



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:08 PM UTC

PDB ID : 4RR2 / pdb\_00004rr2  
Title : Crystal structure of human primase  
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Deposited on : 2014-11-05  
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

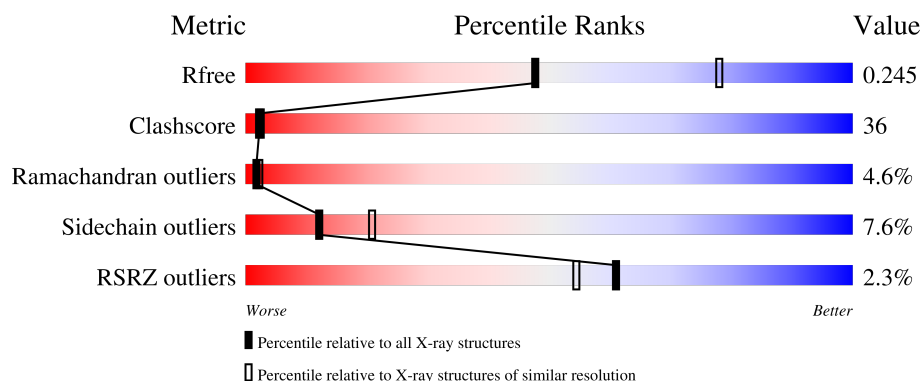
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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                      | 1110 (2.66-2.66)                                      |
| Clashscore            | 190562                      | 1141 (2.66-2.66)                                      |
| Ramachandran outliers | 187476                      | 1126 (2.66-2.66)                                      |
| Sidechain outliers    | 187428                      | 1126 (2.66-2.66)                                      |
| RSRZ outliers         | 180081                      | 1110 (2.66-2.66)                                      |

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     | 420    | <div> <div>43%</div> <div>43%</div> <div>6%</div> <div>7%</div> </div>                |
| 1   | C     | 420    | <div> <div>41%</div> <div>41%</div> <div>9%</div> <div>7%</div> </div>                |
| 2   | B     | 509    | <div> <div>13%</div> <div>22%</div> <div>6%</div> <div>58%</div> </div>               |
| 2   | D     | 509    | <div> <div>4%</div> <div>36%</div> <div>39%</div> <div>8%</div> <div>16%</div> </div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11896 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 DNA primase small subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 389      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3267  | 2101 | 566 | 585 | 15 |         |         |       |
| 1   | C     | 389      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3263  | 2099 | 566 | 583 | 15 |         |         |       |

- Molecule 2 is a protein called DNA primase large subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1755  | 1133 | 299 | 321 | 2  |         |         |       |
| 2   | D     | 429      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3513  | 2249 | 608 | 643 | 13 |         |         |       |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | D     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

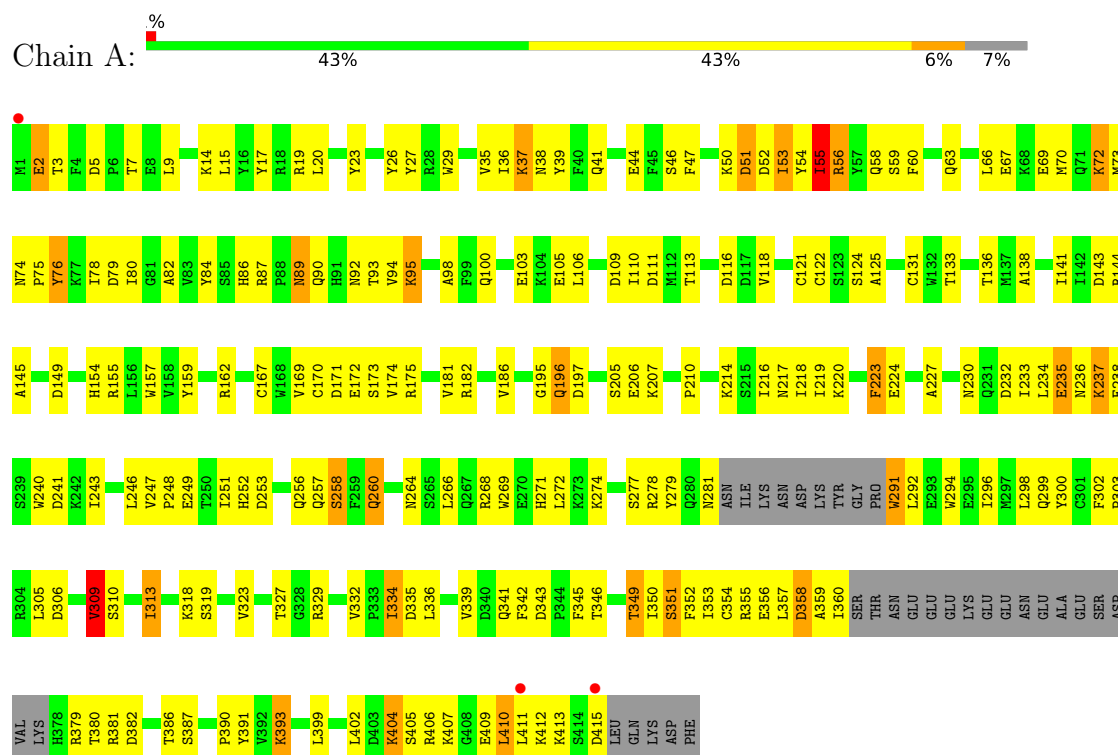
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 5   | B     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 5   | C     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 5   | D     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |

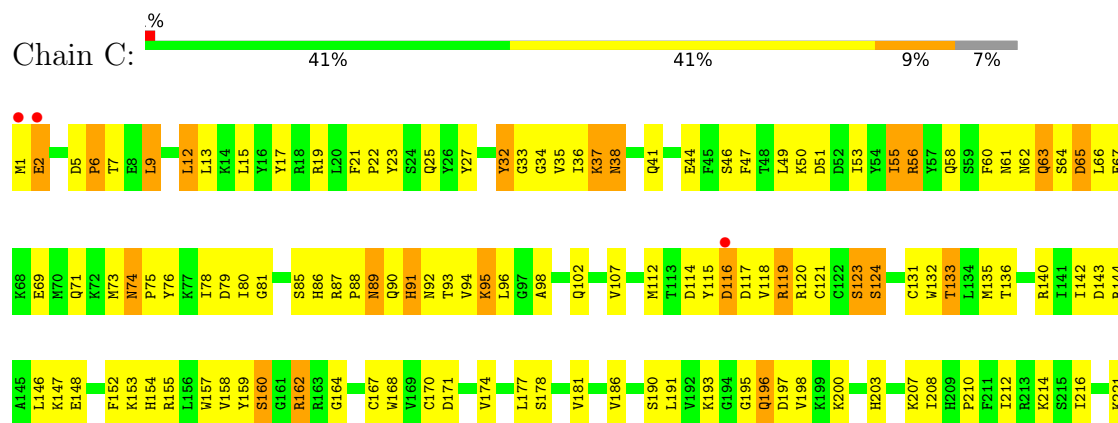
### 3 Residue-property plots

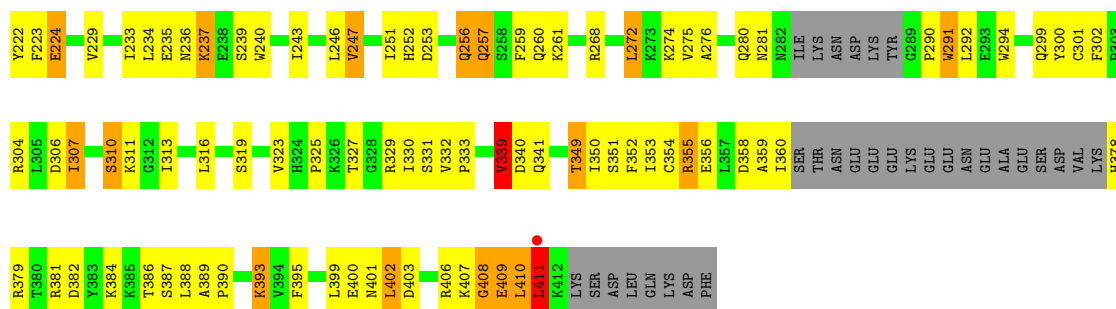
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: DNA primase small subunit

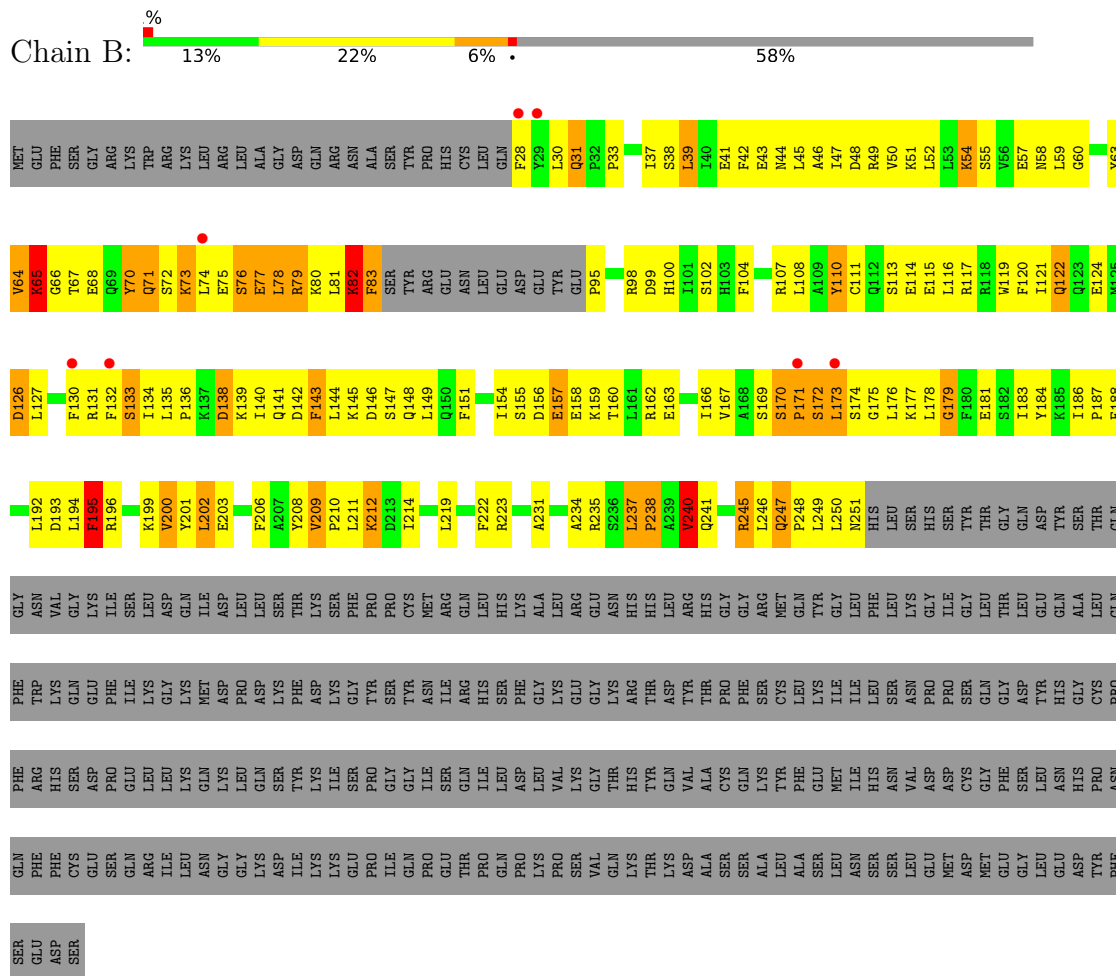


#### • Molecule 1: DNA primase small subunit

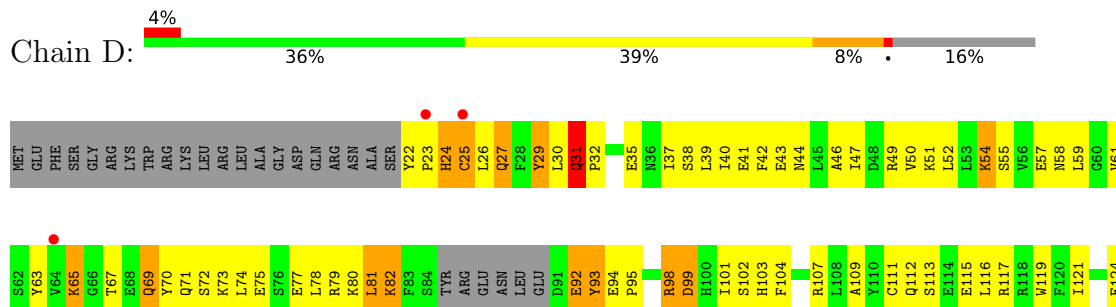




• Molecule 2: DNA primase large subunit



• Molecule 2: DNA primase large subunit





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 86.19Å 88.90Å 94.68Å<br>93.82° 96.57° 111.72°               | Depositor        |
| Resolution (Å)                                                          | 48.48 – 2.65<br>48.48 – 2.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.5 (48.48-2.65)<br>88.5 (48.48-2.65)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.04                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.89 (at 2.61Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.229 , 0.271<br>0.208 , 0.245                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3691 reflections (5.10%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 71.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.392                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 43.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.006 for -k,-h,-l                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 11896                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, SF4

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     | 0.56         | 0/3349      | 1.01        | 12/4514 (0.3%)  |
| 1   | C     | 0.62         | 0/3346      | 1.09        | 18/4512 (0.4%)  |
| 2   | B     | 0.44         | 0/1787      | 1.00        | 11/2402 (0.5%)  |
| 2   | D     | 0.51         | 0/3595      | 1.04        | 22/4838 (0.5%)  |
| All | All   | 0.55         | 0/12077     | 1.04        | 63/16266 (0.4%) |

There are no bond length outliers.

