3383  | 0        | 3310     | 186     | 0            |
| 1   | B     | 3371  | 0        | 3298     | 224     | 0            |
| 1   | C     | 2961  | 0        | 2906     | 215     | 0            |
| 1   | D     | 3006  | 0        | 2920     | 202     | 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     | 198   | 0        | 0        | 29      | 0            |
| 3   | B     | 148   | 0        | 0        | 18      | 0            |
| 3   | C     | 93    | 0        | 0        | 15      | 0            |
| 3   | D     | 63    | 0        | 0        | 14      | 0            |
| All | All   | 13227 | 0        | 12434    | 822     | 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 33.

All (822) 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:11:ARG:CA    | 1:B:89:MSE:HE3   | 1.38                     | 1.49              |
| 1:B:11:ARG:HA    | 1:B:89:MSE:CE    | 1.48                     | 1.43              |
| 1:B:14:PHE:HB3   | 1:B:89:MSE:CE    | 1.65                     | 1.25              |
| 1:B:14:PHE:CB    | 1:B:89:MSE:HE1   | 1.69                     | 1.21              |
| 1:A:139:GLU:HG2  | 1:A:142:ARG:HH21 | 1.05                     | 1.17              |
| 1:B:84:ARG:NH2   | 1:B:163:LEU:HD22 | 1.62                     | 1.14              |
| 1:D:108:SER:HB3  | 1:D:129:SER:HA   | 1.28                     | 1.14              |
| 1:C:436:ALA:HA   | 1:C:439:ARG:HH12 | 1.12                     | 1.13              |
| 1:A:353:THR:HG22 | 1:A:356:GLY:H    | 1.11                     | 1.08              |
| 1:B:84:ARG:HH21  | 1:B:163:LEU:CD2  | 1.67                     | 1.07              |
| 1:B:84:ARG:HH21  | 1:B:163:LEU:HD22 | 0.90                     | 1.03              |
| 1:B:83:ARG:HG2   | 1:B:83:ARG:HH11  | 1.22                     | 1.02              |
| 1:B:14:PHE:HB3   | 1:B:89:MSE:HE1   | 1.23                     | 1.01              |
| 1:C:108:SER:HB3  | 1:C:129:SER:HA   | 1.43                     | 1.00              |
| 1:C:268:LYS:H    | 1:C:268:LYS:NZ   | 1.59                     | 0.99              |
| 1:B:445:GLY:C    | 1:B:446:LEU:HD12 | 1.88                     | 0.96              |
| 1:A:128:THR:HB   | 3:A:671:HOH:O    | 1.68                     | 0.94              |
| 1:C:173:ASN:H    | 1:C:176:GLN:HE21 | 1.16                     | 0.94              |
| 1:B:14:PHE:HB3   | 1:B:89:MSE:HE2   | 1.50                     | 0.94              |
| 1:A:108:SER:HB3  | 1:A:129:SER:HA   | 1.48                     | 0.93              |
| 1:A:139:GLU:HG3  | 1:D:324:MSE:HE3  | 1.47                     | 0.93              |
| 1:C:106:VAL:HG12 | 1:C:131:LEU:HA   | 1.50                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:14:PHE:CB    | 1:B:89:MSE:CE    | 2.37                     | 0.91              |
| 1:A:353:THR:HG22 | 1:A:356:GLY:N    | 1.86                     | 0.90              |
| 1:B:14:PHE:HB2   | 1:B:89:MSE:HE1   | 1.52                     | 0.90              |
| 1:B:89:MSE:HG2   | 1:B:91:MSE:SE    | 2.22                     | 0.89              |
| 1:C:268:LYS:HZ3  | 1:C:268:LYS:N    | 1.70                     | 0.88              |
| 1:B:68:HIS:HA    | 3:B:586:HOH:O    | 1.73                     | 0.87              |
| 1:C:436:ALA:HA   | 1:C:439:ARG:NH1  | 1.89                     | 0.87              |
| 1:A:239:MSE:HE2  | 1:A:244:ILE:HG21 | 1.56                     | 0.87              |
| 1:C:254:PRO:HD3  | 1:C:326:LEU:HD11 | 1.57                     | 0.86              |
| 1:C:268:LYS:H    | 1:C:268:LYS:HZ3  | 0.90                     | 0.86              |
| 1:A:299:THR:HG22 | 1:A:302:GLY:H    | 1.40                     | 0.86              |
| 1:D:154:ILE:HG12 | 1:D:219:GLY:HA2  | 1.57                     | 0.86              |
| 1:A:139:GLU:HG2  | 1:A:142:ARG:NH2  | 1.90                     | 0.85              |
| 1:B:11:ARG:C     | 1:B:89:MSE:HE3   | 2.01                     | 0.84              |
| 1:B:75:THR:OG1   | 1:B:78:GLU:HG3   | 1.77                     | 0.84              |
| 1:C:165:GLU:O    | 1:C:169:GLN:HG2  | 1.77                     | 0.84              |
| 1:B:11:ARG:HH21  | 1:B:90:GLY:HA3   | 1.43                     | 0.84              |
| 1:A:150:ARG:HD3  | 3:A:569:HOH:O    | 1.76                     | 0.83              |
| 1:B:83:ARG:HG2   | 1:B:83:ARG:NH1   | 1.85                     | 0.83              |
| 1:A:173:ASN:C    | 1:A:173:ASN:HD22 | 1.87                     | 0.82              |
| 1:A:49:GLN:H     | 1:A:49:GLN:NE2   | 1.77                     | 0.82              |
| 1:B:11:ARG:CA    | 1:B:89:MSE:CE    | 2.29                     | 0.81              |
| 1:B:224:HIS:CD2  | 1:B:290:GLU:OE1  | 2.34                     | 0.81              |
| 1:B:125:ARG:CZ   | 1:B:294:ARG:NH1  | 2.44                     | 0.81              |
| 1:B:11:ARG:HA    | 1:B:89:MSE:HE3   | 0.80                     | 0.80              |
| 1:A:299:THR:HG21 | 1:A:344:GLY:O    | 1.81                     | 0.79              |
| 1:B:351:ARG:HH11 | 1:B:351:ARG:HB3  | 1.46                     | 0.79              |
| 1:A:232:ILE:H    | 1:A:293:GLN:NE2  | 1.80                     | 0.79              |
| 1:B:365:PRO:HA   | 1:B:446:LEU:HA   | 1.66                     | 0.78              |
| 1:C:6:THR:HG22   | 1:C:9:GLU:OE1    | 1.84                     | 0.78              |
| 1:B:262:LEU:HD21 | 1:B:389:LEU:HG   | 1.63                     | 0.78              |
| 1:C:419:GLU:HG2  | 1:C:425:PRO:HA   | 1.63                     | 0.77              |
| 1:C:136:ILE:HB   | 1:C:142:ARG:HB3  | 1.67                     | 0.77              |
| 1:D:247:LYS:HE2  | 1:D:249:LEU:HB3  | 1.65                     | 0.77              |
| 1:D:144:LYS:HA   | 1:D:144:LYS:HE2  | 1.64                     | 0.77              |
| 1:D:165:GLU:HB3  | 1:D:172:PHE:HZ   | 1.50                     | 0.77              |
| 1:A:85:MSE:HE1   | 1:A:188:PHE:HZ   | 1.49                     | 0.77              |
| 1:B:351:ARG:HH11 | 1:B:351:ARG:CB   | 1.97                     | 0.77              |
| 1:D:91:MSE:HE1   | 1:D:124:PHE:CD2  | 2.22                     | 0.75              |
| 1:D:100:SER:HA   | 1:D:104:VAL:O    | 1.87                     | 0.75              |
| 1:A:232:ILE:H    | 1:A:293:GLN:HE21 | 1.35                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:155:PHE:HB2  | 1:C:160:ARG:NH1  | 2.02                     | 0.74              |
| 1:B:11:ARG:N     | 1:B:89:MSE:HE3   | 2.03                     | 0.74              |
| 1:C:322:HIS:N    | 3:C:555:HOH:O    | 2.21                     | 0.74              |
| 1:C:239:MSE:HB2  | 1:C:240:PRO:HD3  | 1.71                     | 0.73              |
| 1:C:32:LEU:HD22  | 1:C:267:PHE:HZ   | 1.52                     | 0.73              |
| 1:C:132:ARG:HB3  | 1:C:134:GLU:OE2  | 1.88                     | 0.73              |
| 1:C:155:PHE:HB2  | 1:C:160:ARG:HH12 | 1.53                     | 0.73              |
| 1:D:172:PHE:HB3  | 1:D:177:ALA:HB2  | 1.69                     | 0.73              |
| 1:D:431:GLN:O    | 1:D:435:GLU:HG3  | 1.88                     | 0.73              |
| 1:D:99:LEU:HD12  | 1:D:106:VAL:HG23 | 1.70                     | 0.73              |
| 1:D:232:ILE:HG22 | 1:D:293:GLN:NE2  | 2.04                     | 0.72              |
| 1:B:104:VAL:HG12 | 1:B:106:VAL:HG22 | 1.70                     | 0.72              |
| 1:A:240:PRO:HG2  | 3:A:631:HOH:O    | 1.88                     | 0.72              |
| 1:D:221:HIS:HD2  | 3:D:515:HOH:O    | 1.72                     | 0.72              |
| 1:B:299:THR:HG22 | 3:B:517:HOH:O    | 1.90                     | 0.72              |
| 1:B:100:SER:HA   | 1:B:104:VAL:O    | 1.90                     | 0.71              |
| 1:D:193:LEU:HD22 | 1:D:193:LEU:O    | 1.89                     | 0.71              |
| 1:A:351:ARG:HG2  | 1:A:443:ARG:NH2  | 2.04                     | 0.71              |
| 1:C:44:LEU:HD11  | 1:C:60:LEU:HD21  | 1.72                     | 0.71              |
| 1:D:75:THR:HB    | 1:D:77:GLN:HE22  | 1.54                     | 0.71              |
| 1:B:46:ASN:HB3   | 3:B:566:HOH:O    | 1.88                     | 0.71              |
| 1:D:193:LEU:HD13 | 1:D:193:LEU:H    | 1.55                     | 0.71              |
| 1:B:316:GLY:O    | 1:B:318:ASP:N    | 2.23                     | 0.71              |
| 1:C:150:ARG:HH21 | 1:C:151:GLN:NE2  | 1.88                     | 0.71              |
| 1:D:40:ASN:HD22  | 1:D:63:LEU:HD21  | 1.55                     | 0.71              |
| 1:A:6:THR:HG22   | 1:A:9:GLU:HB2    | 1.73                     | 0.70              |
| 1:C:339:LEU:HD12 | 1:C:339:LEU:H    | 1.54                     | 0.70              |
| 1:C:342:GLN:HE21 | 1:C:343:GLN:NE2  | 1.89                     | 0.70              |
| 1:D:106:VAL:HG12 | 1:D:131:LEU:HA   | 1.74                     | 0.70              |
| 1:C:6:THR:HG23   | 1:C:9:GLU:H      | 1.56                     | 0.70              |
| 1:B:148:ILE:HD13 | 1:B:196:VAL:HG11 | 1.72                     | 0.70              |
| 1:C:268:LYS:O    | 1:C:268:LYS:HG2  | 1.92                     | 0.70              |
| 1:C:64:ASN:N     | 1:C:64:ASN:HD22  | 1.87                     | 0.70              |
| 1:B:369:PRO:O    | 1:B:373:ILE:HG13 | 1.92                     | 0.69              |
| 1:D:274:VAL:HB   | 1:D:283:THR:HG22 | 1.74                     | 0.69              |
| 1:A:262:LEU:C    | 1:A:262:LEU:HD12 | 2.17                     | 0.69              |
| 1:A:353:THR:HG21 | 1:A:376:GLY:O    | 1.91                     | 0.69              |
| 1:C:299:THR:HG22 | 1:C:301:LYS:H    | 1.57                     | 0.69              |
| 1:C:83:ARG:HD3   | 1:C:422:LEU:CD2  | 2.23                     | 0.69              |
| 1:C:336:SER:HB3  | 1:C:339:LEU:HD13 | 1.75                     | 0.69              |
| 1:D:165:GLU:HB3  | 1:D:172:PHE:CZ   | 2.28                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:91:MSE:HE3   | 1:B:124:PHE:CD2  | 2.28                     | 0.69              |
| 1:C:150:ARG:HH21 | 1:C:151:GLN:HE22 | 1.41                     | 0.69              |
| 1:A:303:ARG:HG3  | 1:A:303:ARG:HH11 | 1.58                     | 0.68              |
| 1:B:91:MSE:CE    | 1:B:124:PHE:CD2  | 2.76                     | 0.68              |
| 1:C:68:HIS:C     | 1:C:68:HIS:CD2   | 2.72                     | 0.68              |
| 1:C:154:ILE:O    | 1:C:187:THR:HG23 | 1.94                     | 0.68              |
| 1:A:173:ASN:ND2  | 1:A:176:GLN:H    | 1.91                     | 0.68              |
