



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 AM UTC

PDB ID : 3I7O / pdb\_00003i7o  
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of IQWD1  
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.  
Deposited on : 2009-07-08  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

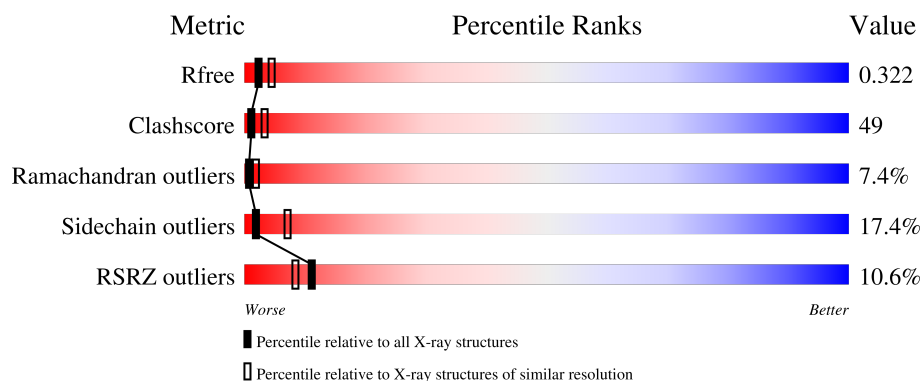
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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     | 1143   |                  |
| 2   | B     | 13     |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8838 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 damage-binding protein 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1114     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8726  | 5529 | 1472 | 1677 | 48 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | GLY      | -      | expression tag | UNP Q16531 |
| A     | -1      | SER      | -      | expression tag | UNP Q16531 |
| A     | 0       | HIS      | -      | expression tag | UNP Q16531 |
| A     | 422     | TYR      | ASP    | SEE REMARK 999 | UNP Q16531 |
| A     | 898     | ASP      | GLU    | SEE REMARK 999 | UNP Q16531 |
| A     | 899     | VAL      | LEU    | SEE REMARK 999 | UNP Q16531 |

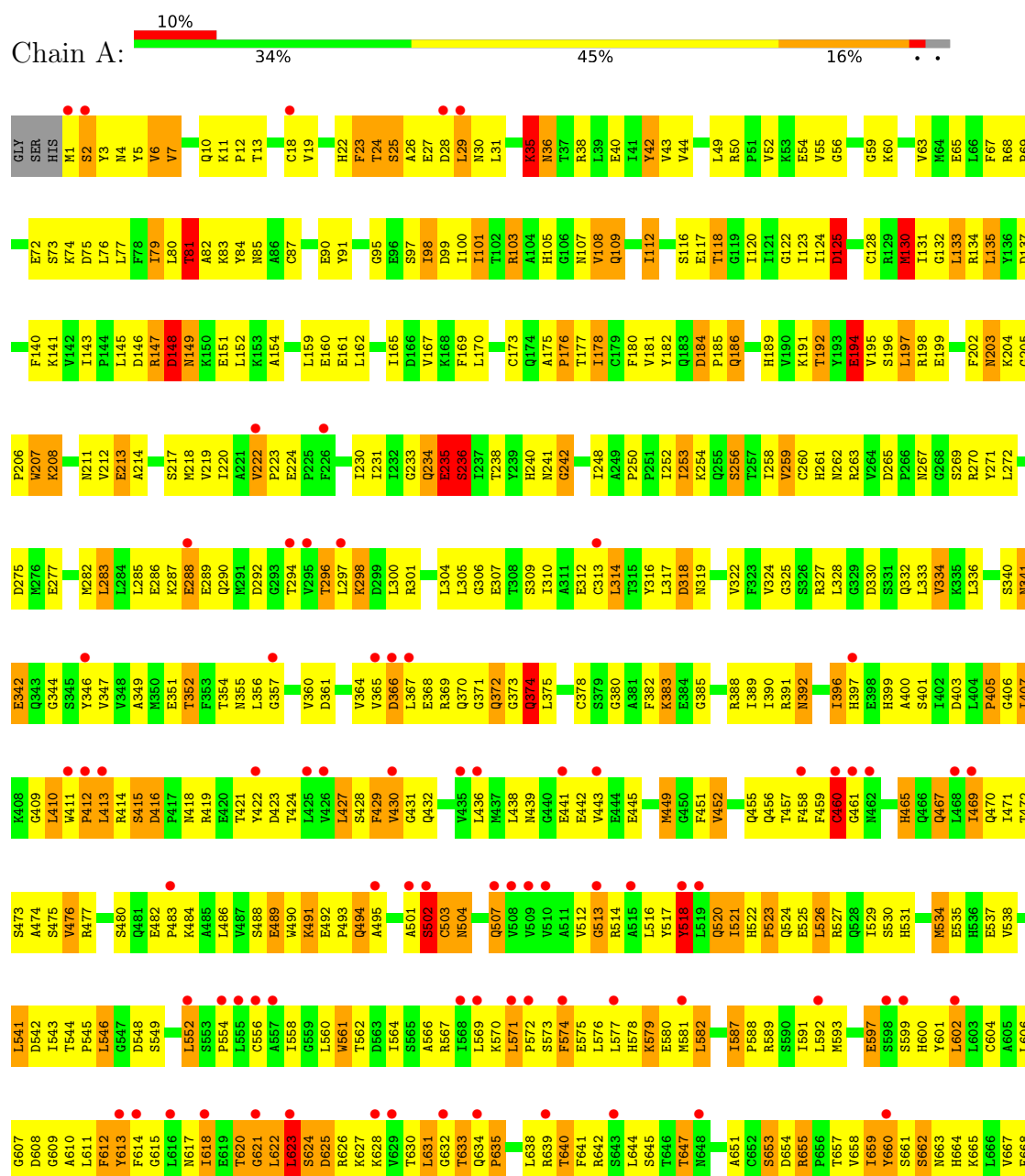
- Molecule 2 is a protein called IQ motif and WD repeat-containing protein 1.

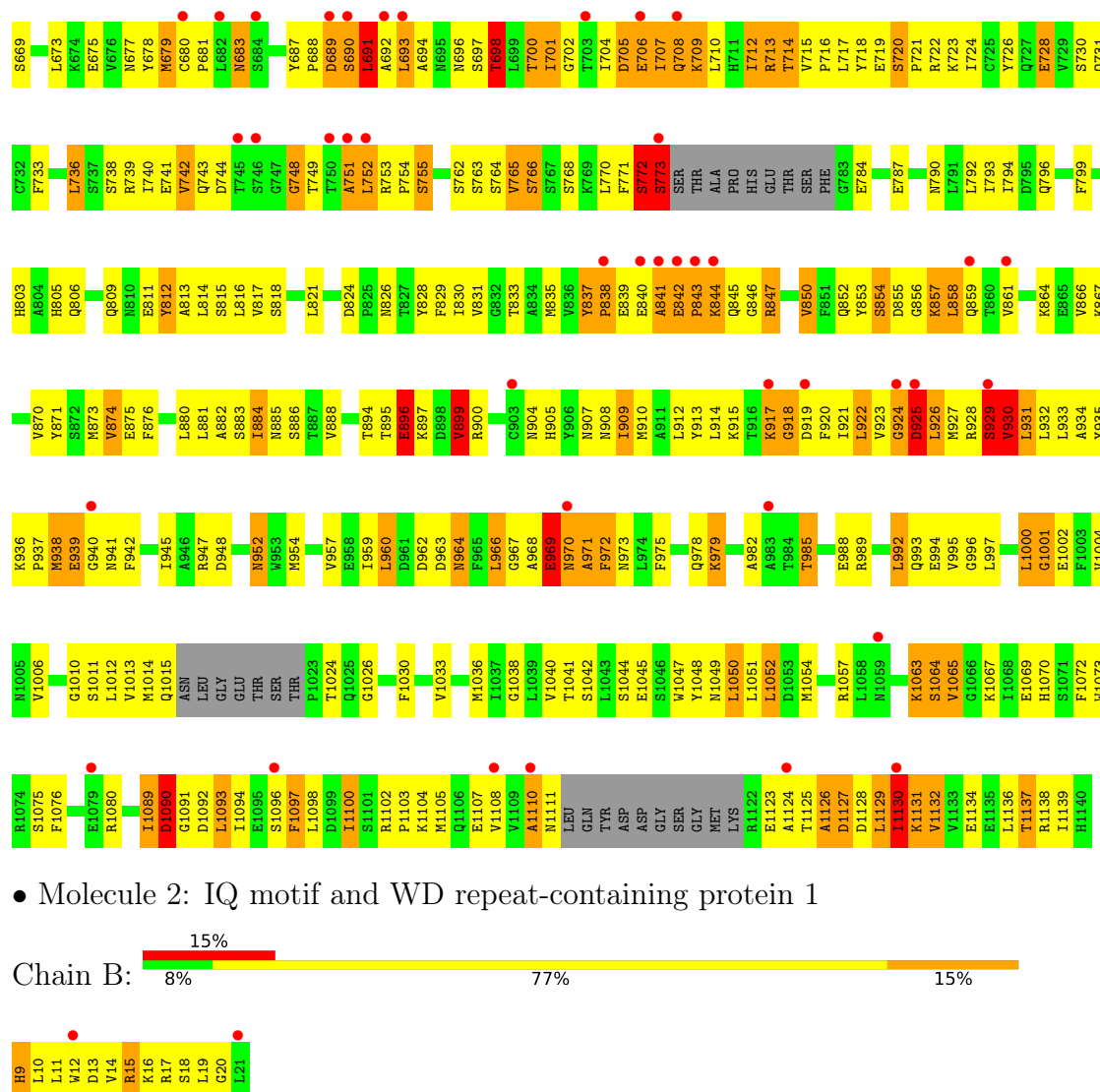
| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2   | B     | 13       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 112   | 73 | 23 | 16 |         |         |       |

### 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 damage-binding protein 1





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 63.76Å 131.94Å 181.27Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 44.46 – 2.80<br>44.46 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 83.3 (44.46-2.80)<br>83.3 (44.46-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.54 (at 2.65Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.256 , 0.320<br>0.265 , 0.322                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1714 reflections (3.75%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 64.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.278                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 56.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 8838                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 83.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

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     | 1.02         | 13/8885 (0.1%) | 1.27        | 73/12034 (0.6%) |
| 2   | B     | 1.89         | 0/114          | 2.04        | 1/152 (0.7%)    |
| All | All   | 1.04         | 13/8999 (0.1%) | 1.28        | 74/12186 (0.6%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 2   | B     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 773 | SER  | C-O   | 29.35 | 1.82        | 1.23     |
| 1   | A     | 899 | VAL  | CA-CB | 9.49  | 1.64        | 1.53     |
| 1   | A     | 925 | ASP  | N-CA  | 6.86  | 1.55        | 1.46     |
| 1   | A     | 924 | GLY  | N-CA  | 6.77  | 1.52        | 1.45     |
| 1   | A     | 928 | ARG  | CA-C  | -6.60 | 1.43        | 1.53     |
| 1   | A     | 970 | ASN  | CA-C  | -6.39 | 1.44        | 1.52     |
| 1   | A     | 971 | ALA  | CA-CB | -6.12 | 1.43        | 1.53     |
| 1   | A     | 720 | SER  | C-O   | -5.79 | 1.17        | 1.24     |
| 1   | A     | 812 | TYR  | CA-C  | -5.57 | 1.45        | 1.52     |
| 1   | A     | 19  | VAL  | CA-CB | 5.41  | 1.61        | 1.55     |
| 1   | A     | 81  | THR  | CA-CB | -5.31 | 1.44        | 1.53     |
| 1   | A     | 969 | GLU  | C-O   | -5.30 | 1.17        | 1.24     |
| 1   | A     | 850 | VAL  | CA-CB | -5.04 | 1.47        | 1.53     |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | A     | 413  | LEU  | N-CA-CB | -18.80 | 79.85       | 109.94   |
| 1   | A     | 29   | LEU  | N-CA-CB | -18.33 | 80.92       | 109.88   |
| 1   | A     | 413  | LEU  | N-CA-C  | 17.12  | 135.20      | 108.67   |
| 1   | A     | 514  | ARG  | N-CA-C  | -16.34 | 94.16       | 114.75   |
| 1   | A     | 561  | TRP  | N-CA-C  | 15.36  | 132.03      | 113.28   |
| 1   | A     | 412  | PRO  | N-CA-C  | 12.67  | 129.58      | 112.48   |
| 1   | A     | 930  | VAL  | N-CA-C  | 12.55  | 135.44      | 109.34   |
| 1   | A     | 971  | ALA  | N-CA-C  | -10.43 | 100.03      | 113.17   |
| 1   | A     | 29   | LEU  | N-CA-C  | 10.10  | 124.79      | 108.63   |
| 1   | A     | 714  | THR  | N-CA-C  | 9.83   | 125.52      | 108.02   |
| 1   | A     | 773  | SER  | CA-C-O  | -9.24  | 105.09      | 120.80   |
| 1   | A     | 929  | SER  | N-CA-C  | 8.54   | 128.99      | 110.80   |
| 1   | A     | 514  | ARG  | N-CA-CB | -8.40  | 98.88       | 111.15   |
| 1   | A     | 207  | TRP  | N-CA-C  | 8.24   | 123.08      | 109.06   |
| 1   | A     | 924  | GLY  | N-CA-C  | 8.16   | 122.66      | 110.75   |
| 1   | A     | 938  | MET  | N-CA-C  | -8.06  | 93.62       | 110.80   |
| 1   | A     | 35   | LYS  | CA-C-N  | -7.71  | 111.00      | 122.56   |
| 1   | A     | 35   | LYS  | C-N-CA  | -7.71  | 111.00      | 122.56   |
| 1   | A     | 130  | MET  | N-CA-C  | 7.42   | 118.39      | 108.38   |
| 1   | A     | 108  | VAL  | N-CA-C  | 7.03   | 118.90      | 112.29   |
| 1   | A     | 969  | GLU  | CA-C-N  | -6.95  | 110.40      | 121.44   |
| 1   | A     | 969  | GLU  | C-N-CA  | -6.95  | 110.40      | 121.44   |
| 1   | A     | 374  | GLN  | N-CA-C  | -6.88  | 99.10       | 110.17   |
| 1   | A     | 409  | GLY  | N-CA-C  | -6.77  | 102.64      | 111.37   |
| 1   | A     | 416  | ASP  | CA-C-N  | 6.64   | 128.15      | 119.84   |
| 1   | A     | 416  | ASP  | C-N-CA  | 6.64   | 128.15      | 119.84   |
| 1   | A     | 837  | TYR  | CA-C-N  | 6.59   | 128.08      | 119.84   |
| 1   | A     | 837  | TYR  | C-N-CA  | 6.59   | 128.08      | 119.84   |
| 1   | A     | 1110 | ALA  | N-CA-C  | -6.46  | 105.98      | 114.31   |
| 1   | A     | 792  | LEU  | CA-C-N  | -6.43  | 114.67      | 122.90   |
| 1   | A     | 792  | LEU  | C-N-CA  | -6.43  | 114.67      | 122.90   |
| 1   | A     | 357  | GLY  | CA-C-N  | -6.39  | 112.37      | 120.23   |
| 1   | A     | 357  | GLY  | C-N-CA  | -6.39  | 112.37      | 120.23   |
| 1   | A     | 691  | LEU  | CA-C-N  | -6.33  | 112.37      | 121.42   |
| 1   | A     | 691  | LEU  | C-N-CA  | -6.33  | 112.37      | 121.42   |
| 1   | A     | 194  | GLU  | N-CA-C  | -6.31  | 101.60      | 110.50   |
| 2   | B     | 16   | LYS  | N-CA-C  | -6.31  | 104.40      | 111.28   |
| 1   | A     | 23   | PHE  | N-CA-C  | -6.26  | 106.28      | 114.04   |
| 1   | A     | 690  | SER  | N-CA-C  | -6.24  | 99.25       | 108.79   |
| 1   | A     | 847  | ARG  | N-CA-C  | 6.14   | 118.51      | 109.24   |
| 1   | A     | 36   | ASN  | N-CA-C  | -6.04  | 103.86      | 112.13   |
| 1   | A     | 213  | GLU  | N-CA-C  | 6.00   | 119.35      | 110.48   |
| 1   | A     | 50   | ARG  | CA-C-N  | 5.99   | 125.92      | 119.76   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 50   | ARG  | C-N-CA  | 5.99  | 125.92      | 119.76   |
| 1   | A     | 1128 | ASP  | N-CA-C  | -5.94 | 105.14      | 112.38   |
| 1   | A     | 773  | SER  | N-CA-C  | -5.89 | 94.50       | 111.00   |
| 1   | A     | 612  | PHE  | N-CA-C  | -5.86 | 99.10       | 109.06   |
| 1   | A     | 712  | ILE  | N-CA-C  | 5.83  | 116.40      | 107.77   |
| 1   | A     | 513  | GLY  | N-CA-C  | 5.74  | 126.79      | 113.18   |
| 1   | A     | 194  | GLU  | CA-C-N  | -5.72 | 115.49      | 123.10   |
| 1   | A     | 194  | GLU  | C-N-CA  | -5.72 | 115.49      | 123.10   |
| 1   | A     | 124  | ILE  | N-CA-C  | 5.68  | 116.46      | 108.17   |
| 1   | A     | 236  | SER  | N-CA-C  | 5.66  | 117.13      | 108.42   |
| 1   | A     | 968  | ALA  | CA-C-N  | -5.64 | 110.77      | 121.54   |
| 1   | A     | 968  | ALA  | C-N-CA  | -5.64 | 110.77      | 121.54   |
| 1   | A     | 899  | VAL  | N-CA-CB | 5.64  | 117.93      | 111.39   |
| 1   | A     | 222  | VAL  | CA-C-N  | 5.61  | 125.93      | 119.92   |
| 1   | A     | 222  | VAL  | C-N-CA  | 5.61  | 125.93      | 119.92   |
| 1   | A     | 736  | LEU  | N-CA-C  | -5.58 | 101.39      | 110.20   |
| 1   | A     | 42   | TYR  | CA-C-N  | -5.54 | 115.95      | 122.93   |
| 1   | A     | 42   | TYR  | C-N-CA  | -5.54 | 115.95      | 122.93   |
| 1   | A     | 1090 | ASP  | N-CA-CB | 5.51  | 118.75      | 109.94   |
| 1   | A     | 258  | ILE  | N-CA-C  | -5.31 | 104.21      | 110.21   |
| 1   | A     | 952  | ASN  | N-CA-C  | 5.29  | 116.77      | 109.15   |
| 1   | A     | 964  | ASN  | N-CA-C  | 5.20  | 117.23      | 108.96   |
| 1   | A     | 125  | ASP  | CA-C-N  | 5.16  | 126.29      | 119.84   |
| 1   | A     | 125  | ASP  | C-N-CA  | 5.16  | 126.29      | 119.84   |
| 1   | A     | 740  | ILE  | N-CA-C  | -5.12 | 101.01      | 108.99   |
| 1   | A     | 556  | CYS  | N-CA-C  | 5.11  | 116.61      | 108.79   |
| 1   | A     | 562  | THR  | CA-C-O  | 5.04  | 125.36      | 119.06   |
| 1   | A     | 184  | ASP  | CA-C-N  | -5.02 | 114.26      | 120.79   |
| 1   | A     | 184  | ASP  | C-N-CA  | -5.02 | 114.26      | 120.79   |
| 1   | A     | 317  | LEU  | CB-CA-C | -5.01 | 109.17      | 116.53   |
| 1   | A     | 1001 | GLY  | N-CA-C  | -5.00 | 108.17      | 115.63   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 194 | GLU  | Mainchain |
| 2   | B     | 20  | GLY  | Peptide   |

## 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     | 8726  | 0        | 8706     | 863     | 0            |
| 2   | B     | 112   | 0        | 120      | 44      | 0            |
| All | All   | 8838  | 0        | 8826     | 869     | 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 49.

All (869) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:365:VAL:HA   | 1:A:366:ASP:CB    | 1.46                     | 1.38              |
| 1:A:365:VAL:CA   | 1:A:366:ASP:HB2   | 1.54                     | 1.35              |
| 1:A:660:TYR:CE1  | 1:A:707:ILE:HG21  | 1.66                     | 1.30              |
| 1:A:660:TYR:HB3  | 1:A:667:VAL:CB    | 1.66                     | 1.25              |
| 1:A:773:SER:O    | 1:A:773:SER:C     | 1.82                     | 1.21              |
| 1:A:660:TYR:CB   | 1:A:667:VAL:HB    | 1.74                     | 1.17              |
| 1:A:365:VAL:CG1  | 1:A:367:LEU:HG    | 1.73                     | 1.17              |
| 1:A:613:TYR:HD1  | 1:A:614:PHE:N     | 1.44                     | 1.16              |
| 1:A:1024:THR:HB  | 1:A:1041:THR:HG21 | 1.20                     | 1.15              |
| 1:A:368:GLU:HG3  | 1:A:370:GLN:NE2   | 1.60                     | 1.15              |
| 1:A:493:PRO:O    | 1:A:494:GLN:HG2   | 1.45                     | 1.15              |
| 1:A:929:SER:CB   | 1:A:952:ASN:HB2   | 1.73                     | 1.15              |
| 1:A:660:TYR:CD1  | 1:A:707:ILE:HG21  | 1.81                     | 1.14              |
| 1:A:660:TYR:CD1  | 1:A:707:ILE:HG12  | 1.83                     | 1.14              |
| 1:A:707:ILE:HG23 | 1:A:708:GLN:H     | 0.99                     | 1.11              |
| 1:A:288:GLU:OE1  | 1:A:298:LYS:HB2   | 1.51                     | 1.10              |
| 1:A:587:ILE:HD13 | 1:A:587:ILE:H     | 1.13                     | 1.09              |
| 1:A:365:VAL:HG13 | 1:A:366:ASP:C     | 1.77                     | 1.09              |