All (63) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 237 | LYS  | N-CA-C | -9.54 | 100.96      | 111.36   |
| 2   | D     | 209 | VAL  | N-CA-C | 8.56  | 117.34      | 107.84   |
| 2   | D     | 261 | ASP  | N-CA-C | -8.07 | 99.65       | 110.55   |
| 2   | B     | 209 | VAL  | N-CA-C | 7.84  | 116.55      | 107.84   |
| 2   | B     | 76  | SER  | N-CA-C | -7.64 | 104.09      | 113.41   |
| 1   | A     | 124 | SER  | N-CA-C | 7.35  | 123.43      | 111.37   |
| 1   | C     | 223 | PHE  | N-CA-C | 7.20  | 119.75      | 111.11   |
| 1   | A     | 92  | ASN  | N-CA-C | -6.96 | 104.59      | 113.23   |
| 1   | A     | 237 | LYS  | N-CA-C | -6.96 | 103.77      | 111.36   |
| 2   | D     | 252 | HIS  | N-CA-C | 6.85  | 125.39      | 110.80   |
| 1   | A     | 76  | TYR  | N-CA-C | -6.79 | 103.68      | 112.23   |
| 2   | D     | 423 | ALA  | N-CA-C | -6.75 | 103.16      | 111.33   |
| 2   | D     | 285 | PRO  | N-CA-C | -6.64 | 104.10      | 110.47   |
| 2   | D     | 71  | GLN  | N-CA-C | 6.62  | 118.58      | 111.36   |
| 1   | C     | 124 | SER  | N-CA-C | 6.58  | 119.28      | 111.71   |
| 2   | B     | 172 | SER  | N-CA-C | -6.47 | 105.49      | 113.19   |
| 1   | C     | 319 | SER  | CA-C-N | -6.46 | 113.01      | 119.92   |
| 1   | C     | 319 | SER  | C-N-CA | -6.46 | 113.01      | 119.92   |
| 2   | B     | 77  | GLU  | N-CA-C | -6.46 | 104.17      | 111.14   |
| 1   | C     | 224 | GLU  | N-CA-C | 6.42  | 117.94      | 111.07   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 230 | ASN  | N-CA-C  | 6.35  | 117.89      | 110.97   |
| 1   | C     | 123 | SER  | N-CA-C  | -6.21 | 102.51      | 110.53   |
| 2   | D     | 263 | SER  | N-CA-C  | -6.16 | 97.68       | 110.80   |
| 2   | B     | 200 | VAL  | CB-CA-C | -6.16 | 105.95      | 111.74   |
| 1   | C     | 198 | VAL  | N-CA-C  | -6.14 | 99.63       | 108.53   |
| 1   | C     | 56  | ARG  | N-CA-C  | 6.09  | 123.78      | 110.80   |
| 2   | D     | 446 | GLN  | N-CA-C  | -6.09 | 104.75      | 111.82   |
| 1   | C     | 339 | VAL  | CB-CA-C | -6.02 | 104.29      | 111.81   |
| 1   | C     | 9   | LEU  | N-CA-C  | 5.98  | 121.67      | 113.77   |
| 2   | D     | 282 | LYS  | N-CA-C  | 5.93  | 119.70      | 112.23   |
| 1   | A     | 223 | PHE  | N-CA-C  | 5.89  | 118.18      | 111.11   |
| 2   | D     | 258 | THR  | N-CA-C  | 5.86  | 118.27      | 107.73   |
| 2   | D     | 109 | ALA  | N-CA-C  | 5.86  | 118.55      | 111.40   |
| 2   | D     | 217 | ILE  | N-CA-C  | -5.83 | 104.94      | 110.42   |
| 2   | D     | 271 | ILE  | N-CA-C  | 5.77  | 117.31      | 108.71   |
| 1   | C     | 389 | ALA  | N-CA-C  | 5.76  | 122.53      | 109.81   |
| 2   | D     | 156 | ASP  | N-CA-C  | -5.74 | 105.37      | 112.38   |
| 2   | D     | 135 | LEU  | N-CA-C  | 5.71  | 116.17      | 109.60   |
| 2   | D     | 422 | VAL  | N-CA-C  | -5.71 | 104.30      | 112.35   |
| 2   | D     | 359 | ARG  | N-CA-C  | -5.70 | 104.97      | 112.72   |
| 1   | C     | 74  | ASN  | CA-C-N  | 5.68  | 125.63      | 119.78   |
| 1   | C     | 74  | ASN  | C-N-CA  | 5.68  | 125.63      | 119.78   |
| 2   | B     | 39  | LEU  | N-CA-C  | -5.65 | 105.49      | 112.38   |
| 2   | D     | 221 | GLU  | N-CA-C  | -5.61 | 105.16      | 111.28   |
| 2   | D     | 373 | SER  | N-CA-C  | 5.56  | 117.08      | 109.18   |
| 1   | C     | 402 | LEU  | N-CA-C  | -5.46 | 105.24      | 111.14   |
| 1   | C     | 310 | SER  | N-CA-C  | 5.45  | 117.30      | 111.36   |
| 2   | B     | 200 | VAL  | N-CA-C  | 5.45  | 114.35      | 107.70   |
| 1   | A     | 182 | ARG  | N-CA-C  | -5.44 | 105.25      | 111.07   |
| 2   | B     | 110 | TYR  | N-CA-C  | 5.32  | 119.48      | 113.15   |
| 2   | D     | 81  | LEU  | N-CA-C  | 5.30  | 119.46      | 113.15   |
| 1   | A     | 235 | GLU  | N-CA-C  | 5.30  | 117.13      | 111.36   |
| 2   | B     | 54  | LYS  | N-CA-C  | -5.20 | 105.79      | 111.82   |
| 1   | C     | 301 | CYS  | N-CA-C  | 5.19  | 121.00      | 114.31   |
| 1   | C     | 76  | TYR  | N-CA-C  | -5.17 | 105.72      | 112.23   |
| 1   | A     | 100 | GLN  | N-CA-C  | 5.17  | 117.10      | 108.99   |
| 2   | B     | 195 | PHE  | N-CA-C  | 5.15  | 117.80      | 111.82   |
| 2   | D     | 262 | TYR  | N-CA-C  | 5.14  | 121.74      | 110.80   |
| 2   | D     | 251 | ASN  | N-CA-C  | 5.13  | 119.90      | 113.43   |
| 1   | A     | 84  | TYR  | N-CA-C  | 5.13  | 118.05      | 110.46   |
| 1   | A     | 55  | ILE  | N-CA-C  | -5.09 | 102.38      | 109.45   |
| 1   | A     | 309 | VAL  | CB-CA-C | -5.07 | 104.64      | 112.05   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 64  | VAL  | N-CA-C | -5.07 | 98.80       | 109.34   |

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     | 3267  | 0        | 3249     | 214     | 0            |
| 1   | C     | 3263  | 0        | 3243     | 204     | 0            |
| 2   | B     | 1755  | 0        | 1801     | 199     | 0            |
| 2   | D     | 3513  | 0        | 3494     | 249     | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 8     | 0        | 0        | 0       | 0            |
| 5   | A     | 23    | 0        | 0        | 11      | 0            |
| 5   | B     | 4     | 0        | 0        | 0       | 0            |
| 5   | C     | 40    | 0        | 0        | 12      | 0            |
| 5   | D     | 21    | 0        | 0        | 3       | 0            |
| All | All   | 11896 | 0        | 11787    | 861     | 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 36.