| 1:A:294:ARG:NH2  | 1:A:387:ASP:O    | 2.27                     | 0.68              |
| 1:C:108:SER:HB3  | 1:C:129:SER:CA   | 2.21                     | 0.68              |
| 1:B:412:ASN:N    | 3:B:580:HOH:O    | 2.27                     | 0.68              |
| 1:C:165:GLU:HA   | 1:C:168:GLN:HB2  | 1.75                     | 0.68              |
| 1:D:75:THR:OG1   | 1:D:78:GLU:HG3   | 1.93                     | 0.67              |
| 1:D:156:THR:HG21 | 1:D:183:GLU:OE2  | 1.94                     | 0.67              |
| 1:B:49:GLN:H     | 1:B:49:GLN:HE21  | 1.43                     | 0.67              |
| 1:B:132:ARG:HB3  | 1:B:134:GLU:OE2  | 1.94                     | 0.67              |
| 1:C:248:ILE:HD13 | 1:C:248:ILE:H    | 1.58                     | 0.67              |
| 1:A:235:VAL:O    | 1:A:239:MSE:HG3  | 1.95                     | 0.67              |
| 1:D:36:VAL:HG12  | 1:D:36:VAL:O     | 1.95                     | 0.67              |
| 1:A:5:ILE:HD11   | 1:A:172:PHE:HB2  | 1.76                     | 0.66              |
| 1:C:67:ARG:HA    | 1:C:226:THR:O    | 1.95                     | 0.66              |
| 1:B:351:ARG:HB3  | 1:B:351:ARG:NH1  | 2.09                     | 0.66              |
| 1:B:47:ASN:C     | 1:B:47:ASN:HD22  | 2.04                     | 0.66              |
| 1:A:299:THR:HG23 | 1:A:301:LYS:H    | 1.61                     | 0.66              |
| 1:D:75:THR:HG22  | 1:D:149:LEU:CD2  | 2.26                     | 0.66              |
| 1:C:89:MSE:CB    | 1:C:91:MSE:HE2   | 2.26                     | 0.66              |
| 1:D:72:ARG:HG3   | 1:D:72:ARG:HH11  | 1.60                     | 0.65              |
| 1:A:160:ARG:HD2  | 3:A:629:HOH:O    | 1.96                     | 0.65              |
| 1:B:299:THR:CG2  | 3:B:517:HOH:O    | 2.43                     | 0.65              |
| 1:D:332:THR:O    | 1:D:334:PRO:HD3  | 1.97                     | 0.65              |
| 1:C:223:ASN:O    | 1:C:224:HIS:HB3  | 1.95                     | 0.65              |
| 1:C:17:ALA:HB1   | 1:C:185:LEU:HD21 | 1.79                     | 0.65              |
| 1:B:239:MSE:HE2  | 1:B:244:ILE:HG21 | 1.78                     | 0.64              |
| 1:C:68:HIS:ND1   | 1:C:388:PHE:HE2  | 1.95                     | 0.64              |
| 1:C:89:MSE:HB2   | 1:C:91:MSE:HE2   | 1.79                     | 0.64              |
| 1:A:270:LEU:C    | 1:A:270:LEU:HD13 | 2.23                     | 0.64              |
| 1:D:47:ASN:HD21  | 1:D:49:GLN:HB2   | 1.63                     | 0.64              |
| 1:B:104:VAL:HG13 | 1:B:210:LEU:HD22 | 1.80                     | 0.64              |
| 1:C:85:MSE:HE1   | 1:C:188:PHE:HZ   | 1.61                     | 0.64              |
| 1:C:342:GLN:HE21 | 1:C:343:GLN:HE21 | 1.43                     | 0.64              |
| 1:A:353:THR:CG2  | 1:A:355:SER:HB3  | 2.28                     | 0.64              |
| 1:B:443:ARG:HG3  | 1:B:443:ARG:HH11 | 1.61                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:64:ASN:HB3   | 3:A:530:HOH:O    | 1.99                     | 0.63              |
| 1:A:349:ARG:HD2  | 1:A:381:GLN:OE1  | 1.97                     | 0.63              |
| 1:B:95:SER:HB2   | 1:B:429:GLU:HG3  | 1.80                     | 0.63              |
| 1:A:353:THR:CG2  | 1:A:356:GLY:H    | 1.99                     | 0.63              |
| 1:D:353:THR:O    | 1:D:357:GLU:HB2  | 1.98                     | 0.63              |
| 1:C:107:HIS:HE1  | 1:C:130:LEU:HD23 | 1.63                     | 0.63              |
| 1:C:347:TRP:HZ3  | 1:C:434:GLN:HG3  | 1.63                     | 0.63              |
| 1:C:83:ARG:HD3   | 1:C:422:LEU:HD22 | 1.81                     | 0.63              |
| 1:C:431:GLN:O    | 1:C:435:GLU:HG3  | 1.97                     | 0.63              |
| 1:B:11:ARG:HB2   | 1:B:89:MSE:O     | 1.98                     | 0.62              |
| 1:C:248:ILE:HD13 | 1:C:248:ILE:N    | 2.14                     | 0.62              |
| 1:D:193:LEU:H    | 1:D:193:LEU:CD1  | 2.11                     | 0.62              |
| 1:B:294:ARG:NH2  | 1:B:387:ASP:O    | 2.32                     | 0.62              |
| 1:B:162:LEU:HD11 | 1:B:179:GLU:HG2  | 1.82                     | 0.62              |
| 1:D:206:ASN:ND2  | 3:D:538:HOH:O    | 2.31                     | 0.62              |
| 1:C:262:LEU:C    | 1:C:262:LEU:HD12 | 2.24                     | 0.62              |
| 1:B:214:VAL:HG13 | 3:B:602:HOH:O    | 2.00                     | 0.62              |
| 1:A:370:GLN:HB3  | 1:A:371:PRO:HD3  | 1.81                     | 0.62              |
| 1:B:91:MSE:CE    | 1:B:124:PHE:HD2  | 2.11                     | 0.62              |
| 1:D:114:ILE:HG21 | 1:D:427:LEU:HD13 | 1.81                     | 0.62              |
| 1:C:35:LEU:HD11  | 1:C:238:MSE:HB3  | 1.80                     | 0.62              |
| 1:B:89:MSE:CG    | 1:B:91:MSE:SE    | 2.97                     | 0.62              |
| 1:B:6:THR:HG23   | 1:B:9:GLU:H      | 1.65                     | 0.62              |
| 1:A:226:THR:CG2  | 1:A:292:GLU:HG2  | 2.29                     | 0.61              |
| 1:A:6:THR:HG23   | 1:A:9:GLU:H      | 1.64                     | 0.61              |
| 1:C:160:ARG:O    | 1:C:164:GLU:HB2  | 1.99                     | 0.61              |
| 1:C:208:HIS:HB3  | 1:C:211:ILE:HG13 | 1.81                     | 0.61              |
| 1:A:268:LYS:HE2  | 1:A:286:ALA:HB1  | 1.82                     | 0.61              |
| 1:D:267:PHE:CZ   | 1:D:289:GLY:HA3  | 2.35                     | 0.61              |
| 1:A:249:LEU:O    | 1:A:265:THR:HG23 | 2.00                     | 0.61              |
| 1:B:83:ARG:HH11  | 1:B:83:ARG:CG    | 2.02                     | 0.61              |
| 1:A:250:ILE:HG12 | 1:A:265:THR:OG1  | 2.01                     | 0.61              |
| 1:A:253:PRO:HG3  | 1:A:260:ILE:HG13 | 1.81                     | 0.61              |
| 1:A:368:ASP:O    | 1:A:371:PRO:HD2  | 2.01                     | 0.61              |
| 1:B:84:ARG:HE    | 1:B:163:LEU:HD21 | 1.64                     | 0.61              |
| 1:B:267:PHE:HB3  | 3:B:526:HOH:O    | 2.00                     | 0.61              |
| 1:B:173:ASN:OD1  | 1:B:176:GLN:HG3  | 2.01                     | 0.61              |
| 1:A:248:ILE:HD13 | 1:A:248:ILE:H    | 1.65                     | 0.61              |
| 1:B:248:ILE:CG2  | 1:B:320:LEU:HG   | 2.31                     | 0.61              |
| 1:B:352:LEU:HD23 | 1:B:378:VAL:HG22 | 1.83                     | 0.61              |
| 1:D:91:MSE:HE1   | 1:D:124:PHE:HD2  | 1.64                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:152:ARG:HH21 | 1:D:154:ILE:CG1  | 2.13                     | 0.60              |
| 1:D:152:ARG:HH21 | 1:D:154:ILE:HB   | 1.66                     | 0.60              |
| 1:D:86:PHE:HB3   | 1:D:91:MSE:HB2   | 1.82                     | 0.60              |
| 1:D:32:LEU:O     | 1:D:36:VAL:HG23  | 2.02                     | 0.60              |
| 1:D:155:PHE:HD2  | 1:D:160:ARG:HB3  | 1.66                     | 0.60              |
| 1:B:348:PHE:O    | 1:B:437:GLU:HG3  | 2.02                     | 0.60              |
| 1:D:175:THR:O    | 1:D:179:GLU:HB2  | 2.00                     | 0.60              |
| 1:D:353:THR:CG2  | 1:D:354:PRO:HD2  | 2.32                     | 0.60              |
| 1:A:173:ASN:HD21 | 1:A:176:GLN:HG3  | 1.67                     | 0.60              |
| 1:B:132:ARG:HA   | 3:B:533:HOH:O    | 2.01                     | 0.60              |
| 1:D:39:VAL:HG21  | 1:D:235:VAL:HG22 | 1.83                     | 0.60              |
| 1:B:193:LEU:HD13 | 1:B:194:ALA:O    | 2.02                     | 0.60              |
| 1:C:173:ASN:H    | 1:C:176:GLN:NE2  | 1.94                     | 0.60              |
| 1:A:85:MSE:HE1   | 1:A:188:PHE:CZ   | 2.35                     | 0.59              |
| 1:A:210:LEU:C    | 1:A:210:LEU:HD23 | 2.27                     | 0.59              |
| 1:C:247:LYS:HB2  | 3:C:538:HOH:O    | 2.01                     | 0.59              |
| 1:C:60:LEU:HD13  | 1:C:60:LEU:O     | 2.02                     | 0.59              |
| 1:B:319:ASN:HB2  | 1:B:321:THR:HG23 | 1.84                     | 0.59              |
| 1:A:210:LEU:O    | 1:A:214:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:11:ARG:O     | 1:B:89:MSE:CE    | 2.51                     | 0.59              |
| 1:D:21:MSE:SE    | 1:D:189:ARG:HG2  | 2.51                     | 0.59              |
| 1:C:173:ASN:N    | 1:C:176:GLN:HE21 | 1.96                     | 0.59              |
| 1:D:294:ARG:NH2  | 1:D:387:ASP:O    | 2.35                     | 0.59              |
| 1:C:299:THR:HG23 | 1:C:300:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:357:GLU:O    | 1:A:360:ARG:HB2  | 2.02                     | 0.58              |
| 1:D:5:ILE:N      | 1:D:5:ILE:HD13   | 2.18                     | 0.58              |
| 1:D:353:THR:HG23 | 1:D:354:PRO:HD2  | 1.84                     | 0.58              |
| 1:C:207:GLU:HB3  | 1:C:211:ILE:HD12 | 1.84                     | 0.58              |
| 1:D:60:LEU:HD23  | 1:D:60:LEU:O     | 2.03                     | 0.58              |
| 1:A:439:ARG:NH2  | 3:A:608:HOH:O    | 2.34                     | 0.58              |
| 1:C:294:ARG:HH21 | 1:C:386:GLU:C    | 2.12                     | 0.58              |
| 1:D:232:ILE:HG22 | 1:D:293:GLN:HE21 | 1.68                     | 0.58              |
| 1:D:348:PHE:HA   | 1:D:382:PRO:HA   | 1.84                     | 0.58              |
| 1:B:11:ARG:C     | 1:B:89:MSE:CE    | 2.71                     | 0.58              |
| 1:C:298:LEU:C    | 1:C:347:TRP:HE1  | 2.11                     | 0.58              |
| 1:D:355:SER:C    | 1:D:357:GLU:H    | 2.11                     | 0.58              |
| 1:B:226:THR:OG1  | 1:B:290:GLU:HB3  | 2.04                     | 0.58              |
| 1:C:294:ARG:NH2  | 1:C:387:ASP:O    | 2.36                     | 0.58              |
| 1:C:339:LEU:H    | 1:C:339:LEU:CD1  | 2.17                     | 0.58              |
| 1:B:68:HIS:HE1   | 3:B:629:HOH:O    | 1.84                     | 0.58              |
| 1:C:10:ILE:HG22  | 1:C:89:MSE:HG2   | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:271:GLU:OE1  | 1:A:284:HIS:HD2  | 1.86                     | 0.58              |
| 1:C:136:ILE:CB   | 1:C:142:ARG:HB3  | 2.34                     | 0.58              |
| 1:C:138:ASN:HD21 | 1:C:140:ILE:HD12 | 1.68                     | 0.58              |