| 1:A:365:VAL:HG11 | 1:A:367:LEU:CD2   | 1.81                     | 1.09              |
| 1:A:812:TYR:HD1  | 2:B:15:ARG:NH2    | 1.51                     | 1.08              |
| 1:A:197:LEU:H    | 1:A:197:LEU:CD2   | 1.62                     | 1.07              |
| 1:A:368:GLU:HG2  | 1:A:370:GLN:HG3   | 1.09                     | 1.07              |
| 1:A:368:GLU:HG2  | 1:A:370:GLN:CG    | 1.85                     | 1.06              |
| 1:A:812:TYR:CE1  | 2:B:15:ARG:NH1    | 2.24                     | 1.04              |
| 1:A:659:ILE:O    | 1:A:659:ILE:HG22  | 1.56                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:969:GLU:HG2  | 1:A:970:ASN:N    | 1.72                     | 1.04              |
| 1:A:365:VAL:HG11 | 1:A:367:LEU:HG   | 1.39                     | 1.03              |
| 1:A:365:VAL:CG1  | 1:A:366:ASP:C    | 2.32                     | 1.02              |
| 1:A:365:VAL:HG11 | 1:A:367:LEU:CG   | 1.89                     | 1.02              |
| 1:A:197:LEU:H    | 1:A:197:LEU:HD23 | 0.87                     | 1.02              |
| 1:A:969:GLU:CG   | 1:A:970:ASN:H    | 1.72                     | 1.02              |
| 1:A:626:ARG:O    | 1:A:627:LYS:HG3  | 1.59                     | 1.01              |
| 1:A:639:ARG:HG3  | 1:A:640:THR:H    | 1.25                     | 1.01              |
| 1:A:707:ILE:HG23 | 1:A:708:GLN:N    | 1.72                     | 1.01              |
| 1:A:98:ILE:HD13  | 1:A:98:ILE:H     | 1.17                     | 1.01              |
| 1:A:482:GLU:HB2  | 1:A:483:PRO:HD3  | 1.40                     | 1.01              |
| 1:A:2:SER:HB3    | 1:A:995:VAL:HG23 | 1.44                     | 1.00              |
| 1:A:197:LEU:HD23 | 1:A:197:LEU:N    | 1.72                     | 1.00              |
| 1:A:929:SER:HB3  | 1:A:952:ASN:HB2  | 1.38                     | 1.00              |
| 1:A:660:TYR:CG   | 1:A:707:ILE:HG12 | 1.97                     | 0.99              |
| 1:A:256:SER:HB3  | 1:A:275:ASP:OD2  | 1.62                     | 0.99              |
| 1:A:929:SER:OG   | 1:A:952:ASN:HB2  | 1.60                     | 0.99              |
| 1:A:660:TYR:HD2  | 1:A:667:VAL:HG23 | 1.25                     | 0.98              |
| 1:A:910:MET:SD   | 2:B:10:LEU:HD12  | 2.03                     | 0.98              |
| 1:A:382:PHE:H    | 1:A:720:SER:HB3  | 1.24                     | 0.98              |
| 1:A:969:GLU:CD   | 1:A:970:ASN:H    | 1.72                     | 0.98              |
| 1:A:613:TYR:CD1  | 1:A:613:TYR:C    | 2.37                     | 0.97              |
| 1:A:641:PHE:HA   | 1:A:681:PRO:HG3  | 1.42                     | 0.97              |
| 1:A:707:ILE:CG2  | 1:A:708:GLN:H    | 1.76                     | 0.97              |
| 1:A:175:ALA:HB3  | 1:A:194:GLU:HG2  | 1.43                     | 0.96              |
| 1:A:632:GLY:HA3  | 1:A:653:SER:HB3  | 1.46                     | 0.95              |
| 1:A:660:TYR:HB3  | 1:A:667:VAL:HB   | 0.97                     | 0.95              |
| 1:A:103:ARG:HH11 | 1:A:103:ARG:HB3  | 1.29                     | 0.95              |
| 1:A:365:VAL:HG12 | 1:A:367:LEU:HG   | 1.46                     | 0.94              |
| 1:A:613:TYR:HD1  | 1:A:613:TYR:C    | 1.73                     | 0.94              |
| 1:A:289:GLU:HG2  | 1:A:290:GLN:H    | 1.32                     | 0.93              |
| 1:A:396:ILE:HD13 | 1:A:396:ILE:O    | 1.68                     | 0.93              |
| 1:A:969:GLU:CG   | 1:A:970:ASN:N    | 2.30                     | 0.93              |
| 1:A:613:TYR:CD1  | 1:A:614:PHE:N    | 2.36                     | 0.93              |
| 1:A:614:PHE:CE2  | 1:A:625:ASP:O    | 2.22                     | 0.93              |
| 1:A:838:PRO:HA   | 2:B:9:HIS:HE2    | 1.31                     | 0.93              |
| 1:A:25:SER:HB2   | 1:A:28:ASP:OD1   | 1.68                     | 0.92              |
| 1:A:587:ILE:H    | 1:A:587:ILE:CD1  | 1.81                     | 0.92              |
| 1:A:632:GLY:HA3  | 1:A:653:SER:CB   | 1.99                     | 0.92              |
| 1:A:660:TYR:HB2  | 1:A:707:ILE:HG12 | 1.50                     | 0.91              |
| 1:A:396:ILE:HD11 | 1:A:673:LEU:HD21 | 1.52                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:840:GLU:O    | 2:B:9:HIS:CE1    | 2.23                     | 0.91              |
| 1:A:1024:THR:HB  | 1:A:1041:THR:CG2 | 2.00                     | 0.90              |
| 1:A:614:PHE:HE2  | 1:A:625:ASP:O    | 1.53                     | 0.89              |
| 1:A:713:ARG:CG   | 1:A:713:ARG:HH11 | 1.82                     | 0.89              |
| 1:A:660:TYR:CD2  | 1:A:667:VAL:CG2  | 2.55                     | 0.89              |
| 1:A:660:TYR:HB2  | 1:A:707:ILE:CG1  | 2.02                     | 0.89              |
| 1:A:876:PHE:HZ   | 1:A:920:PHE:HA   | 1.35                     | 0.89              |
| 1:A:571:LEU:HB3  | 1:A:572:PRO:HD3  | 1.55                     | 0.89              |
| 1:A:660:TYR:CD2  | 1:A:667:VAL:HG23 | 2.07                     | 0.88              |
| 1:A:400:ALA:H    | 1:A:701:ILE:HD11 | 1.38                     | 0.88              |
| 1:A:690:SER:C    | 1:A:691:LEU:HD23 | 1.99                     | 0.88              |
| 1:A:876:PHE:CZ   | 1:A:920:PHE:HA   | 2.09                     | 0.87              |
| 1:A:382:PHE:N    | 1:A:720:SER:HB3  | 1.90                     | 0.87              |
| 1:A:513:GLY:O    | 1:A:537:GLU:HA   | 1.74                     | 0.87              |
| 1:A:617:ASN:HB2  | 1:A:621:GLY:H    | 1.38                     | 0.87              |
| 1:A:626:ARG:O    | 1:A:627:LYS:CG   | 2.22                     | 0.87              |
| 1:A:309:SER:H    | 1:A:332:GLN:HE22 | 1.23                     | 0.87              |
| 1:A:660:TYR:HB3  | 1:A:667:VAL:CG2  | 2.05                     | 0.87              |
| 1:A:812:TYR:HE1  | 2:B:15:ARG:NH1   | 1.71                     | 0.87              |
| 1:A:288:GLU:OE1  | 1:A:298:LYS:CB   | 2.23                     | 0.86              |
| 1:A:660:TYR:CB   | 1:A:707:ILE:HG12 | 2.05                     | 0.86              |
| 1:A:644:LEU:HG   | 1:A:645:SER:H    | 1.39                     | 0.86              |
| 1:A:844:LYS:HE2  | 1:A:845:GLN:HG2  | 1.55                     | 0.86              |
| 1:A:929:SER:HB3  | 1:A:952:ASN:CB   | 2.05                     | 0.86              |
| 1:A:469:ILE:HD11 | 1:A:471:ILE:HG13 | 1.54                     | 0.86              |
| 1:A:289:GLU:HG2  | 1:A:290:GLN:N    | 1.90                     | 0.86              |
| 1:A:812:TYR:HD1  | 2:B:15:ARG:HH22  | 0.86                     | 0.85              |
| 1:A:365:VAL:CG1  | 1:A:367:LEU:CG   | 2.50                     | 0.85              |
| 1:A:368:GLU:CG   | 1:A:370:GLN:NE2  | 2.39                     | 0.84              |
| 1:A:267:ASN:HD21 | 1:A:269:SER:HB3  | 1.42                     | 0.84              |
| 1:A:365:VAL:HG13 | 1:A:366:ASP:O    | 1.76                     | 0.84              |
| 1:A:98:ILE:H     | 1:A:98:ILE:CD1   | 1.91                     | 0.84              |
| 1:A:771:PHE:O    | 1:A:772:SER:HB2  | 1.78                     | 0.84              |
| 1:A:969:GLU:HG2  | 1:A:970:ASN:H    | 1.31                     | 0.84              |
| 1:A:368:GLU:HG3  | 1:A:370:GLN:HE21 | 1.40                     | 0.83              |
| 1:A:655:ARG:HG3  | 1:A:655:ARG:HH11 | 1.43                     | 0.83              |
| 1:A:414:ARG:HA   | 1:A:422:TYR:HA   | 1.60                     | 0.83              |
| 1:A:309:SER:H    | 1:A:332:GLN:NE2  | 1.77                     | 0.83              |
| 1:A:660:TYR:CD1  | 1:A:707:ILE:CG2  | 2.62                     | 0.83              |
| 1:A:364:VAL:HG21 | 1:A:1010:GLY:HA3 | 1.61                     | 0.82              |
| 1:A:365:VAL:HA   | 1:A:366:ASP:CG   | 2.04                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:744:ASP:N    | 1:A:748:GLY:O    | 2.12                     | 0.82              |
| 1:A:841:ALA:HA   | 2:B:9:HIS:ND1    | 1.95                     | 0.82              |
| 1:A:883:SER:C    | 1:A:884:ILE:HD12 | 2.05                     | 0.82              |
| 1:A:714:THR:O    | 1:A:716:PRO:HD3  | 1.81                     | 0.81              |
| 1:A:1063:LYS:H   | 1:A:1063:LYS:HD3 | 1.45                     | 0.80              |
| 1:A:660:TYR:HD2  | 1:A:667:VAL:CG2  | 1.94                     | 0.80              |
| 1:A:884:ILE:HD12 | 1:A:884:ILE:N    | 1.97                     | 0.80              |
| 1:A:938:MET:HG2  | 1:A:939:GLU:H    | 1.46                     | 0.80              |
| 1:A:493:PRO:O    | 1:A:494:GLN:CG   | 2.30                     | 0.79              |
| 1:A:484:LYS:O    | 1:A:484:LYS:HG3  | 1.79                     | 0.79              |
| 1:A:660:TYR:CD1  | 1:A:707:ILE:CG1  | 2.65                     | 0.79              |
| 1:A:396:ILE:CD1  | 1:A:673:LEU:HD21 | 2.12                     | 0.79              |
| 1:A:742:VAL:O    | 1:A:749:THR:HA   | 1.81                     | 0.79              |
| 1:A:639:ARG:HG3  | 1:A:640:THR:N    | 1.99                     | 0.78              |
| 1:A:579:LYS:NZ   | 1:A:581:MET:SD   | 2.56                     | 0.78              |
| 1:A:23:PHE:H     | 1:A:30:ASN:ND2   | 1.82                     | 0.77              |
| 1:A:838:PRO:HA   | 2:B:9:HIS:NE2    | 1.99                     | 0.77              |
| 1:A:289:GLU:CG   | 1:A:290:GLN:H    | 1.97                     | 0.77              |
| 1:A:812:TYR:CD1  | 2:B:15:ARG:NH2   | 2.42                     | 0.77              |
| 1:A:1044:SER:HG  | 1:A:1047:TRP:CD1 | 2.03                     | 0.77              |
| 1:A:854:SER:HB2  | 1:A:857:LYS:HG3  | 1.66                     | 0.77              |
| 1:A:69:PRO:HD2   | 1:A:72:GLU:HG3   | 1.65                     | 0.77              |
| 1:A:192:THR:HB   | 1:A:205:GLY:HA3  | 1.67                     | 0.76              |
| 1:A:364:VAL:HG12 | 1:A:365:VAL:N    | 1.98                     | 0.76              |
| 1:A:883:SER:HB3  | 1:A:914:LEU:HD11 | 1.68                     | 0.76              |
| 1:A:365:VAL:HG12 | 1:A:367:LEU:N    | 2.01                     | 0.76              |
| 1:A:365:VAL:O    | 1:A:373:GLY:HA2  | 1.85                     | 0.76              |
| 1:A:570:LYS:NZ   | 1:A:572:PRO:HD2  | 2.00                     | 0.75              |
| 1:A:611:LEU:O    | 1:A:628:LYS:HA   | 1.85                     | 0.75              |
| 1:A:871:TYR:CE2  | 2:B:11:LEU:HD21  | 2.22                     | 0.75              |
| 1:A:365:VAL:HG12 | 1:A:366:ASP:C    | 2.09                     | 0.75              |
| 1:A:84:TYR:CE2   | 1:A:135:LEU:HD12 | 2.20                     | 0.75              |
| 1:A:587:ILE:HD13 | 1:A:587:ILE:N    | 1.97                     | 0.75              |
| 1:A:492:GLU:C    | 1:A:492:GLU:OE1  | 2.30                     | 0.74              |
| 1:A:267:ASN:ND2  | 1:A:269:SER:HB3  | 2.01                     | 0.74              |
| 1:A:365:VAL:CB   | 1:A:366:ASP:HB2  | 2.16                     | 0.74              |
| 1:A:27:GLU:C     | 1:A:28:ASP:OD1   | 2.30                     | 0.74              |
| 1:A:612:PHE:CE2  | 1:A:628:LYS:HB2  | 2.23                     | 0.74              |
| 1:A:660:TYR:CD2  | 1:A:667:VAL:HG21 | 2.22                     | 0.74              |
| 1:A:894:THR:HB   | 1:A:896:GLU:HG3  | 1.70                     | 0.74              |