All (861) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:82:LYS:HE2   | 2:D:98:ARG:HD3   | 1.36                     | 1.07              |
| 2:D:117:ARG:HG2  | 2:D:230:LEU:HD13 | 1.38                     | 1.05              |
| 2:B:68:GLU:HA    | 2:B:71:GLN:HB3   | 1.42                     | 1.02              |
| 2:B:82:LYS:HG2   | 2:B:98:ARG:HD3   | 1.42                     | 1.01              |
| 1:C:50:LYS:H     | 1:C:50:LYS:HD2   | 1.25                     | 1.00              |
| 1:A:95:LYS:H     | 1:A:95:LYS:HD3   | 1.27                     | 0.98              |
| 2:B:237:LEU:HD13 | 2:B:241:GLN:HE22 | 1.25                     | 0.98              |
| 2:B:79:ARG:HH11  | 2:B:79:ARG:HB3   | 1.27                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:ILE:H     | 1:A:53:ILE:HD12  | 1.27                     | 0.96              |
| 2:B:72:SER:HA    | 2:B:75:GLU:HG2   | 1.48                     | 0.96              |
| 1:A:37:LYS:HD2   | 1:A:38:ASN:H     | 1.28                     | 0.95              |
| 2:D:94:GLU:HB3   | 2:D:95:PRO:HD3   | 1.49                     | 0.94              |
| 2:D:44:ASN:HA    | 2:D:47:ILE:HD12  | 1.50                     | 0.92              |
| 1:C:233:ILE:HD12 | 1:C:243:ILE:HD11 | 1.51                     | 0.91              |
| 2:D:43:GLU:O     | 2:D:47:ILE:HG13  | 1.70                     | 0.91              |
| 1:C:49:LEU:HB3   | 1:C:50:LYS:HD2   | 1.53                     | 0.91              |
| 1:C:349:THR:HG22 | 1:C:351:SER:H    | 1.32                     | 0.91              |
| 2:B:154:ILE:CG2  | 2:B:158:GLU:HB2  | 2.01                     | 0.91              |
| 1:C:379:ARG:HA   | 5:C:1034:HOH:O   | 1.72                     | 0.90              |
| 1:C:144:ARG:HG2  | 1:C:144:ARG:HH21 | 1.36                     | 0.89              |
| 2:D:113:SER:HB3  | 2:D:116:LEU:HG   | 1.55                     | 0.88              |
| 1:C:353:ILE:HB   | 1:C:386:THR:HG21 | 1.54                     | 0.88              |
| 2:D:262:TYR:HB2  | 2:D:264:THR:H    | 1.39                     | 0.88              |
| 2:B:170:SER:HB3  | 2:B:171:PRO:HD2  | 1.55                     | 0.87              |
| 2:D:82:LYS:HE2   | 2:D:98:ARG:CD    | 2.04                     | 0.87              |
| 1:C:154:HIS:ND1  | 1:C:402:LEU:HD12 | 1.89                     | 0.86              |
| 1:C:247:VAL:HG22 | 1:C:292:LEU:HD13 | 1.57                     | 0.85              |
| 1:A:247:VAL:HG22 | 1:A:292:LEU:HD11 | 1.57                     | 0.85              |
| 1:C:37:LYS:HD2   | 1:C:38:ASN:H     | 1.42                     | 0.85              |
| 1:C:355:ARG:HG3  | 1:C:355:ARG:HH11 | 1.41                     | 0.85              |
| 2:D:82:LYS:HG3   | 2:D:98:ARG:HD3   | 1.59                     | 0.85              |
| 1:C:38:ASN:HB3   | 1:C:41:GLN:HB2   | 1.57                     | 0.84              |
| 2:B:82:LYS:CG    | 2:B:98:ARG:HD3   | 2.06                     | 0.84              |
| 2:B:49:ARG:CG    | 2:B:102:SER:HB3  | 2.08                     | 0.84              |
| 1:A:51:ASP:H     | 1:A:53:ILE:HD11  | 1.40                     | 0.84              |
| 2:B:154:ILE:HG21 | 2:B:158:GLU:HB2  | 1.60                     | 0.84              |
| 1:A:353:ILE:HB   | 1:A:386:THR:HG21 | 1.60                     | 0.84              |
| 1:A:410:LEU:HD23 | 1:A:411:LEU:N    | 1.93                     | 0.83              |
| 1:C:260:GLN:HB2  | 5:C:1002:HOH:O   | 1.77                     | 0.83              |
| 1:C:349:THR:HG22 | 1:C:351:SER:N    | 1.93                     | 0.82              |
| 1:A:232:ASP:OD2  | 1:A:235:GLU:HB2  | 1.80                     | 0.82              |
| 2:D:67:THR:HG22  | 2:D:69:GLN:H     | 1.43                     | 0.81              |
| 2:B:113:SER:HB2  | 2:B:116:LEU:HG   | 1.62                     | 0.81              |
| 1:A:349:THR:HG22 | 1:A:351:SER:H    | 1.46                     | 0.81              |
| 1:C:36:ILE:HG22  | 1:C:37:LYS:HG3   | 1.63                     | 0.81              |
| 1:A:379:ARG:HB3  | 1:A:382:ASP:OD1  | 1.80                     | 0.80              |
| 1:A:327:THR:OG1  | 1:A:329:ARG:HG2  | 1.81                     | 0.80              |
| 1:A:38:ASN:HB3   | 1:A:41:GLN:HB2   | 1.64                     | 0.79              |
| 1:C:276:ALA:O    | 1:C:280:GLN:HG2  | 1.82                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:37:LYS:CD    | 1:A:38:ASN:H     | 1.96                     | 0.78              |
| 1:A:172:GLU:HA   | 1:A:175:ARG:NH1  | 1.99                     | 0.78              |
| 2:D:425:GLN:O    | 2:D:429:GLU:HG3  | 1.85                     | 0.78              |
| 1:A:51:ASP:H     | 1:A:53:ILE:CD1   | 1.97                     | 0.77              |
| 1:A:235:GLU:HG2  | 1:A:236:ASN:ND2  | 1.99                     | 0.77              |
| 2:D:170:SER:HB3  | 2:D:171:PRO:HD2  | 1.66                     | 0.77              |
| 1:A:260:GLN:HA   | 1:A:260:GLN:NE2  | 2.00                     | 0.77              |
| 2:D:77:GLU:CD    | 2:D:418:THR:HG21 | 2.09                     | 0.77              |
| 2:D:155:SER:OG   | 2:D:157:GLU:HB2  | 1.85                     | 0.77              |
| 2:D:421:GLN:O    | 2:D:425:GLN:HG3  | 1.83                     | 0.77              |
| 2:B:247:GLN:N    | 2:B:247:GLN:HE21 | 1.83                     | 0.77              |
| 1:C:353:ILE:HB   | 1:C:386:THR:CG2  | 2.13                     | 0.77              |
| 1:C:349:THR:CG2  | 1:C:351:SER:HB3  | 2.16                     | 0.76              |
| 2:B:144:LEU:O    | 2:B:147:SER:HB3  | 1.86                     | 0.76              |
| 1:A:66:LEU:HG    | 1:A:70:MET:HE3   | 1.67                     | 0.76              |
| 2:B:59:LEU:HD21  | 2:B:73:LYS:HG2   | 1.66                     | 0.75              |
| 2:D:82:LYS:CE    | 2:D:98:ARG:HD3   | 2.16                     | 0.75              |
| 2:B:199:LYS:O    | 2:B:200:VAL:HG13 | 1.87                     | 0.75              |
| 1:C:46:SER:HB3   | 1:C:79:ASP:HB2   | 1.69                     | 0.75              |
| 2:B:46:ALA:O     | 2:B:50:VAL:HG23  | 1.86                     | 0.75              |
| 2:D:273:LEU:HD11 | 2:D:326:PHE:HB2  | 1.68                     | 0.74              |
| 1:C:62:ASN:OD1   | 1:C:64:SER:HB3   | 1.87                     | 0.74              |
| 1:A:407:LYS:HG3  | 1:A:411:LEU:HD12 | 1.67                     | 0.74              |
| 2:B:171:PRO:HG2  | 2:B:173:LEU:HB2  | 1.68                     | 0.74              |
| 1:C:95:LYS:HD3   | 1:C:98:ALA:HB2   | 1.67                     | 0.74              |
| 1:A:334:ILE:HD12 | 1:A:342:PHE:CE2  | 2.22                     | 0.74              |
| 1:C:89:ASN:HD22  | 1:C:89:ASN:C     | 1.95                     | 0.74              |
| 1:A:349:THR:HG22 | 1:A:351:SER:N    | 2.02                     | 0.73              |
| 1:A:386:THR:HG22 | 1:A:387:SER:N    | 2.01                     | 0.73              |
| 1:C:85:SER:HA    | 1:C:102:GLN:NE2  | 2.03                     | 0.73              |
| 1:C:144:ARG:HG2  | 1:C:144:ARG:NH2  | 2.00                     | 0.73              |
| 2:B:30:LEU:HG    | 2:B:31:GLN:HG3   | 1.70                     | 0.73              |
| 2:D:80:LYS:NZ    | 2:D:418:THR:HG22 | 2.04                     | 0.73              |
| 2:D:125:MET:HE1  | 2:D:223:ARG:HH21 | 1.52                     | 0.73              |
| 2:B:238:PRO:HA   | 2:B:241:GLN:HG2  | 1.70                     | 0.73              |
| 2:D:320:LEU:HD11 | 2:D:350:ARG:HA   | 1.70                     | 0.73              |
| 1:C:55:ILE:HD12  | 1:C:58:GLN:NE2   | 2.04                     | 0.72              |
| 2:B:113:SER:H    | 2:B:116:LEU:HD12 | 1.54                     | 0.72              |
| 2:B:173:LEU:HD23 | 2:B:173:LEU:O    | 1.90                     | 0.72              |
| 2:B:151:PHE:HB3  | 2:B:186:ILE:HG22 | 1.72                     | 0.72              |
| 2:B:163:GLU:O    | 2:B:167:VAL:HG23 | 1.90                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:212:LYS:HD3  | 2:B:212:LYS:C    | 2.14                     | 0.72              |
| 1:A:196:GLN:HG2  | 1:A:196:GLN:O    | 1.88                     | 0.72              |
| 1:A:247:VAL:HG22 | 1:A:292:LEU:HD21 | 1.71                     | 0.71              |
| 1:C:393:LYS:HE3  | 1:C:393:LYS:HA   | 1.72                     | 0.71              |
| 1:A:355:ARG:HG3  | 1:A:355:ARG:HH11 | 1.56                     | 0.71              |
| 2:D:265:GLN:HA   | 2:D:265:GLN:HE21 | 1.56                     | 0.71              |
| 2:D:418:THR:HG22 | 2:D:418:THR:O    | 1.91                     | 0.71              |
| 1:C:51:ASP:HB2   | 1:C:53:ILE:HD13  | 1.72                     | 0.71              |
| 1:C:355:ARG:HG3  | 1:C:355:ARG:NH1  | 2.06                     | 0.70              |
| 2:D:25:CYS:HB3   | 2:D:131:ARG:HD3  | 1.73                     | 0.70              |
| 2:B:50:VAL:O     | 2:B:54:LYS:HB2   | 1.90                     | 0.70              |
| 2:B:240:VAL:HG13 | 2:B:246:LEU:CD1  | 2.21                     | 0.70              |
| 2:D:358:LYS:HG3  | 2:D:363:THR:OG1  | 1.92                     | 0.70              |
| 1:A:5:ASP:OD1    | 1:A:7:THR:HB     | 1.90                     | 0.70              |
| 2:B:110:TYR:HB3  | 2:B:116:LEU:HB3  | 1.74                     | 0.70              |
| 2:D:178:LEU:HD11 | 2:D:183:ILE:HD11 | 1.72                     | 0.70              |
| 1:C:386:THR:HG22 | 1:C:387:SER:N    | 2.07                     | 0.70              |
| 1:C:299:GLN:O    | 1:C:304:ARG:NH2  | 2.26                     | 0.69              |
| 1:C:73:MET:HG3   | 5:C:1033:HOH:O   | 1.92                     | 0.69              |
| 1:C:49:LEU:HD13  | 1:C:50:LYS:NZ    | 2.08                     | 0.69              |
| 1:C:386:THR:HG22 | 1:C:388:LEU:H    | 1.57                     | 0.69              |
| 2:D:268:VAL:HG12 | 2:D:269:GLY:N    | 2.07                     | 0.69              |
| 1:A:237:LYS:HE2  | 1:A:241:ASP:OD1  | 1.93                     | 0.69              |
| 2:D:358:LYS:HE3  | 2:D:360:THR:HA   | 1.74                     | 0.69              |
| 2:B:163:GLU:HG3  | 2:B:178:LEU:HB2  | 1.74                     | 0.68              |
| 2:D:199:LYS:O    | 2:D:200:VAL:HG13 | 1.92                     | 0.68              |
| 1:A:118:VAL:HG13 | 1:A:300:TYR:CD2  | 2.28                     | 0.68              |
| 2:D:24:HIS:CE1   | 2:D:92:GLU:HB2   | 2.28                     | 0.68              |
| 2:D:92:GLU:HG2   | 2:D:93:TYR:H     | 1.59                     | 0.68              |
| 1:C:120:ARG:NH2  | 1:C:235:GLU:OE1  | 2.25                     | 0.68              |
| 2:D:80:LYS:HZ3   | 2:D:418:THR:HG22 | 1.57                     | 0.68              |
| 2:D:30:LEU:HG    | 2:D:31:GLN:HG3   | 1.74                     | 0.68              |
| 2:B:95:PRO:N     | 2:B:98:ARG:HD2   | 2.08                     | 0.68              |
| 2:B:184:TYR:HE1  | 2:B:211:LEU:HB2  | 1.58                     | 0.68              |
| 2:B:49:ARG:HG3   | 2:B:102:SER:HB3  | 1.75                     | 0.68              |
| 2:B:77:GLU:HA    | 2:B:80:LYS:HE3   | 1.75                     | 0.68              |
| 1:A:29:TRP:HB2   | 1:A:399:LEU:HD21 | 1.77                     | 0.67              |
| 2:B:151:PHE:CB   | 2:B:186:ILE:HG22 | 2.24                     | 0.67              |
| 1:A:393:LYS:HA   | 1:A:393:LYS:HE3  | 1.77                     | 0.66              |
| 1:C:207:LYS:NZ   | 2:D:167:VAL:O    | 2.28                     | 0.66              |
| 2:D:30:LEU:HD12  | 2:D:31:GLN:H     | 1.59                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:359:ALA:O    | 1:A:360:ILE:HD13 | 1.95                     | 0.66              |
| 2:B:238:PRO:HA   | 2:B:241:GLN:CG   | 2.25                     | 0.66              |
| 2:D:244:GLU:O    | 2:D:247:GLN:HG2  | 1.94                     | 0.66              |
| 1:A:353:ILE:HB   | 1:A:386:THR:CG2  | 2.26                     | 0.66              |
| 2:B:64:VAL:C     | 2:B:66:GLY:H     | 2.04                     | 0.66              |
| 2:D:63:TYR:OH    | 2:D:73:LYS:NZ    | 2.26                     | 0.66              |
| 2:B:156:ASP:HA   | 2:B:159:LYS:HB2  | 1.77                     | 0.66              |
| 1:A:37:LYS:HD2   | 1:A:38:ASN:N     | 2.09                     | 0.65              |
| 1:A:247:VAL:HG13 | 1:A:248:PRO:HD2  | 1.78                     | 0.65              |
| 2:B:72:SER:HA    | 2:B:75:GLU:CG    | 2.26                     | 0.65              |
| 2:D:26:LEU:HD12  | 2:D:135:LEU:HD12 | 1.78                     | 0.65              |
| 1:A:224:GLU:OE2  | 1:C:381:ARG:HD2  | 1.96                     | 0.65              |
| 2:D:107:ARG:O    | 2:D:111:CYS:HB3  | 1.96                     | 0.65              |
| 1:C:349:THR:CG2  | 1:C:351:SER:H    | 2.07                     | 0.65              |
| 1:C:237:LYS:HA   | 1:C:240:TRP:CE2  | 2.31                     | 0.65              |
| 1:C:37:LYS:HB2   | 1:C:38:ASN:HD22  | 1.63                     | 0.64              |
| 1:C:112:MET:HG3  | 1:C:119:ARG:NH1  | 2.11                     | 0.64              |
| 1:C:191:LEU:HD11 | 1:C:212:ILE:HG12 | 1.78                     | 0.64              |
| 2:D:271:ILE:HD13 | 2:D:316:ILE:HD12 | 1.79                     | 0.64              |
| 2:D:163:GLU:O    | 2:D:167:VAL:HG23 | 1.98                     | 0.64              |
| 1:A:266:LEU:HD13 | 1:C:384:LYS:HD3  | 1.79                     | 0.64              |
| 2:B:79:ARG:HH11  | 2:B:79:ARG:CB    | 2.07                     | 0.64              |
| 2:D:42:PHE:HE2   | 2:D:249:LEU:HD13 | 1.61                     | 0.64              |
| 2:B:81:LEU:O     | 2:B:82:LYS:CB    | 2.45                     | 0.64              |
| 2:D:268:VAL:HG12 | 2:D:269:GLY:O    | 1.97                     | 0.64              |
| 2:D:29:TYR:HE2   | 2:D:99:ASP:OD1   | 1.81                     | 0.63              |
| 2:D:214:ILE:O    | 2:D:218:ILE:HG13 | 1.98                     | 0.63              |
| 1:C:410:LEU:HG   | 1:C:411:LEU:HD23 | 1.81                     | 0.63              |
| 2:D:173:LEU:HD23 | 2:D:174:SER:O    | 1.98                     | 0.63              |
| 2:D:243:ASP:OD1  | 2:D:245:ARG:HD2  | 1.99                     | 0.63              |
| 1:A:260:GLN:HA   | 1:A:260:GLN:HE21 | 1.63                     | 0.63              |
| 2:D:307:MET:HA   | 2:D:307:MET:HE3  | 1.79                     | 0.63              |
| 2:D:421:GLN:NE2  | 2:D:441:LEU:O    | 2.31                     | 0.63              |
| 2:B:130:PHE:CZ   | 2:B:134:ILE:HD11 | 2.34                     | 0.62              |
| 2:D:293:LYS:O    | 2:D:297:GLU:HG3  | 1.99                     | 0.62              |
| 2:D:268:VAL:HG12 | 2:D:269:GLY:H    | 1.64                     | 0.62              |
| 2:D:337:ASP:HB3  | 2:D:340:LYS:CB   | 2.28                     | 0.62              |
| 2:D:337:ASP:HB3  | 2:D:340:LYS:HB2  | 1.81                     | 0.62              |
| 1:C:234:LEU:CD2  | 1:C:243:ILE:HD12 | 2.30                     | 0.62              |
| 1:C:25:GLN:OE1   | 1:C:25:GLN:N     | 2.31                     | 0.62              |
| 2:D:261:ASP:HB2  | 2:D:442:ASN:HD21 | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:265:GLN:HA   | 2:D:265:GLN:NE2  | 2.15                     | 0.62              |
| 2:B:37:ILE:HB    | 2:B:41:GLU:HG3   | 1.82                     | 0.61              |
| 2:B:131:ARG:O    | 2:B:135:LEU:HG   | 2.00                     | 0.61              |
| 1:C:49:LEU:HD13  | 1:C:50:LYS:HZ1   | 1.65                     | 0.61              |
| 1:C:349:THR:HG21 | 1:C:351:SER:HB3  | 1.81                     | 0.61              |
| 2:D:37:ILE:HB    | 2:D:41:GLU:HB3   | 1.83                     | 0.61              |
| 1:C:118:VAL:CG1  | 5:C:1032:HOH:O   | 2.49                     | 0.61              |
| 1:A:343:ASP:CG   | 1:A:346:THR:HG23 | 2.25                     | 0.61              |
| 2:D:39:LEU:HB3   | 2:D:43:GLU:OE1   | 2.01                     | 0.61              |
| 2:D:178:LEU:O    | 2:D:179:GLY:O    | 2.17                     | 0.61              |
| 2:D:290:GLN:NE2  | 2:D:385:PRO:HG3  | 2.16                     | 0.61              |
| 2:D:387:ARG:HD2  | 2:D:420:TYR:CZ   | 2.35                     | 0.61              |
| 2:D:26:LEU:HD12  | 2:D:135:LEU:CD1  | 2.31                     | 0.61              |
| 2:D:442:ASN:C    | 2:D:442:ASN:HD22 | 2.06                     | 0.61              |
| 1:A:53:ILE:HD12  | 1:A:53:ILE:N     | 2.09                     | 0.61              |
| 1:C:181:VAL:HG21 | 5:C:1023:HOH:O   | 2.01                     | 0.61              |
| 1:C:9:LEU:HD11   | 1:C:325:PRO:HA   | 1.83                     | 0.61              |
| 1:A:233:ILE:HD12 | 1:A:243:ILE:HD11 | 1.83                     | 0.61              |
| 2:B:192:LEU:O    | 2:B:196:ARG:HG2  | 2.01                     | 0.61              |
| 1:C:290:PRO:O    | 1:C:291:TRP:HB2  | 2.00                     | 0.61              |
| 2:D:82:LYS:CG    | 2:D:98:ARG:HD3   | 2.29                     | 0.61              |
| 2:D:176:LEU:HB3  | 5:D:1108:HOH:O   | 2.00                     | 0.61              |
| 1:C:190:SER:O    | 2:D:198:ARG:NH2  | 2.33                     | 0.61              |
| 1:A:402:LEU:HA   | 5:A:919:HOH:O    | 2.01                     | 0.60              |
| 1:A:55:ILE:HD12  | 1:A:58:GLN:OE1   | 2.02                     | 0.60              |
| 2:B:64:VAL:O     | 2:B:66:GLY:N     | 2.32                     | 0.60              |
| 2:B:169:SER:OG   | 2:B:201:TYR:HB2  | 2.00                     | 0.60              |
| 2:B:75:GLU:HB2   | 2:B:79:ARG:HH21  | 1.65                     | 0.60              |
| 2:B:75:GLU:HB3   | 2:B:130:PHE:HZ   | 1.64                     | 0.60              |
| 1:A:247:VAL:CG2  | 1:A:292:LEU:HD11 | 2.28                     | 0.60              |
| 2:B:178:LEU:HD21 | 2:B:183:ILE:HD12 | 1.84                     | 0.60              |
| 2:D:246:LEU:HD23 | 2:D:249:LEU:HD12 | 1.83                     | 0.60              |
| 2:D:44:ASN:HA    | 2:D:47:ILE:CD1   | 2.30                     | 0.60              |
| 2:D:147:SER:O    | 2:D:148:GLN:HB2  | 2.00                     | 0.60              |
| 1:A:103:GLU:HG2  | 1:A:175:ARG:O    | 2.01                     | 0.60              |
| 2:D:113:SER:HB3  | 2:D:116:LEU:CG   | 2.31                     | 0.59              |
| 2:D:140:ILE:O    | 2:D:144:LEU:HG   | 2.00                     | 0.59              |
| 1:A:237:LYS:HA   | 1:A:240:TRP:CE2  | 2.38                     | 0.59              |
| 1:A:336:LEU:O    | 1:A:339:VAL:HG23 | 2.02                     | 0.59              |
| 1:C:216:ILE:HD13 | 1:C:294:TRP:CD2  | 2.37                     | 0.59              |
| 2:B:58:ASN:C     | 2:B:60:GLY:H     | 2.10                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:407:LYS:O    | 1:C:411:LEU:HB2  | 2.01                     | 0.59              |
| 1:A:386:THR:HG22 | 1:A:387:SER:H    | 1.68                     | 0.59              |
| 2:B:247:GLN:HE21 | 2:B:247:GLN:CA   | 2.14                     | 0.59              |
| 2:B:113:SER:HB2  | 2:B:116:LEU:CG   | 2.31                     | 0.59              |
| 2:D:444:PRO:O    | 2:D:447:PHE:HB3  | 2.01                     | 0.59              |
| 2:B:30:LEU:HD12  | 2:B:31:GLN:H     | 1.66                     | 0.59              |
| 2:B:68:GLU:CA    | 2:B:71:GLN:HB3   | 2.27                     | 0.59              |
| 2:B:114:GLU:OE1  | 2:B:117:ARG:HD3  | 2.03                     | 0.59              |
| 1:A:266:LEU:CD1  | 1:C:384:LYS:HD3  | 2.32                     | 0.59              |
| 2:B:75:GLU:O     | 2:B:79:ARG:NE    | 2.35                     | 0.59              |
| 1:A:181:VAL:HG21 | 5:A:903:HOH:O    | 2.02                     | 0.58              |
| 1:C:234:LEU:HD21 | 1:C:243:ILE:HD12 | 1.85                     | 0.58              |
| 2:D:69:GLN:O     | 2:D:73:LYS:HG3   | 2.03                     | 0.58              |
| 1:A:110:ILE:HD13 | 1:A:138:ALA:HB1  | 1.85                     | 0.58              |
| 1:C:33:GLY:O     | 1:C:35:VAL:N     | 2.36                     | 0.58              |
| 2:D:24:HIS:NE2   | 2:D:92:GLU:HB3   | 2.18                     | 0.58              |
| 2:D:293:LYS:HE2  | 2:D:297:GLU:OE2  | 2.03                     | 0.58              |
| 1:A:19:ARG:NH1   | 1:A:379:ARG:HH11 | 2.00                     | 0.58              |
| 1:C:195:GLY:O    | 1:C:197:ASP:N    | 2.36                     | 0.58              |
| 1:A:35:VAL:HG12  | 1:A:35:VAL:O     | 2.03                     | 0.58              |
| 2:B:82:LYS:HB2   | 2:B:82:LYS:NZ    | 2.19                     | 0.58              |
| 1:A:247:VAL:HG22 | 1:A:292:LEU:CD1  | 2.29                     | 0.58              |
| 2:B:81:LEU:O     | 2:B:82:LYS:HB2   | 2.03                     | 0.58              |
| 2:B:240:VAL:HG13 | 2:B:246:LEU:HD12 | 1.85                     | 0.58              |
| 2:D:418:THR:HG23 | 2:D:420:TYR:CE2  | 2.39                     | 0.58              |
| 2:D:201:TYR:CE1  | 2:D:203:GLU:HB2  | 2.39                     | 0.58              |
| 1:C:37:LYS:CD    | 1:C:38:ASN:H     | 2.12                     | 0.58              |
| 2:D:163:GLU:CD   | 2:D:178:LEU:HB3  | 2.28                     | 0.58              |
| 1:C:19:ARG:CZ    | 1:C:379:ARG:HD2  | 2.33                     | 0.57              |
| 2:D:22:TYR:HB2   | 2:D:24:HIS:NE2   | 2.19                     | 0.57              |
| 2:D:22:TYR:HB2   | 2:D:24:HIS:CD2   | 2.39                     | 0.57              |
| 1:C:410:LEU:HG   | 1:C:411:LEU:N    | 2.18                     | 0.57              |
| 1:A:413:LYS:C    | 1:A:415:ASP:H    | 2.13                     | 0.57              |
| 1:C:216:ILE:HD13 | 1:C:294:TRP:CG   | 2.40                     | 0.57              |
| 1:C:33:GLY:C     | 1:C:35:VAL:H     | 2.12                     | 0.57              |
| 2:B:144:LEU:HB3  | 2:B:151:PHE:CE2  | 2.40                     | 0.57              |
| 1:A:35:VAL:O     | 1:A:36:ILE:HD13  | 2.04                     | 0.57              |
| 1:A:141:ILE:HG21 | 1:A:302:PHE:CE2  | 2.39                     | 0.57              |
| 2:D:358:LYS:HG2  | 2:D:360:THR:N    | 2.20                     | 0.57              |
| 1:C:349:THR:HG22 | 1:C:351:SER:HB3  | 1.86                     | 0.57              |
| 1:A:247:VAL:HG13 | 1:A:292:LEU:HD21 | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:19:ARG:HH12  | 1:A:379:ARG:HH11 | 1.53                     | 0.56              |
| 1:A:195:GLY:O    | 1:A:197:ASP:N    | 2.39                     | 0.56              |
| 1:A:386:THR:CG2  | 1:A:387:SER:N    | 2.68                     | 0.56              |
| 2:B:72:SER:CA    | 2:B:75:GLU:HG2   | 2.29                     | 0.56              |
| 2:B:104:PHE:CE1  | 2:B:107:ARG:NH1  | 2.73                     | 0.56              |
| 2:B:64:VAL:HG12  | 2:B:65:LYS:H     | 1.69                     | 0.56              |
| 1:C:329:ARG:HG3  | 5:C:1036:HOH:O   | 2.03                     | 0.56              |
| 2:D:130:PHE:CE2  | 2:D:134:ILE:HD11 | 2.40                     | 0.56              |
| 2:D:192:LEU:HD12 | 2:D:192:LEU:O    | 2.05                     | 0.56              |
| 2:D:342:ASP:HA   | 2:D:346:SER:HB2  | 1.86                     | 0.56              |
| 2:D:24:HIS:CE1   | 2:D:92:GLU:CB    | 2.89                     | 0.56              |
| 2:D:77:GLU:OE1   | 2:D:418:THR:HG21 | 2.05                     | 0.56              |
| 2:B:33:PRO:HD3   | 2:B:104:PHE:CD2  | 2.41                     | 0.56              |
| 2:D:287:CYS:SG   | 2:D:288:MET:N    | 2.79                     | 0.56              |
| 2:B:195:PHE:CD1  | 2:B:195:PHE:C    | 2.83                     | 0.56              |
| 1:C:144:ARG:NH2  | 1:C:148:GLU:HB2  | 2.20                     | 0.56              |
| 2:D:22:TYR:HB3   | 2:D:23:PRO:HD2   | 1.88                     | 0.56              |
| 1:A:355:ARG:HG3  | 1:A:355:ARG:NH1  | 2.20                     | 0.56              |
| 2:B:192:LEU:C    | 2:B:192:LEU:HD23 | 2.31                     | 0.56              |
| 1:A:38:ASN:HA    | 1:A:41:GLN:OE1   | 2.05                     | 0.56              |
| 1:A:260:GLN:HE21 | 1:A:260:GLN:CA   | 2.17                     | 0.56              |
| 1:A:19:ARG:HH12  | 1:A:379:ARG:NH1  | 2.03                     | 0.55              |
| 1:C:51:ASP:HB2   | 1:C:53:ILE:CD1   | 2.36                     | 0.55              |
| 1:C:379:ARG:HB3  | 1:C:382:ASP:OD2  | 2.06                     | 0.55              |
| 2:B:59:LEU:HD13  | 2:B:74:LEU:HB2   | 1.88                     | 0.55              |
| 1:C:38:ASN:HA    | 1:C:41:GLN:OE1   | 2.05                     | 0.55              |
| 1:A:111:ASP:OD2  | 1:A:113:THR:HG23 | 2.05                     | 0.55              |
| 1:A:9:LEU:HD23   | 1:A:76:TYR:HE2   | 1.72                     | 0.55              |
| 1:C:89:ASN:C     | 1:C:89:ASN:ND2   | 2.62                     | 0.55              |
| 1:C:200:LYS:HE2  | 1:C:246:LEU:O    | 2.07                     | 0.55              |
| 1:C:38:ASN:HD22  | 1:C:38:ASN:N     | 2.05                     | 0.55              |
| 1:C:61:ASN:HB2   | 1:C:65:ASP:OD1   | 2.07                     | 0.55              |
| 1:A:172:GLU:HA   | 1:A:175:ARG:CZ   | 2.36                     | 0.55              |
| 2:D:32:PRO:HA    | 2:D:104:PHE:CE1  | 2.42                     | 0.55              |