| 1:C:339:LEU:HD12 | 1:C:339:LEU:N    | 2.17                     | 0.58              |
| 1:A:109:THR:CG2  | 3:A:671:HOH:O    | 2.53                     | 0.57              |
| 1:B:299:THR:HG23 | 1:B:300:PRO:HD2  | 1.85                     | 0.57              |
| 1:D:79:LEU:HD23  | 1:D:421:ALA:O    | 2.04                     | 0.57              |
| 1:D:152:ARG:HH21 | 1:D:154:ILE:CB   | 2.16                     | 0.57              |
| 1:A:153:ASP:HA   | 3:A:517:HOH:O    | 2.05                     | 0.57              |
| 1:B:11:ARG:HA    | 1:B:89:MSE:SE    | 2.53                     | 0.57              |
| 1:D:78:GLU:OE2   | 1:D:154:ILE:HD12 | 2.04                     | 0.57              |
| 1:A:322:HIS:N    | 3:A:502:HOH:O    | 2.37                     | 0.57              |
| 1:B:150:ARG:NE   | 3:B:584:HOH:O    | 2.36                     | 0.57              |
| 1:B:370:GLN:HB3  | 1:B:371:PRO:HD3  | 1.85                     | 0.57              |
| 1:D:40:ASN:ND2   | 1:D:63:LEU:HD21  | 2.19                     | 0.57              |
| 1:D:75:THR:HG22  | 1:D:149:LEU:HD23 | 1.86                     | 0.57              |
| 1:D:157:PRO:HA   | 1:D:160:ARG:HG3  | 1.87                     | 0.57              |
| 1:D:239:MSE:HE2  | 1:D:244:ILE:HG21 | 1.86                     | 0.57              |
| 1:C:132:ARG:HB3  | 1:C:135:LEU:HD23 | 1.87                     | 0.57              |
| 1:D:56:ASN:C     | 1:D:58:ASP:H     | 2.12                     | 0.57              |
| 1:D:60:LEU:HD21  | 3:D:543:HOH:O    | 2.03                     | 0.57              |
| 1:B:235:VAL:HG11 | 1:B:291:ILE:HD13 | 1.87                     | 0.57              |
| 1:D:32:LEU:HD13  | 1:D:239:MSE:HE3  | 1.86                     | 0.57              |
| 1:A:117:ALA:HB3  | 3:A:679:HOH:O    | 2.04                     | 0.57              |
| 1:C:224:HIS:CE1  | 3:C:567:HOH:O    | 2.57                     | 0.57              |
| 1:B:62:ARG:HD3   | 1:B:66:GLU:OE2   | 2.05                     | 0.56              |
| 1:D:153:ASP:HB2  | 1:D:155:PHE:CE1  | 2.40                     | 0.56              |
| 1:A:226:THR:HG22 | 1:A:292:GLU:HG2  | 1.87                     | 0.56              |
| 1:B:72:ARG:NH1   | 1:B:210:LEU:HD12 | 2.19                     | 0.56              |
| 1:A:431:GLN:O    | 1:A:435:GLU:HG3  | 2.06                     | 0.56              |
| 1:B:319:ASN:HD22 | 1:B:319:ASN:H    | 1.53                     | 0.56              |
| 1:C:41:LEU:C     | 1:C:41:LEU:HD23  | 2.30                     | 0.56              |
| 1:D:193:LEU:HD13 | 1:D:193:LEU:N    | 2.20                     | 0.56              |
| 1:A:41:LEU:C     | 1:A:41:LEU:HD23  | 2.29                     | 0.56              |
| 1:A:89:MSE:SE    | 1:A:91:MSE:CE    | 3.03                     | 0.56              |
| 1:A:248:ILE:HD13 | 1:A:248:ILE:N    | 2.20                     | 0.56              |
| 1:C:39:VAL:HG21  | 1:C:235:VAL:HG22 | 1.87                     | 0.56              |
| 1:D:429:GLU:HG3  | 1:D:430:PHE:H    | 1.71                     | 0.56              |
| 1:A:63:LEU:CD2   | 1:A:230:LEU:HD21 | 2.36                     | 0.56              |
| 1:A:95:SER:HB2   | 1:A:429:GLU:HG2  | 1.88                     | 0.56              |
| 1:A:100:SER:C    | 1:A:102:ALA:H    | 2.12                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:299:THR:CG2  | 1:B:300:PRO:HD2  | 2.36                     | 0.56              |
| 1:B:319:ASN:HD22 | 1:B:319:ASN:N    | 2.02                     | 0.56              |
| 1:B:319:ASN:H    | 1:B:319:ASN:ND2  | 2.03                     | 0.56              |
| 1:C:232:ILE:H    | 1:C:293:GLN:NE2  | 2.04                     | 0.56              |
| 1:B:101:GLN:OE1  | 1:B:101:GLN:N    | 2.38                     | 0.56              |
| 1:B:137:GLU:HB2  | 1:B:207:GLU:OE2  | 2.06                     | 0.56              |
| 1:C:5:ILE:HD12   | 1:C:9:GLU:HB3    | 1.88                     | 0.56              |
| 1:C:254:PRO:HD3  | 1:C:326:LEU:CD1  | 2.33                     | 0.56              |
| 1:A:357:GLU:CD   | 1:A:360:ARG:HH12 | 2.13                     | 0.56              |
| 1:A:191:HIS:HD2  | 1:B:308:ASP:OD2  | 1.88                     | 0.55              |
| 1:D:232:ILE:HD11 | 1:D:265:THR:OG1  | 2.06                     | 0.55              |
| 1:A:369:PRO:O    | 1:A:373:ILE:HG13 | 2.05                     | 0.55              |
| 1:B:173:ASN:O    | 1:B:174:GLU:C    | 2.49                     | 0.55              |
| 1:C:68:HIS:CD2   | 1:C:68:HIS:O     | 2.59                     | 0.55              |
| 1:A:229:THR:HG22 | 1:A:292:GLU:O    | 2.07                     | 0.55              |
| 1:C:419:GLU:CG   | 1:C:425:PRO:HA   | 2.35                     | 0.55              |
| 1:D:207:GLU:HB3  | 3:D:538:HOH:O    | 2.06                     | 0.55              |
| 1:D:56:ASN:C     | 1:D:58:ASP:N     | 2.64                     | 0.55              |
| 1:A:292:GLU:OE2  | 1:A:294:ARG:HD2  | 2.06                     | 0.55              |
| 1:A:365:PRO:HA   | 1:A:446:LEU:HA   | 1.88                     | 0.55              |
| 1:D:148:ILE:O    | 1:D:152:ARG:HG2  | 2.06                     | 0.55              |
| 1:A:239:MSE:HB3  | 1:A:244:ILE:HB   | 1.87                     | 0.55              |
| 1:B:72:ARG:CZ    | 1:B:210:LEU:CD1  | 2.85                     | 0.55              |
| 1:C:88:ILE:HG23  | 1:C:166:TYR:CE1  | 2.42                     | 0.55              |
| 1:B:378:VAL:HG12 | 1:B:379:VAL:N    | 2.21                     | 0.55              |
| 1:C:256:ARG:NH2  | 1:C:335:ASP:HA   | 2.21                     | 0.55              |
| 1:D:262:LEU:C    | 1:D:262:LEU:HD12 | 2.32                     | 0.55              |
| 1:C:240:PRO:C    | 1:C:242:CYS:H    | 2.13                     | 0.55              |
| 1:D:260:ILE:HG22 | 1:D:340:MSE:HE1  | 1.88                     | 0.55              |
| 1:B:104:VAL:CG1  | 1:B:106:VAL:HG22 | 2.37                     | 0.55              |
| 1:D:98:ASP:O     | 1:D:101:GLN:HG3  | 2.07                     | 0.55              |
| 1:D:134:GLU:HG2  | 3:D:542:HOH:O    | 2.06                     | 0.54              |
| 1:A:331:ARG:HD3  | 3:A:699:HOH:O    | 2.07                     | 0.54              |
| 1:C:229:THR:HG22 | 1:C:292:GLU:O    | 2.07                     | 0.54              |
| 1:D:85:MSE:HG3   | 1:D:180:PHE:CZ   | 2.41                     | 0.54              |
| 1:D:41:LEU:HD11  | 1:D:45:GLU:HG3   | 1.90                     | 0.54              |
| 1:B:84:ARG:NH2   | 1:B:163:LEU:CD2  | 2.44                     | 0.54              |
| 1:B:116:ASP:OD2  | 1:B:439:ARG:HD2  | 2.07                     | 0.54              |
| 1:B:446:LEU:HD12 | 1:B:446:LEU:N    | 2.20                     | 0.54              |
| 1:D:75:THR:HB    | 1:D:77:GLN:NE2   | 2.21                     | 0.54              |
| 1:D:78:GLU:OE2   | 1:D:152:ARG:NH2  | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:172:PHE:CB   | 1:D:177:ALA:HB2  | 2.36                     | 0.54              |
| 1:A:303:ARG:HG3  | 1:A:303:ARG:NH1  | 2.21                     | 0.54              |
| 1:C:64:ASN:N     | 1:C:64:ASN:ND2   | 2.55                     | 0.54              |
| 1:D:420:GLN:C    | 1:D:422:LEU:H    | 2.14                     | 0.54              |
| 1:A:341:ARG:NE   | 3:A:511:HOH:O    | 2.22                     | 0.54              |
| 1:B:240:PRO:HG2  | 3:B:628:HOH:O    | 2.08                     | 0.54              |
| 1:A:324:MSE:HG3  | 3:A:624:HOH:O    | 2.07                     | 0.54              |
| 1:A:348:PHE:O    | 1:A:437:GLU:HG3  | 2.06                     | 0.54              |
| 1:B:235:VAL:HG11 | 1:B:291:ILE:CD1  | 2.38                     | 0.54              |
| 1:B:353:THR:HG22 | 1:B:355:SER:H    | 1.72                     | 0.54              |
| 1:C:232:ILE:HG22 | 1:C:293:GLN:NE2  | 2.23                     | 0.54              |
| 1:D:185:LEU:HD13 | 1:D:185:LEU:O    | 2.08                     | 0.54              |
| 1:D:270:LEU:HA   | 3:D:541:HOH:O    | 2.07                     | 0.54              |
| 1:B:75:THR:HB    | 1:B:77:GLN:NE2   | 2.23                     | 0.54              |
| 1:C:41:LEU:HD23  | 1:C:42:ALA:N     | 2.23                     | 0.54              |
| 1:C:207:GLU:OE2  | 1:C:207:GLU:HA   | 2.07                     | 0.54              |
| 1:D:114:ILE:HG21 | 1:D:427:LEU:CD1  | 2.38                     | 0.54              |
| 1:D:152:ARG:HG3  | 1:D:152:ARG:HH11 | 1.73                     | 0.54              |
| 1:D:152:ARG:HE   | 1:D:154:ILE:HG13 | 1.73                     | 0.54              |
| 1:D:156:THR:HG21 | 1:D:183:GLU:HG3  | 1.88                     | 0.54              |
| 1:D:156:THR:O    | 1:D:159:CYS:HB3  | 2.08                     | 0.54              |
| 1:C:150:ARG:NH2  | 3:C:551:HOH:O    | 2.41                     | 0.54              |
| 1:B:10:ILE:C     | 1:B:89:MSE:HE3   | 2.33                     | 0.53              |
| 1:B:270:LEU:HD22 | 1:B:271:GLU:N    | 2.23                     | 0.53              |
| 1:C:256:ARG:HH22 | 1:C:335:ASP:HA   | 1.73                     | 0.53              |
| 1:C:35:LEU:O     | 1:C:39:VAL:HG23  | 2.09                     | 0.53              |
| 1:C:39:VAL:HG11  | 1:C:235:VAL:HG23 | 1.89                     | 0.53              |
| 1:A:362:ALA:HA   | 3:A:521:HOH:O    | 2.08                     | 0.53              |
| 1:B:351:ARG:NH2  | 1:B:381:GLN:HE22 | 2.07                     | 0.53              |
| 1:A:51:HIS:O     | 1:A:55:VAL:HG23  | 2.09                     | 0.53              |
| 1:A:311:ARG:HG3  | 1:A:311:ARG:HH11 | 1.74                     | 0.53              |
| 1:B:60:LEU:HD23  | 1:B:60:LEU:O     | 2.08                     | 0.53              |
| 1:B:442:ARG:C    | 1:B:444:CYS:H    | 2.16                     | 0.53              |
| 1:B:317:GLN:O    | 1:B:318:ASP:HB2  | 2.09                     | 0.53              |
| 1:B:35:LEU:HD11  | 1:B:238:MSE:HB3  | 1.89                     | 0.53              |
| 1:B:260:ILE:O    | 1:B:261:LEU:C    | 2.52                     | 0.53              |
| 1:B:353:THR:HG23 | 1:B:354:PRO:HD2  | 1.91                     | 0.53              |
| 1:C:43:VAL:HG13  | 3:C:532:HOH:O    | 2.08                     | 0.53              |
| 1:D:64:ASN:N     | 1:D:64:ASN:HD22  | 2.07                     | 0.53              |
| 1:B:173:ASN:O    | 1:B:175:THR:N    | 2.42                     | 0.52              |
| 1:C:97:TYR:HE2   | 1:C:388:PHE:O    | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:ARG:CZ   | 3:C:551:HOH:O    | 2.56                     | 0.52              |