| 1:A:853:TYR:HA   | 1:A:857:LYS:O    | 1.88                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1125:THR:HG22 | 1:A:1126:ALA:N    | 2.03                     | 0.73              |
| 1:A:55:VAL:HG11   | 1:A:100:ILE:HD12  | 1.70                     | 0.73              |
| 1:A:385:GLY:HA3   | 1:A:719:GLU:O     | 1.88                     | 0.73              |
| 1:A:469:ILE:CD1   | 1:A:471:ILE:HG13  | 2.17                     | 0.73              |
| 1:A:708:GLN:HG3   | 1:A:710:LEU:O     | 1.88                     | 0.73              |
| 1:A:98:ILE:HD13   | 1:A:98:ILE:N      | 1.99                     | 0.73              |
| 1:A:197:LEU:CD2   | 1:A:197:LEU:N     | 2.36                     | 0.73              |
| 1:A:480:SER:HB3   | 1:A:483:PRO:HD2   | 1.71                     | 0.73              |
| 1:A:610:ALA:CB    | 1:A:628:LYS:HD2   | 2.18                     | 0.73              |
| 1:A:658:VAL:HG12  | 1:A:659:ILE:N     | 2.03                     | 0.73              |
| 1:A:713:ARG:HH11  | 1:A:713:ARG:HG3   | 1.52                     | 0.72              |
| 1:A:923:VAL:HG13  | 1:A:923:VAL:O     | 1.89                     | 0.72              |
| 1:A:1044:SER:HG   | 1:A:1047:TRP:HD1  | 1.32                     | 0.72              |
| 1:A:886:SER:O     | 1:A:908:ASN:HB2   | 1.89                     | 0.72              |
| 1:A:288:GLU:OE1   | 1:A:298:LYS:CA    | 2.37                     | 0.72              |
| 1:A:482:GLU:HB2   | 1:A:483:PRO:CD    | 2.19                     | 0.72              |
| 2:B:9:HIS:N       | 2:B:9:HIS:CD2     | 2.56                     | 0.72              |
| 1:A:692:ALA:C     | 1:A:693:LEU:HD12  | 2.14                     | 0.72              |
| 1:A:932:LEU:C     | 1:A:933:LEU:HD12  | 2.14                     | 0.72              |
| 1:A:367:LEU:HD12  | 1:A:374:GLN:HG3   | 1.71                     | 0.72              |
| 1:A:722:ARG:HH12  | 2:B:15:ARG:CZ     | 2.02                     | 0.72              |
| 1:A:1024:THR:CB   | 1:A:1041:THR:HG21 | 2.11                     | 0.72              |
| 1:A:917:LYS:O     | 1:A:919:ASP:N     | 2.23                     | 0.72              |
| 1:A:1030:PHE:CZ   | 1:A:1038:GLY:HA3  | 2.25                     | 0.72              |
| 1:A:235:GLU:HB3   | 1:A:254:LYS:HG3   | 1.72                     | 0.72              |
| 1:A:602:LEU:HD23  | 1:A:614:PHE:HB2   | 1.72                     | 0.72              |
| 1:A:920:PHE:HB3   | 1:A:935:TYR:HB3   | 1.72                     | 0.71              |
| 1:A:1097:PHE:O    | 1:A:1100:ILE:HB   | 1.89                     | 0.71              |
| 1:A:929:SER:HB2   | 1:A:954:MET:SD    | 2.29                     | 0.71              |
| 1:A:117:GLU:O     | 1:A:118:THR:HB    | 1.88                     | 0.71              |
| 1:A:614:PHE:HE2   | 1:A:625:ASP:C     | 1.98                     | 0.71              |
| 1:A:504:ASN:HD21  | 1:A:507:GLN:HB3   | 1.56                     | 0.71              |
| 1:A:969:GLU:CD    | 1:A:970:ASN:N     | 2.48                     | 0.70              |
| 1:A:309:SER:N     | 1:A:332:GLN:HE22  | 1.89                     | 0.70              |
| 1:A:707:ILE:O     | 1:A:708:GLN:C     | 2.33                     | 0.70              |
| 1:A:469:ILE:HD11  | 1:A:471:ILE:CG1   | 2.22                     | 0.70              |
| 1:A:812:TYR:CD1   | 2:B:15:ARG:NH1    | 2.54                     | 0.70              |
| 1:A:854:SER:N     | 1:A:857:LYS:O     | 2.23                     | 0.70              |
| 1:A:175:ALA:CB    | 1:A:194:GLU:HG2   | 2.21                     | 0.70              |
| 1:A:374:GLN:OE1   | 1:A:391:ARG:HG3   | 1.92                     | 0.70              |
| 1:A:844:LYS:H     | 1:A:844:LYS:HD3   | 1.56                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:365:VAL:HA    | 1:A:366:ASP:HB2  | 0.75                     | 0.70              |
| 1:A:81:THR:HG23   | 1:A:82:ALA:N     | 2.06                     | 0.69              |
| 1:A:2:SER:CB      | 1:A:995:VAL:HG23 | 2.20                     | 0.69              |
| 1:A:368:GLU:CG    | 1:A:370:GLN:HG3  | 2.04                     | 0.69              |
| 1:A:287:LYS:O     | 1:A:288:GLU:HB2  | 1.92                     | 0.69              |
| 1:A:691:LEU:HD23  | 1:A:691:LEU:N    | 2.06                     | 0.69              |
| 1:A:256:SER:CB    | 1:A:277:GLU:HG2  | 2.23                     | 0.69              |
| 1:A:368:GLU:CG    | 1:A:370:GLN:CD   | 2.65                     | 0.69              |
| 1:A:871:TYR:CE2   | 2:B:11:LEU:CD2   | 2.75                     | 0.69              |
| 1:A:591:ILE:HD12  | 1:A:604:CYS:HB2  | 1.75                     | 0.69              |
| 1:A:920:PHE:O     | 1:A:934:ALA:HA   | 1.93                     | 0.69              |
| 1:A:701:ILE:N     | 1:A:701:ILE:HD13 | 2.07                     | 0.69              |
| 1:A:841:ALA:HA    | 2:B:9:HIS:HB3    | 1.75                     | 0.68              |
| 1:A:688:PRO:O     | 1:A:689:ASP:C    | 2.36                     | 0.68              |
| 1:A:844:LYS:HD3   | 1:A:844:LYS:N    | 2.08                     | 0.68              |
| 1:A:669:SER:OG    | 1:A:709:LYS:HA   | 1.94                     | 0.68              |
| 1:A:40:GLU:HG3    | 1:A:54:GLU:HG2   | 1.75                     | 0.68              |
| 1:A:103:ARG:HH11  | 1:A:103:ARG:CB   | 2.03                     | 0.68              |
| 1:A:202:PHE:O     | 1:A:203:ASN:HB2  | 1.94                     | 0.68              |
| 1:A:661:SER:HA    | 1:A:665:LYS:O    | 1.94                     | 0.68              |
| 1:A:68:ARG:NH1    | 1:A:73:SER:O     | 2.27                     | 0.67              |
| 1:A:391:ARG:NH2   | 1:A:705:ASP:OD2  | 2.27                     | 0.67              |
| 1:A:597:GLU:OE1   | 1:A:664:HIS:HA   | 1.95                     | 0.67              |
| 1:A:763:SER:C     | 1:A:803:HIS:HE1  | 2.01                     | 0.67              |
| 1:A:1000:LEU:HD13 | 1:A:1002:GLU:HB2 | 1.75                     | 0.67              |
| 1:A:679:MET:SD    | 1:A:679:MET:C    | 2.78                     | 0.67              |
| 1:A:693:LEU:HD12  | 1:A:693:LEU:N    | 2.10                     | 0.67              |
| 1:A:762:SER:O     | 1:A:763:SER:HB3  | 1.93                     | 0.67              |
| 1:A:630:THR:O     | 1:A:631:LEU:HD23 | 1.95                     | 0.66              |
| 1:A:626:ARG:C     | 1:A:627:LYS:HG3  | 2.19                     | 0.66              |
| 1:A:659:ILE:HA    | 1:A:667:VAL:O    | 1.94                     | 0.66              |
| 1:A:803:HIS:CD2   | 1:A:858:LEU:HB2  | 2.30                     | 0.66              |
| 1:A:971:ALA:O     | 1:A:972:PHE:HB2  | 1.95                     | 0.66              |
| 1:A:507:GLN:HE22  | 1:A:552:LEU:HG   | 1.60                     | 0.66              |
| 1:A:613:TYR:O     | 1:A:614:PHE:CD2  | 2.48                     | 0.66              |
| 1:A:641:PHE:HB3   | 1:A:679:MET:CE   | 2.26                     | 0.66              |
| 1:A:985:THR:HB    | 1:A:989:ARG:HE   | 1.61                     | 0.66              |
| 1:A:708:GLN:O     | 1:A:709:LYS:C    | 2.39                     | 0.66              |
| 1:A:365:VAL:HG11  | 1:A:367:LEU:HD23 | 1.74                     | 0.66              |
| 1:A:885:ASN:C     | 1:A:885:ASN:HD22 | 2.03                     | 0.66              |
| 1:A:289:GLU:CG    | 1:A:290:GLN:N    | 2.58                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1011:SER:OG   | 1:A:1013:VAL:HG22 | 1.96                     | 0.66              |
| 1:A:654:ASP:HA    | 1:A:675:GLU:HG3   | 1.76                     | 0.66              |
| 1:A:611:LEU:O     | 1:A:628:LYS:HG3   | 1.96                     | 0.65              |
| 1:A:571:LEU:HB3   | 1:A:572:PRO:CD    | 2.26                     | 0.65              |
| 1:A:98:ILE:CD1    | 1:A:98:ILE:N      | 2.58                     | 0.65              |
| 1:A:639:ARG:CG    | 1:A:640:THR:H     | 2.04                     | 0.65              |
| 1:A:1051:LEU:HD23 | 1:A:1054:MET:HE2  | 1.78                     | 0.65              |
| 1:A:610:ALA:HB1   | 1:A:628:LYS:HD2   | 1.78                     | 0.65              |
| 1:A:27:GLU:N      | 1:A:27:GLU:OE2    | 2.30                     | 0.65              |
| 1:A:969:GLU:OE2   | 1:A:970:ASN:N     | 2.30                     | 0.65              |
| 1:A:996:GLY:O     | 1:A:997:LEU:HD23  | 1.96                     | 0.65              |
| 1:A:118:THR:O     | 1:A:118:THR:CG2   | 2.45                     | 0.65              |
| 2:B:10:LEU:O      | 2:B:14:VAL:N      | 2.23                     | 0.65              |
| 1:A:342:GLU:C     | 1:A:344:GLY:H     | 2.06                     | 0.64              |
| 1:A:492:GLU:OE1   | 1:A:494:GLN:N     | 2.30                     | 0.64              |
| 1:A:455:GLN:HB3   | 1:A:472:THR:OG1   | 1.97                     | 0.64              |
| 1:A:1127:ASP:O    | 1:A:1130:ILE:HG22 | 1.98                     | 0.64              |
| 1:A:840:GLU:O     | 2:B:9:HIS:ND1     | 2.29                     | 0.64              |
| 1:A:660:TYR:CG    | 1:A:661:SER:N     | 2.62                     | 0.64              |
| 1:A:660:TYR:HD1   | 1:A:707:ILE:HG12  | 1.55                     | 0.64              |
| 1:A:482:GLU:CB    | 1:A:483:PRO:HD3   | 2.24                     | 0.64              |
| 1:A:726:TYR:CE2   | 1:A:728:GLU:HB2   | 2.33                     | 0.64              |
| 1:A:330:ASP:CG    | 1:A:388:ARG:HH22  | 2.05                     | 0.63              |
| 1:A:884:ILE:HG22  | 1:A:884:ILE:O     | 1.98                     | 0.63              |
| 1:A:969:GLU:OE2   | 1:A:971:ALA:N     | 2.24                     | 0.63              |
| 1:A:173:CYS:HB3   | 1:A:175:ALA:O     | 1.98                     | 0.63              |
| 1:A:642:ARG:NH2   | 1:A:683:ASN:HB2   | 2.14                     | 0.63              |
| 1:A:929:SER:CB    | 1:A:954:MET:SD    | 2.87                     | 0.63              |
| 1:A:143:ILE:HG12  | 1:A:154:ALA:HB2   | 1.80                     | 0.62              |
| 1:A:431:GLY:HA2   | 1:A:456:GLN:HB2   | 1.79                     | 0.62              |
| 1:A:1026:GLY:O    | 1:A:1041:THR:HG23 | 1.99                     | 0.62              |
| 1:A:364:VAL:CG1   | 1:A:365:VAL:N     | 2.61                     | 0.62              |
| 1:A:713:ARG:HH11  | 1:A:713:ARG:HG2   | 1.61                     | 0.62              |
| 1:A:659:ILE:O     | 1:A:659:ILE:CG2   | 2.30                     | 0.62              |
| 1:A:871:TYR:HE2   | 2:B:11:LEU:CD2    | 2.12                     | 0.62              |
| 1:A:368:GLU:HG2   | 1:A:370:GLN:CD    | 2.24                     | 0.62              |
| 1:A:368:GLU:CD    | 1:A:368:GLU:H     | 2.06                     | 0.62              |
| 1:A:118:THR:O     | 1:A:118:THR:HG22  | 1.99                     | 0.62              |
| 1:A:330:ASP:OD1   | 1:A:388:ARG:NH2   | 2.33                     | 0.62              |
| 1:A:356:LEU:HD21  | 1:A:712:ILE:HD13  | 1.82                     | 0.62              |
| 1:A:365:VAL:HG11  | 1:A:367:LEU:HD21  | 1.79                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:367:LEU:HB2  | 1:A:368:GLU:OE1  | 1.99                     | 0.62              |
| 1:A:573:SER:O    | 1:A:574:PHE:HB2  | 1.98                     | 0.62              |
| 1:A:936:LYS:C    | 1:A:938:MET:H    | 2.06                     | 0.62              |
| 1:A:105:HIS:HA   | 1:A:152:LEU:HD12 | 1.82                     | 0.62              |
| 1:A:658:VAL:CG1  | 1:A:659:ILE:N    | 2.62                     | 0.61              |