| 2:D:262:TYR:N    | 2:D:262:TYR:CD2  | 2.74                     | 0.55              |
| 1:A:402:LEU:HB3  | 1:A:406:ARG:HH21 | 1.72                     | 0.55              |
| 2:B:54:LYS:O     | 2:B:57:GLU:HB3   | 2.07                     | 0.55              |
| 1:C:21:PHE:O     | 1:C:23:TYR:N     | 2.35                     | 0.55              |
| 2:D:245:ARG:O    | 2:D:248:PRO:HD2  | 2.07                     | 0.55              |
| 2:D:70:TYR:CD1   | 2:D:70:TYR:C     | 2.85                     | 0.54              |
| 2:D:65:LYS:H     | 2:D:65:LYS:HD2   | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:437:CYS:HB2  | 2:D:439:PHE:CE2  | 2.42                     | 0.54              |
| 2:B:49:ARG:C     | 2:B:51:LYS:N     | 2.63                     | 0.54              |
| 1:C:36:ILE:CG2   | 1:C:37:LYS:HG3   | 2.36                     | 0.54              |
| 1:A:409:GLU:O    | 1:A:413:LYS:HB2  | 2.07                     | 0.54              |
| 2:B:64:VAL:HG12  | 2:B:65:LYS:N     | 2.23                     | 0.54              |
| 2:B:154:ILE:N    | 2:B:154:ILE:HD12 | 2.21                     | 0.54              |
| 2:B:192:LEU:O    | 2:B:192:LEU:HD23 | 2.07                     | 0.54              |
| 2:B:194:LEU:HD13 | 2:B:200:VAL:HG11 | 1.90                     | 0.54              |
| 2:B:237:LEU:HB3  | 2:B:241:GLN:NE2  | 2.23                     | 0.54              |
| 2:B:166:ILE:HD13 | 2:B:183:ILE:HD13 | 1.88                     | 0.54              |
| 1:C:12:LEU:CD1   | 1:C:351:SER:HA   | 2.36                     | 0.54              |
| 1:A:14:LYS:HG2   | 1:A:74:ASN:ND2   | 2.22                     | 0.54              |
| 2:B:47:ILE:O     | 2:B:51:LYS:HG3   | 2.08                     | 0.54              |
| 1:C:50:LYS:O     | 1:C:53:ILE:HD13  | 2.08                     | 0.54              |
| 1:C:112:MET:HG3  | 1:C:119:ARG:CZ   | 2.37                     | 0.54              |
| 1:C:193:LYS:HE2  | 5:C:1013:HOH:O   | 2.08                     | 0.54              |
| 2:D:261:ASP:HB2  | 2:D:442:ASN:OD1  | 2.07                     | 0.54              |
| 1:A:302:PHE:CD2  | 1:A:303:PRO:HD2  | 2.43                     | 0.54              |
| 2:D:129:ARG:HG2  | 2:D:219:LEU:HD11 | 1.89                     | 0.54              |
| 1:A:51:ASP:N     | 1:A:53:ILE:CD1   | 2.68                     | 0.54              |
| 1:A:232:ASP:CG   | 1:A:235:GLU:HB2  | 2.32                     | 0.54              |
| 1:C:50:LYS:H     | 1:C:50:LYS:CD    | 2.04                     | 0.54              |
| 1:C:81:GLY:CA    | 1:C:316:LEU:HD23 | 2.38                     | 0.54              |
| 1:A:233:ILE:HG13 | 1:A:234:LEU:HG   | 1.90                     | 0.54              |
| 1:C:280:GLN:HE22 | 1:C:290:PRO:CD   | 2.21                     | 0.54              |
| 1:A:272:LEU:HD12 | 1:A:272:LEU:O    | 2.08                     | 0.54              |
| 2:D:54:LYS:O     | 2:D:57:GLU:HB3   | 2.08                     | 0.54              |
| 2:B:141:GLN:HE21 | 2:B:145:LYS:HE3  | 1.73                     | 0.53              |
| 1:C:153:LYS:HE2  | 1:C:153:LYS:HA   | 1.90                     | 0.53              |
| 2:B:78:LEU:HD23  | 2:B:79:ARG:HH22  | 1.73                     | 0.53              |
| 1:A:121:CYS:SG   | 1:A:131:CYS:HB3  | 2.47                     | 0.53              |
| 1:A:224:GLU:HB2  | 5:A:907:HOH:O    | 2.08                     | 0.53              |
| 1:A:247:VAL:HG22 | 1:A:292:LEU:CD2  | 2.38                     | 0.53              |
| 1:A:292:LEU:O    | 1:A:296:ILE:HG13 | 2.09                     | 0.53              |
| 1:A:412:LYS:O    | 1:A:412:LYS:HG2  | 2.08                     | 0.53              |
| 2:D:94:GLU:OE2   | 2:D:94:GLU:HA    | 2.07                     | 0.53              |
| 2:D:358:LYS:CE   | 2:D:360:THR:HA   | 2.37                     | 0.53              |
| 1:A:306:ASP:HB3  | 1:A:309:VAL:HG23 | 1.90                     | 0.53              |
| 2:B:75:GLU:HB3   | 2:B:130:PHE:CZ   | 2.44                     | 0.53              |
| 1:C:381:ARG:NH1  | 1:C:384:LYS:HZ1  | 2.06                     | 0.53              |
| 2:D:273:LEU:HD13 | 2:D:322:GLN:HB3  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:67:GLU:O     | 1:C:71:GLN:HG3   | 2.09                     | 0.53              |
| 2:D:424:CYS:HB3  | 2:D:441:LEU:HD23 | 1.89                     | 0.53              |
| 1:A:66:LEU:CG    | 1:A:70:MET:HE3   | 2.37                     | 0.53              |
| 1:C:257:GLN:O    | 1:C:261:LYS:HG3  | 2.08                     | 0.53              |
| 2:D:358:LYS:HG2  | 2:D:360:THR:H    | 1.74                     | 0.53              |
| 1:A:118:VAL:HG11 | 1:A:300:TYR:O    | 2.08                     | 0.53              |
| 2:B:237:LEU:CD1  | 2:B:241:GLN:HE22 | 2.10                     | 0.53              |
| 1:C:401:ASN:N    | 1:C:401:ASN:HD22 | 2.05                     | 0.53              |
| 2:D:261:ASP:HB2  | 2:D:442:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:402:LEU:CA   | 5:A:919:HOH:O    | 2.57                     | 0.53              |
| 1:C:118:VAL:HG12 | 5:C:1032:HOH:O   | 2.09                     | 0.53              |
| 2:B:64:VAL:C     | 2:B:66:GLY:N     | 2.65                     | 0.53              |
| 2:D:264:THR:OG1  | 2:D:265:GLN:N    | 2.42                     | 0.53              |
| 2:D:121:ILE:HG12 | 2:D:226:LEU:HD23 | 1.91                     | 0.53              |
| 2:D:280:SER:HA   | 2:D:284:PHE:CD2  | 2.45                     | 0.52              |
| 1:A:238:GLU:HG2  | 1:A:238:GLU:O    | 2.09                     | 0.52              |
| 2:B:59:LEU:HD21  | 2:B:73:LYS:CG    | 2.38                     | 0.52              |
| 1:C:400:GLU:O    | 1:C:403:ASP:N    | 2.42                     | 0.52              |
| 2:D:192:LEU:HA   | 2:D:195:PHE:CE2  | 2.43                     | 0.52              |
| 2:B:235:ARG:NH1  | 2:B:235:ARG:HG2  | 2.25                     | 0.52              |
| 1:C:116:ASP:CG   | 1:C:124:SER:OG   | 2.53                     | 0.52              |
| 2:D:263:SER:OG   | 2:D:445:ASN:HB2  | 2.10                     | 0.52              |
| 1:A:237:LYS:HD2  | 1:A:240:TRP:HE1  | 1.75                     | 0.52              |
| 2:B:39:LEU:HD23  | 2:B:39:LEU:O     | 2.09                     | 0.52              |
| 2:B:49:ARG:NH2   | 2:B:124:GLU:OE1  | 2.42                     | 0.52              |
| 2:B:132:PHE:O    | 2:B:133:SER:C    | 2.53                     | 0.52              |
| 2:B:201:TYR:CE1  | 2:B:203:GLU:HB2  | 2.45                     | 0.52              |
| 2:D:74:LEU:HD12  | 2:D:74:LEU:O     | 2.08                     | 0.52              |
| 1:A:53:ILE:H     | 1:A:53:ILE:CD1   | 2.06                     | 0.52              |
| 2:B:140:ILE:O    | 2:B:143:PHE:HD1  | 1.93                     | 0.52              |
| 1:A:356:GLU:O    | 1:A:360:ILE:HG12 | 2.09                     | 0.52              |
| 1:C:2:GLU:O      | 1:C:2:GLU:HG2    | 2.09                     | 0.52              |
| 2:D:263:SER:CB   | 2:D:445:ASN:HB3  | 2.40                     | 0.52              |
| 2:B:117:ARG:NH2  | 2:B:231:ALA:HA   | 2.25                     | 0.52              |
| 2:D:113:SER:H    | 2:D:116:LEU:HD12 | 1.74                     | 0.52              |
| 1:C:19:ARG:NH2   | 1:C:379:ARG:NH2  | 2.57                     | 0.52              |
| 1:C:132:TRP:CZ3  | 1:C:135:MET:HG3  | 2.45                     | 0.52              |
| 2:B:136:PRO:O    | 2:B:140:ILE:HG13 | 2.09                     | 0.52              |
| 2:B:71:GLN:HG2   | 2:B:72:SER:N     | 2.24                     | 0.51              |
| 1:C:44:GLU:OE1   | 1:C:56:ARG:HG2   | 2.10                     | 0.51              |
| 2:D:94:GLU:HB3   | 2:D:95:PRO:CD    | 2.31                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:311:LEU:CD1  | 2:D:363:THR:H    | 2.23                     | 0.51              |
| 1:A:118:VAL:CG1  | 1:A:118:VAL:O    | 2.57                     | 0.51              |
| 1:C:1:MET:HB3    | 5:C:1011:HOH:O   | 2.09                     | 0.51              |
| 1:C:86:HIS:CD2   | 1:C:94:VAL:HG11  | 2.45                     | 0.51              |
| 2:D:24:HIS:O     | 2:D:25:CYS:C     | 2.53                     | 0.51              |
| 1:A:20:LEU:HD13  | 1:A:353:ILE:HD12 | 1.91                     | 0.51              |
| 2:D:49:ARG:HB2   | 2:D:102:SER:HB2  | 1.91                     | 0.51              |
| 2:D:237:LEU:HD12 | 2:D:240:VAL:HG12 | 1.92                     | 0.51              |
| 1:A:19:ARG:NH1   | 1:A:379:ARG:NH1  | 2.58                     | 0.51              |
| 1:A:349:THR:CG2  | 1:A:351:SER:H    | 2.21                     | 0.51              |
| 2:D:268:VAL:CG1  | 2:D:269:GLY:N    | 2.73                     | 0.51              |
| 1:C:47:PHE:CE1   | 1:C:78:ILE:HG23  | 2.45                     | 0.51              |
| 1:C:81:GLY:HA3   | 1:C:316:LEU:HD23 | 1.92                     | 0.51              |
| 1:C:208:ILE:HD11 | 1:C:291:TRP:CD1  | 2.46                     | 0.51              |
| 1:A:27:TYR:HB2   | 1:A:63:GLN:HG3   | 1.92                     | 0.51              |
| 1:C:280:GLN:NE2  | 1:C:290:PRO:HD2  | 2.25                     | 0.51              |
| 1:C:395:PHE:O    | 1:C:399:LEU:HG   | 2.10                     | 0.51              |
| 2:D:247:GLN:O    | 2:D:251:ASN:HB2  | 2.11                     | 0.51              |
| 1:A:251:ILE:HG22 | 1:A:251:ILE:O    | 2.10                     | 0.51              |
| 2:B:237:LEU:HD22 | 2:B:241:GLN:NE2  | 2.26                     | 0.51              |
| 1:A:79:ASP:OD2   | 1:A:318:LYS:HA   | 2.11                     | 0.51              |
| 2:B:52:LEU:HD22  | 2:B:83:PHE:CE1   | 2.46                     | 0.51              |
| 2:B:58:ASN:C     | 2:B:60:GLY:N     | 2.68                     | 0.51              |
| 2:D:252:HIS:HD2  | 2:D:257:TYR:HE2  | 1.59                     | 0.51              |
| 1:C:386:THR:CG2  | 1:C:387:SER:N    | 2.72                     | 0.51              |
| 1:A:41:GLN:CD    | 1:A:41:GLN:H     | 2.18                     | 0.50              |
| 1:A:44:GLU:OE1   | 1:A:56:ARG:NE    | 2.40                     | 0.50              |
| 2:B:38:SER:OG    | 2:B:41:GLU:HG2   | 2.11                     | 0.50              |
| 2:B:72:SER:HA    | 2:B:75:GLU:OE2   | 2.11                     | 0.50              |
| 2:B:126:ASP:N    | 2:B:126:ASP:OD2  | 2.44                     | 0.50              |
| 2:B:237:LEU:N    | 2:B:238:PRO:CD   | 2.73                     | 0.50              |
| 1:C:154:HIS:ND1  | 1:C:402:LEU:CD1  | 2.70                     | 0.50              |
| 1:A:89:ASN:HD22  | 1:A:90:GLN:N     | 2.09                     | 0.50              |
| 1:C:178:SER:OG   | 1:C:181:VAL:HG23 | 2.12                     | 0.50              |
| 2:D:252:HIS:CB   | 2:D:256:SER:HB2  | 2.42                     | 0.50              |
| 1:A:248:PRO:HG3  | 1:A:279:TYR:CE2  | 2.46                     | 0.50              |
| 1:A:402:LEU:HD23 | 5:A:919:HOH:O    | 2.10                     | 0.50              |
| 2:B:95:PRO:CA    | 2:B:98:ARG:HD2   | 2.42                     | 0.50              |
| 2:B:219:LEU:O    | 2:B:222:PHE:HB3  | 2.11                     | 0.50              |
| 1:C:155:ARG:HG3  | 1:C:155:ARG:HH11 | 1.75                     | 0.50              |
| 1:A:404:LYS:O    | 1:A:405:SER:C    | 2.54                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:49:ARG:HH22  | 2:B:124:GLU:CD   | 2.19                     | 0.50              |
| 2:B:238:PRO:C    | 2:B:240:VAL:H    | 2.19                     | 0.50              |
| 2:D:352:SER:HA   | 2:D:362:TYR:CD2  | 2.46                     | 0.50              |
| 1:A:334:ILE:HD13 | 1:A:334:ILE:N    | 2.26                     | 0.50              |
| 2:B:145:LYS:C    | 2:B:147:SER:N    | 2.67                     | 0.50              |
| 1:C:160:SER:OG   | 1:C:164:GLY:C    | 2.55                     | 0.50              |
| 1:A:172:GLU:CA   | 1:A:175:ARG:NH1  | 2.74                     | 0.50              |
| 2:B:144:LEU:HB3  | 2:B:151:PHE:CZ   | 2.47                     | 0.50              |
| 2:B:237:LEU:HD13 | 2:B:241:GLN:NE2  | 2.09                     | 0.50              |
| 1:C:115:TYR:C    | 1:C:117:ASP:H    | 2.20                     | 0.50              |
| 2:D:46:ALA:O     | 2:D:50:VAL:HG23  | 2.12                     | 0.50              |
| 1:C:210:PRO:O    | 1:C:214:LYS:HG3  | 2.12                     | 0.50              |
| 1:C:329:ARG:CG   | 5:C:1036:HOH:O   | 2.59                     | 0.50              |
| 2:D:265:GLN:HB3  | 2:D:356:GLU:HA   | 1.93                     | 0.50              |
| 2:B:120:PHE:O    | 2:B:124:GLU:HB2  | 2.11                     | 0.50              |
| 1:C:80:ILE:HB    | 1:C:168:TRP:HH2  | 1.77                     | 0.50              |
| 1:A:154:HIS:ND1  | 1:A:402:LEU:HD23 | 2.27                     | 0.49              |
| 1:C:154:HIS:N    | 1:C:154:HIS:CD2  | 2.79                     | 0.49              |
| 2:D:311:LEU:HD13 | 2:D:363:THR:H    | 1.77                     | 0.49              |
| 1:A:118:VAL:O    | 1:A:118:VAL:HG12 | 2.11                     | 0.49              |
| 2:D:43:GLU:O     | 2:D:47:ILE:CG1   | 2.53                     | 0.49              |
| 2:D:268:VAL:CG1  | 2:D:269:GLY:H    | 2.23                     | 0.49              |
| 1:A:113:THR:HA   | 1:A:116:ASP:OD1  | 2.11                     | 0.49              |
| 1:A:186:VAL:HG21 | 1:A:310:SER:HB2  | 1.93                     | 0.49              |
| 1:A:217:ASN:O    | 1:A:220:LYS:HB2  | 2.12                     | 0.49              |
| 2:B:68:GLU:O     | 2:B:72:SER:N     | 2.45                     | 0.49              |
| 2:D:365:PHE:N    | 5:D:1105:HOH:O   | 2.38                     | 0.49              |
| 2:B:49:ARG:HG2   | 2:B:102:SER:HB3  | 1.93                     | 0.49              |
| 2:B:177:LYS:C    | 2:B:179:GLY:H    | 2.20                     | 0.49              |
| 2:D:49:ARG:HD3   | 2:D:102:SER:OG   | 2.11                     | 0.49              |
| 2:D:243:ASP:O    | 2:D:247:GLN:NE2  | 2.35                     | 0.49              |
| 2:D:288:MET:HG3  | 2:D:312:PHE:CD2  | 2.48                     | 0.49              |
| 2:B:74:LEU:O     | 2:B:74:LEU:HD23  | 2.12                     | 0.49              |
| 2:B:171:PRO:C    | 2:B:173:LEU:H    | 2.18                     | 0.49              |
| 2:D:286:PRO:O    | 2:D:290:GLN:HB2  | 2.13                     | 0.49              |
| 1:A:278:ARG:HG2  | 1:A:278:ARG:HH11 | 1.78                     | 0.49              |
| 1:C:38:ASN:N     | 1:C:38:ASN:ND2   | 2.61                     | 0.49              |
| 1:C:15:LEU:HD23  | 1:C:354:CYS:SG   | 2.53                     | 0.49              |
| 2:D:113:SER:OG   | 2:D:115:GLU:HB2  | 2.12                     | 0.49              |
| 2:D:221:GLU:OE1  | 2:D:225:LYS:HE3  | 2.13                     | 0.49              |
| 2:D:272:SER:H    | 2:D:275:GLN:NE2  | 2.10                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:349:THR:CG2  | 1:A:351:SER:HB3  | 2.43                     | 0.49              |
| 1:C:91:HIS:ND1   | 1:C:92:ASN:N     | 2.61                     | 0.49              |
| 2:D:237:LEU:HB3  | 2:D:238:PRO:HD3  | 1.95                     | 0.49              |
| 1:A:73:MET:O     | 1:A:74:ASN:C     | 2.56                     | 0.49              |
| 2:D:82:LYS:CG    | 2:D:82:LYS:O     | 2.60                     | 0.49              |
| 2:D:192:LEU:HD12 | 2:D:192:LEU:C    | 2.38                     | 0.49              |
| 1:A:118:VAL:HG11 | 1:A:300:TYR:HA   | 1.95                     | 0.49              |
| 1:A:205:SER:O    | 1:A:206:GLU:C    | 2.54                     | 0.49              |
| 1:C:143:ASP:OD1  | 1:C:155:ARG:NE   | 2.42                     | 0.48              |
| 1:C:191:LEU:HD12 | 1:C:302:PHE:CE2  | 2.47                     | 0.48              |
| 2:D:57:GLU:O     | 2:D:61:VAL:HG23  | 2.13                     | 0.48              |
| 2:D:337:ASP:HB3  | 2:D:340:LYS:HB3  | 1.94                     | 0.48              |
| 1:A:170:CYS:O    | 1:A:175:ARG:NH1  | 2.45                     | 0.48              |
| 1:A:247:VAL:HG22 | 1:A:292:LEU:CG   | 2.43                     | 0.48              |
| 1:C:339:VAL:O    | 1:C:341:GLN:N    | 2.46                     | 0.48              |
| 2:D:103:HIS:HE1  | 2:D:124:GLU:HG2  | 1.77                     | 0.48              |
| 2:D:164:GLN:HE22 | 2:D:176:LEU:HD22 | 1.77                     | 0.48              |
| 1:A:402:LEU:N    | 5:A:919:HOH:O    | 2.46                     | 0.48              |
| 2:B:138:ASP:OD2  | 2:B:138:ASP:N    | 2.43                     | 0.48              |
| 2:B:145:LYS:O    | 2:B:147:SER:N    | 2.46                     | 0.48              |
| 2:B:235:ARG:HG2  | 2:B:235:ARG:HH11 | 1.77                     | 0.48              |
| 1:C:60:PHE:HB3   | 1:C:65:ASP:HB2   | 1.95                     | 0.48              |
| 2:D:219:LEU:O    | 2:D:222:PHE:HB3  | 2.13                     | 0.48              |
| 2:D:229:ALA:O    | 2:D:233:THR:HG23 | 2.12                     | 0.48              |
| 2:D:259:GLY:O    | 2:D:260:GLN:HG2  | 2.13                     | 0.48              |
| 2:D:320:LEU:HD13 | 2:D:353:PHE:CD1  | 2.47                     | 0.48              |
| 2:B:119:TRP:O    | 2:B:122:GLN:HB3  | 2.14                     | 0.48              |
| 2:D:155:SER:C    | 2:D:157:GLU:N    | 2.67                     | 0.48              |
| 2:D:335:LYS:HD2  | 2:D:335:LYS:N    | 2.28                     | 0.48              |
| 1:A:386:THR:CG2  | 1:A:387:SER:H    | 2.27                     | 0.48              |
| 2:B:249:LEU:C    | 2:B:251:ASN:H    | 2.21                     | 0.48              |
| 1:C:381:ARG:NH1  | 1:C:384:LYS:NZ   | 2.61                     | 0.48              |
| 2:D:418:THR:O    | 2:D:418:THR:CG2  | 2.61                     | 0.48              |
| 1:A:210:PRO:O    | 1:A:214:LYS:HG3  | 2.13                     | 0.48              |
| 2:B:115:GLU:O    | 2:B:119:TRP:HB2  | 2.14                     | 0.48              |
| 2:D:324:LEU:HD23 | 2:D:349:ILE:HG21 | 1.95                     | 0.48              |
| 2:B:104:PHE:HE1  | 2:B:107:ARG:NH1  | 2.12                     | 0.48              |
| 2:D:35:GLU:OE2   | 2:D:101:ILE:HD11 | 2.13                     | 0.48              |
| 2:D:173:LEU:HD23 | 2:D:173:LEU:C    | 2.38                     | 0.48              |
| 1:A:216:ILE:HD13 | 1:A:294:TRP:CD2  | 2.49                     | 0.48              |
| 1:C:95:LYS:HD3   | 1:C:98:ALA:CB    | 2.40                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:110:TYR:CD2  | 2:B:116:LEU:HD22 | 2.49                     | 0.48              |
| 2:B:134:ILE:O    | 2:B:135:LEU:C    | 2.55                     | 0.48              |
| 1:C:69:GLU:O     | 1:C:73:MET:HG2   | 2.14                     | 0.48              |
| 1:A:358:ASP:C    | 1:A:360:ILE:H    | 2.22                     | 0.47              |
| 2:D:117:ARG:CG   | 2:D:230:LEU:HD13 | 2.27                     | 0.47              |
| 2:D:424:CYS:HB3  | 2:D:441:LEU:CD2  | 2.44                     | 0.47              |
| 1:A:133:THR:O    | 1:A:136:THR:HB   | 2.13                     | 0.47              |
| 1:C:140:ARG:HG2  | 1:C:140:ARG:HH11 | 1.79                     | 0.47              |
| 2:B:155:SER:C    | 2:B:157:GLU:N    | 2.68                     | 0.47              |
| 2:B:178:LEU:HD11 | 2:B:183:ILE:HD11 | 1.96                     | 0.47              |
| 2:D:288:MET:CG   | 2:D:312:PHE:CD2  | 2.97                     | 0.47              |
| 1:A:41:GLN:HB3   | 1:A:87:ARG:NH1   | 2.29                     | 0.47              |
| 2:B:110:TYR:HA   | 2:B:116:LEU:HD13 | 1.97                     | 0.47              |
| 2:D:32:PRO:HG3   | 2:D:104:PHE:HE1  | 1.79                     | 0.47              |
| 2:D:129:ARG:HE   | 2:D:219:LEU:HD13 | 1.79                     | 0.47              |
| 2:B:111:CYS:O    | 2:B:234:ALA:HB2  | 2.14                     | 0.47              |
| 2:D:94:GLU:CB    | 2:D:95:PRO:HD3   | 2.33                     | 0.47              |
| 1:A:69:GLU:OE2   | 1:A:72:LYS:HE3   | 2.14                     | 0.47              |
| 1:A:145:ALA:O    | 1:A:149:ASP:HB2  | 2.15                     | 0.47              |
| 1:A:359:ALA:C    | 1:A:360:ILE:HD13 | 2.40                     | 0.47              |
| 1:C:147:LYS:NZ   | 5:C:1008:HOH:O   | 2.48                     | 0.47              |
| 1:C:280:GLN:HE22 | 1:C:290:PRO:HD2  | 1.80                     | 0.47              |
| 1:C:360:ILE:O    | 1:C:360:ILE:HG22 | 2.15                     | 0.47              |
| 2:D:72:SER:HA    | 2:D:75:GLU:HG2   | 1.97                     | 0.47              |
| 2:D:80:LYS:NZ    | 2:D:418:THR:CG2  | 2.76                     | 0.47              |
| 2:D:329:GLN:C    | 2:D:329:GLN:CD   | 2.82                     | 0.47              |
| 2:D:362:TYR:O    | 2:D:363:THR:OG1  | 2.29                     | 0.47              |
| 2:B:37:ILE:HB    | 2:B:41:GLU:CB    | 2.45                     | 0.47              |
| 2:D:262:TYR:HB2  | 2:D:264:THR:N    | 2.20                     | 0.47              |
| 2:B:37:ILE:HB    | 2:B:41:GLU:CG    | 2.43                     | 0.47              |
| 1:C:49:LEU:HD13  | 1:C:50:LYS:HZ2   | 1.80                     | 0.47              |
| 1:C:160:SER:OG   | 1:C:164:GLY:O    | 2.32                     | 0.47              |
| 2:D:159:LYS:HE3  | 2:D:183:ILE:HD12 | 1.97                     | 0.47              |
| 1:A:15:LEU:HD23  | 1:A:354:CYS:HB3  | 1.97                     | 0.47              |
| 2:D:166:ILE:HG21 | 2:D:183:ILE:HD13 | 1.97                     | 0.47              |
| 1:A:159:TYR:HB2  | 1:A:334:ILE:HD11 | 1.97                     | 0.46              |
| 2:B:202:LEU:HA   | 2:B:206:PHE:O    | 2.15                     | 0.46              |
| 1:C:140:ARG:HD3  | 5:C:1025:HOH:O   | 2.14                     | 0.46              |
| 1:C:158:VAL:HG12 | 1:C:159:TYR:N    | 2.30                     | 0.46              |
| 1:C:390:PRO:O    | 1:C:393:LYS:HB3  | 2.15                     | 0.46              |
| 2:D:431:ILE:HG13 | 2:D:432:HIS:ND1  | 2.28                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:47:PHE:CE1   | 1:A:78:ILE:HG23  | 2.50                     | 0.46              |
| 1:A:249:GLU:HA   | 1:A:252:HIS:CD2  | 2.51                     | 0.46              |
| 1:C:118:VAL:HG11 | 1:C:300:TYR:O    | 2.15                     | 0.46              |
| 1:C:358:ASP:C    | 1:C:360:ILE:H    | 2.23                     | 0.46              |
| 2:D:263:SER:CB   | 2:D:445:ASN:CB   | 2.93                     | 0.46              |
| 2:D:359:ARG:HB2  | 2:D:362:TYR:HB2  | 1.97                     | 0.46              |
| 2:D:373:SER:C    | 2:D:375:PRO:HD3  | 2.40                     | 0.46              |
| 1:A:402:LEU:HB3  | 1:A:406:ARG:NH2  | 2.30                     | 0.46              |
| 2:B:141:GLN:O    | 2:B:145:LYS:HG3  | 2.14                     | 0.46              |
| 2:D:200:VAL:HG12 | 2:D:209:VAL:HG12 | 1.98                     | 0.46              |
| 1:A:214:LYS:NZ   | 5:A:914:HOH:O    | 2.47                     | 0.46              |
| 1:A:379:ARG:O    | 1:A:381:ARG:N    | 2.47                     | 0.46              |
| 2:D:442:ASN:C    | 2:D:442:ASN:ND2  | 2.74                     | 0.46              |
| 1:A:249:GLU:HG2  | 1:A:252:HIS:CE1  | 2.50                     | 0.46              |
| 2:B:65:LYS:HE3   | 2:B:65:LYS:O     | 2.15                     | 0.46              |
| 1:C:95:LYS:H     | 1:C:95:LYS:HG3   | 1.46                     | 0.46              |
| 1:C:171:ASP:OD2  | 1:C:171:ASP:N    | 2.48                     | 0.46              |
| 2:D:125:MET:HE3  | 2:D:129:ARG:NH2  | 2.30                     | 0.46              |
| 2:B:170:SER:HB3  | 2:B:171:PRO:CD   | 2.35                     | 0.46              |
| 1:A:323:VAL:HG21 | 1:A:350:ILE:HD12 | 1.98                     | 0.46              |
| 1:A:415:ASP:OD1  | 1:A:415:ASP:C    | 2.59                     | 0.46              |
| 2:D:29:TYR:HB3   | 2:D:104:PHE:HE2  | 1.80                     | 0.46              |
| 1:A:217:ASN:O    | 1:A:218:ILE:C    | 2.56                     | 0.46              |
| 2:B:39:LEU:O     | 2:B:43:GLU:HB2   | 2.15                     | 0.46              |
| 2:B:175:GLY:O    | 2:B:176:LEU:HD23 | 2.16                     | 0.46              |
| 1:C:162:ARG:HG3  | 1:C:327:THR:CG2  | 2.46                     | 0.46              |
| 1:C:196:GLN:O    | 1:C:196:GLN:HG2  | 2.16                     | 0.46              |
| 1:C:200:LYS:HG2  | 1:C:203:HIS:CE1  | 2.51                     | 0.46              |
| 2:D:184:TYR:N    | 2:D:184:TYR:CD1  | 2.83                     | 0.46              |
| 2:D:288:MET:HG2  | 2:D:312:PHE:CG   | 2.50                     | 0.46              |
| 2:B:192:LEU:C    | 2:B:192:LEU:CD2  | 2.89                     | 0.46              |
| 1:C:152:PHE:CE1  | 1:C:174:VAL:HG22 | 2.51                     | 0.46              |
| 2:D:58:ASN:O     | 2:D:59:LEU:C     | 2.58                     | 0.46              |
| 2:D:263:SER:HB3  | 2:D:445:ASN:HB3  | 1.97                     | 0.46              |
| 1:A:157:TRP:CZ3  | 1:A:167:CYS:HB2  | 2.51                     | 0.46              |