| 1:D:270:LEU:HD12 | 3:D:541:HOH:O    | 2.08                     | 0.52              |
| 1:A:49:GLN:NE2   | 1:A:49:GLN:N     | 2.53                     | 0.52              |
| 1:B:133:LEU:C    | 1:B:135:LEU:H    | 2.16                     | 0.52              |
| 1:C:64:ASN:HD22  | 1:C:64:ASN:H     | 1.56                     | 0.52              |
| 1:C:97:TYR:N     | 1:C:97:TYR:CD1   | 2.76                     | 0.52              |
| 1:C:106:VAL:CG1  | 1:C:131:LEU:HA   | 2.32                     | 0.52              |
| 1:D:132:ARG:NH1  | 3:D:542:HOH:O    | 2.42                     | 0.52              |
| 1:A:49:GLN:H     | 1:A:49:GLN:CD    | 2.18                     | 0.52              |
| 1:B:239:MSE:N    | 1:B:240:PRO:HD2  | 2.25                     | 0.52              |
| 1:C:141:LEU:HD21 | 1:C:203:ALA:HB1  | 1.91                     | 0.52              |
| 1:D:11:ARG:NH1   | 1:D:123:PRO:N    | 2.57                     | 0.52              |
| 1:D:85:MSE:HG3   | 1:D:180:PHE:HZ   | 1.74                     | 0.52              |
| 1:A:299:THR:HG22 | 1:A:302:GLY:N    | 2.17                     | 0.52              |
| 1:D:212:ALA:O    | 1:D:216:CYS:HB2  | 2.09                     | 0.52              |
| 1:A:162:LEU:HD11 | 1:A:179:GLU:HG2  | 1.91                     | 0.52              |
| 1:B:310:LEU:HD23 | 1:B:326:LEU:HD21 | 1.91                     | 0.52              |
| 1:C:44:LEU:O     | 1:C:45:GLU:HG3   | 2.10                     | 0.52              |
| 1:C:163:LEU:C    | 1:C:163:LEU:HD13 | 2.35                     | 0.52              |
| 1:B:215:VAL:O    | 1:B:215:VAL:HG12 | 2.08                     | 0.52              |
| 1:A:353:THR:HG23 | 1:A:355:SER:H    | 1.75                     | 0.52              |
| 1:B:8:ASP:O      | 1:B:12:GLU:HG2   | 2.10                     | 0.52              |
| 1:B:262:LEU:CD2  | 1:B:389:LEU:HG   | 2.37                     | 0.52              |
| 1:C:141:LEU:HD12 | 1:C:204:LEU:HD23 | 1.92                     | 0.52              |
| 1:D:84:ARG:O     | 1:D:88:ILE:HG13  | 2.10                     | 0.52              |
| 1:A:49:GLN:H     | 1:A:49:GLN:HE21  | 1.55                     | 0.52              |
| 1:C:239:MSE:C    | 1:C:244:ILE:O    | 2.53                     | 0.52              |
| 1:C:160:ARG:HG3  | 1:C:160:ARG:HH11 | 1.76                     | 0.51              |
| 1:C:299:THR:HA   | 1:C:347:TRP:HE1  | 1.75                     | 0.51              |
| 1:D:268:LYS:HA   | 1:D:288:PHE:CD1  | 2.45                     | 0.51              |
| 1:B:91:MSE:HE1   | 1:B:124:PHE:CE2  | 2.46                     | 0.51              |
| 1:D:173:ASN:HD21 | 1:D:176:GLN:HB2  | 1.75                     | 0.51              |
| 1:B:173:ASN:O    | 1:B:176:GLN:N    | 2.43                     | 0.51              |
| 1:A:165:GLU:O    | 1:A:169:GLN:HG3  | 2.11                     | 0.51              |
| 1:A:178:GLN:HB3  | 3:A:575:HOH:O    | 2.10                     | 0.51              |
| 1:A:208:HIS:HB3  | 1:A:211:ILE:HD12 | 1.91                     | 0.51              |
| 1:D:97:TYR:N     | 1:D:97:TYR:CD1   | 2.78                     | 0.51              |
| 1:D:152:ARG:HH21 | 1:D:154:ILE:HG13 | 1.75                     | 0.51              |
| 1:D:226:THR:OG1  | 1:D:290:GLU:HB3  | 2.10                     | 0.51              |
| 1:A:269:ALA:O    | 1:A:270:LEU:HB2  | 2.11                     | 0.51              |
| 1:B:91:MSE:HE3   | 1:B:124:PHE:HD2  | 1.73                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:149:LEU:O    | 1:B:152:ARG:HG2  | 2.11                     | 0.51              |
| 1:D:232:ILE:H    | 1:D:293:GLN:NE2  | 2.09                     | 0.51              |
| 1:B:136:ILE:HG23 | 1:B:207:GLU:HG2  | 1.93                     | 0.51              |
| 1:B:248:ILE:HG22 | 1:B:320:LEU:HG   | 1.91                     | 0.51              |
| 1:D:11:ARG:HH22  | 1:D:118:SER:HB2  | 1.76                     | 0.51              |
| 1:A:27:PRO:O     | 1:A:30:GLY:N     | 2.41                     | 0.50              |
| 1:A:100:SER:C    | 1:A:102:ALA:N    | 2.69                     | 0.50              |
| 1:A:241:GLU:HB2  | 3:A:631:HOH:O    | 2.11                     | 0.50              |
| 1:B:441:LYS:O    | 1:B:444:CYS:HB2  | 2.10                     | 0.50              |
| 1:D:125:ARG:NH2  | 1:D:294:ARG:HD2  | 2.26                     | 0.50              |
| 1:D:322:HIS:HA   | 3:D:551:HOH:O    | 2.09                     | 0.50              |
| 1:D:271:GLU:OE1  | 1:D:284:HIS:HB3  | 2.12                     | 0.50              |
| 1:B:340:MSE:HE2  | 1:B:346:ALA:HB2  | 1.93                     | 0.50              |
| 1:C:100:SER:HA   | 1:C:104:VAL:O    | 2.10                     | 0.50              |
| 1:D:41:LEU:CD1   | 1:D:45:GLU:HG3   | 2.42                     | 0.50              |
| 1:A:173:ASN:HD22 | 1:A:176:GLN:H    | 1.59                     | 0.50              |
| 1:A:239:MSE:SE   | 1:A:246:PRO:HB3  | 2.60                     | 0.50              |
| 1:A:353:THR:O    | 1:A:354:PRO:C    | 2.53                     | 0.50              |
| 1:B:141:LEU:HD21 | 1:B:203:ALA:CB   | 2.41                     | 0.50              |
| 1:B:213:ASP:OD1  | 1:B:221:HIS:HE1  | 1.95                     | 0.50              |
| 1:C:133:LEU:C    | 1:C:135:LEU:H    | 2.20                     | 0.50              |
| 1:C:113:PRO:HB2  | 1:C:119:LEU:CD2  | 2.42                     | 0.50              |
| 1:C:299:THR:HA   | 1:C:347:TRP:NE1  | 2.27                     | 0.50              |
| 1:B:443:ARG:HG3  | 1:B:443:ARG:NH1  | 2.24                     | 0.50              |
| 1:C:173:ASN:HB2  | 1:C:176:GLN:HB2  | 1.93                     | 0.50              |
| 1:D:104:VAL:HG12 | 1:D:106:VAL:HG22 | 1.92                     | 0.50              |
| 1:C:46:ASN:N     | 1:C:46:ASN:HD22  | 2.09                     | 0.50              |
| 1:C:83:ARG:HA    | 1:C:111:PHE:CE2  | 2.47                     | 0.50              |
| 1:D:47:ASN:C     | 1:D:47:ASN:HD22  | 2.20                     | 0.50              |
| 1:A:49:GLN:N     | 1:A:49:GLN:HE21  | 2.09                     | 0.49              |
| 1:A:412:ASN:C    | 1:A:414:SER:H    | 2.19                     | 0.49              |
| 1:C:27:PRO:HD2   | 3:C:518:HOH:O    | 2.11                     | 0.49              |
| 1:C:266:SER:HA   | 1:C:289:GLY:O    | 2.11                     | 0.49              |
| 1:D:239:MSE:HG3  | 3:D:505:HOH:O    | 2.11                     | 0.49              |
| 1:A:63:LEU:HD22  | 1:A:230:LEU:HD21 | 1.94                     | 0.49              |
| 1:B:141:LEU:HD11 | 1:B:203:ALA:HB1  | 1.94                     | 0.49              |
| 1:C:6:THR:HG21   | 3:C:540:HOH:O    | 2.12                     | 0.49              |
| 1:C:333:PHE:HE1  | 1:C:340:MSE:HE3  | 1.75                     | 0.49              |
| 1:D:47:ASN:ND2   | 1:D:49:GLN:HB2   | 2.26                     | 0.49              |
| 1:A:6:THR:HB     | 3:A:645:HOH:O    | 2.11                     | 0.49              |
| 1:B:323:GLN:O    | 1:B:327:GLN:HG3  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:62:ARG:HD3   | 1:C:66:GLU:OE2   | 2.11                     | 0.49              |
| 1:C:64:ASN:ND2   | 1:C:64:ASN:H     | 2.10                     | 0.49              |
| 1:A:310:LEU:C    | 1:A:312:ASN:H    | 2.19                     | 0.49              |
| 1:B:10:ILE:O     | 1:B:89:MSE:CE    | 2.60                     | 0.49              |
| 1:D:236:GLN:HA   | 1:D:239:MSE:HG3  | 1.95                     | 0.49              |
| 1:A:5:ILE:HD11   | 1:A:172:PHE:CB   | 2.42                     | 0.49              |
| 1:B:90:GLY:O     | 1:B:92:TYR:CE2   | 2.66                     | 0.49              |
| 1:C:169:GLN:HE22 | 1:C:176:GLN:HE22 | 1.59                     | 0.49              |
| 1:A:108:SER:CB   | 1:A:128:THR:O    | 2.61                     | 0.49              |
| 1:A:299:THR:HG23 | 1:A:301:LYS:N    | 2.25                     | 0.49              |
| 1:C:134:GLU:HG2  | 1:C:135:LEU:HD22 | 1.95                     | 0.49              |
| 1:C:187:THR:HG22 | 1:C:187:THR:O    | 2.12                     | 0.49              |
| 1:D:14:PHE:HB2   | 1:D:89:MSE:HE1   | 1.94                     | 0.49              |
| 1:D:255:ARG:O    | 1:D:256:ARG:HG3  | 2.12                     | 0.49              |
| 1:A:68:HIS:C     | 1:A:68:HIS:CD2   | 2.91                     | 0.49              |
| 1:A:139:GLU:HG3  | 1:D:324:MSE:CE   | 2.31                     | 0.49              |
| 1:B:347:TRP:HB3  | 1:B:383:ILE:HD12 | 1.94                     | 0.49              |
| 1:B:378:VAL:CG1  | 1:B:379:VAL:N    | 2.75                     | 0.49              |
| 1:C:248:ILE:H    | 1:C:248:ILE:CD1  | 2.24                     | 0.49              |
| 1:A:67:ARG:HA    | 1:A:226:THR:O    | 2.13                     | 0.49              |
| 1:B:370:GLN:HE21 | 1:B:374:GLU:CD   | 2.20                     | 0.49              |
| 1:C:163:LEU:O    | 1:C:163:LEU:HD22 | 2.13                     | 0.49              |
| 1:D:177:ALA:C    | 1:D:179:GLU:N    | 2.69                     | 0.49              |
| 1:B:287:ARG:HB3  | 3:B:632:HOH:O    | 2.11                     | 0.49              |
| 1:C:19:SER:HA    | 1:C:225:LEU:CD1  | 2.43                     | 0.49              |
| 1:C:72:ARG:CZ    | 1:C:223:ASN:ND2  | 2.76                     | 0.49              |
| 1:D:152:ARG:HG3  | 1:D:152:ARG:NH1  | 2.28                     | 0.49              |
| 1:D:154:ILE:CG1  | 1:D:219:GLY:HA2  | 2.34                     | 0.49              |
| 1:A:48:PRO:O     | 1:A:52:GLU:HG3   | 2.13                     | 0.49              |
| 1:B:108:SER:HB3  | 1:B:128:THR:O    | 2.13                     | 0.49              |
| 1:B:142:ARG:O    | 1:B:145:ALA:HB3  | 2.13                     | 0.49              |
| 1:C:105:PRO:O    | 1:C:106:VAL:HG13 | 2.12                     | 0.49              |
| 1:A:239:MSE:N    | 1:A:240:PRO:HD2  | 2.28                     | 0.48              |
| 1:A:415:ARG:O    | 1:A:419:GLU:HG3  | 2.12                     | 0.48              |
| 1:B:91:MSE:HE1   | 1:B:124:PHE:CD2  | 2.48                     | 0.48              |
| 1:B:166:TYR:HB2  | 1:B:172:PHE:CZ   | 2.47                     | 0.48              |
| 1:D:160:ARG:HD3  | 1:D:161:GLN:N    | 2.28                     | 0.48              |
| 1:D:195:THR:HG22 | 1:D:195:THR:O    | 2.13                     | 0.48              |