| 1:A:558:ILE:O    | 1:A:566:ALA:HA   | 2.00                     | 0.61              |
| 1:A:830:ILE:HD13 | 1:A:880:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:846:GLY:O    | 1:A:866:VAL:HG22 | 2.00                     | 0.61              |
| 1:A:364:VAL:HG12 | 1:A:365:VAL:H    | 1.65                     | 0.61              |
| 1:A:835:MET:HB2  | 1:A:845:GLN:HG3  | 1.83                     | 0.61              |
| 1:A:1076:PHE:C   | 1:A:1076:PHE:CD2 | 2.79                     | 0.61              |
| 1:A:615:GLY:H    | 1:A:624:SER:CB   | 2.14                     | 0.61              |
| 1:A:691:LEU:O    | 1:A:693:LEU:CD1  | 2.49                     | 0.61              |
| 1:A:731:GLN:HA   | 1:A:796:GLN:NE2  | 2.15                     | 0.61              |
| 1:A:634:GLN:O    | 1:A:635:PRO:C    | 2.42                     | 0.61              |
| 1:A:818:SER:HA   | 1:A:828:TYR:O    | 2.01                     | 0.61              |
| 1:A:361:ASP:OD1  | 1:A:723:LYS:HD2  | 2.00                     | 0.61              |
| 1:A:400:ALA:N    | 1:A:701:ILE:HD11 | 2.14                     | 0.61              |
| 1:A:938:MET:C    | 1:A:940:GLY:H    | 2.08                     | 0.61              |
| 1:A:1044:SER:OG  | 1:A:1047:TRP:HD1 | 1.83                     | 0.61              |
| 1:A:1100:ILE:O   | 1:A:1105:MET:CE  | 2.49                     | 0.61              |
| 1:A:476:VAL:HG13 | 1:A:490:TRP:HB3  | 1.82                     | 0.61              |
| 1:A:923:VAL:HA   | 1:A:931:LEU:O    | 2.00                     | 0.61              |
| 1:A:591:ILE:HD12 | 1:A:604:CYS:CB   | 2.30                     | 0.61              |
| 1:A:134:ARG:HD2  | 1:A:134:ARG:C    | 2.25                     | 0.60              |
| 1:A:884:ILE:N    | 1:A:884:ILE:CD1  | 2.64                     | 0.60              |
| 1:A:122:GLY:O    | 1:A:123:ILE:HG23 | 2.01                     | 0.60              |
| 1:A:368:GLU:CG   | 1:A:370:GLN:CG   | 2.70                     | 0.60              |
| 1:A:314:LEU:HD11 | 1:A:324:VAL:HG22 | 1.83                     | 0.60              |
| 1:A:929:SER:CB   | 1:A:952:ASN:CB   | 2.62                     | 0.60              |
| 1:A:971:ALA:O    | 1:A:972:PHE:CB   | 2.48                     | 0.60              |
| 1:A:364:VAL:O    | 1:A:365:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:368:GLU:OE1  | 1:A:368:GLU:N    | 2.30                     | 0.60              |
| 1:A:458:PHE:CE2  | 1:A:473:SER:HA   | 2.36                     | 0.60              |
| 1:A:812:TYR:O    | 1:A:833:THR:HA   | 2.01                     | 0.60              |
| 1:A:250:PRO:HB2  | 1:A:252:ILE:HG22 | 1.83                     | 0.60              |
| 1:A:416:ASP:HB3  | 1:A:419:ARG:HG2  | 1.82                     | 0.60              |
| 1:A:718:TYR:HB2  | 1:A:755:SER:HA   | 1.82                     | 0.60              |
| 1:A:812:TYR:CD1  | 2:B:15:ARG:CZ    | 2.85                     | 0.60              |
| 1:A:844:LYS:H    | 1:A:844:LYS:CD   | 2.14                     | 0.60              |
| 1:A:372:GLN:H    | 1:A:372:GLN:HE21 | 1.50                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:909:ILE:HG22 | 1:A:925:ASP:OD2  | 2.02                     | 0.60              |
| 1:A:546:LEU:HD11 | 1:A:593:MET:SD   | 2.42                     | 0.60              |
| 1:A:614:PHE:CE2  | 1:A:626:ARG:HA   | 2.36                     | 0.60              |
| 1:A:644:LEU:CG   | 1:A:645:SER:H    | 2.13                     | 0.60              |
| 1:A:917:LYS:NZ   | 1:A:917:LYS:HB3  | 2.17                     | 0.60              |
| 1:A:412:PRO:O    | 1:A:422:TYR:CD2  | 2.55                     | 0.59              |
| 1:A:707:ILE:O    | 1:A:708:GLN:O    | 2.20                     | 0.59              |
| 1:A:81:THR:CG2   | 1:A:83:LYS:H     | 2.15                     | 0.59              |
| 1:A:313:CYS:HB3  | 1:A:325:GLY:HA3  | 1.84                     | 0.59              |
| 1:A:701:ILE:HD13 | 1:A:701:ILE:H    | 1.68                     | 0.59              |
| 1:A:925:ASP:OD2  | 1:A:926:LEU:N    | 2.36                     | 0.59              |
| 1:A:1123:GLU:HG2 | 1:A:1124:ALA:H   | 1.66                     | 0.59              |
| 1:A:364:VAL:CG1  | 1:A:365:VAL:H    | 2.15                     | 0.59              |
| 1:A:389:ILE:HD12 | 1:A:389:ILE:N    | 2.18                     | 0.59              |
| 1:A:23:PHE:H     | 1:A:30:ASN:HD22  | 1.51                     | 0.59              |
| 1:A:81:THR:CG2   | 1:A:82:ALA:N     | 2.60                     | 0.59              |
| 1:A:715:VAL:HG21 | 1:A:799:PHE:HB3  | 1.84                     | 0.59              |
| 1:A:570:LYS:HZ1  | 1:A:572:PRO:HD2  | 1.65                     | 0.58              |
| 1:A:885:ASN:O    | 1:A:886:SER:HB3  | 2.02                     | 0.58              |
| 1:A:642:ARG:HH21 | 1:A:683:ASN:HB2  | 1.67                     | 0.58              |
| 1:A:161:GLU:CD   | 1:A:191:LYS:HZ3  | 2.10                     | 0.58              |
| 1:A:241:ASN:O    | 1:A:242:GLY:C    | 2.46                     | 0.58              |
| 1:A:662:SER:HB3  | 1:A:665:LYS:HB2  | 1.84                     | 0.58              |
| 1:A:751:ALA:O    | 1:A:752:LEU:C    | 2.44                     | 0.58              |
| 1:A:452:VAL:HG13 | 1:A:477:ARG:NH1  | 2.18                     | 0.58              |
| 1:A:488:SER:O    | 1:A:489:GLU:HB3  | 2.03                     | 0.58              |
| 1:A:108:VAL:O    | 1:A:141:LYS:NZ   | 2.35                     | 0.58              |
| 1:A:314:LEU:CD1  | 1:A:324:VAL:HG22 | 2.34                     | 0.58              |
| 1:A:614:PHE:CE2  | 1:A:625:ASP:C    | 2.78                     | 0.58              |
| 1:A:368:GLU:O    | 1:A:369:ARG:C    | 2.46                     | 0.58              |
| 1:A:122:GLY:HA2  | 1:A:133:LEU:HD12 | 1.85                     | 0.58              |
| 1:A:288:GLU:CD   | 1:A:298:LYS:HB2  | 2.29                     | 0.58              |
| 1:A:364:VAL:O    | 1:A:365:VAL:CG2  | 2.52                     | 0.58              |
| 1:A:458:PHE:HE2  | 1:A:473:SER:HA   | 1.66                     | 0.58              |
| 1:A:571:LEU:CB   | 1:A:572:PRO:HD3  | 2.31                     | 0.58              |
| 1:A:692:ALA:HA   | 1:A:700:THR:O    | 2.04                     | 0.57              |
| 1:A:885:ASN:C    | 1:A:885:ASN:ND2  | 2.61                     | 0.57              |
| 1:A:1136:LEU:C   | 1:A:1138:ARG:N   | 2.60                     | 0.57              |
| 1:A:296:THR:OG1  | 1:A:297:LEU:N    | 2.37                     | 0.57              |
| 1:A:856:GLY:H    | 1:A:857:LYS:HG2  | 1.68                     | 0.57              |
| 1:A:905:HIS:HD2  | 1:A:908:ASN:ND2  | 2.03                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:84:TYR:HE2   | 1:A:135:LEU:HD12  | 1.63                     | 0.57              |
| 1:A:38:ARG:NH1   | 1:A:56:GLY:HA3    | 2.19                     | 0.57              |
| 1:A:614:PHE:HE2  | 1:A:626:ARG:HA    | 1.68                     | 0.57              |
| 1:A:641:PHE:HB3  | 1:A:679:MET:HE1   | 1.86                     | 0.57              |
| 1:A:167:VAL:HG13 | 1:A:180:PHE:HB3   | 1.85                     | 0.57              |
| 1:A:917:LYS:HB2  | 1:A:959:ILE:HG21  | 1.87                     | 0.57              |
| 1:A:68:ARG:NH1   | 1:A:74:LYS:HA     | 2.19                     | 0.57              |
| 1:A:480:SER:CB   | 1:A:483:PRO:HD2   | 2.33                     | 0.57              |
| 1:A:22:HIS:HB3   | 1:A:25:SER:O      | 2.03                     | 0.57              |
| 1:A:375:LEU:HB2  | 1:A:1012:LEU:HD21 | 1.86                     | 0.57              |
| 1:A:518:TYR:C    | 1:A:518:TYR:CD2   | 2.83                     | 0.57              |
| 1:A:185:PRO:O    | 1:A:186:GLN:HG3   | 2.04                     | 0.57              |
| 1:A:518:TYR:C    | 1:A:518:TYR:HD2   | 2.13                     | 0.57              |
| 1:A:265:ASP:OD2  | 1:A:270:ARG:HB2   | 2.05                     | 0.57              |
| 1:A:787:GLU:OE1  | 2:B:12:TRP:CZ3    | 2.58                     | 0.56              |
| 1:A:947:ARG:O    | 1:A:992:LEU:HD12  | 2.05                     | 0.56              |
| 1:A:1090:ASP:HB2 | 1:A:1092:ASP:HB2  | 1.87                     | 0.56              |
| 1:A:24:THR:H     | 1:A:30:ASN:ND2    | 2.03                     | 0.56              |
| 1:A:176:PRO:O    | 1:A:195:VAL:N     | 2.36                     | 0.56              |
| 1:A:787:GLU:HG3  | 2:B:12:TRP:HH2    | 1.69                     | 0.56              |
| 1:A:871:TYR:HE2  | 2:B:11:LEU:HD23   | 1.70                     | 0.56              |
| 1:A:11:LYS:HZ3   | 1:A:38:ARG:HE     | 1.54                     | 0.56              |
| 1:A:660:TYR:CE1  | 1:A:707:ILE:CG2   | 2.62                     | 0.56              |
| 1:A:693:LEU:N    | 1:A:700:THR:O     | 2.31                     | 0.56              |
| 1:A:1049:ASN:O   | 1:A:1050:LEU:C    | 2.47                     | 0.56              |
| 1:A:1136:LEU:O   | 1:A:1138:ARG:N    | 2.38                     | 0.56              |
| 1:A:549:SER:HB2  | 1:A:552:LEU:O     | 2.06                     | 0.56              |
| 1:A:365:VAL:CA   | 1:A:366:ASP:CB    | 2.30                     | 0.56              |
| 1:A:614:PHE:CD2  | 1:A:625:ASP:O     | 2.56                     | 0.56              |
| 1:A:812:TYR:N    | 1:A:812:TYR:HD2   | 2.04                     | 0.56              |
| 1:A:996:GLY:C    | 1:A:997:LEU:HD23  | 2.30                     | 0.56              |
| 1:A:194:GLU:O    | 1:A:202:PHE:O     | 2.23                     | 0.56              |
| 1:A:332:GLN:HB2  | 1:A:351:GLU:O     | 2.06                     | 0.56              |
| 1:A:600:HIS:CD2  | 1:A:618:ILE:HG12  | 2.40                     | 0.56              |
| 1:A:469:ILE:HD13 | 1:A:470:GLN:N     | 2.20                     | 0.55              |
| 1:A:736:LEU:HD13 | 1:A:813:ALA:HB1   | 1.88                     | 0.55              |
| 1:A:198:ARG:HG3  | 1:A:198:ARG:HH11  | 1.72                     | 0.55              |
| 1:A:365:VAL:CG1  | 1:A:366:ASP:CA    | 2.84                     | 0.55              |
| 1:A:938:MET:HG2  | 1:A:939:GLU:N     | 2.19                     | 0.55              |
| 1:A:964:ASN:OD1  | 1:A:978:GLN:NE2   | 2.40                     | 0.55              |
| 1:A:660:TYR:CD1  | 1:A:707:ILE:CB    | 2.90                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:763:SER:HA    | 1:A:803:HIS:CE1  | 2.42                     | 0.55              |
| 1:A:655:ARG:HH11  | 1:A:655:ARG:CG   | 2.16                     | 0.55              |
| 1:A:912:LEU:HB2   | 1:A:913:TYR:CE1  | 2.42                     | 0.55              |
| 1:A:38:ARG:HH11   | 1:A:56:GLY:HA3   | 1.71                     | 0.55              |
| 1:A:610:ALA:HB3   | 1:A:628:LYS:HD2  | 1.88                     | 0.55              |
| 1:A:812:TYR:N     | 1:A:812:TYR:CD2  | 2.73                     | 0.55              |
| 1:A:914:LEU:O     | 1:A:915:LYS:HG2  | 2.07                     | 0.55              |
| 1:A:364:VAL:C     | 1:A:365:VAL:HG23 | 2.32                     | 0.55              |
| 1:A:475:SER:HB2   | 1:A:490:TRP:O    | 2.06                     | 0.55              |
| 1:A:688:PRO:O     | 1:A:690:SER:HB3  | 2.06                     | 0.55              |
| 1:A:803:HIS:HD2   | 1:A:858:LEU:HG   | 1.71                     | 0.55              |
| 1:A:24:THR:H      | 1:A:30:ASN:HD21  | 1.55                     | 0.54              |