| 1:A:235:GLU:HG2  | 1:A:236:ASN:HD21 | 1.78                     | 0.46              |
| 1:A:336:LEU:HA   | 1:A:339:VAL:HG22 | 1.98                     | 0.46              |
| 2:B:49:ARG:C     | 2:B:51:LYS:H     | 2.24                     | 0.46              |
| 1:C:90:GLN:O     | 1:C:93:THR:HB    | 2.15                     | 0.46              |
| 1:A:237:LYS:HE2  | 1:A:241:ASP:CG   | 2.40                     | 0.45              |
| 1:A:334:ILE:CD1  | 1:A:342:PHE:CE2  | 2.97                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:407:LYS:O   | 1:A:411:LEU:HB2  | 2.15                     | 0.45              |
| 2:B:49:ARG:NH1  | 2:B:99:ASP:OD2   | 2.49                     | 0.45              |
| 2:D:78:LEU:HD11 | 2:D:127:LEU:HD11 | 1.97                     | 0.45              |
| 1:A:143:ASP:CG  | 1:A:155:ARG:HE   | 2.24                     | 0.45              |
| 1:A:264:ASN:O   | 1:A:268:ARG:HG3  | 2.17                     | 0.45              |
| 2:B:49:ARG:CD   | 2:B:102:SER:HB3  | 2.46                     | 0.45              |
| 2:B:199:LYS:O   | 2:B:200:VAL:CG1  | 2.62                     | 0.45              |
| 1:C:89:ASN:O    | 1:C:90:GLN:HG3   | 2.15                     | 0.45              |
| 2:D:49:ARG:HH11 | 2:D:124:GLU:CD   | 2.23                     | 0.45              |
| 2:D:342:ASP:HA  | 2:D:346:SER:CB   | 2.47                     | 0.45              |
| 1:A:413:LYS:C   | 1:A:415:ASP:N    | 2.74                     | 0.45              |
| 2:B:48:ASP:O    | 2:B:51:LYS:HB2   | 2.15                     | 0.45              |
| 2:B:172:SER:O   | 2:B:174:SER:N    | 2.49                     | 0.45              |
| 2:B:222:PHE:O   | 2:B:223:ARG:C    | 2.58                     | 0.45              |
| 1:C:5:ASP:OD1   | 1:C:7:THR:OG1    | 2.25                     | 0.45              |
| 2:D:47:ILE:HG13 | 2:D:47:ILE:H     | 1.59                     | 0.45              |
| 2:D:251:ASN:HB3 | 2:D:252:HIS:ND1  | 2.31                     | 0.45              |
| 2:D:275:GLN:O   | 2:D:276:ILE:C    | 2.60                     | 0.45              |
| 2:D:377:SER:O   | 2:D:378:GLN:C    | 2.58                     | 0.45              |
| 1:A:327:THR:CB  | 1:A:329:ARG:HG2  | 2.47                     | 0.45              |
| 2:B:113:SER:HB2 | 2:B:116:LEU:CD1  | 2.47                     | 0.45              |
| 1:C:66:LEU:HD12 | 1:C:66:LEU:HA    | 1.81                     | 0.45              |
| 2:D:336:MET:HG3 | 5:D:1111:HOH:O   | 2.16                     | 0.45              |
| 2:D:343:LYS:O   | 2:D:343:LYS:HG2  | 2.17                     | 0.45              |
| 2:B:38:SER:H    | 2:B:41:GLU:HG3   | 1.81                     | 0.45              |
| 1:C:153:LYS:N   | 1:C:171:ASP:OD1  | 2.36                     | 0.45              |
| 1:C:339:VAL:C   | 1:C:341:GLN:N    | 2.74                     | 0.45              |
| 2:D:38:SER:C    | 2:D:40:ILE:N     | 2.73                     | 0.45              |
| 2:D:265:GLN:CB  | 2:D:356:GLU:HA   | 2.46                     | 0.45              |
| 1:A:73:MET:HG3  | 5:A:922:HOH:O    | 2.16                     | 0.45              |
| 2:B:28:PHE:O    | 2:B:28:PHE:CG    | 2.70                     | 0.45              |
| 2:B:247:GLN:CA  | 2:B:247:GLN:NE2  | 2.79                     | 0.45              |
| 1:C:50:LYS:HD2  | 1:C:50:LYS:N     | 2.10                     | 0.45              |
| 1:C:140:ARG:HG2 | 1:C:140:ARG:NH1  | 2.31                     | 0.45              |
| 2:D:259:GLY:C   | 2:D:260:GLN:HG2  | 2.42                     | 0.45              |
| 2:D:272:SER:HB2 | 2:D:275:GLN:HG3  | 1.99                     | 0.45              |
| 2:D:375:PRO:HA  | 2:D:376:PRO:HD2  | 1.82                     | 0.45              |
| 1:A:26:TYR:OH   | 1:A:80:ILE:HD11  | 2.16                     | 0.45              |
| 1:A:237:LYS:HE3 | 1:A:256:GLN:OE1  | 2.17                     | 0.45              |
| 2:B:247:GLN:N   | 2:B:248:PRO:CD   | 2.80                     | 0.45              |
| 1:C:12:LEU:HD13 | 1:C:351:SER:HA   | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:82:LYS:HG3   | 2:D:98:ARG:CD    | 2.37                     | 0.45              |
| 2:D:414:LEU:HD13 | 2:D:422:VAL:HG12 | 1.97                     | 0.45              |
| 1:A:258:SER:HB3  | 1:A:271:HIS:ND1  | 2.31                     | 0.45              |
| 1:A:302:PHE:CG   | 1:A:303:PRO:HD2  | 2.52                     | 0.45              |
| 1:C:224:GLU:O    | 1:C:229:VAL:HG23 | 2.17                     | 0.45              |
| 2:D:57:GLU:OE1   | 2:D:119:TRP:NE1  | 2.48                     | 0.45              |
| 2:B:44:ASN:O     | 2:B:45:LEU:C     | 2.60                     | 0.45              |
| 1:C:19:ARG:NH2   | 1:C:379:ARG:HH21 | 2.13                     | 0.45              |
| 2:D:65:LYS:HD2   | 2:D:65:LYS:N     | 2.32                     | 0.45              |
| 2:D:272:SER:C    | 2:D:274:ASP:H    | 2.24                     | 0.45              |
| 1:A:379:ARG:HD3  | 1:A:382:ASP:OD2  | 2.16                     | 0.44              |
| 2:B:49:ARG:O     | 2:B:51:LYS:N     | 2.50                     | 0.44              |
| 2:B:181:GLU:OE2  | 2:B:210:PRO:HB2  | 2.16                     | 0.44              |
| 2:B:247:GLN:O    | 2:B:248:PRO:C    | 2.59                     | 0.44              |
| 1:C:272:LEU:HD12 | 1:C:272:LEU:O    | 2.17                     | 0.44              |
| 1:C:349:THR:HG22 | 1:C:351:SER:CA   | 2.47                     | 0.44              |
| 2:D:192:LEU:O    | 2:D:196:ARG:HG2  | 2.16                     | 0.44              |
| 2:D:354:GLY:HA3  | 2:D:359:ARG:NH1  | 2.32                     | 0.44              |
| 1:A:38:ASN:O     | 1:A:39:TYR:C     | 2.60                     | 0.44              |
| 2:D:265:GLN:HB3  | 2:D:355:LYS:O    | 2.16                     | 0.44              |
| 2:D:295:LEU:HG   | 2:D:330:GLU:HG2  | 1.99                     | 0.44              |
| 2:D:154:ILE:HB   | 2:D:158:GLU:HB2  | 1.99                     | 0.44              |
| 1:A:332:VAL:HB   | 1:A:391:TYR:CD2  | 2.52                     | 0.44              |
| 2:B:42:PHE:CZ    | 2:B:249:LEU:HD22 | 2.52                     | 0.44              |
| 2:B:117:ARG:O    | 2:B:121:ILE:HG13 | 2.18                     | 0.44              |
| 2:B:145:LYS:C    | 2:B:147:SER:H    | 2.25                     | 0.44              |
| 2:D:248:PRO:HB3  | 2:D:253:LEU:HB2  | 1.99                     | 0.44              |
| 2:B:75:GLU:HB2   | 2:B:79:ARG:NH2   | 2.32                     | 0.44              |
| 2:B:201:TYR:HD1  | 2:B:208:TYR:HD2  | 1.64                     | 0.44              |
| 1:C:191:LEU:HD21 | 1:C:212:ILE:HD11 | 1.98                     | 0.44              |
| 2:D:82:LYS:CD    | 2:D:98:ARG:HD3   | 2.47                     | 0.44              |
| 2:D:418:THR:HG23 | 2:D:420:TYR:CZ   | 2.52                     | 0.44              |
| 1:C:27:TYR:CD1   | 1:C:63:GLN:HB2   | 2.52                     | 0.44              |
| 1:C:56:ARG:HG2   | 1:C:56:ARG:O     | 2.16                     | 0.44              |
| 2:D:263:SER:OG   | 2:D:445:ASN:CB   | 2.65                     | 0.44              |
| 1:A:144:ARG:CZ   | 1:A:214:LYS:HD2  | 2.47                     | 0.44              |
| 1:C:87:ARG:HD3   | 1:C:90:GLN:NE2   | 2.33                     | 0.44              |
| 1:A:253:ASP:O    | 1:A:257:GLN:HG3  | 2.18                     | 0.44              |
| 2:B:237:LEU:C    | 2:B:241:GLN:HE21 | 2.26                     | 0.44              |
| 1:C:35:VAL:O     | 1:C:35:VAL:HG12  | 2.16                     | 0.44              |
| 2:D:232:LEU:O    | 2:D:235:ARG:HB3  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:125:ALA:HB1  | 1:A:162:ARG:NH1  | 2.33                     | 0.44              |
| 2:B:162:ARG:O    | 2:B:163:GLU:C    | 2.61                     | 0.44              |
| 2:B:171:PRO:C    | 2:B:173:LEU:N    | 2.76                     | 0.44              |
| 1:A:80:ILE:HG13  | 1:A:319:SER:HB2  | 1.99                     | 0.43              |
| 2:B:45:LEU:O     | 2:B:46:ALA:C     | 2.60                     | 0.43              |
| 1:C:259:PHE:HA   | 1:C:268:ARG:HG2  | 2.00                     | 0.43              |
| 2:D:288:MET:HE3  | 2:D:312:PHE:HB2  | 2.00                     | 0.43              |
| 2:D:392:GLU:OE2  | 2:D:392:GLU:HA   | 2.16                     | 0.43              |
| 1:C:19:ARG:HH21  | 1:C:379:ARG:NH2  | 2.15                     | 0.43              |
| 2:D:52:LEU:CD1   | 2:D:78:LEU:HD12  | 2.48                     | 0.43              |
| 2:D:82:LYS:HE2   | 2:D:98:ARG:NE    | 2.32                     | 0.43              |
| 2:D:420:TYR:O    | 2:D:423:ALA:HB3  | 2.17                     | 0.43              |
| 1:A:264:ASN:C    | 1:A:264:ASN:OD1  | 2.61                     | 0.43              |
| 1:A:409:GLU:OE1  | 5:A:920:HOH:O    | 2.21                     | 0.43              |
| 2:B:154:ILE:HG23 | 2:B:158:GLU:OE1  | 2.18                     | 0.43              |
| 2:D:42:PHE:CE2   | 2:D:249:LEU:HD13 | 2.49                     | 0.43              |
| 1:A:379:ARG:HB3  | 1:A:382:ASP:CG   | 2.41                     | 0.43              |
| 2:B:113:SER:O    | 2:B:116:LEU:HB2  | 2.18                     | 0.43              |
| 2:B:141:GLN:HA   | 2:B:144:LEU:HD12 | 2.00                     | 0.43              |
| 2:B:200:VAL:HG11 | 2:B:209:VAL:CG1  | 2.48                     | 0.43              |
| 1:C:65:ASP:OD2   | 1:C:65:ASP:N     | 2.48                     | 0.43              |
| 2:D:75:GLU:O     | 2:D:79:ARG:HB2   | 2.18                     | 0.43              |
| 2:D:112:GLN:HE21 | 2:D:112:GLN:HB2  | 1.56                     | 0.43              |
| 1:A:82:ALA:HB2   | 1:A:313:ILE:O    | 2.18                     | 0.43              |
| 1:A:237:LYS:HA   | 1:A:240:TRP:NE1  | 2.33                     | 0.43              |
| 2:B:37:ILE:HD12  | 2:B:41:GLU:CB    | 2.49                     | 0.43              |
| 2:B:158:GLU:HB3  | 2:B:162:ARG:NH2  | 2.33                     | 0.43              |
| 1:C:323:VAL:HG21 | 1:C:350:ILE:HD12 | 2.01                     | 0.43              |
| 2:D:366:SER:O    | 2:D:370:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:66:LEU:HD11  | 1:A:70:MET:CE    | 2.48                     | 0.43              |
| 1:A:248:PRO:HD2  | 1:A:292:LEU:CD2  | 2.49                     | 0.43              |
| 1:C:5:ASP:HA     | 1:C:6:PRO:HD2    | 1.79                     | 0.43              |
| 1:C:37:LYS:CG    | 1:C:38:ASN:H     | 2.31                     | 0.43              |
| 1:C:177:LEU:HD22 | 1:C:181:VAL:HG11 | 2.01                     | 0.43              |
| 2:D:350:ARG:C    | 2:D:352:SER:N    | 2.76                     | 0.43              |
| 1:A:19:ARG:HD2   | 1:A:357:LEU:HD21 | 2.01                     | 0.43              |
| 2:B:132:PHE:CE2  | 2:B:219:LEU:HD21 | 2.53                     | 0.43              |
| 1:C:132:TRP:O    | 1:C:135:MET:N    | 2.52                     | 0.43              |
| 2:D:266:GLY:O    | 2:D:267:ASN:C    | 2.62                     | 0.43              |
| 1:A:95:LYS:HE2   | 1:A:98:ALA:CB    | 2.48                     | 0.43              |
| 1:A:329:ARG:HH22 | 1:A:345:PHE:C    | 2.27                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:410:LEU:HD23 | 1:A:411:LEU:CA   | 2.49                     | 0.43              |
| 2:B:42:PHE:CE2   | 2:B:249:LEU:HD22 | 2.54                     | 0.43              |
| 2:B:74:LEU:HD23  | 2:B:74:LEU:C     | 2.43                     | 0.43              |
| 1:C:133:THR:O    | 1:C:136:THR:HB   | 2.19                     | 0.43              |
| 2:D:81:LEU:O     | 2:D:82:LYS:CB    | 2.66                     | 0.43              |
| 1:A:154:HIS:CD2  | 5:A:919:HOH:O    | 2.71                     | 0.43              |
| 1:A:246:LEU:HD12 | 1:A:296:ILE:HG23 | 2.01                     | 0.43              |
| 1:C:74:ASN:N     | 1:C:75:PRO:HD3   | 2.33                     | 0.43              |
| 1:A:278:ARG:HH11 | 1:A:278:ARG:CG   | 2.32                     | 0.43              |
| 1:A:291:TRP:HA   | 1:A:291:TRP:CE3  | 2.53                     | 0.43              |
| 1:A:334:ILE:HD12 | 1:A:342:PHE:CD2  | 2.51                     | 0.43              |
| 2:B:178:LEU:O    | 2:B:179:GLY:C    | 2.62                     | 0.43              |
| 2:B:237:LEU:N    | 2:B:238:PRO:HD2  | 2.33                     | 0.43              |
| 1:C:13:LEU:HD22  | 1:C:17:TYR:CE2   | 2.54                     | 0.43              |
| 1:C:94:VAL:HG12  | 1:C:98:ALA:HB3   | 2.00                     | 0.43              |
| 1:C:251:ILE:HG23 | 1:C:275:VAL:HG11 | 2.01                     | 0.43              |
| 2:D:245:ARG:H    | 2:D:245:ARG:HG3  | 1.57                     | 0.42              |
| 2:D:291:LEU:HD21 | 2:D:382:HIS:HA   | 2.00                     | 0.42              |
| 2:D:386:PHE:HE2  | 2:D:424:CYS:SG   | 2.42                     | 0.42              |
| 1:C:157:TRP:CE3  | 1:C:167:CYS:HB2  | 2.54                     | 0.42              |
| 1:C:353:ILE:CB   | 1:C:386:THR:CG2  | 2.93                     | 0.42              |
| 2:D:38:SER:O     | 2:D:39:LEU:C     | 2.62                     | 0.42              |
| 1:A:90:GLN:O     | 1:A:93:THR:HB    | 2.20                     | 0.42              |
| 1:C:200:LYS:HD2  | 1:C:246:LEU:HB3  | 2.02                     | 0.42              |
| 2:D:265:GLN:NE2  | 2:D:265:GLN:CA   | 2.80                     | 0.42              |
| 2:D:426:LYS:HG3  | 2:D:430:MET:HE2  | 2.01                     | 0.42              |
| 1:A:106:LEU:HB3  | 1:A:169:VAL:HB   | 2.01                     | 0.42              |
| 1:A:118:VAL:HG21 | 1:A:299:GLN:O    | 2.20                     | 0.42              |
| 2:B:37:ILE:HD12  | 2:B:41:GLU:HB2   | 2.01                     | 0.42              |
| 1:C:36:ILE:HG22  | 1:C:37:LYS:N     | 2.32                     | 0.42              |
| 1:A:95:LYS:HD3   | 1:A:95:LYS:N     | 2.12                     | 0.42              |
| 1:C:356:GLU:OE1  | 1:C:387:SER:N    | 2.48                     | 0.42              |
| 1:C:378:HIS:O    | 1:C:379:ARG:HG3  | 2.19                     | 0.42              |
| 2:D:27:GLN:HE21  | 2:D:27:GLN:HB3   | 1.57                     | 0.42              |
| 2:D:51:LYS:O     | 2:D:55:SER:OG    | 2.36                     | 0.42              |
| 2:D:67:THR:CG2   | 2:D:69:GLN:HE21  | 2.32                     | 0.42              |
| 1:A:54:TYR:CE2   | 1:A:56:ARG:HB2   | 2.55                     | 0.42              |
| 1:A:412:LYS:O    | 1:A:415:ASP:OD1  | 2.37                     | 0.42              |
| 2:B:49:ARG:NH2   | 2:B:124:GLU:OE2  | 2.53                     | 0.42              |
| 1:C:32:TYR:O     | 1:C:406:ARG:NE   | 2.53                     | 0.42              |
| 1:C:186:VAL:HG21 | 1:C:310:SER:HB2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:341:PHE:O    | 2:D:345:TYR:N    | 2.53                     | 0.42              |
| 2:D:441:LEU:HD12 | 2:D:441:LEU:HA   | 1.79                     | 0.42              |
| 1:A:224:GLU:HG3  | 1:A:266:LEU:CD2  | 2.50                     | 0.42              |
| 2:B:154:ILE:HG23 | 2:B:158:GLU:HB2  | 1.98                     | 0.42              |
| 1:C:140:ARG:NE   | 1:C:222:TYR:OH   | 2.53                     | 0.42              |
| 1:C:155:ARG:HG3  | 1:C:155:ARG:NH1  | 2.35                     | 0.42              |
| 1:C:280:GLN:OE1  | 1:C:292:LEU:HG   | 2.20                     | 0.42              |
| 2:D:261:ASP:HB2  | 2:D:442:ASN:CG   | 2.44                     | 0.42              |
| 2:D:416:LYS:HE2  | 2:D:416:LYS:HB3  | 1.85                     | 0.42              |
| 1:A:59:SER:C     | 1:A:60:PHE:CD1   | 2.98                     | 0.42              |
| 1:A:269:TRP:CZ3  | 1:A:272:LEU:HD23 | 2.54                     | 0.42              |
| 2:B:49:ARG:O     | 2:B:50:VAL:C     | 2.63                     | 0.42              |
| 2:B:159:LYS:O    | 2:B:163:GLU:N    | 2.53                     | 0.42              |
| 2:D:271:ILE:CD1  | 2:D:316:ILE:HD12 | 2.47                     | 0.42              |
| 2:B:80:LYS:C     | 2:B:82:LYS:H     | 2.26                     | 0.42              |
| 1:C:170:CYS:O    | 1:C:171:ASP:C    | 2.59                     | 0.42              |
| 2:D:155:SER:C    | 2:D:157:GLU:H    | 2.28                     | 0.42              |
| 2:D:170:SER:HB3  | 2:D:171:PRO:CD   | 2.44                     | 0.42              |
| 1:A:51:ASP:O     | 1:A:52:ASP:CB    | 2.68                     | 0.42              |
| 1:A:247:VAL:CG2  | 1:A:292:LEU:HD21 | 2.47                     | 0.42              |
| 1:A:335:ASP:OD2  | 1:A:335:ASP:C    | 2.62                     | 0.42              |
| 1:A:390:PRO:O    | 1:A:393:LYS:HB3  | 2.18                     | 0.42              |
| 1:C:27:TYR:CD2   | 1:C:27:TYR:C     | 2.97                     | 0.42              |
| 1:C:114:ASP:O    | 1:C:304:ARG:HD2  | 2.20                     | 0.42              |
| 1:C:236:ASN:HB2  | 1:C:239:SER:H    | 1.85                     | 0.42              |
| 1:C:307:ILE:O    | 1:C:311:LYS:HB3  | 2.20                     | 0.42              |
| 1:C:330:ILE:O    | 1:C:332:VAL:HG13 | 2.19                     | 0.42              |
| 2:D:50:VAL:O     | 2:D:54:LYS:HB2   | 2.20                     | 0.42              |
| 2:D:173:LEU:HD23 | 2:D:173:LEU:O    | 2.20                     | 0.42              |
| 2:D:358:LYS:C    | 2:D:360:THR:H    | 2.28                     | 0.42              |
| 1:A:46:SER:HB3   | 1:A:79:ASP:HB2   | 2.01                     | 0.41              |
| 1:A:272:LEU:HD12 | 1:A:272:LEU:C    | 2.44                     | 0.41              |
| 1:A:277:SER:O    | 1:A:281:ASN:ND2  | 2.53                     | 0.41              |
| 2:B:39:LEU:HD12  | 2:B:245:ARG:HD3  | 2.01                     | 0.41              |
| 2:B:95:PRO:HA    | 2:B:98:ARG:HD2   | 2.02                     | 0.41              |
| 2:B:148:GLN:NE2  | 2:B:148:GLN:HA   | 2.35                     | 0.41              |
| 2:B:65:LYS:O     | 2:B:65:LYS:HG3   | 2.20                     | 0.41              |
| 2:B:79:ARG:H     | 2:B:79:ARG:HG2   | 1.65                     | 0.41              |
| 2:D:247:GLN:N    | 2:D:248:PRO:CD   | 2.83                     | 0.41              |
| 1:A:412:LYS:O    | 1:A:415:ASP:CG   | 2.64                     | 0.41              |
| 2:D:138:ASP:OD2  | 2:D:138:ASP:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:ASP:O    | 1:A:174:VAL:N    | 2.53                     | 0.41              |
| 1:A:349:THR:HG22 | 1:A:352:PHE:H    | 1.86                     | 0.41              |
| 2:B:110:TYR:CB   | 2:B:116:LEU:HB3  | 2.45                     | 0.41              |
| 2:B:188:PHE:CD1  | 2:B:188:PHE:C    | 2.99                     | 0.41              |
| 2:B:201:TYR:CZ   | 2:B:203:GLU:HB2  | 2.56                     | 0.41              |
| 1:C:257:GLN:HE21 | 1:C:257:GLN:HB3  | 1.53                     | 0.41              |
| 1:C:349:THR:HG22 | 1:C:352:PHE:H    | 1.85                     | 0.41              |
| 2:D:237:LEU:HG   | 2:D:241:GLN:HG3  | 2.01                     | 0.41              |
| 1:A:86:HIS:CG    | 1:A:94:VAL:HG21  | 2.56                     | 0.41              |
| 1:A:105:GLU:H    | 1:A:105:GLU:CD   | 2.27                     | 0.41              |
| 2:B:43:GLU:O     | 2:B:47:ILE:HG13  | 2.21                     | 0.41              |
| 2:B:49:ARG:NH2   | 2:B:124:GLU:CD   | 2.78                     | 0.41              |
| 2:B:51:LYS:O     | 2:B:55:SER:N     | 2.53                     | 0.41              |
| 2:B:82:LYS:HB2   | 2:B:82:LYS:HZ2   | 1.85                     | 0.41              |
| 1:C:313:ILE:O    | 1:C:313:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:109:ASP:C    | 1:A:109:ASP:OD1  | 2.63                     | 0.41              |
| 1:C:158:VAL:HG12 | 1:C:159:TYR:O    | 2.21                     | 0.41              |
| 2:D:374:ASN:O    | 2:D:375:PRO:C    | 2.61                     | 0.41              |
| 1:A:2:GLU:HG2    | 1:A:3:THR:N      | 2.33                     | 0.41              |
| 1:A:35:VAL:O     | 1:A:35:VAL:CG1   | 2.68                     | 0.41              |
| 1:A:223:PHE:O    | 1:A:227:ALA:HB3  | 2.21                     | 0.41              |
| 2:B:70:TYR:CD1   | 2:B:70:TYR:C     | 2.98                     | 0.41              |
| 1:C:121:CYS:SG   | 1:C:131:CYS:HB3  | 2.61                     | 0.41              |
| 1:A:23:TYR:CG    | 1:A:67:GLU:HG2   | 2.56                     | 0.41              |
| 1:A:66:LEU:CD1   | 1:A:70:MET:HE3   | 2.50                     | 0.41              |
| 2:B:78:LEU:HD23  | 2:B:79:ARG:NH2   | 2.35                     | 0.41              |
| 2:B:113:SER:N    | 2:B:116:LEU:HD12 | 2.30                     | 0.41              |
| 2:B:139:LYS:HD3  | 2:B:142:ASP:OD2  | 2.21                     | 0.41              |
| 2:B:141:GLN:NE2  | 2:B:145:LYS:HE3  | 2.33                     | 0.41              |
| 1:C:36:ILE:O     | 1:C:37:LYS:C     | 2.63                     | 0.41              |
| 1:C:233:ILE:HD12 | 1:C:243:ILE:CD1  | 2.35                     | 0.41              |
| 1:C:349:THR:HG22 | 1:C:351:SER:CB   | 2.50                     | 0.41              |
| 2:D:422:VAL:O    | 2:D:423:ALA:C    | 2.62                     | 0.41              |
| 1:A:234:LEU:HD21 | 1:A:243:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:313:ILE:O    | 1:A:313:ILE:CG1  | 2.68                     | 0.41              |
| 1:A:409:GLU:O    | 1:A:413:LYS:N    | 2.49                     | 0.41              |
| 2:B:74:LEU:HD13  | 2:B:130:PHE:CD1  | 2.56                     | 0.41              |
| 2:B:148:GLN:O    | 2:B:149:LEU:C    | 2.62                     | 0.41              |
| 1:C:142:ILE:HB   | 1:C:157:TRP:HH2  | 1.86                     | 0.41              |
| 1:C:349:THR:C    | 1:C:351:SER:N    | 2.78                     | 0.41              |
| 1:C:378:HIS:ND1  | 1:C:378:HIS:C    | 2.78                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:135:LEU:HB3  | 2:D:139:LYS:HB3  | 2.03                     | 0.41              |
| 2:D:200:VAL:HG12 | 2:D:209:VAL:CG1  | 2.51                     | 0.41              |
| 1:A:171:ASP:HB2  | 1:A:174:VAL:CG2  | 2.51                     | 0.41              |
| 1:A:237:LYS:CD   | 1:A:256:GLN:OE1  | 2.69                     | 0.41              |
| 1:A:305:LEU:HA   | 5:A:918:HOH:O    | 2.20                     | 0.41              |
| 2:B:30:LEU:O     | 2:B:31:GLN:HB2   | 2.21                     | 0.41              |
| 2:B:178:LEU:HD12 | 2:B:178:LEU:HA   | 1.91                     | 0.41              |
| 1:C:381:ARG:HH11 | 1:C:384:LYS:NZ   | 2.18                     | 0.41              |
| 2:D:99:ASP:OD1   | 2:D:99:ASP:C     | 2.63                     | 0.41              |
| 2:D:58:ASN:O     | 2:D:61:VAL:N     | 2.55                     | 0.40              |
| 2:D:328:LYS:HA   | 2:D:341:PHE:CE1  | 2.56                     | 0.40              |
| 1:A:413:LYS:HE2  | 1:A:413:LYS:HB3  | 1.91                     | 0.40              |
| 1:C:146:LEU:O    | 1:C:152:PHE:HB2  | 2.20                     | 0.40              |
| 2:D:30:LEU:O     | 2:D:31:GLN:CB    | 2.70                     | 0.40              |
| 2:D:358:LYS:HE3  | 2:D:360:THR:CA   | 2.48                     | 0.40              |
| 1:A:17:TYR:CE2   | 1:A:75:PRO:HD2   | 2.57                     | 0.40              |
| 1:A:36:ILE:O     | 1:A:37:LYS:C     | 2.63                     | 0.40              |
| 1:A:36:ILE:HG22  | 1:A:37:LYS:HG3   | 2.03                     | 0.40              |
| 1:A:219:ILE:HD12 | 1:A:298:LEU:HD23 | 2.03                     | 0.40              |
| 1:A:306:ASP:HB3  | 1:A:309:VAL:CG2  | 2.50                     | 0.40              |
| 2:B:107:ARG:O    | 2:B:108:LEU:C    | 2.65                     | 0.40              |
| 2:D:92:GLU:O     | 2:D:95:PRO:HD2   | 2.21                     | 0.40              |
| 1:A:51:ASP:O     | 1:A:52:ASP:HB3   | 2.21                     | 0.40              |
| 2:B:76:SER:O     | 2:B:80:LYS:HB3   | 2.22                     | 0.40              |
| 1:C:36:ILE:CG2   | 1:C:37:LYS:N     | 2.84                     | 0.40              |
| 1:C:251:ILE:HD13 | 1:C:251:ILE:HA   | 1.93                     | 0.40              |
| 1:C:408:GLY:O    | 1:C:409:GLU:C    | 2.63                     | 0.40              |
| 2:D:184:TYR:CZ   | 2:D:211:LEU:HD13 | 2.56                     | 0.40              |
| 2:B:49:ARG:HD3   | 2:B:102:SER:HB3  | 2.02                     | 0.40              |
| 2:B:127:LEU:HG   | 2:B:131:ARG:HH11 | 1.87                     | 0.40              |
| 1:C:256:GLN:HE21 | 1:C:256:GLN:HB2  | 1.53                     | 0.40              |
| 1:C:306:ASP:OD1  | 1:C:306:ASP:C    | 2.65                     | 0.40              |
| 2:D:212:LYS:H    | 2:D:212:LYS:HG3  | 1.63                     | 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     | 383/420 (91%)   | 331 (86%)  | 45 (12%)  | 7 (2%)   | 6           | 11 |
| 1   | C     | 383/420 (91%)   | 327 (85%)  | 36 (9%)   | 20 (5%)  | 1           | 2  |
| 2   | B     | 209/509 (41%)   | 156 (75%)  | 37 (18%)  | 16 (8%)  | 1           | 0  |
| 2   | D     | 425/509 (84%)   | 346 (81%)  | 58 (14%)  | 21 (5%)  | 1           | 2  |
| All | All   | 1400/1858 (75%) | 1160 (83%) | 176 (13%) | 64 (5%)  | 2           | 2  |