| 1:A:347:TRP:HB3  | 1:A:383:ILE:HD12 | 1.95                     | 0.48              |
| 1:C:113:PRO:O    | 1:C:119:LEU:HD21 | 2.12                     | 0.48              |
| 1:D:244:ILE:HG23 | 1:D:267:PHE:CD2  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:268:LYS:HE3  | 1:D:271:GLU:HG2  | 1.95                     | 0.48              |
| 1:C:104:VAL:HG12 | 1:C:106:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:140:ILE:H    | 1:C:140:ILE:HG13 | 1.44                     | 0.48              |
| 1:B:283:THR:OG1  | 1:B:284:HIS:N    | 2.47                     | 0.48              |
| 1:C:426:VAL:HG11 | 3:C:576:HOH:O    | 2.12                     | 0.48              |
| 1:A:173:ASN:ND2  | 1:A:176:GLN:HG3  | 2.29                     | 0.48              |
| 1:D:10:ILE:O     | 1:D:89:MSE:HE2   | 2.12                     | 0.48              |
| 1:A:68:HIS:NE2   | 1:A:224:HIS:HE1  | 2.11                     | 0.48              |
| 1:C:83:ARG:HD3   | 1:C:422:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:6:THR:CG2    | 1:A:9:GLU:HB2    | 2.42                     | 0.48              |
| 1:B:420:GLN:O    | 1:B:420:GLN:HG2  | 2.14                     | 0.48              |
| 1:C:224:HIS:CD2  | 1:C:224:HIS:O    | 2.66                     | 0.48              |
| 1:A:50:LEU:HD23  | 1:A:50:LEU:C     | 2.38                     | 0.48              |
| 1:A:226:THR:HG21 | 1:A:292:GLU:HG2  | 1.95                     | 0.48              |
| 1:A:309:LEU:HD22 | 1:A:329:THR:HG22 | 1.96                     | 0.48              |
| 1:C:234:ARG:O    | 1:C:238:MSE:HG2  | 2.13                     | 0.48              |
| 1:D:35:LEU:C     | 1:D:37:ALA:H     | 2.22                     | 0.48              |
| 1:A:173:ASN:C    | 1:A:173:ASN:ND2  | 2.61                     | 0.48              |
| 1:D:274:VAL:HB   | 1:D:283:THR:CG2  | 2.42                     | 0.48              |
| 1:B:229:THR:HG22 | 1:B:292:GLU:O    | 2.13                     | 0.48              |
| 1:D:73:VAL:HG23  | 1:D:130:LEU:HD12 | 1.96                     | 0.48              |
| 1:D:226:THR:HG23 | 1:D:290:GLU:O    | 2.12                     | 0.48              |
| 1:D:231:ASP:OD1  | 1:D:233:ASP:HB2  | 2.13                     | 0.48              |
| 1:B:106:VAL:HG11 | 1:B:210:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:5:ILE:N      | 1:A:5:ILE:HD13   | 2.29                     | 0.47              |
| 1:A:88:ILE:O     | 1:A:88:ILE:HG22  | 2.14                     | 0.47              |
| 1:A:355:SER:HG   | 1:A:377:TRP:CD1  | 2.32                     | 0.47              |
| 1:C:232:ILE:HB   | 1:C:293:GLN:HB2  | 1.95                     | 0.47              |
| 1:C:328:GLU:O    | 1:C:331:ARG:HG3  | 2.13                     | 0.47              |
| 1:D:98:ASP:OD2   | 1:D:100:SER:OG   | 2.29                     | 0.47              |
| 1:B:156:THR:O    | 1:B:159:CYS:HB3  | 2.15                     | 0.47              |
| 1:C:301:LYS:HE2  | 1:C:343:GLN:O    | 2.14                     | 0.47              |
| 1:D:173:ASN:ND2  | 1:D:176:GLN:HB2  | 2.29                     | 0.47              |
| 1:A:429:GLU:H    | 1:A:429:GLU:HG3  | 1.50                     | 0.47              |
| 1:C:209:ARG:NH2  | 3:C:549:HOH:O    | 2.47                     | 0.47              |
| 1:C:230:LEU:HD12 | 1:C:230:LEU:N    | 2.29                     | 0.47              |
| 1:D:99:LEU:HD12  | 1:D:106:VAL:CG2  | 2.42                     | 0.47              |
| 1:D:147:GLU:OE2  | 1:D:150:ARG:NH1  | 2.48                     | 0.47              |
| 1:D:177:ALA:C    | 1:D:179:GLU:H    | 2.22                     | 0.47              |
| 1:B:248:ILE:HG21 | 1:B:320:LEU:HG   | 1.95                     | 0.47              |
| 1:A:330:PHE:C    | 1:A:332:THR:N    | 2.71                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:225:LEU:HD23 | 1:B:225:LEU:HA   | 1.70                     | 0.47              |
| 1:B:270:LEU:HD13 | 1:B:270:LEU:C    | 2.39                     | 0.47              |
| 1:C:86:PHE:HD1   | 1:C:91:MSE:HE3   | 1.80                     | 0.47              |
| 1:C:89:MSE:HB2   | 1:C:91:MSE:CE    | 2.44                     | 0.47              |
| 1:D:16:GLN:NE2   | 1:D:16:GLN:HA    | 2.30                     | 0.47              |
| 1:D:420:GLN:C    | 1:D:422:LEU:N    | 2.71                     | 0.47              |
| 1:A:239:MSE:HE2  | 1:A:244:ILE:CG2  | 2.38                     | 0.47              |
| 1:B:47:ASN:C     | 1:B:47:ASN:ND2   | 2.71                     | 0.47              |
| 1:B:319:ASN:CB   | 1:B:321:THR:HG23 | 2.44                     | 0.47              |
| 1:C:45:GLU:C     | 1:C:46:ASN:HD22  | 2.23                     | 0.47              |
| 1:D:57:ALA:HB3   | 1:D:59:GLU:HG2   | 1.97                     | 0.47              |
| 1:B:220:CYS:SG   | 1:B:220:CYS:O    | 2.73                     | 0.47              |
| 1:B:319:ASN:CG   | 1:B:321:THR:HG23 | 2.39                     | 0.47              |
| 1:C:326:LEU:HD13 | 1:C:326:LEU:C    | 2.40                     | 0.47              |
| 1:D:96:TYR:CE1   | 1:D:107:HIS:HB2  | 2.49                     | 0.47              |
| 1:B:35:LEU:HD11  | 1:B:238:MSE:CB   | 2.45                     | 0.47              |
| 1:C:106:VAL:HG12 | 1:C:130:LEU:O    | 2.15                     | 0.47              |
| 1:C:113:PRO:HB2  | 1:C:119:LEU:HD23 | 1.97                     | 0.47              |
| 1:D:14:PHE:CD1   | 1:D:89:MSE:HE1   | 2.50                     | 0.47              |
| 1:D:157:PRO:O    | 1:D:161:GLN:HB2  | 2.15                     | 0.47              |
| 1:C:83:ARG:HH11  | 1:C:83:ARG:HG2   | 1.80                     | 0.47              |
| 1:C:227:PRO:HG2  | 1:C:291:ILE:CD1  | 2.44                     | 0.47              |
| 1:D:225:LEU:HD21 | 3:D:544:HOH:O    | 2.15                     | 0.47              |
| 1:D:32:LEU:CD1   | 1:D:239:MSE:HE3  | 2.45                     | 0.46              |
| 1:D:168:GLN:HG2  | 3:D:565:HOH:O    | 2.14                     | 0.46              |
| 1:D:207:GLU:O    | 1:D:207:GLU:HG3  | 2.15                     | 0.46              |
| 1:A:83:ARG:HH21  | 1:A:423:GLY:HA3  | 1.80                     | 0.46              |
| 1:B:112:ARG:HB3  | 1:B:125:ARG:HG2  | 1.97                     | 0.46              |
| 1:C:19:SER:HA    | 1:C:225:LEU:HD11 | 1.98                     | 0.46              |
| 1:D:173:ASN:OD1  | 1:D:176:GLN:N    | 2.37                     | 0.46              |
| 1:A:109:THR:HG22 | 3:A:671:HOH:O    | 2.14                     | 0.46              |
| 1:A:143:GLN:HA   | 1:A:143:GLN:OE1  | 2.15                     | 0.46              |
| 1:A:249:LEU:HA   | 3:A:598:HOH:O    | 2.14                     | 0.46              |
| 1:A:220:CYS:HB3  | 3:A:586:HOH:O    | 2.15                     | 0.46              |
| 1:B:92:TYR:HB3   | 1:B:93:PRO:HD2   | 1.97                     | 0.46              |
| 1:B:299:THR:HG22 | 1:B:300:PRO:N    | 2.30                     | 0.46              |
| 1:C:296:VAL:HA   | 1:C:384:THR:HA   | 1.96                     | 0.46              |
| 1:C:299:THR:O    | 1:C:300:PRO:C    | 2.58                     | 0.46              |
| 1:B:115:ASP:HB2  | 3:B:576:HOH:O    | 2.16                     | 0.46              |
| 1:B:125:ARG:CZ   | 1:B:294:ARG:HH11 | 2.25                     | 0.46              |
| 1:B:133:LEU:O    | 1:B:136:ILE:HG13 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:370:GLN:N    | 1:B:371:PRO:CD   | 2.78                     | 0.46              |
| 1:B:6:THR:CG2    | 1:B:9:GLU:HB2    | 2.46                     | 0.46              |
| 1:B:125:ARG:N    | 3:B:586:HOH:O    | 2.23                     | 0.46              |
| 1:D:14:PHE:CE2   | 1:D:18:MSE:HE2   | 2.50                     | 0.46              |
| 1:D:54:MSE:HE2   | 1:D:59:GLU:OE2   | 2.16                     | 0.46              |
| 1:D:204:LEU:HD13 | 1:D:211:ILE:HG22 | 1.98                     | 0.46              |
| 1:D:72:ARG:HE    | 1:D:210:LEU:HD12 | 1.81                     | 0.46              |
| 1:D:251:GLU:O    | 1:D:263:ARG:HA   | 2.16                     | 0.46              |
| 1:A:210:LEU:HD23 | 1:A:210:LEU:O    | 2.16                     | 0.46              |
| 1:A:412:ASN:C    | 1:A:414:SER:N    | 2.72                     | 0.46              |
| 1:A:412:ASN:OD1  | 1:A:413:ALA:N    | 2.48                     | 0.46              |
| 1:B:178:GLN:O    | 1:B:182:GLN:HG2  | 2.15                     | 0.46              |
| 1:B:270:LEU:HD22 | 1:B:271:GLU:H    | 1.80                     | 0.46              |
| 1:A:250:ILE:HG21 | 1:A:263:ARG:NH2  | 2.31                     | 0.46              |
| 1:C:43:VAL:HA    | 3:C:532:HOH:O    | 2.16                     | 0.46              |
| 1:D:316:GLY:O    | 1:D:317:GLN:C    | 2.59                     | 0.46              |
| 1:C:239:MSE:CB   | 1:C:246:PRO:HD3  | 2.46                     | 0.45              |
| 1:C:136:ILE:HB   | 1:C:142:ARG:CB   | 2.44                     | 0.45              |
| 1:B:32:LEU:HD11  | 1:B:291:ILE:HD12 | 1.98                     | 0.45              |
| 1:B:207:GLU:O    | 1:B:208:HIS:HB2  | 2.16                     | 0.45              |
| 1:B:250:ILE:HG12 | 1:B:265:THR:OG1  | 2.16                     | 0.45              |
| 1:D:72:ARG:HB3   | 1:D:214:VAL:HG22 | 1.98                     | 0.45              |
| 1:A:45:GLU:HB2   | 3:A:520:HOH:O    | 2.17                     | 0.45              |
| 1:B:154:ILE:HG22 | 1:B:219:GLY:HA2  | 1.98                     | 0.45              |
| 1:A:6:THR:HA     | 3:A:692:HOH:O    | 2.17                     | 0.45              |
| 1:B:226:THR:HG23 | 1:B:291:ILE:HA   | 1.99                     | 0.45              |
| 1:C:62:ARG:HG3   | 1:C:63:LEU:N     | 2.31                     | 0.45              |
| 1:C:115:ASP:O    | 1:C:117:ALA:N    | 2.50                     | 0.45              |
| 1:D:238:MSE:O    | 1:D:241:GLU:HB2  | 2.16                     | 0.45              |
| 1:B:149:LEU:HD12 | 1:B:149:LEU:HA   | 1.81                     | 0.45              |
| 1:B:445:GLY:C    | 1:B:446:LEU:CD1  | 2.76                     | 0.45              |
| 1:C:188:PHE:CD1  | 1:C:188:PHE:N    | 2.84                     | 0.45              |
| 1:D:160:ARG:HD3  | 1:D:160:ARG:C    | 2.42                     | 0.45              |
| 1:D:341:ARG:HD2  | 1:D:350:TYR:CE1  | 2.52                     | 0.45              |
| 1:A:109:THR:HG23 | 3:A:671:HOH:O    | 2.12                     | 0.45              |