| 1:A:587:ILE:CD1   | 1:A:587:ILE:N    | 2.60                     | 0.54              |
| 1:A:424:THR:HA    | 1:A:436:LEU:O    | 2.07                     | 0.54              |
| 1:A:982:ALA:HB1   | 1:A:988:GLU:OE1  | 2.07                     | 0.54              |
| 1:A:610:ALA:HB1   | 1:A:628:LYS:CD   | 2.38                     | 0.54              |
| 1:A:632:GLY:HA3   | 1:A:653:SER:HB2  | 1.85                     | 0.54              |
| 1:A:793:ILE:HD12  | 1:A:829:PHE:HE2  | 1.73                     | 0.54              |
| 1:A:1102:ARG:N    | 1:A:1103:PRO:HD2 | 2.22                     | 0.54              |
| 1:A:365:VAL:CG1   | 1:A:367:LEU:CD2  | 2.70                     | 0.54              |
| 1:A:993:GLN:O     | 1:A:995:VAL:HG13 | 2.07                     | 0.54              |
| 1:A:1064:SER:O    | 1:A:1065:VAL:C   | 2.50                     | 0.54              |
| 1:A:971:ALA:O     | 1:A:972:PHE:CD1  | 2.60                     | 0.54              |
| 1:A:477:ARG:HA    | 1:A:489:GLU:HA   | 1.89                     | 0.54              |
| 1:A:909:ILE:HG12  | 1:A:927:MET:HE3  | 1.88                     | 0.54              |
| 1:A:256:SER:OG    | 1:A:277:GLU:HG2  | 2.06                     | 0.54              |
| 1:A:365:VAL:CG1   | 1:A:367:LEU:N    | 2.65                     | 0.54              |
| 1:A:517:TYR:O     | 1:A:518:TYR:HB2  | 2.07                     | 0.54              |
| 1:A:610:ALA:HB1   | 1:A:628:LYS:CG   | 2.38                     | 0.54              |
| 1:A:1033:VAL:HG22 | 2:B:18:SER:O     | 2.08                     | 0.54              |
| 1:A:1090:ASP:OD2  | 1:A:1090:ASP:N   | 2.38                     | 0.54              |
| 1:A:609:GLY:HA2   | 1:A:632:GLY:O    | 2.08                     | 0.53              |
| 1:A:630:THR:HG22  | 1:A:1134:GLU:OE2 | 2.07                     | 0.53              |
| 1:A:753:ARG:HB2   | 1:A:754:PRO:HD2  | 1.90                     | 0.53              |
| 1:A:793:ILE:HD12  | 1:A:829:PHE:CE2  | 2.43                     | 0.53              |
| 1:A:841:ALA:HA    | 2:B:9:HIS:CG     | 2.43                     | 0.53              |
| 1:A:184:ASP:OD1   | 1:A:186:GLN:HB2  | 2.08                     | 0.53              |
| 1:A:503:CYS:SG    | 1:A:504:ASN:N    | 2.81                     | 0.53              |
| 1:A:741:GLU:HB3   | 1:A:749:THR:HB   | 1.90                     | 0.53              |
| 1:A:1125:THR:HG22 | 1:A:1126:ALA:H   | 1.71                     | 0.53              |
| 1:A:400:ALA:HB2   | 1:A:687:TYR:OH   | 2.09                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:917:LYS:HE3  | 1:A:962:ASP:HA    | 1.90                     | 0.53              |
| 1:A:407:ILE:HG21 | 1:A:410:LEU:HD23  | 1.91                     | 0.53              |
| 1:A:84:TYR:CD2   | 1:A:135:LEU:HD12  | 2.43                     | 0.53              |
| 1:A:107:ASN:OD1  | 1:A:109:GLN:HG2   | 2.08                     | 0.53              |
| 1:A:256:SER:HB2  | 1:A:277:GLU:HG2   | 1.90                     | 0.53              |
| 1:A:365:VAL:HG13 | 1:A:366:ASP:CB    | 2.38                     | 0.53              |
| 1:A:365:VAL:O    | 1:A:374:GLN:N     | 2.37                     | 0.53              |
| 1:A:415:SER:HB2  | 1:A:423:ASP:OD2   | 2.08                     | 0.53              |
| 1:A:480:SER:HB2  | 1:A:484:LYS:H     | 1.73                     | 0.53              |
| 1:A:971:ALA:C    | 1:A:972:PHE:CG    | 2.85                     | 0.53              |
| 1:A:1104:LYS:O   | 1:A:1108:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:392:ASN:ND2  | 1:A:710:LEU:HD23  | 2.24                     | 0.53              |
| 1:A:439:ASN:HB3  | 1:A:442:GLU:HB3   | 1.90                     | 0.53              |
| 1:A:701:ILE:N    | 1:A:701:ILE:CD1   | 2.71                     | 0.53              |
| 2:B:17:ARG:C     | 2:B:19:LEU:N      | 2.65                     | 0.53              |
| 1:A:140:PHE:HB2  | 1:A:159:LEU:HD12  | 1.90                     | 0.53              |
| 1:A:660:TYR:HB2  | 1:A:707:ILE:CD1   | 2.39                     | 0.52              |
| 1:A:938:MET:CG   | 1:A:939:GLU:H     | 2.18                     | 0.52              |
| 1:A:283:LEU:HD21 | 1:A:300:LEU:HD12  | 1.89                     | 0.52              |
| 1:A:923:VAL:O    | 1:A:923:VAL:CG1   | 2.58                     | 0.52              |
| 1:A:383:LYS:HA   | 1:A:718:TYR:O     | 2.09                     | 0.52              |
| 1:A:494:GLN:O    | 1:A:495:ALA:HB3   | 2.08                     | 0.52              |
| 1:A:814:LEU:CD2  | 2:B:15:ARG:NH2    | 2.72                     | 0.52              |
| 1:A:512:VAL:HG12 | 1:A:512:VAL:O     | 2.09                     | 0.52              |
| 1:A:490:TRP:O    | 1:A:491:LYS:HB2   | 2.09                     | 0.52              |
| 1:A:538:VAL:HG11 | 1:A:541:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:842:GLU:O    | 1:A:842:GLU:HG2   | 2.09                     | 0.52              |
| 1:A:378:CYS:HB3  | 1:A:721:PRO:HB2   | 1.91                     | 0.52              |
| 1:A:811:GLU:C    | 1:A:812:TYR:HD2   | 2.18                     | 0.52              |
| 1:A:1093:LEU:O   | 1:A:1094:ILE:C    | 2.52                     | 0.52              |
| 1:A:55:VAL:CG1   | 1:A:100:ILE:HD12  | 2.39                     | 0.52              |
| 1:A:396:ILE:HG13 | 1:A:673:LEU:HD11  | 1.90                     | 0.52              |
| 1:A:131:ILE:HG13 | 1:A:145:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:206:PRO:HB2  | 1:A:207:TRP:CE3   | 2.45                     | 0.52              |
| 1:A:365:VAL:HG13 | 1:A:366:ASP:CA    | 2.38                     | 0.52              |
| 1:A:476:VAL:HG22 | 1:A:476:VAL:O     | 2.09                     | 0.52              |
| 1:A:513:GLY:O    | 1:A:538:VAL:N     | 2.41                     | 0.52              |
| 1:A:841:ALA:HA   | 2:B:9:HIS:CB      | 2.39                     | 0.52              |
| 1:A:842:GLU:O    | 1:A:843:PRO:C     | 2.53                     | 0.52              |
| 1:A:713:ARG:CG   | 1:A:713:ARG:NH1   | 2.55                     | 0.52              |
| 1:A:18:CYS:N     | 1:A:313:CYS:SG    | 2.83                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:660:TYR:CD2   | 1:A:661:SER:N     | 2.61                     | 0.52              |
| 1:A:693:LEU:N     | 1:A:693:LEU:CD1   | 2.72                     | 0.52              |
| 1:A:731:GLN:HA    | 1:A:796:GLN:HE21  | 1.74                     | 0.52              |
| 1:A:936:LYS:C     | 1:A:938:MET:N     | 2.68                     | 0.52              |
| 1:A:6:VAL:HG12    | 1:A:1040:VAL:HG22 | 1.92                     | 0.51              |
| 1:A:932:LEU:O     | 1:A:933:LEU:HD12  | 2.10                     | 0.51              |
| 1:A:429:PHE:HB3   | 1:A:432:GLN:HB2   | 1.92                     | 0.51              |
| 1:A:578:HIS:CE1   | 1:A:623:LEU:HG    | 2.45                     | 0.51              |
| 1:A:876:PHE:HZ    | 1:A:920:PHE:CA    | 2.15                     | 0.51              |
| 1:A:1057:ARG:HH22 | 1:A:1111:ASN:H    | 1.58                     | 0.51              |
| 1:A:1134:GLU:O    | 1:A:1137:THR:OG1  | 2.28                     | 0.51              |
| 1:A:367:LEU:HD12  | 1:A:374:GLN:CG    | 2.37                     | 0.51              |
| 1:A:68:ARG:HD3    | 1:A:74:LYS:C      | 2.36                     | 0.51              |
| 1:A:234:GLN:O     | 1:A:236:SER:N     | 2.44                     | 0.51              |
| 1:A:411:TRP:CB    | 1:A:460:CYS:HB3   | 2.41                     | 0.51              |
| 1:A:1136:LEU:C    | 1:A:1138:ARG:H    | 2.18                     | 0.51              |
| 1:A:925:ASP:CG    | 1:A:926:LEU:H     | 2.19                     | 0.51              |
| 1:A:133:LEU:HB3   | 1:A:135:LEU:CD2   | 2.40                     | 0.51              |
| 1:A:578:HIS:CG    | 1:A:579:LYS:N     | 2.78                     | 0.51              |
| 1:A:739:ARG:NH1   | 1:A:790:ASN:HD21  | 2.09                     | 0.51              |
| 1:A:513:GLY:O     | 1:A:537:GLU:CA    | 2.53                     | 0.51              |
| 1:A:81:THR:HG21   | 1:A:85:ASN:OD1    | 2.11                     | 0.51              |
| 1:A:588:PRO:HA    | 1:A:606:LEU:HA    | 1.93                     | 0.51              |
| 1:A:633:THR:N     | 1:A:654:ASP:OD1   | 2.43                     | 0.51              |
| 1:A:841:ALA:CA    | 2:B:9:HIS:ND1     | 2.72                     | 0.51              |
| 1:A:6:VAL:CG1     | 1:A:1040:VAL:HG22 | 2.41                     | 0.51              |
| 1:A:641:PHE:HB3   | 1:A:679:MET:HE3   | 1.92                     | 0.51              |
| 1:A:708:GLN:O     | 1:A:710:LEU:N     | 2.44                     | 0.51              |
| 1:A:910:MET:CE    | 1:A:912:LEU:HD21  | 2.41                     | 0.51              |
| 1:A:921:ILE:HG23  | 1:A:932:LEU:HD11  | 1.93                     | 0.51              |
| 1:A:1:MET:HB2     | 1:A:3:TYR:OH      | 2.11                     | 0.50              |
| 1:A:81:THR:HG23   | 1:A:83:LYS:H      | 1.75                     | 0.50              |
| 1:A:591:ILE:HD12  | 1:A:604:CYS:SG    | 2.51                     | 0.50              |
| 1:A:934:ALA:HB2   | 1:A:945:ILE:HD11  | 1.93                     | 0.50              |
| 1:A:60:LYS:NZ     | 1:A:1001:GLY:O    | 2.42                     | 0.50              |
| 1:A:135:LEU:N     | 1:A:135:LEU:HD22  | 2.27                     | 0.50              |
| 1:A:492:GLU:C     | 1:A:492:GLU:CD    | 2.80                     | 0.50              |
| 1:A:569:LEU:HG    | 1:A:576:LEU:HA    | 1.92                     | 0.50              |
| 1:A:602:LEU:CD2   | 1:A:614:PHE:HB2   | 2.41                     | 0.50              |
| 1:A:610:ALA:HA    | 1:A:630:THR:HA    | 1.92                     | 0.50              |
| 1:A:630:THR:HG22  | 1:A:1134:GLU:CD   | 2.37                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:691:LEU:O     | 1:A:693:LEU:HD12 | 2.12                     | 0.50              |
| 1:A:765:VAL:HG23  | 1:A:806:GLN:HB3  | 1.93                     | 0.50              |
| 1:A:842:GLU:O     | 1:A:843:PRO:O    | 2.30                     | 0.50              |
| 1:A:414:ARG:CA    | 1:A:422:TYR:HA   | 2.39                     | 0.50              |
| 1:A:963:ASP:HA    | 1:A:979:LYS:HD3  | 1.93                     | 0.50              |
| 1:A:452:VAL:HG22  | 1:A:477:ARG:HD2  | 1.93                     | 0.50              |
| 1:A:492:GLU:OE2   | 1:A:494:GLN:HB2  | 2.11                     | 0.50              |
| 1:A:1014:MET:SD   | 1:A:1015:GLN:N   | 2.85                     | 0.50              |
| 1:A:578:HIS:NE2   | 1:A:623:LEU:HG   | 2.27                     | 0.50              |
| 1:A:763:SER:C     | 1:A:803:HIS:CE1  | 2.87                     | 0.50              |
| 1:A:1057:ARG:HH12 | 1:A:1110:ALA:HB3 | 1.77                     | 0.50              |
| 1:A:1125:THR:CG2  | 1:A:1126:ALA:N   | 2.72                     | 0.50              |
| 1:A:411:TRP:HB2   | 1:A:460:CYS:HB3  | 1.94                     | 0.50              |
| 1:A:939:GLU:O     | 1:A:940:GLY:C    | 2.55                     | 0.50              |
| 1:A:5:TYR:CZ      | 1:A:1091:GLY:HA3 | 2.47                     | 0.49              |
| 1:A:231:ILE:HD13  | 1:A:240:HIS:HD2  | 1.76                     | 0.49              |
| 1:A:411:TRP:HH2   | 1:A:428:SER:HB2  | 1.77                     | 0.49              |