All (64) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | LYS  |
| 1   | A     | 50  | LYS  |
| 1   | A     | 95  | LYS  |
| 1   | A     | 196 | GLN  |
| 1   | A     | 380 | THR  |
| 2   | B     | 82  | LYS  |
| 2   | B     | 173 | LEU  |
| 1   | C     | 37  | LYS  |
| 1   | C     | 196 | GLN  |
| 2   | D     | 25  | CYS  |
| 2   | D     | 179 | GLY  |
| 2   | D     | 264 | THR  |
| 2   | D     | 267 | ASN  |
| 2   | B     | 179 | GLY  |
| 1   | C     | 32  | TYR  |
| 1   | C     | 34  | GLY  |
| 1   | C     | 63  | GLN  |
| 1   | C     | 252 | HIS  |
| 1   | C     | 281 | ASN  |
| 1   | C     | 340 | ASP  |
| 1   | C     | 410 | LEU  |
| 2   | D     | 24  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 93  | TYR  |
| 2   | D     | 171 | PRO  |
| 2   | D     | 252 | HIS  |
| 2   | D     | 276 | ILE  |
| 1   | A     | 404 | LYS  |
| 2   | B     | 71  | GLN  |
| 2   | B     | 122 | GLN  |
| 2   | B     | 146 | ASP  |
| 2   | B     | 157 | GLU  |
| 2   | B     | 171 | PRO  |
| 1   | C     | 96  | LEU  |
| 1   | C     | 409 | GLU  |
| 1   | C     | 411 | LEU  |
| 2   | D     | 29  | TYR  |
| 2   | D     | 157 | GLU  |
| 2   | D     | 263 | SER  |
| 2   | D     | 273 | LEU  |
| 2   | D     | 355 | LYS  |
| 2   | D     | 360 | THR  |
| 2   | B     | 67  | THR  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 100 | HIS  |
| 2   | B     | 133 | SER  |
| 2   | B     | 170 | SER  |
| 2   | B     | 240 | VAL  |
| 2   | B     | 250 | LEU  |
| 1   | C     | 22  | PRO  |
| 1   | C     | 116 | ASP  |
| 1   | C     | 133 | THR  |
| 1   | C     | 253 | ASP  |
| 1   | C     | 291 | TRP  |
| 1   | A     | 410 | LEU  |
| 2   | B     | 65  | LYS  |
| 1   | C     | 359 | ALA  |
| 2   | D     | 244 | GLU  |
| 2   | D     | 260 | GLN  |
| 2   | D     | 357 | GLY  |
| 1   | C     | 6   | PRO  |
| 2   | D     | 31  | GLN  |
| 1   | C     | 408 | GLY  |
| 2   | D     | 344 | GLY  |
| 2   | D     | 363 | THR  |