| 1:C:8:ASP:HB3    | 1:C:121:ARG:HD3  | 1.98                     | 0.45              |
| 1:C:324:MSE:O    | 1:C:327:GLN:HB3  | 2.16                     | 0.45              |
| 1:D:46:ASN:HD22  | 1:D:46:ASN:HA    | 1.61                     | 0.45              |
| 1:D:162:LEU:O    | 1:D:165:GLU:HB3  | 2.16                     | 0.45              |
| 1:A:65:VAL:O     | 1:A:67:ARG:HD3   | 2.15                     | 0.45              |
| 1:A:208:HIS:HB3  | 1:A:211:ILE:CD1  | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:262:LEU:C    | 1:A:262:LEU:CD1  | 2.89                     | 0.45              |
| 1:A:270:LEU:HD13 | 1:A:271:GLU:N    | 2.32                     | 0.45              |
| 1:B:262:LEU:N    | 1:B:262:LEU:HD23 | 2.32                     | 0.45              |
| 1:C:32:LEU:HD22  | 1:C:267:PHE:CZ   | 2.43                     | 0.45              |
| 1:A:193:LEU:HD11 | 1:B:309:LEU:HD23 | 1.97                     | 0.45              |
| 1:A:248:ILE:H    | 1:A:248:ILE:CD1  | 2.19                     | 0.45              |
| 1:B:424:CYS:HB2  | 1:B:425:PRO:HD2  | 1.98                     | 0.45              |
| 1:B:49:GLN:H     | 1:B:49:GLN:NE2   | 2.13                     | 0.45              |
| 1:B:106:VAL:CG1  | 1:B:210:LEU:HD21 | 2.47                     | 0.45              |
| 1:C:72:ARG:O     | 1:C:220:CYS:HB3  | 2.16                     | 0.45              |
| 1:C:136:ILE:HD12 | 1:C:142:ARG:HB2  | 1.98                     | 0.44              |
| 1:A:107:HIS:CG   | 1:A:132:ARG:HD2  | 2.52                     | 0.44              |
| 1:B:133:LEU:C    | 1:B:135:LEU:N    | 2.75                     | 0.44              |
| 1:C:298:LEU:C    | 1:C:347:TRP:NE1  | 2.75                     | 0.44              |
| 1:D:157:PRO:C    | 1:D:159:CYS:H    | 2.25                     | 0.44              |
| 1:D:239:MSE:N    | 1:D:240:PRO:HD2  | 2.33                     | 0.44              |
| 1:D:355:SER:C    | 1:D:357:GLU:N    | 2.75                     | 0.44              |
| 1:D:428:ASP:O    | 1:D:429:GLU:C    | 2.60                     | 0.44              |
| 1:A:268:LYS:HE2  | 1:A:286:ALA:CB   | 2.47                     | 0.44              |
| 1:C:62:ARG:HG3   | 1:C:63:LEU:H     | 1.83                     | 0.44              |
| 1:C:164:GLU:HG2  | 1:C:168:GLN:NE2  | 2.32                     | 0.44              |
| 1:C:219:GLY:N    | 3:C:527:HOH:O    | 2.36                     | 0.44              |
| 1:A:137:GLU:OE1  | 1:A:137:GLU:HA   | 2.17                     | 0.44              |
| 1:A:424:CYS:HB2  | 1:A:425:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:66:GLU:CD    | 1:B:228:ARG:HD2  | 2.42                     | 0.44              |
| 1:C:85:MSE:HE1   | 1:C:188:PHE:CZ   | 2.48                     | 0.44              |
| 1:B:68:HIS:CD2   | 1:B:68:HIS:C     | 2.94                     | 0.44              |
| 1:B:123:PRO:O    | 1:B:125:ARG:HG3  | 2.18                     | 0.44              |
| 1:B:332:THR:HG22 | 1:B:332:THR:O    | 2.17                     | 0.44              |
| 1:A:322:HIS:HA   | 3:A:665:HOH:O    | 2.17                     | 0.44              |
| 1:B:14:PHE:HB2   | 1:B:89:MSE:CE    | 2.30                     | 0.44              |
| 1:B:62:ARG:HG3   | 1:B:63:LEU:N     | 2.33                     | 0.44              |
| 1:C:236:GLN:O    | 1:C:236:GLN:HG2  | 2.17                     | 0.44              |
| 1:D:94:VAL:HA    | 1:D:427:LEU:HB2  | 1.98                     | 0.44              |
| 1:D:107:HIS:HE1  | 1:D:130:LEU:HD23 | 1.83                     | 0.44              |
| 1:C:222:ILE:HG22 | 1:C:224:HIS:N    | 2.33                     | 0.44              |
| 1:D:28:GLN:NE2   | 1:D:244:ILE:HG12 | 2.32                     | 0.44              |
| 1:D:47:ASN:C     | 1:D:47:ASN:ND2   | 2.75                     | 0.44              |
| 1:D:67:ARG:HB3   | 1:D:225:LEU:HD21 | 2.00                     | 0.44              |
| 1:B:370:GLN:O    | 1:B:374:GLU:HG2  | 2.17                     | 0.44              |
| 1:C:68:HIS:C     | 1:C:68:HIS:HD2   | 2.25                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:ARG:HH21 | 1:C:151:GLN:CD   | 2.25                     | 0.44              |
| 1:C:233:ASP:HB3  | 3:C:548:HOH:O    | 2.17                     | 0.44              |
| 1:C:269:ALA:HB3  | 1:C:287:ARG:O    | 2.18                     | 0.44              |
| 1:C:339:LEU:O    | 1:C:343:GLN:HG2  | 2.18                     | 0.44              |
| 1:D:387:ASP:OD1  | 1:D:429:GLU:HB3  | 2.18                     | 0.44              |
| 1:A:244:ILE:O    | 1:A:246:PRO:HD3  | 2.17                     | 0.43              |
| 1:C:150:ARG:NH2  | 1:C:151:GLN:HE22 | 2.11                     | 0.43              |
| 1:C:223:ASN:O    | 1:C:224:HIS:CB   | 2.66                     | 0.43              |
| 1:D:105:PRO:O    | 1:D:106:VAL:HG13 | 2.18                     | 0.43              |
| 1:B:5:ILE:HA     | 3:B:516:HOH:O    | 2.18                     | 0.43              |
| 1:B:16:GLN:HE21  | 1:B:16:GLN:HA    | 1.82                     | 0.43              |
| 1:C:40:ASN:OD1   | 1:C:230:LEU:HD13 | 2.18                     | 0.43              |
| 1:D:283:THR:HG23 | 1:D:284:HIS:N    | 2.32                     | 0.43              |
| 1:A:193:LEU:HD12 | 1:B:308:ASP:HB3  | 1.99                     | 0.43              |
| 1:A:300:PRO:HD2  | 3:A:683:HOH:O    | 2.18                     | 0.43              |
| 1:A:360:ARG:NH2  | 3:A:518:HOH:O    | 2.34                     | 0.43              |
| 1:B:419:GLU:OE2  | 1:B:426:VAL:HG22 | 2.18                     | 0.43              |
| 1:C:136:ILE:CG2  | 1:C:142:ARG:HB3  | 2.48                     | 0.43              |
| 1:C:153:ASP:OD1  | 1:C:160:ARG:NH1  | 2.51                     | 0.43              |
| 1:A:30:GLY:HA3   | 3:A:590:HOH:O    | 2.18                     | 0.43              |
| 1:A:83:ARG:HG3   | 1:A:422:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:108:SER:HB2  | 1:A:128:THR:O    | 2.18                     | 0.43              |
| 1:B:105:PRO:C    | 1:B:106:VAL:HG13 | 2.43                     | 0.43              |
| 1:B:319:ASN:N    | 1:B:319:ASN:ND2  | 2.62                     | 0.43              |
| 1:B:11:ARG:HB2   | 1:B:89:MSE:HG3   | 1.99                     | 0.43              |
| 1:D:64:ASN:N     | 1:D:64:ASN:ND2   | 2.67                     | 0.43              |
| 1:A:353:THR:HG23 | 1:A:355:SER:N    | 2.33                     | 0.43              |
| 1:C:202:ARG:HG3  | 1:C:202:ARG:HH11 | 1.83                     | 0.43              |
| 1:D:236:GLN:N    | 3:D:505:HOH:O    | 2.52                     | 0.43              |
| 1:D:320:LEU:C    | 1:D:322:HIS:H    | 2.26                     | 0.43              |
| 1:A:66:GLU:HG3   | 1:A:123:PRO:HG2  | 2.01                     | 0.43              |
| 1:B:84:ARG:NE    | 1:B:163:LEU:HD21 | 2.33                     | 0.43              |
| 1:C:443:ARG:C    | 1:C:445:GLY:H    | 2.25                     | 0.43              |
| 1:C:126:VAL:O    | 1:C:126:VAL:HG12 | 2.18                     | 0.43              |
| 1:A:35:LEU:HD11  | 1:A:238:MSE:CB   | 2.49                     | 0.43              |
| 1:A:265:THR:HG22 | 1:A:266:SER:N    | 2.33                     | 0.43              |
| 1:A:269:ALA:O    | 1:A:270:LEU:CB   | 2.67                     | 0.43              |
| 1:D:178:GLN:O    | 1:D:178:GLN:NE2  | 2.52                     | 0.43              |
| 1:A:264:GLN:HE21 | 1:A:389:LEU:HD12 | 1.84                     | 0.43              |
| 1:C:61:ALA:HB2   | 3:C:515:HOH:O    | 2.18                     | 0.43              |
| 1:D:39:VAL:HG21  | 1:D:235:VAL:CG2  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:267:PHE:CZ   | 1:A:289:GLY:HA3  | 2.54                     | 0.42              |
| 1:B:125:ARG:NE   | 1:B:294:ARG:NH1  | 2.67                     | 0.42              |
| 1:B:241:GLU:HG2  | 3:B:630:HOH:O    | 2.19                     | 0.42              |
| 1:B:299:THR:CG2  | 1:B:300:PRO:CD   | 2.97                     | 0.42              |
| 1:C:185:LEU:HD12 | 1:C:185:LEU:HA   | 1.89                     | 0.42              |
| 1:C:340:MSE:HE2  | 1:C:346:ALA:HB2  | 2.01                     | 0.42              |
| 1:D:162:LEU:HD22 | 1:D:172:PHE:HE1  | 1.84                     | 0.42              |
| 1:D:174:GLU:H    | 1:D:174:GLU:CD   | 2.27                     | 0.42              |
| 1:D:250:ILE:HG12 | 1:D:265:THR:OG1  | 2.19                     | 0.42              |
| 1:D:294:ARG:HH21 | 1:D:386:GLU:C    | 2.27                     | 0.42              |
| 1:B:260:ILE:HG22 | 1:B:340:MSE:HE1  | 2.01                     | 0.42              |
| 1:C:89:MSE:HB3   | 1:C:91:MSE:HE2   | 2.00                     | 0.42              |
| 1:C:222:ILE:HG22 | 1:C:224:HIS:H    | 1.84                     | 0.42              |
| 1:D:106:VAL:HG13 | 1:D:210:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:183:GLU:O    | 1:B:186:GLU:HB2  | 2.19                     | 0.42              |
| 1:B:379:VAL:O    | 1:B:379:VAL:HG13 | 2.19                     | 0.42              |
| 1:C:272:GLU:HG3  | 1:C:273:THR:N    | 2.35                     | 0.42              |
| 1:D:247:LYS:HE2  | 1:D:249:LEU:CB   | 2.42                     | 0.42              |
| 1:D:224:HIS:C    | 1:D:224:HIS:CD2  | 2.97                     | 0.42              |
| 1:A:156:THR:OG1  | 1:A:159:CYS:HB2  | 2.19                     | 0.42              |
| 1:A:262:LEU:HD12 | 1:A:262:LEU:O    | 2.19                     | 0.42              |
| 1:B:72:ARG:CZ    | 1:B:210:LEU:HD11 | 2.49                     | 0.42              |
| 1:B:115:ASP:HB3  | 1:B:118:SER:HB2  | 2.02                     | 0.42              |
| 1:B:133:LEU:O    | 1:B:135:LEU:N    | 2.52                     | 0.42              |
| 1:B:299:THR:HG21 | 3:B:542:HOH:O    | 2.19                     | 0.42              |
| 1:D:48:PRO:HA    | 3:D:540:HOH:O    | 2.20                     | 0.42              |
| 1:D:324:MSE:O    | 1:D:327:GLN:HB3  | 2.18                     | 0.42              |
| 1:A:108:SER:HB3  | 1:A:129:SER:CA   | 2.35                     | 0.42              |
| 1:B:213:ASP:OD1  | 1:B:221:HIS:CE1  | 2.72                     | 0.42              |
| 1:C:15:SER:C     | 1:C:67:ARG:HH21  | 2.27                     | 0.42              |
| 1:C:230:LEU:O    | 1:C:231:ASP:HB3  | 2.19                     | 0.42              |
| 1:C:326:LEU:HD13 | 1:C:326:LEU:O    | 2.19                     | 0.42              |