| 1:A:803:HIS:HD2   | 1:A:858:LEU:HB2  | 1.77                     | 0.49              |
| 1:A:960:LEU:HD12  | 1:A:964:ASN:HB3  | 1.94                     | 0.49              |
| 1:A:141:LYS:HD2   | 1:A:154:ALA:HB3  | 1.93                     | 0.49              |
| 1:A:372:GLN:O     | 1:A:372:GLN:NE2  | 2.45                     | 0.49              |
| 1:A:812:TYR:OH    | 2:B:12:TRP:CZ2   | 2.60                     | 0.49              |
| 1:A:81:THR:CG2    | 1:A:83:LYS:N     | 2.75                     | 0.49              |
| 1:A:743:GLN:HB3   | 1:A:784:GLU:HB2  | 1.93                     | 0.49              |
| 1:A:288:GLU:HG2   | 1:A:296:THR:HG23 | 1.93                     | 0.49              |
| 1:A:660:TYR:O     | 1:A:661:SER:OG   | 2.30                     | 0.49              |
| 1:A:170:LEU:HD12  | 1:A:177:THR:HG22 | 1.94                     | 0.49              |
| 1:A:261:HIS:HA    | 1:A:272:LEU:O    | 2.12                     | 0.49              |
| 1:A:449:MET:HG3   | 1:A:484:LYS:HG3  | 1.94                     | 0.49              |
| 1:A:612:PHE:CZ    | 1:A:628:LYS:HD3  | 2.47                     | 0.49              |
| 1:A:905:HIS:CD2   | 1:A:908:ASN:ND2  | 2.80                     | 0.49              |
| 1:A:459:PHE:CD2   | 1:A:460:CYS:N    | 2.78                     | 0.49              |
| 1:A:11:LYS:NZ     | 1:A:54:GLU:OE2   | 2.46                     | 0.49              |
| 1:A:130:MET:HE1   | 1:A:195:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:263:ARG:HB2   | 1:A:271:TYR:CE2  | 2.48                     | 0.49              |
| 1:A:722:ARG:HH22  | 2:B:15:ARG:HH11  | 1.60                     | 0.49              |
| 1:A:811:GLU:OE2   | 1:A:847:ARG:NE   | 2.45                     | 0.49              |
| 1:A:1098:LEU:C    | 1:A:1100:ILE:H   | 2.20                     | 0.49              |
| 1:A:288:GLU:OE1   | 1:A:298:LYS:N    | 2.45                     | 0.49              |
| 1:A:429:PHE:HD1   | 1:A:430:VAL:H    | 1.59                     | 0.49              |
| 1:A:492:GLU:OE1   | 1:A:492:GLU:O    | 2.30                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:882:ALA:O    | 1:A:884:ILE:CD1   | 2.60                     | 0.49              |
| 1:A:910:MET:HE1  | 2:B:10:LEU:HB3    | 1.93                     | 0.49              |
| 1:A:704:ILE:O    | 1:A:705:ASP:O     | 2.30                     | 0.49              |
| 1:A:874:VAL:HG22 | 1:A:875:GLU:O     | 2.13                     | 0.49              |
| 1:A:814:LEU:CD2  | 2:B:15:ARG:HH21   | 2.26                     | 0.49              |
| 1:A:341:ASN:O    | 1:A:342:GLU:C     | 2.56                     | 0.48              |
| 1:A:895:THR:C    | 1:A:897:LYS:H     | 2.21                     | 0.48              |
| 1:A:26:ALA:HB3   | 1:A:27:GLU:OE2    | 2.13                     | 0.48              |
| 1:A:27:GLU:O     | 1:A:28:ASP:OD1    | 2.30                     | 0.48              |
| 1:A:105:HIS:CA   | 1:A:152:LEU:HD12  | 2.43                     | 0.48              |
| 1:A:364:VAL:CG2  | 1:A:1010:GLY:HA3  | 2.38                     | 0.48              |
| 1:A:480:SER:CB   | 1:A:484:LYS:H     | 2.26                     | 0.48              |
| 1:A:120:ILE:HG12 | 1:A:135:LEU:HD13  | 1.95                     | 0.48              |
| 1:A:492:GLU:CD   | 1:A:494:GLN:HB2   | 2.38                     | 0.48              |
| 1:A:516:LEU:O    | 1:A:531:HIS:HA    | 2.14                     | 0.48              |
| 1:A:644:LEU:HG   | 1:A:645:SER:N     | 2.19                     | 0.48              |
| 1:A:824:ASP:OD1  | 1:A:826:ASN:HB2   | 2.12                     | 0.48              |
| 1:A:939:GLU:HG3  | 1:A:941:ASN:HB2   | 1.95                     | 0.48              |
| 1:A:1070:HIS:C   | 1:A:1070:HIS:CD2  | 2.89                     | 0.48              |
| 1:A:43:VAL:HG23  | 1:A:52:VAL:HG21   | 1.96                     | 0.48              |
| 1:A:389:ILE:HD12 | 1:A:389:ILE:H     | 1.78                     | 0.48              |
| 1:A:591:ILE:CD1  | 1:A:604:CYS:HB2   | 2.41                     | 0.48              |
| 1:A:632:GLY:C    | 1:A:634:GLN:N     | 2.68                     | 0.48              |
| 1:A:917:LYS:O    | 1:A:918:GLY:C     | 2.56                     | 0.48              |
| 1:A:930:VAL:O    | 1:A:930:VAL:HG23  | 2.13                     | 0.48              |
| 1:A:287:LYS:O    | 1:A:288:GLU:CB    | 2.59                     | 0.48              |
| 1:A:715:VAL:CG2  | 1:A:799:PHE:HB3   | 2.43                     | 0.48              |
| 1:A:1105:MET:SD  | 1:A:1130:ILE:HD12 | 2.53                     | 0.48              |
| 1:A:538:VAL:HG11 | 1:A:541:LEU:CD1   | 2.44                     | 0.48              |
| 1:A:921:ILE:HA   | 1:A:933:LEU:O     | 2.14                     | 0.48              |
| 1:A:27:GLU:O     | 1:A:28:ASP:CG     | 2.56                     | 0.48              |
| 1:A:116:SER:OG   | 1:A:134:ARG:CZ    | 2.62                     | 0.48              |
| 1:A:161:GLU:OE1  | 1:A:191:LYS:NZ    | 2.45                     | 0.48              |
| 1:A:256:SER:HB3  | 1:A:275:ASP:CG    | 2.37                     | 0.48              |
| 1:A:340:SER:HB3  | 1:A:346:TYR:CE1   | 2.49                     | 0.48              |
| 1:A:342:GLU:C    | 1:A:344:GLY:N     | 2.71                     | 0.48              |
| 1:A:632:GLY:O    | 1:A:634:GLN:N     | 2.46                     | 0.48              |
| 1:A:662:SER:OG   | 1:A:663:ASN:N     | 2.46                     | 0.48              |
| 1:A:123:ILE:N    | 1:A:132:GLY:O     | 2.41                     | 0.48              |
| 1:A:507:GLN:NE2  | 1:A:552:LEU:HA    | 2.29                     | 0.48              |
| 1:A:717:LEU:C    | 1:A:719:GLU:H     | 2.22                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1136:LEU:O    | 1:A:1139:ILE:HG13 | 2.14                     | 0.48              |
| 1:A:397:HIS:O     | 1:A:702:GLY:HA3   | 2.14                     | 0.48              |
| 1:A:660:TYR:CD2   | 1:A:661:SER:C     | 2.92                     | 0.48              |
| 1:A:852:GLN:O     | 1:A:859:GLN:N     | 2.34                     | 0.48              |
| 1:A:912:LEU:HB2   | 1:A:913:TYR:CD1   | 2.49                     | 0.48              |
| 1:A:196:SER:OG    | 1:A:198:ARG:HB3   | 2.14                     | 0.47              |
| 1:A:222:VAL:HG13  | 1:A:223:PRO:HD2   | 1.95                     | 0.47              |
| 1:A:336:LEU:HD23  | 1:A:347:VAL:HG22  | 1.95                     | 0.47              |
| 1:A:365:VAL:CG1   | 1:A:366:ASP:HB2   | 2.44                     | 0.47              |
| 1:A:467:GLN:HE22  | 1:A:524:GLN:HA    | 1.79                     | 0.47              |
| 1:A:521:ILE:HD13  | 1:A:526:LEU:HD23  | 1.96                     | 0.47              |
| 1:A:67:PHE:HD1    | 1:A:128:CYS:SG    | 2.37                     | 0.47              |
| 1:A:677:ASN:HB3   | 1:A:678:TYR:CE1   | 2.49                     | 0.47              |
| 1:A:985:THR:HB    | 1:A:989:ARG:HH21  | 1.79                     | 0.47              |
| 1:A:146:ASP:O     | 1:A:147:ARG:C     | 2.55                     | 0.47              |
| 1:A:304:LEU:HD12  | 1:A:306:GLY:H     | 1.78                     | 0.47              |
| 1:A:340:SER:HB3   | 1:A:346:TYR:CD1   | 2.48                     | 0.47              |
| 1:A:828:TYR:CE2   | 1:A:861:VAL:HG21  | 2.49                     | 0.47              |
| 1:A:230:ILE:C     | 1:A:231:ILE:HD12  | 2.39                     | 0.47              |
| 1:A:116:SER:HB3   | 1:A:137:ASP:OD1   | 2.13                     | 0.47              |
| 1:A:334:VAL:HG13  | 1:A:347:VAL:HG13  | 1.96                     | 0.47              |
| 1:A:328:LEU:O     | 1:A:380:GLY:HA2   | 2.14                     | 0.47              |
| 1:A:365:VAL:CG1   | 1:A:367:LEU:HD23  | 2.42                     | 0.47              |
| 1:A:765:VAL:HG13  | 1:A:766:SER:O     | 2.13                     | 0.47              |
| 1:A:821:LEU:O     | 1:A:824:ASP:HB3   | 2.14                     | 0.47              |
| 1:A:913:TYR:O     | 1:A:914:LEU:HD23  | 2.15                     | 0.47              |
| 1:A:79:ILE:HB     | 1:A:87:CYS:SG     | 2.55                     | 0.47              |
| 1:A:429:PHE:O     | 1:A:431:GLY:N     | 2.48                     | 0.47              |
| 1:A:938:MET:C     | 1:A:940:GLY:N     | 2.70                     | 0.47              |
| 1:A:236:SER:N     | 1:A:253:ILE:HD11  | 2.30                     | 0.47              |
| 2:B:9:HIS:O       | 2:B:10:LEU:C      | 2.58                     | 0.47              |
| 1:A:316:TYR:HA    | 1:A:322:VAL:HG22  | 1.97                     | 0.47              |
| 1:A:910:MET:CE    | 2:B:10:LEU:HD12   | 2.45                     | 0.47              |
| 1:A:1090:ASP:C    | 1:A:1092:ASP:N    | 2.69                     | 0.47              |
| 1:A:403:ASP:OD2   | 1:A:403:ASP:N     | 2.45                     | 0.46              |
| 1:A:542:ASP:O     | 1:A:593:MET:HE3   | 2.14                     | 0.46              |
| 1:A:1041:THR:HG22 | 1:A:1042:SER:N    | 2.31                     | 0.46              |
| 1:A:1063:LYS:H    | 1:A:1063:LYS:CD   | 2.19                     | 0.46              |
| 1:A:411:TRP:CH2   | 1:A:428:SER:HB2   | 2.50                     | 0.46              |
| 1:A:722:ARG:HH22  | 2:B:15:ARG:NH1    | 2.12                     | 0.46              |
| 1:A:399:HIS:HB2   | 1:A:687:TYR:HE1   | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:660:TYR:CB    | 1:A:667:VAL:CG2   | 2.84                     | 0.46              |
| 1:A:719:GLU:OE2   | 1:A:755:SER:HB2   | 2.14                     | 0.46              |
| 1:A:969:GLU:O     | 1:A:970:ASN:OD1   | 2.33                     | 0.46              |
| 1:A:472:THR:O     | 1:A:473:SER:C     | 2.57                     | 0.46              |
| 1:A:690:SER:HA    | 1:A:702:GLY:O     | 2.14                     | 0.46              |
| 1:A:38:ARG:NE     | 1:A:54:GLU:OE2    | 2.48                     | 0.46              |
| 1:A:81:THR:HG22   | 1:A:84:TYR:H      | 1.81                     | 0.46              |
| 1:A:369:ARG:O     | 1:A:369:ARG:HG2   | 2.16                     | 0.46              |
| 1:A:1048:TYR:CE2  | 1:A:1052:LEU:HD12 | 2.51                     | 0.46              |
| 1:A:235:GLU:HB3   | 1:A:254:LYS:CG    | 2.44                     | 0.46              |
| 1:A:667:VAL:HG12  | 1:A:668:PHE:N     | 2.31                     | 0.46              |
| 1:A:1063:LYS:HD3  | 1:A:1063:LYS:N    | 2.23                     | 0.46              |
| 1:A:593:MET:HA    | 1:A:601:TYR:O     | 2.16                     | 0.46              |
| 1:A:706:GLU:HG3   | 1:A:707:ILE:N     | 2.31                     | 0.46              |
| 1:A:846:GLY:C     | 1:A:866:VAL:HG22  | 2.41                     | 0.46              |
| 1:A:413:LEU:C     | 1:A:422:TYR:HB3   | 2.41                     | 0.46              |
| 1:A:905:HIS:CE1   | 1:A:907:ASN:HB3   | 2.51                     | 0.46              |
| 1:A:4:ASN:O       | 1:A:1089:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:364:VAL:HG21  | 1:A:1010:GLY:CA   | 2.39                     | 0.46              |
| 1:A:542:ASP:OD2   | 1:A:592:LEU:HD12  | 2.16                     | 0.46              |
| 1:A:651:ALA:HB3   | 1:A:657:THR:HB    | 1.97                     | 0.46              |
| 1:A:707:ILE:CG2   | 1:A:708:GLN:N     | 2.44                     | 0.46              |
| 1:A:910:MET:HE2   | 1:A:912:LEU:HD21  | 1.96                     | 0.46              |