### 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     | 364/393 (93%)   | 342 (94%)  | 22 (6%)  | 17          | 30 |
| 1   | C     | 363/393 (92%)   | 335 (92%)  | 28 (8%)  | 12          | 20 |
| 2   | B     | 194/459 (42%)   | 171 (88%)  | 23 (12%) | 5           | 7  |
| 2   | D     | 389/459 (85%)   | 362 (93%)  | 27 (7%)  | 14          | 24 |
| All | All   | 1310/1704 (77%) | 1210 (92%) | 100 (8%) | 12          | 21 |

All (100) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | GLU  |
| 1   | A     | 51  | ASP  |
| 1   | A     | 53  | ILE  |
| 1   | A     | 55  | ILE  |
| 1   | A     | 56  | ARG  |
| 1   | A     | 72  | LYS  |
| 1   | A     | 89  | ASN  |
| 1   | A     | 122 | CYS  |
| 1   | A     | 173 | SER  |
| 1   | A     | 207 | LYS  |
| 1   | A     | 258 | SER  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 274 | LYS  |
| 1   | A     | 291 | TRP  |
| 1   | A     | 309 | VAL  |
| 1   | A     | 313 | ILE  |
| 1   | A     | 334 | ILE  |
| 1   | A     | 341 | GLN  |
| 1   | A     | 349 | THR  |
| 1   | A     | 351 | SER  |
| 1   | A     | 358 | ASP  |
| 1   | A     | 393 | LYS  |
| 2   | B     | 31  | GLN  |
| 2   | B     | 63  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 65  | LYS  |
| 2   | B     | 70  | TYR  |
| 2   | B     | 73  | LYS  |
| 2   | B     | 79  | ARG  |
| 2   | B     | 82  | LYS  |
| 2   | B     | 83  | PHE  |
| 2   | B     | 126 | ASP  |
| 2   | B     | 138 | ASP  |
| 2   | B     | 143 | PHE  |
| 2   | B     | 160 | THR  |
| 2   | B     | 187 | PRO  |
| 2   | B     | 193 | ASP  |
| 2   | B     | 195 | PHE  |
| 2   | B     | 202 | LEU  |
| 2   | B     | 212 | LYS  |
| 2   | B     | 214 | ILE  |
| 2   | B     | 237 | LEU  |
| 2   | B     | 238 | PRO  |
| 2   | B     | 240 | VAL  |
| 2   | B     | 245 | ARG  |
| 2   | B     | 247 | GLN  |
| 1   | C     | 2   | GLU  |
| 1   | C     | 12  | LEU  |
| 1   | C     | 38  | ASN  |
| 1   | C     | 55  | ILE  |
| 1   | C     | 65  | ASP  |
| 1   | C     | 88  | PRO  |
| 1   | C     | 89  | ASN  |
| 1   | C     | 91  | HIS  |
| 1   | C     | 95  | LYS  |
| 1   | C     | 107 | VAL  |
| 1   | C     | 119 | ARG  |
| 1   | C     | 123 | SER  |
| 1   | C     | 160 | SER  |
| 1   | C     | 162 | ARG  |
| 1   | C     | 221 | LYS  |
| 1   | C     | 247 | VAL  |
| 1   | C     | 256 | GLN  |
| 1   | C     | 257 | GLN  |
| 1   | C     | 272 | LEU  |
| 1   | C     | 274 | LYS  |
| 1   | C     | 307 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 331 | SER  |
| 1   | C     | 333 | PRO  |
| 1   | C     | 339 | VAL  |
| 1   | C     | 349 | THR  |
| 1   | C     | 355 | ARG  |
| 1   | C     | 393 | LYS  |
| 1   | C     | 411 | LEU  |
| 2   | D     | 27  | GLN  |
| 2   | D     | 31  | GLN  |
| 2   | D     | 54  | LYS  |
| 2   | D     | 65  | LYS  |
| 2   | D     | 69  | GLN  |
| 2   | D     | 82  | LYS  |
| 2   | D     | 92  | GLU  |
| 2   | D     | 98  | ARG  |
| 2   | D     | 99  | ASP  |
| 2   | D     | 138 | ASP  |
| 2   | D     | 139 | LYS  |
| 2   | D     | 165 | GLU  |
| 2   | D     | 169 | SER  |
| 2   | D     | 173 | LEU  |
| 2   | D     | 240 | VAL  |
| 2   | D     | 244 | GLU  |
| 2   | D     | 245 | ARG  |
| 2   | D     | 262 | TYR  |
| 2   | D     | 264 | THR  |
| 2   | D     | 288 | MET  |
| 2   | D     | 321 | GLU  |
| 2   | D     | 359 | ARG  |
| 2   | D     | 378 | GLN  |
| 2   | D     | 387 | ARG  |
| 2   | D     | 391 | PRO  |
| 2   | D     | 397 | LYS  |
| 2   | D     | 442 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | ASN  |
| 1   | A     | 89  | ASN  |
| 1   | A     | 90  | GLN  |
| 1   | A     | 92  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 102 | GLN  |
| 1   | A     | 236 | ASN  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 281 | ASN  |
| 1   | A     | 337 | GLN  |
| 1   | A     | 341 | GLN  |
| 1   | A     | 378 | HIS  |
| 1   | A     | 401 | ASN  |
| 2   | B     | 31  | GLN  |
| 2   | B     | 44  | ASN  |
| 2   | B     | 69  | GLN  |
| 2   | B     | 71  | GLN  |
| 2   | B     | 123 | GLN  |
| 2   | B     | 141 | GLN  |
| 2   | B     | 148 | GLN  |
| 2   | B     | 150 | GLN  |
| 2   | B     | 164 | GLN  |
| 2   | B     | 241 | GLN  |
| 2   | B     | 247 | GLN  |
| 1   | C     | 38  | ASN  |
| 1   | C     | 58  | GLN  |
| 1   | C     | 86  | HIS  |
| 1   | C     | 89  | ASN  |
| 1   | C     | 90  | GLN  |
| 1   | C     | 102 | GLN  |
| 1   | C     | 166 | HIS  |
| 1   | C     | 203 | HIS  |
| 1   | C     | 236 | ASN  |
| 1   | C     | 257 | GLN  |
| 1   | C     | 260 | GLN  |
| 1   | C     | 267 | GLN  |
| 1   | C     | 280 | GLN  |
| 1   | C     | 337 | GLN  |
| 1   | C     | 341 | GLN  |
| 1   | C     | 401 | ASN  |
| 2   | D     | 27  | GLN  |
| 2   | D     | 31  | GLN  |
| 2   | D     | 69  | GLN  |
| 2   | D     | 71  | GLN  |
| 2   | D     | 100 | HIS  |
| 2   | D     | 112 | GLN  |
| 2   | D     | 141 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 148 | GLN  |
| 2   | D     | 150 | GLN  |
| 2   | D     | 164 | GLN  |
| 2   | D     | 260 | GLN  |
| 2   | D     | 265 | GLN  |
| 2   | D     | 275 | GLN  |
| 2   | D     | 290 | GLN  |
| 2   | D     | 298 | ASN  |
| 2   | D     | 329 | GLN  |
| 2   | D     | 351 | HIS  |
| 2   | D     | 396 | GLN  |
| 2   | D     | 399 | GLN  |
| 2   | D     | 421 | GLN  |
| 2   | D     | 442 | ASN  |
| 2   | D     | 452 | GLN  |
| 2   | D     | 456 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SF4  | D     | 1000 | 2    | 0,12,12      | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 4   | SF4  | D     | 1000 | 2    | -       | -        | 0/6/5/5 |