| 1:B:11:ARG:O     | 1:B:89:MSE:HE2   | 2.20                     | 0.42              |
| 1:B:428:ASP:C    | 1:B:428:ASP:OD1  | 2.63                     | 0.42              |
| 1:A:232:ILE:HG23 | 1:A:233:ASP:N    | 2.35                     | 0.42              |
| 1:B:125:ARG:NH2  | 1:B:294:ARG:HH11 | 2.17                     | 0.42              |
| 1:B:257:GLU:HB2  | 1:B:335:ASP:OD2  | 2.19                     | 0.42              |
| 1:C:17:ALA:CB    | 1:C:185:LEU:HD21 | 2.49                     | 0.42              |
| 1:C:125:ARG:HD3  | 1:C:386:GLU:O    | 2.19                     | 0.42              |
| 1:C:190:TRP:CZ2  | 1:C:272:GLU:HG2  | 2.54                     | 0.42              |
| 1:D:157:PRO:C    | 1:D:159:CYS:N    | 2.76                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:226:THR:HA   | 1:D:227:PRO:HD3  | 1.72                     | 0.42              |
| 1:A:83:ARG:HB3   | 1:A:83:ARG:NH1   | 2.35                     | 0.42              |
| 1:A:147:GLU:HA   | 1:A:150:ARG:NH1  | 2.35                     | 0.42              |
| 1:B:141:LEU:O    | 1:B:145:ALA:N    | 2.53                     | 0.42              |
| 1:B:253:PRO:O    | 1:B:263:ARG:NE   | 2.52                     | 0.42              |
| 1:B:274:VAL:HB   | 1:B:283:THR:HG23 | 2.01                     | 0.42              |
| 1:D:60:LEU:HD23  | 1:D:60:LEU:C     | 2.45                     | 0.42              |
| 1:D:107:HIS:CE1  | 1:D:130:LEU:HD23 | 2.55                     | 0.42              |
| 1:D:156:THR:CG2  | 1:D:183:GLU:HG3  | 2.49                     | 0.42              |
| 1:D:414:SER:O    | 1:D:417:ALA:HB3  | 2.20                     | 0.42              |
| 1:A:118:SER:N    | 3:A:679:HOH:O    | 2.52                     | 0.42              |
| 1:B:47:ASN:ND2   | 1:B:50:LEU:H     | 2.18                     | 0.42              |
| 1:C:68:HIS:HB2   | 1:C:125:ARG:HB2  | 2.02                     | 0.42              |
| 1:C:114:ILE:HG22 | 1:C:432:LEU:HD13 | 2.02                     | 0.42              |
| 1:C:211:ILE:O    | 1:C:215:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:254:PRO:O    | 1:A:256:ARG:HG3  | 2.19                     | 0.41              |
| 1:B:10:ILE:O     | 1:B:89:MSE:HE3   | 2.17                     | 0.41              |
| 1:B:141:LEU:HD21 | 1:B:203:ALA:HB1  | 2.02                     | 0.41              |
| 1:B:253:PRO:HG3  | 1:B:260:ILE:HG13 | 2.02                     | 0.41              |
| 1:C:106:VAL:HG12 | 1:C:131:LEU:CA   | 2.36                     | 0.41              |
| 1:D:5:ILE:N      | 1:D:5:ILE:CD1    | 2.83                     | 0.41              |
| 1:D:6:THR:OG1    | 1:D:9:GLU:HG3    | 2.20                     | 0.41              |
| 1:D:57:ALA:O     | 1:D:58:ASP:C     | 2.62                     | 0.41              |
| 1:C:239:MSE:HB2  | 1:C:240:PRO:CD   | 2.46                     | 0.41              |
| 1:A:26:VAL:O     | 1:A:29:TYR:HB3   | 2.20                     | 0.41              |
| 1:B:162:LEU:HD13 | 1:B:180:PHE:HA   | 2.02                     | 0.41              |
| 1:B:247:LYS:HB3  | 1:B:266:SER:O    | 2.20                     | 0.41              |
| 1:D:165:GLU:O    | 1:D:169:GLN:HG2  | 2.19                     | 0.41              |
| 1:A:49:GLN:O     | 1:A:50:LEU:C     | 2.64                     | 0.41              |
| 1:A:353:THR:HB   | 1:A:377:TRP:O    | 2.20                     | 0.41              |
| 1:B:350:TYR:O    | 1:B:440:SER:HB2  | 2.21                     | 0.41              |
| 1:C:96:TYR:HA    | 3:C:576:HOH:O    | 2.20                     | 0.41              |
| 1:C:166:TYR:CE1  | 1:C:171:GLY:HA2  | 2.55                     | 0.41              |
| 1:C:299:THR:CG2  | 1:C:300:PRO:HD2  | 2.49                     | 0.41              |
| 1:C:303:ARG:O    | 1:C:306:TYR:HB3  | 2.21                     | 0.41              |
| 1:D:14:PHE:HB2   | 1:D:89:MSE:CE    | 2.49                     | 0.41              |
| 1:D:166:TYR:C    | 1:D:168:GLN:N    | 2.79                     | 0.41              |
| 1:D:302:GLY:HA3  | 1:D:345:LEU:O    | 2.21                     | 0.41              |
| 1:D:319:ASN:C    | 1:D:321:THR:N    | 2.78                     | 0.41              |
| 1:B:29:TYR:CE2   | 1:B:33:LEU:HD11  | 2.55                     | 0.41              |
| 1:B:198:GLU:HA   | 1:B:276:PHE:CE1  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:TYR:HE1   | 1:C:418:PHE:HB2  | 1.85                     | 0.41              |
| 1:A:5:ILE:HG13   | 1:A:177:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:49:GLN:O     | 1:A:52:GLU:N     | 2.54                     | 0.41              |
| 1:A:89:MSE:HB2   | 1:A:91:MSE:HE3   | 2.03                     | 0.41              |
| 1:A:123:PRO:O    | 1:A:124:PHE:C    | 2.63                     | 0.41              |
| 1:A:169:GLN:HG3  | 1:A:169:GLN:H    | 1.69                     | 0.41              |
| 1:C:12:GLU:HB2   | 1:C:122:ASN:HD22 | 1.85                     | 0.41              |
| 1:C:36:VAL:HG12  | 1:C:37:ALA:N     | 2.34                     | 0.41              |
| 1:A:311:ARG:HG3  | 1:A:311:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:104:VAL:HG13 | 1:B:210:LEU:CD2  | 2.49                     | 0.41              |
| 1:C:240:PRO:C    | 1:C:242:CYS:N    | 2.79                     | 0.41              |
| 1:D:70:ALA:HA    | 1:D:127:PHE:O    | 2.20                     | 0.41              |
| 1:D:353:THR:HG22 | 1:D:355:SER:H    | 1.86                     | 0.41              |
| 1:C:88:ILE:HD11  | 1:C:163:LEU:HD23 | 2.03                     | 0.41              |
| 1:D:247:LYS:CE   | 1:D:249:LEU:HB3  | 2.44                     | 0.41              |
| 1:D:415:ARG:HH21 | 1:D:426:VAL:CG2  | 2.33                     | 0.41              |
| 1:A:35:LEU:HD11  | 1:A:238:MSE:HB2  | 2.02                     | 0.41              |
| 1:A:330:PHE:C    | 1:A:332:THR:H    | 2.29                     | 0.41              |
| 1:B:16:GLN:HA    | 1:B:16:GLN:NE2   | 2.36                     | 0.41              |
| 1:B:72:ARG:CZ    | 1:B:210:LEU:HD12 | 2.51                     | 0.41              |
| 1:B:112:ARG:CB   | 1:B:125:ARG:HG2  | 2.51                     | 0.41              |
| 1:C:35:LEU:HD21  | 1:C:238:MSE:HB2  | 2.03                     | 0.41              |
| 1:C:66:GLU:CD    | 1:C:228:ARG:HD2  | 2.46                     | 0.41              |
| 1:C:72:ARG:CZ    | 1:C:223:ASN:HD21 | 2.34                     | 0.41              |
| 1:C:86:PHE:CZ    | 1:C:126:VAL:HG11 | 2.56                     | 0.41              |
| 1:C:388:PHE:O    | 1:C:389:LEU:C    | 2.63                     | 0.41              |
| 1:D:149:LEU:HD23 | 1:D:150:ARG:N    | 2.36                     | 0.41              |
| 1:A:27:PRO:C     | 1:A:29:TYR:N     | 2.78                     | 0.41              |
| 1:C:62:ARG:O     | 1:C:63:LEU:C     | 2.64                     | 0.41              |
| 1:A:86:PHE:HB3   | 1:A:91:MSE:HB2   | 2.04                     | 0.40              |
| 1:A:250:ILE:HG22 | 3:A:512:HOH:O    | 2.21                     | 0.40              |
| 1:C:34:GLU:O     | 1:C:35:LEU:C     | 2.64                     | 0.40              |
| 1:C:300:PRO:HD3  | 1:C:347:TRP:HZ2  | 1.87                     | 0.40              |
| 1:C:423:GLY:O    | 1:C:424:CYS:HB3  | 2.21                     | 0.40              |
| 1:D:36:VAL:HG13  | 1:D:229:THR:HB   | 2.01                     | 0.40              |
| 1:D:318:ASP:O    | 1:D:319:ASN:O    | 2.39                     | 0.40              |
| 1:A:106:VAL:HG12 | 1:A:131:LEU:HD12 | 2.02                     | 0.40              |
| 1:A:270:LEU:C    | 1:A:270:LEU:CD1  | 2.93                     | 0.40              |
| 1:A:353:THR:O    | 1:A:356:GLY:N    | 2.55                     | 0.40              |
| 1:B:105:PRO:O    | 1:B:106:VAL:CG1  | 2.69                     | 0.40              |
| 1:B:226:THR:HA   | 1:B:227:PRO:HD2  | 1.96                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:353:THR:O    | 1:B:354:PRO:C    | 2.63                     | 0.40              |
| 1:C:169:GLN:HE22 | 1:C:176:GLN:NE2  | 2.18                     | 0.40              |
| 1:C:253:PRO:HD2  | 1:C:262:LEU:O    | 2.21                     | 0.40              |
| 1:D:6:THR:C      | 1:D:8:ASP:N      | 2.79                     | 0.40              |
| 1:D:149:LEU:HD23 | 1:D:149:LEU:C    | 2.46                     | 0.40              |
| 1:A:49:GLN:O     | 1:A:52:GLU:HB2   | 2.22                     | 0.40              |
| 1:A:133:LEU:O    | 1:A:142:ARG:HD3  | 2.21                     | 0.40              |
| 1:B:98:ASP:O     | 1:B:101:GLN:HG2  | 2.22                     | 0.40              |
| 1:B:169:GLN:OE1  | 1:B:176:GLN:OE1  | 2.39                     | 0.40              |
| 1:B:296:VAL:HG22 | 1:B:297:ALA:N    | 2.35                     | 0.40              |
| 1:C:281:GLN:HA   | 1:C:281:GLN:NE2  | 2.36                     | 0.40              |
| 1:D:210:LEU:O    | 1:D:214:VAL:HG23 | 2.22                     | 0.40              |
| 1:D:264:GLN:HA   | 1:D:291:ILE:O    | 2.22                     | 0.40              |
| 1:B:246:PRO:HA   | 3:B:526:HOH:O    | 2.21                     | 0.40              |
| 1:B:333:PHE:HE1  | 1:B:340:MSE:HE3  | 1.86                     | 0.40              |
| 1:C:89:MSE:SE    | 1:C:91:MSE:CE    | 3.20                     | 0.40              |
| 1:A:123:PRO:O    | 1:A:125:ARG:HG3  | 2.22                     | 0.40              |
| 1:A:270:LEU:HD13 | 1:A:271:GLU:C    | 2.46                     | 0.40              |
| 1:B:419:GLU:OE2  | 1:B:426:VAL:N    | 2.40                     | 0.40              |
| 1:C:249:LEU:HD23 | 1:C:249:LEU:C    | 2.46                     | 0.40              |
| 1:D:178:GLN:NE2  | 1:D:178:GLN:C    | 2.80                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 412/455 (90%) | 380 (92%) | 27 (7%)  | 5 (1%)   | 10          | 23 |
| 1   | B     | 412/455 (90%) | 385 (93%) | 22 (5%)  | 5 (1%)   | 10          | 23 |
| 1   | C     | 354/455 (78%) | 304 (86%) | 40 (11%) | 10 (3%)  | 4           | 6  |
| 1   | D     | 358/455 (79%) | 305 (85%) | 43 (12%) | 10 (3%)  | 4           | 6  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| All | All   | 1536/1820 (84%) | 1374 (90%) | 132 (9%) | 30 (2%)  | 6           | 12 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | PRO  |
| 1   | B     | 174 | GLU  |
| 1   | B     | 317 | GLN  |
| 1   | B     | 318 | ASP  |
| 1   | D     | 218 | PRO  |
| 1   | D     | 236 | GLN  |