| 1:A:925:ASP:CG    | 1:A:926:LEU:N     | 2.74                     | 0.46              |
| 1:A:27:GLU:C      | 1:A:28:ASP:CG     | 2.84                     | 0.46              |
| 1:A:660:TYR:CG    | 1:A:667:VAL:CG2   | 2.99                     | 0.46              |
| 1:A:1139:ILE:HG22 | 1:A:1139:ILE:O    | 2.16                     | 0.46              |
| 1:A:262:ASN:ND2   | 1:A:316:TYR:H     | 2.14                     | 0.45              |
| 1:A:620:THR:OG1   | 1:A:622:LEU:HD12  | 2.16                     | 0.45              |
| 1:A:817:VAL:HG22  | 1:A:830:ILE:HB    | 1.97                     | 0.45              |
| 1:A:880:LEU:HD23  | 1:A:899:VAL:HG11  | 1.96                     | 0.45              |
| 2:B:17:ARG:O      | 2:B:18:SER:C      | 2.58                     | 0.45              |
| 1:A:354:THR:HG22  | 1:A:388:ARG:HH12  | 1.81                     | 0.45              |
| 1:A:537:GLU:O     | 1:A:561:TRP:HB2   | 2.16                     | 0.45              |
| 1:A:570:LYS:HZ3   | 1:A:572:PRO:HD2   | 1.80                     | 0.45              |
| 1:A:405:PRO:HA    | 1:A:696:ASN:O     | 2.16                     | 0.45              |
| 1:A:697:SER:O     | 1:A:698:THR:CB    | 2.63                     | 0.45              |
| 1:A:787:GLU:OE1   | 2:B:12:TRP:HZ3    | 2.00                     | 0.45              |
| 1:A:1047:TRP:O    | 1:A:1048:TYR:C    | 2.60                     | 0.45              |
| 1:A:840:GLU:C     | 2:B:9:HIS:ND1     | 2.75                     | 0.45              |
| 1:A:599:SER:HB2   | 1:A:664:HIS:CE1   | 2.52                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:620:THR:OG1   | 1:A:622:LEU:CD1  | 2.64                     | 0.45              |
| 1:A:630:THR:O     | 1:A:631:LEU:CD2  | 2.63                     | 0.45              |
| 1:A:921:ILE:CG2   | 1:A:932:LEU:HD11 | 2.47                     | 0.45              |
| 1:A:926:LEU:HG    | 1:A:927:MET:N    | 2.24                     | 0.45              |
| 1:A:5:TYR:CZ      | 1:A:1091:GLY:CA  | 3.00                     | 0.45              |
| 1:A:169:PHE:CE2   | 1:A:178:ILE:HG23 | 2.52                     | 0.45              |
| 1:A:606:LEU:HB2   | 1:A:608:ASP:OD2  | 2.17                     | 0.45              |
| 1:A:181:VAL:HG23  | 1:A:219:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:844:LYS:O     | 1:A:867:LYS:HA   | 2.17                     | 0.45              |
| 1:A:122:GLY:CA    | 1:A:133:LEU:HD12 | 2.47                     | 0.45              |
| 1:A:134:ARG:C     | 1:A:134:ARG:CD   | 2.90                     | 0.45              |
| 1:A:1129:LEU:C    | 1:A:1131:LYS:N   | 2.75                     | 0.45              |
| 1:A:22:HIS:O      | 1:A:75:ASP:HB2   | 2.17                     | 0.44              |
| 1:A:334:VAL:HG22  | 1:A:349:ALA:HA   | 1.99                     | 0.44              |
| 1:A:731:GLN:CA    | 1:A:796:GLN:HE21 | 2.30                     | 0.44              |
| 1:A:881:LEU:HD11  | 1:A:888:VAL:CG1  | 2.46                     | 0.44              |
| 1:A:1075:SER:O    | 1:A:1076:PHE:C   | 2.59                     | 0.44              |
| 1:A:534:MET:O     | 1:A:535:GLU:C    | 2.59                     | 0.44              |
| 1:A:830:ILE:HG12  | 1:A:850:VAL:HG22 | 1.98                     | 0.44              |
| 1:A:1093:LEU:HD22 | 1:A:1096:SER:OG  | 2.17                     | 0.44              |
| 1:A:181:VAL:HG13  | 1:A:212:VAL:HG21 | 1.98                     | 0.44              |
| 1:A:764:SER:HB2   | 1:A:805:HIS:HA   | 1.99                     | 0.44              |
| 1:A:1103:PRO:O    | 1:A:1107:GLU:HG3 | 2.17                     | 0.44              |
| 1:A:367:LEU:CD1   | 1:A:374:GLN:HG3  | 2.44                     | 0.44              |
| 1:A:924:GLY:O     | 1:A:925:ASP:HB2  | 2.17                     | 0.44              |
| 1:A:971:ALA:O     | 1:A:972:PHE:CG   | 2.70                     | 0.44              |
| 1:A:223:PRO:HG2   | 1:A:267:ASN:O    | 2.18                     | 0.44              |
| 1:A:370:GLN:HB2   | 1:A:372:GLN:NE2  | 2.33                     | 0.44              |
| 1:A:378:CYS:SG    | 1:A:724:ILE:CG2  | 3.05                     | 0.44              |
| 1:A:520:GLN:OE1   | 1:A:527:ARG:O    | 2.36                     | 0.44              |
| 1:A:564:ILE:HG22  | 1:A:564:ILE:O    | 2.17                     | 0.44              |
| 1:A:763:SER:CA    | 1:A:803:HIS:CE1  | 3.00                     | 0.44              |
| 1:A:816:LEU:CD1   | 1:A:831:VAL:HG22 | 2.47                     | 0.44              |
| 1:A:29:LEU:O      | 1:A:44:VAL:HG23  | 2.17                     | 0.44              |
| 1:A:38:ARG:HH11   | 1:A:56:GLY:CA    | 2.31                     | 0.44              |
| 1:A:76:LEU:CD2    | 1:A:90:GLU:HG3   | 2.48                     | 0.44              |
| 1:A:837:TYR:HA    | 1:A:838:PRO:HD3  | 1.87                     | 0.44              |
| 1:A:341:ASN:O     | 1:A:342:GLU:O    | 2.35                     | 0.44              |
| 1:A:492:GLU:OE1   | 1:A:494:GLN:HB2  | 2.18                     | 0.44              |
| 1:A:571:LEU:O     | 1:A:572:PRO:C    | 2.59                     | 0.44              |
| 1:A:615:GLY:N     | 1:A:624:SER:OG   | 2.49                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1076:PHE:C   | 1:A:1076:PHE:HD2  | 2.25                     | 0.44              |
| 1:A:135:LEU:CD2  | 1:A:135:LEU:N     | 2.81                     | 0.44              |
| 1:A:220:ILE:HB   | 1:A:230:ILE:HB    | 1.98                     | 0.44              |
| 1:A:406:GLY:O    | 1:A:407:ILE:C     | 2.61                     | 0.44              |
| 1:A:427:LEU:HD12 | 1:A:427:LEU:O     | 2.17                     | 0.44              |
| 1:A:742:VAL:HG23 | 1:A:743:GLN:O     | 2.18                     | 0.44              |
| 1:A:837:TYR:O    | 2:B:9:HIS:CE1     | 2.71                     | 0.44              |
| 1:A:839:GLU:OE1  | 1:A:839:GLU:HA    | 2.18                     | 0.44              |
| 1:A:12:PRO:HD3   | 1:A:1036:MET:HG3  | 1.99                     | 0.43              |
| 1:A:112:ILE:HD12 | 1:A:112:ILE:HA    | 1.75                     | 0.43              |
| 1:A:917:LYS:HZ3  | 1:A:921:ILE:HD12  | 1.82                     | 0.43              |
| 1:A:40:GLU:HB3   | 1:A:42:TYR:CE1    | 2.53                     | 0.43              |
| 1:A:63:VAL:HB    | 1:A:80:LEU:HB3    | 1.99                     | 0.43              |
| 1:A:342:GLU:OE1  | 1:A:342:GLU:HA    | 2.18                     | 0.43              |
| 1:A:610:ALA:HB1  | 1:A:628:LYS:HG2   | 2.00                     | 0.43              |
| 1:A:677:ASN:HB2  | 1:A:694:ALA:O     | 2.18                     | 0.43              |
| 1:A:542:ASP:OD2  | 1:A:593:MET:HG2   | 2.18                     | 0.43              |
| 1:A:763:SER:HA   | 1:A:803:HIS:ND1   | 2.32                     | 0.43              |
| 1:A:921:ILE:C    | 1:A:922:LEU:HD12  | 2.43                     | 0.43              |
| 1:A:1047:TRP:HZ3 | 1:A:1132:VAL:HG13 | 1.84                     | 0.43              |
| 1:A:125:ASP:OD2  | 1:A:128:CYS:N     | 2.51                     | 0.43              |
| 1:A:486:LEU:HD11 | 1:A:489:GLU:HB2   | 1.99                     | 0.43              |
| 1:A:582:LEU:H    | 1:A:582:LEU:HG    | 1.59                     | 0.43              |
| 1:A:787:GLU:HG3  | 2:B:12:TRP:CH2    | 2.52                     | 0.43              |
| 1:A:634:GLN:O    | 1:A:635:PRO:O     | 2.35                     | 0.43              |
| 1:A:660:TYR:CE2  | 1:A:661:SER:O     | 2.71                     | 0.43              |
| 1:A:1136:LEU:O   | 1:A:1137:THR:C    | 2.60                     | 0.43              |
| 1:A:342:GLU:O    | 1:A:344:GLY:N     | 2.51                     | 0.43              |
| 1:A:816:LEU:HD12 | 1:A:831:VAL:HG22  | 2.00                     | 0.43              |
| 1:A:864:LYS:HD3  | 1:A:899:VAL:O     | 2.19                     | 0.43              |
| 1:A:7:VAL:HG13   | 1:A:1091:GLY:HA3  | 2.01                     | 0.43              |
| 1:A:65:GLU:O     | 1:A:77:LEU:HD12   | 2.18                     | 0.43              |
| 1:A:5:TYR:CE2    | 1:A:7:VAL:HG22    | 2.53                     | 0.43              |
| 1:A:81:THR:HB    | 1:A:85:ASN:HB2    | 2.01                     | 0.43              |
| 1:A:130:MET:HE1  | 1:A:195:VAL:CG1   | 2.48                     | 0.43              |
| 1:A:318:ASP:HB3  | 1:A:319:ASN:H     | 1.58                     | 0.43              |
| 1:A:130:MET:HE3  | 1:A:176:PRO:HB3   | 2.00                     | 0.43              |
| 1:A:465:HIS:N    | 1:A:465:HIS:ND1   | 2.67                     | 0.43              |
| 1:A:517:TYR:O    | 1:A:518:TYR:CB    | 2.66                     | 0.43              |
| 1:A:38:ARG:HH11  | 1:A:38:ARG:HD3    | 1.69                     | 0.43              |
| 1:A:609:GLY:CA   | 1:A:632:GLY:O     | 2.67                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:391:ARG:HG3   | 1:A:391:ARG:HH11 | 1.84                     | 0.42              |
| 1:A:507:GLN:HE22  | 1:A:552:LEU:HA   | 1.83                     | 0.42              |
| 1:A:611:LEU:O     | 1:A:628:LYS:CA   | 2.61                     | 0.42              |
| 1:A:885:ASN:O     | 1:A:886:SER:CB   | 2.67                     | 0.42              |
| 1:A:13:THR:HB     | 1:A:355:ASN:HA   | 2.00                     | 0.42              |
| 1:A:81:THR:HG22   | 1:A:83:LYS:N     | 2.34                     | 0.42              |
| 1:A:285:LEU:O     | 1:A:286:GLU:C    | 2.61                     | 0.42              |
| 1:A:457:THR:CG2   | 1:A:459:PHE:O    | 2.67                     | 0.42              |
| 1:A:660:TYR:HB2   | 1:A:707:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:934:ALA:HB2   | 1:A:945:ILE:CD1  | 2.48                     | 0.42              |
| 1:A:105:HIS:CD2   | 1:A:1067:LYS:HB2 | 2.55                     | 0.42              |
| 1:A:501:ALA:O     | 1:A:502:SER:HB2  | 2.19                     | 0.42              |
| 1:A:948:ASP:OD1   | 1:A:948:ASP:C    | 2.62                     | 0.42              |
| 1:A:131:ILE:HG22  | 1:A:133:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:213:GLU:CD    | 1:A:233:GLY:HA3  | 2.44                     | 0.42              |
| 1:A:611:LEU:HG    | 1:A:612:PHE:H    | 1.84                     | 0.42              |
| 1:A:632:GLY:O     | 1:A:633:THR:C    | 2.62                     | 0.42              |
| 1:A:522:HIS:O     | 1:A:523:PRO:C    | 2.63                     | 0.42              |
| 1:A:843:PRO:HG2   | 2:B:11:LEU:CD1   | 2.49                     | 0.42              |
| 1:A:1013:VAL:HB   | 1:A:1014:MET:H   | 1.70                     | 0.42              |
| 1:A:607:GLY:HA2   | 1:A:635:PRO:HA   | 2.01                     | 0.42              |
| 1:A:706:GLU:HG3   | 1:A:707:ILE:HG22 | 2.01                     | 0.42              |
| 1:A:954:MET:HE1   | 1:A:975:PHE:CZ   | 2.54                     | 0.42              |
| 1:A:733:PHE:HE1   | 1:A:799:PHE:CZ   | 2.37                     | 0.42              |
| 1:A:1052:LEU:HD23 | 1:A:1052:LEU:O   | 2.20                     | 0.42              |
| 1:A:312:GLU:HG3   | 1:A:327:ARG:HB3  | 2.01                     | 0.42              |
| 1:A:449:MET:HG3   | 1:A:484:LYS:O    | 2.20                     | 0.42              |
| 1:A:451:PHE:HA    | 1:A:470:GLN:OE1  | 2.19                     | 0.42              |
| 1:A:571:LEU:CB    | 1:A:572:PRO:CD   | 2.93                     | 0.42              |