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 389/420 (92%)   | -0.47  | 3 (0%) 82 79  | 13, 42, 78, 100       | 0     |
| 1   | C     | 389/420 (92%)   | -0.58  | 4 (1%) 79 76  | 14, 37, 75, 95        | 0     |
| 2   | B     | 213/509 (41%)   | 0.14   | 7 (3%) 49 40  | 23, 77, 100, 109      | 0     |
| 2   | D     | 429/509 (84%)   | -0.12  | 18 (4%) 40 32 | 15, 61, 95, 107       | 0     |
| All | All   | 1420/1858 (76%) | -0.30  | 32 (2%) 61 54 | 13, 50, 93, 109       | 0     |

All (32) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 360 | THR  | 5.7  |
| 2   | B     | 29  | TYR  | 5.2  |
| 2   | D     | 358 | LYS  | 4.6  |
| 2   | D     | 359 | ARG  | 4.6  |
| 2   | D     | 361 | ASP  | 4.1  |
| 1   | C     | 2   | GLU  | 3.7  |
| 2   | B     | 173 | LEU  | 3.7  |
| 1   | A     | 411 | LEU  | 3.6  |
| 2   | D     | 261 | ASP  | 3.5  |
| 2   | D     | 258 | THR  | 3.4  |
| 2   | B     | 28  | PHE  | 3.4  |
| 2   | B     | 74  | LEU  | 3.4  |
| 2   | D     | 253 | LEU  | 3.4  |
| 1   | C     | 116 | ASP  | 3.4  |
| 2   | D     | 25  | CYS  | 3.3  |
| 2   | D     | 23  | PRO  | 3.3  |
| 1   | C     | 411 | LEU  | 3.0  |
| 2   | D     | 64  | VAL  | 2.9  |
| 2   | D     | 257 | TYR  | 2.8  |
| 2   | D     | 173 | LEU  | 2.8  |
| 2   | B     | 171 | PRO  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 1   | MET  | 2.6  |
| 1   | C     | 1   | MET  | 2.6  |
| 2   | B     | 132 | PHE  | 2.5  |
| 2   | B     | 130 | PHE  | 2.4  |
| 2   | D     | 255 | HIS  | 2.4  |
| 2   | D     | 252 | HIS  | 2.2  |
| 2   | D     | 267 | ASN  | 2.2  |
| 2   | D     | 262 | TYR  | 2.2  |
| 2   | D     | 355 | LYS  | 2.2  |
| 2   | D     | 268 | VAL  | 2.0  |
| 1   | A     | 415 | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | ZN   | A     | 800  | 1/1   | 0.99 | 0.02 | 34,34,34,34                 | 0     |
| 4   | SF4  | D     | 1000 | 8/8   | 0.99 | 0.03 | 17,26,32,38                 | 0     |
| 3   | ZN   | C     | 900  | 1/1   | 1.00 | 0.02 | 26,26,26,26                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.