| 1   | D     | 319 | ASN  |
| 1   | A     | 137 | GLU  |
| 1   | A     | 248 | ILE  |
| 1   | B     | 208 | HIS  |
| 1   | C     | 116 | ASP  |
| 1   | C     | 224 | HIS  |
| 1   | C     | 391 | VAL  |
| 1   | B     | 134 | GLU  |
| 1   | C     | 137 | GLU  |
| 1   | C     | 241 | GLU  |
| 1   | C     | 330 | PHE  |
| 1   | D     | 317 | GLN  |
| 1   | D     | 318 | ASP  |
| 1   | A     | 270 | LEU  |
| 1   | C     | 45  | GLU  |
| 1   | C     | 173 | ASN  |
| 1   | D     | 231 | ASP  |
| 1   | C     | 240 | PRO  |
| 1   | D     | 152 | ARG  |
| 1   | A     | 219 | GLY  |
| 1   | D     | 208 | HIS  |
| 1   | D     | 36  | VAL  |
| 1   | D     | 334 | PRO  |
| 1   | C     | 105 | 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     | 361/380 (95%)   | 326 (90%)  | 35 (10%) | 8           | 17 |
| 1   | B     | 360/380 (95%)   | 335 (93%)  | 25 (7%)  | 14          | 32 |
| 1   | C     | 317/380 (83%)   | 288 (91%)  | 29 (9%)  | 9           | 19 |
| 1   | D     | 322/380 (85%)   | 300 (93%)  | 22 (7%)  | 14          | 32 |
| All | All   | 1360/1520 (90%) | 1249 (92%) | 111 (8%) | 10          | 24 |

All (111) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | ILE  |
| 1   | A     | 49  | GLN  |
| 1   | A     | 62  | ARG  |
| 1   | A     | 68  | HIS  |
| 1   | A     | 83  | ARG  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 107 | HIS  |
| 1   | A     | 115 | ASP  |
| 1   | A     | 139 | GLU  |
| 1   | A     | 143 | GLN  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 164 | GLU  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 172 | PHE  |
| 1   | A     | 173 | ASN  |
| 1   | A     | 174 | GLU  |
| 1   | A     | 175 | THR  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 218 | PRO  |
| 1   | A     | 225 | LEU  |
| 1   | A     | 248 | ILE  |
| 1   | A     | 255 | ARG  |
| 1   | A     | 257 | GLU  |
| 1   | A     | 262 | LEU  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 299 | THR  |
| 1   | A     | 303 | ARG  |
| 1   | A     | 326 | LEU  |
| 1   | A     | 336 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 353 | THR  |
| 1   | A     | 391 | VAL  |
| 1   | A     | 420 | GLN  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 429 | GLU  |
| 1   | B     | 49  | GLN  |
| 1   | B     | 77  | GLN  |
| 1   | B     | 83  | ARG  |
| 1   | B     | 85  | MSE  |
| 1   | B     | 91  | MSE  |
| 1   | B     | 100 | SER  |
| 1   | B     | 107 | HIS  |
| 1   | B     | 118 | SER  |
| 1   | B     | 135 | LEU  |
| 1   | B     | 149 | LEU  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 230 | LEU  |
| 1   | B     | 257 | GLU  |
| 1   | B     | 270 | LEU  |
| 1   | B     | 300 | PRO  |
| 1   | B     | 319 | ASN  |
| 1   | B     | 320 | LEU  |
| 1   | B     | 322 | HIS  |
| 1   | B     | 326 | LEU  |
| 1   | B     | 351 | ARG  |
| 1   | B     | 353 | THR  |
| 1   | B     | 422 | LEU  |
| 1   | B     | 429 | GLU  |
| 1   | B     | 443 | ARG  |
| 1   | B     | 446 | LEU  |
| 1   | C     | 18  | MSE  |
| 1   | C     | 41  | LEU  |
| 1   | C     | 44  | LEU  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 68  | HIS  |
| 1   | C     | 97  | TYR  |
| 1   | C     | 107 | HIS  |
| 1   | C     | 116 | ASP  |
| 1   | C     | 140 | ILE  |
| 1   | C     | 141 | LEU  |
| 1   | C     | 142 | ARG  |
| 1   | C     | 149 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 156 | THR  |
| 1   | C     | 163 | LEU  |
| 1   | C     | 176 | GLN  |
| 1   | C     | 185 | LEU  |
| 1   | C     | 193 | LEU  |
| 1   | C     | 195 | THR  |
| 1   | C     | 207 | GLU  |
| 1   | C     | 230 | LEU  |
| 1   | C     | 239 | MSE  |
| 1   | C     | 248 | ILE  |
| 1   | C     | 268 | LYS  |
| 1   | C     | 271 | GLU  |
| 1   | C     | 273 | THR  |
| 1   | C     | 310 | LEU  |
| 1   | C     | 328 | GLU  |
| 1   | C     | 422 | LEU  |
| 1   | C     | 429 | GLU  |
| 1   | D     | 5   | ILE  |
| 1   | D     | 46  | ASN  |
| 1   | D     | 49  | GLN  |
| 1   | D     | 68  | HIS  |
| 1   | D     | 75  | THR  |
| 1   | D     | 97  | TYR  |
| 1   | D     | 107 | HIS  |
| 1   | D     | 108 | SER  |
| 1   | D     | 144 | LYS  |
| 1   | D     | 178 | GLN  |
| 1   | D     | 179 | GLU  |
| 1   | D     | 193 | LEU  |
| 1   | D     | 225 | LEU  |
| 1   | D     | 257 | GLU  |
| 1   | D     | 262 | LEU  |
| 1   | D     | 322 | HIS  |
| 1   | D     | 326 | LEU  |
| 1   | D     | 334 | PRO  |
| 1   | D     | 357 | GLU  |
| 1   | D     | 391 | VAL  |
| 1   | D     | 415 | ARG  |
| 1   | D     | 416 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | GLN  |
| 1   | A     | 16  | GLN  |
| 1   | A     | 46  | ASN  |
| 1   | A     | 47  | ASN  |
| 1   | A     | 49  | GLN  |
| 1   | A     | 56  | ASN  |
| 1   | A     | 77  | GLN  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 168 | GLN  |
| 1   | A     | 173 | ASN  |
| 1   | A     | 191 | HIS  |
| 1   | A     | 192 | GLN  |
| 1   | A     | 205 | HIS  |
| 1   | A     | 224 | HIS  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 281 | GLN  |
| 1   | A     | 284 | HIS  |
| 1   | A     | 293 | GLN  |
| 1   | A     | 323 | GLN  |
| 1   | A     | 343 | GLN  |
| 1   | A     | 364 | HIS  |
| 1   | B     | 16  | GLN  |
| 1   | B     | 46  | ASN  |
| 1   | B     | 47  | ASN  |
| 1   | B     | 49  | GLN  |
| 1   | B     | 77  | GLN  |
| 1   | B     | 168 | GLN  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 192 | GLN  |
| 1   | B     | 221 | HIS  |
| 1   | B     | 281 | GLN  |
| 1   | B     | 319 | ASN  |
| 1   | B     | 323 | GLN  |
| 1   | B     | 327 | GLN  |
| 1   | B     | 342 | GLN  |
| 1   | B     | 381 | GLN  |
| 1   | B     | 420 | GLN  |
| 1   | C     | 28  | GLN  |
| 1   | C     | 46  | ASN  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 151 | GLN  |
| 1   | C     | 168 | GLN  |
| 1   | C     | 169 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 173 | ASN  |
| 1   | C     | 176 | GLN  |
| 1   | C     | 205 | HIS  |
| 1   | C     | 221 | HIS  |
| 1   | C     | 223 | ASN  |
| 1   | C     | 224 | HIS  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 281 | GLN  |
| 1   | C     | 293 | GLN  |
| 1   | C     | 343 | GLN  |
| 1   | C     | 431 | GLN  |
| 1   | D     | 16  | GLN  |
| 1   | D     | 28  | GLN  |
| 1   | D     | 40  | ASN  |
| 1   | D     | 46  | ASN  |
| 1   | D     | 47  | ASN  |
| 1   | D     | 64  | ASN  |
| 1   | D     | 77  | GLN  |
| 1   | D     | 143 | GLN  |
| 1   | D     | 178 | GLN  |
| 1   | D     | 192 | GLN  |
| 1   | D     | 224 | HIS  |
| 1   | D     | 279 | GLN  |
| 1   | D     | 293 | GLN  |
| 1   | D     | 342 | GLN  |
| 1   | D     | 343 | 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     | 408/455 (89%)   | -0.08  | 3 (0%) 84 82  | 11, 27, 44, 66        | 0     |
| 1   | B     | 408/455 (89%)   | 0.23   | 12 (2%) 53 48 | 12, 34, 55, 64        | 0     |
| 1   | C     | 355/455 (78%)   | 0.66   | 13 (3%) 45 39 | 15, 54, 76, 87        | 0     |
| 1   | D     | 362/455 (79%)   | 1.13   | 52 (14%) 6 5  | 21, 66, 93, 102       | 0     |
| All | All   | 1533/1820 (84%) | 0.46   | 80 (5%) 33 27 | 11, 42, 81, 102       | 0     |

All (80) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 317 | GLN  | 8.5  |
| 1   | D     | 134 | GLU  | 3.9  |
| 1   | D     | 141 | LEU  | 3.8  |
| 1   | C     | 245 | GLU  | 3.7  |
| 1   | D     | 133 | LEU  | 3.7  |
| 1   | D     | 166 | TYR  | 3.7  |
| 1   | D     | 172 | PHE  | 3.7  |
| 1   | A     | 413 | ALA  | 3.6  |
| 1   | B     | 446 | LEU  | 3.6  |
| 1   | D     | 321 | THR  | 3.6  |
| 1   | D     | 55  | VAL  | 3.5  |
| 1   | D     | 185 | LEU  | 3.4  |
| 1   | D     | 180 | PHE  | 3.4  |
| 1   | D     | 318 | ASP  | 3.4  |
| 1   | B     | 319 | ASN  | 3.4  |
| 1   | D     | 189 | ARG  | 3.2  |
| 1   | B     | 362 | ALA  | 3.2  |
| 1   | D     | 60  | LEU  | 3.2  |
| 1   | D     | 186 | GLU  | 3.1  |
| 1   | D     | 123 | PRO  | 3.1  |
| 1   | C     | 246 | PRO  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 320 | LEU  | 3.0  |
| 1   | D     | 17  | ALA  | 3.0  |
| 1   | A     | 446 | LEU  | 3.0  |
| 1   | D     | 155 | PHE  | 2.9  |
| 1   | D     | 5   | ILE  | 2.9  |
| 1   | D     | 95  | SER  | 2.9  |
| 1   | D     | 174 | GLU  | 2.8  |
| 1   | C     | 163 | LEU  | 2.8  |
| 1   | D     | 92  | TYR  | 2.7  |
| 1   | D     | 184 | ALA  | 2.7  |
| 1   | B     | 412 | ASN  | 2.7  |
| 1   | D     | 383 | ILE  | 2.6  |
| 1   | D     | 427 | LEU  | 2.6  |
| 1   | A     | 412 | ASN  | 2.6  |
| 1   | D     | 274 | VAL  | 2.6  |
| 1   | D     | 317 | GLN  | 2.6  |
| 1   | D     | 158 | ARG  | 2.5  |
| 1   | D     | 414 | SER  | 2.5  |
| 1   | D     | 211 | ILE  | 2.5  |
| 1   | B     | 316 | GLY  | 2.5  |
| 1   | D     | 178 | GLN  | 2.5  |
| 1   | D     | 90  | GLY  | 2.5  |
| 1   | D     | 193 | LEU  | 2.4  |
| 1   | D     | 70  | ALA  | 2.4  |
| 1   | D     | 421 | ALA  | 2.4  |
| 1   | D     | 160 | ARG  | 2.4  |
| 1   | D     | 181 | VAL  | 2.4  |
| 1   | D     | 42  | ALA  | 2.4  |
| 1   | D     | 15  | SER  | 2.3  |
| 1   | D     | 316 | GLY  | 2.3  |
| 1   | D     | 275 | LEU  | 2.3  |
| 1   | D     | 223 | ASN  | 2.3  |
| 1   | D     | 182 | GLN  | 2.3  |
| 1   | B     | 38  | ASP  | 2.3  |
| 1   | C     | 172 | PHE  | 2.2  |
| 1   | C     | 241 | GLU  | 2.2  |
| 1   | D     | 115 | ASP  | 2.2  |
| 1   | D     | 170 | GLY  | 2.2  |
| 1   | B     | 223 | ASN  | 2.2  |
| 1   | D     | 315 | THR  | 2.2  |
| 1   | C     | 433 | TYR  | 2.2  |
| 1   | C     | 230 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 63  | LEU  | 2.2  |
| 1   | D     | 248 | ILE  | 2.2  |
| 1   | D     | 417 | ALA  | 2.1  |
| 1   | C     | 28  | GLN  | 2.1  |
| 1   | C     | 446 | LEU  | 2.1  |
| 1   | B     | 140 | ILE  | 2.1  |
| 1   | D     | 204 | LEU  | 2.1  |
| 1   | D     | 320 | LEU  | 2.1  |
| 1   | C     | 61  | ALA  | 2.1  |
| 1   | B     | 328 | GLU  | 2.1  |
| 1   | D     | 157 | PRO  | 2.1  |
| 1   | D     | 44  | LEU  | 2.1  |
| 1   | C     | 137 | GLU  | 2.0  |
| 1   | D     | 88  | ILE  | 2.0  |
| 1   | C     | 311 | ARG  | 2.0  |
| 1   | B     | 321 | THR  | 2.0  |
| 1   | C     | 235 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | ZN   | A     | 501 | 1/1   | 0.93 | 0.21 | 22,22,22,22                | 0     |
| 2   | ZN   | C     | 503 | 1/1   | 0.96 | 0.33 | 22,22,22,22                | 0     |
| 2   | ZN   | D     | 504 | 1/1   | 0.96 | 0.35 | 22,22,22,22                | 0     |
| 2   | ZN   | B     | 502 | 1/1   | 0.97 | 0.24 | 22,22,22,22                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.