| 1:A:575:GLU:O     | 1:A:577:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:185:PRO:O     | 1:A:186:GLN:CG   | 2.67                     | 0.42              |
| 1:A:207:TRP:O     | 1:A:208:LYS:C    | 2.62                     | 0.42              |
| 1:A:476:VAL:O     | 1:A:476:VAL:CG2  | 2.68                     | 0.42              |
| 1:A:655:ARG:CG    | 1:A:655:ARG:NH1  | 2.80                     | 0.42              |
| 1:A:680:CYS:O     | 1:A:691:LEU:HA   | 2.20                     | 0.42              |
| 1:A:122:GLY:O     | 1:A:123:ILE:CG2  | 2.67                     | 0.42              |
| 1:A:537:GLU:HB3   | 1:A:561:TRP:CD1  | 2.55                     | 0.42              |
| 1:A:304:LEU:HD12  | 1:A:305:LEU:N    | 2.35                     | 0.41              |
| 1:A:679:MET:SD    | 1:A:679:MET:O    | 2.77                     | 0.41              |
| 1:A:938:MET:O     | 1:A:940:GLY:N    | 2.40                     | 0.41              |
| 1:A:148:ASP:HB2   | 1:A:149:ASN:H    | 1.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:580:GLU:HG3  | 1:A:582:LEU:HD23 | 2.00                     | 0.41              |
| 1:A:645:SER:C    | 1:A:647:THR:H    | 2.26                     | 0.41              |
| 1:A:706:GLU:HA   | 1:A:706:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:917:LYS:HB3  | 1:A:917:LYS:HZ2  | 1.85                     | 0.41              |
| 1:A:36:ASN:CG    | 1:A:60:LYS:HZ1   | 2.27                     | 0.41              |
| 1:A:118:THR:HG21 | 1:A:165:ILE:O    | 2.20                     | 0.41              |
| 1:A:218:MET:SD   | 1:A:261:HIS:HD2  | 2.43                     | 0.41              |
| 1:A:275:ASP:C    | 1:A:277:GLU:H    | 2.27                     | 0.41              |
| 1:A:764:SER:OG   | 1:A:803:HIS:CE1  | 2.73                     | 0.41              |
| 1:A:971:ALA:HB3  | 1:A:973:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:256:SER:CB   | 1:A:275:ASP:OD2  | 2.52                     | 0.41              |
| 1:A:282:MET:HB2  | 1:A:305:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:133:LEU:HB3  | 1:A:135:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:275:ASP:C    | 1:A:277:GLU:N    | 2.77                     | 0.41              |
| 1:A:449:MET:H    | 1:A:449:MET:HG2  | 1.48                     | 0.41              |
| 1:A:663:ASN:OD1  | 1:A:665:LYS:HG3  | 2.21                     | 0.41              |
| 1:A:966:LEU:HD23 | 1:A:967:GLY:H    | 1.86                     | 0.41              |
| 1:A:332:GLN:HG3  | 1:A:334:VAL:HG23 | 2.02                     | 0.41              |
| 1:A:613:TYR:HD1  | 1:A:614:PHE:CA   | 2.26                     | 0.41              |
| 1:A:920:PHE:O    | 1:A:935:TYR:N    | 2.53                     | 0.41              |
| 1:A:936:LYS:O    | 1:A:940:GLY:HA2  | 2.21                     | 0.41              |
| 2:B:17:ARG:O     | 2:B:19:LEU:N     | 2.54                     | 0.41              |
| 1:A:80:LEU:HD11  | 1:A:84:TYR:HA    | 2.02                     | 0.41              |
| 1:A:80:LEU:HD23  | 1:A:120:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:336:LEU:CD2  | 1:A:347:VAL:HG22 | 2.51                     | 0.41              |
| 1:A:803:HIS:CD2  | 1:A:858:LEU:CB   | 3.02                     | 0.41              |
| 1:A:222:VAL:CG1  | 1:A:223:PRO:HD2  | 2.51                     | 0.41              |
| 1:A:396:ILE:HD13 | 1:A:396:ILE:C    | 2.40                     | 0.41              |
| 1:A:492:GLU:OE1  | 1:A:493:PRO:C    | 2.64                     | 0.41              |
| 1:A:824:ASP:OD1  | 1:A:824:ASP:C    | 2.64                     | 0.41              |
| 1:A:840:GLU:C    | 2:B:9:HIS:CE1    | 2.96                     | 0.41              |
| 1:A:1013:VAL:O   | 1:A:1014:MET:HG3 | 2.20                     | 0.41              |
| 1:A:365:VAL:HG13 | 1:A:366:ASP:HB2  | 2.03                     | 0.41              |
| 1:A:416:ASP:HB3  | 1:A:419:ARG:CG   | 2.51                     | 0.41              |
| 1:A:492:GLU:HA   | 1:A:493:PRO:HD3  | 1.92                     | 0.41              |
| 1:A:921:ILE:HG23 | 1:A:932:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:713:ARG:HG2  | 1:A:713:ARG:NH1  | 2.32                     | 0.40              |
| 1:A:809:GLN:HE21 | 1:A:809:GLN:HB2  | 1.62                     | 0.40              |
| 1:A:10:GLN:HG3   | 1:A:11:LYS:O     | 2.20                     | 0.40              |
| 1:A:81:THR:HG22  | 1:A:84:TYR:N     | 2.36                     | 0.40              |
| 1:A:161:GLU:HG2  | 1:A:182:TYR:CD2  | 2.55                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:324:VAL:HB    | 1:A:332:GLN:HG2  | 2.03                     | 0.40              |
| 1:A:632:GLY:C     | 1:A:634:GLN:H    | 2.30                     | 0.40              |
| 1:A:1004:VAL:HG13 | 1:A:1030:PHE:HB2 | 2.02                     | 0.40              |
| 1:A:23:PHE:CE2    | 1:A:91:TYR:HB2   | 2.56                     | 0.40              |
| 1:A:59:GLY:HA2    | 1:A:1073:TRP:CZ3 | 2.56                     | 0.40              |
| 1:A:90:GLU:HB3    | 1:A:101:ILE:HG22 | 2.03                     | 0.40              |
| 1:A:189:HIS:HD2   | 1:A:211:ASN:OD1  | 2.03                     | 0.40              |
| 1:A:352:THR:O     | 1:A:352:THR:HG22 | 2.18                     | 0.40              |
| 1:A:467:GLN:OE1   | 1:A:521:ILE:HG22 | 2.21                     | 0.40              |
| 1:A:667:VAL:CG1   | 1:A:668:PHE:N    | 2.85                     | 0.40              |
| 1:A:997:LEU:HB3   | 1:A:1076:PHE:HB2 | 2.04                     | 0.40              |
| 1:A:105:HIS:O     | 1:A:151:GLU:HA   | 2.20                     | 0.40              |
| 1:A:488:SER:O     | 1:A:489:GLU:CB   | 2.69                     | 0.40              |
| 1:A:673:LEU:CD1   | 1:A:693:LEU:CD2  | 3.00                     | 0.40              |
| 1:A:828:TYR:HE2   | 1:A:861:VAL:HG21 | 1.84                     | 0.40              |
| 1:A:852:GLN:O     | 1:A:858:LEU:HA   | 2.22                     | 0.40              |
| 1:A:930:VAL:CG1   | 1:A:954:MET:HE2  | 2.52                     | 0.40              |
| 1:A:948:ASP:HB2   | 1:A:992:LEU:HD12 | 2.04                     | 0.40              |
| 1:A:1057:ARG:HH12 | 1:A:1110:ALA:H   | 1.70                     | 0.40              |
| 1:A:1069:GLU:HG3  | 1:A:1072:PHE:H   | 1.86                     | 0.40              |
| 1:A:364:VAL:C     | 1:A:365:VAL:CG2  | 2.94                     | 0.40              |
| 1:A:793:ILE:CD1   | 1:A:829:PHE:CE2  | 3.04                     | 0.40              |
| 1:A:813:ALA:HA    | 1:A:833:THR:HG22 | 2.03                     | 0.40              |
| 1:A:941:ASN:CG    | 1:A:942:PHE:H    | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles                         |
|-----|-------|-----------------|-----------|-----------|----------|-------------------------------------|
| 1   | A     | 1106/1143 (97%) | 851 (77%) | 172 (16%) | 83 (8%)  | <a href="#">1</a> <a href="#">2</a> |

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| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|-----------|-----------|----------|-------------|-----|
| 2   | B     | 11/13 (85%)     | 10 (91%)  | 1 (9%)    | 0        | 100         | 100 |
| All | All   | 1117/1156 (97%) | 861 (77%) | 173 (16%) | 83 (7%)  | 1           | 2   |

All (83) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 148  | ASP  |
| 1   | A     | 186  | GLN  |
| 1   | A     | 235  | GLU  |
| 1   | A     | 242  | GLY  |
| 1   | A     | 366  | ASP  |
| 1   | A     | 407  | ILE  |
| 1   | A     | 430  | VAL  |
| 1   | A     | 460  | CYS  |
| 1   | A     | 494  | GLN  |
| 1   | A     | 502  | SER  |
| 1   | A     | 518  | TYR  |
| 1   | A     | 546  | LEU  |
| 1   | A     | 554  | PRO  |
| 1   | A     | 571  | LEU  |
| 1   | A     | 647  | THR  |
| 1   | A     | 662  | SER  |
| 1   | A     | 698  | THR  |
| 1   | A     | 705  | ASP  |
| 1   | A     | 707  | ILE  |
| 1   | A     | 708  | GLN  |
| 1   | A     | 752  | LEU  |
| 1   | A     | 768  | SER  |
| 1   | A     | 772  | SER  |
| 1   | A     | 841  | ALA  |
| 1   | A     | 843  | PRO  |
| 1   | A     | 918  | GLY  |
| 1   | A     | 1065 | VAL  |
| 1   | A     | 1080 | ARG  |
| 1   | A     | 288  | GLU  |
| 1   | A     | 292  | ASP  |
| 1   | A     | 318  | ASP  |
| 1   | A     | 342  | GLU  |
| 1   | A     | 461  | GLY  |
| 1   | A     | 474  | ALA  |
| 1   | A     | 623  | LEU  |
| 1   | A     | 660  | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 683  | ASN  |
| 1   | A     | 689  | ASP  |
| 1   | A     | 706  | GLU  |
| 1   | A     | 709  | LYS  |
| 1   | A     | 751  | ALA  |
| 1   | A     | 925  | ASP  |
| 1   | A     | 939  | GLU  |
| 1   | A     | 1126 | ALA  |
| 1   | A     | 1137 | THR  |
| 1   | A     | 35   | LYS  |
| 1   | A     | 118  | THR  |
| 1   | A     | 217  | SER  |
| 1   | A     | 341  | ASN  |
| 1   | A     | 491  | LYS  |
| 1   | A     | 503  | CYS  |
| 1   | A     | 574  | PHE  |
| 1   | A     | 635  | PRO  |
| 1   | A     | 748  | GLY  |
| 1   | A     | 770  | LEU  |
| 1   | A     | 929  | SER  |
| 1   | A     | 972  | PHE  |
| 1   | A     | 1127 | ASP  |
| 1   | A     | 149  | ASN  |
| 1   | A     | 214  | ALA  |
| 1   | A     | 489  | GLU  |
| 1   | A     | 523  | PRO  |
| 1   | A     | 631  | LEU  |
| 1   | A     | 633  | THR  |
| 1   | A     | 896  | GLU  |
| 1   | A     | 994  | GLU  |
| 1   | A     | 203  | ASN  |
| 1   | A     | 208  | LYS  |
| 1   | A     | 371  | GLY  |
| 1   | A     | 624  | SER  |
| 1   | A     | 838  | PRO  |
| 1   | A     | 930  | VAL  |
| 1   | A     | 1097 | PHE  |
| 1   | A     | 224  | GLU  |
| 1   | A     | 545  | PRO  |
| 1   | A     | 842  | GLU  |
| 1   | A     | 259  | VAL  |
| 1   | A     | 176  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 621  | GLY  |
| 1   | A     | 1130 | ILE  |
| 1   | A     | 405  | PRO  |
| 1   | A     | 937  | PRO  |
| 1   | A     | 95   | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | A     | 977/1001 (98%) | 808 (83%) | 169 (17%) | 2           | 7 |
| 2   | B     | 12/12 (100%)   | 9 (75%)   | 3 (25%)   | 0           | 2 |
| All | All   | 989/1013 (98%) | 817 (83%) | 172 (17%) | 2           | 7 |

All (172) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | SER  |
| 1   | A     | 6   | VAL  |
| 1   | A     | 7   | VAL  |
| 1   | A     | 24  | THR  |
| 1   | A     | 25  | SER  |
| 1   | A     | 31  | LEU  |
| 1   | A     | 35  | LYS  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 79  | ILE  |
| 1   | A     | 81  | THR  |
| 1   | A     | 97  | SER  |
| 1   | A     | 98  | ILE  |
| 1   | A     | 99  | ASP  |
| 1   | A     | 101 | ILE  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 109 | GLN  |
| 1   | A     | 112 | ILE  |
| 1   | A     | 125 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 130 | MET  |
| 1   | A     | 133 | LEU  |
| 1   | A     | 135 | LEU  |
| 1   | A     | 147 | ARG  |
| 1   | A     | 148 | ASP  |
| 1   | A     | 160 | GLU  |
| 1   | A     | 162 | LEU  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 192 | THR  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 199 | GLU  |
| 1   | A     | 204 | LYS  |
| 1   | A     | 234 | GLN  |
| 1   | A     | 235 | GLU  |
| 1   | A     | 236 | SER  |
| 1   | A     | 238 | THR  |
| 1   | A     | 248 | ILE  |
| 1   | A     | 253 | ILE  |
| 1   | A     | 256 | SER  |
| 1   | A     | 259 | VAL  |
| 1   | A     | 260 | CYS  |
| 1   | A     | 283 | LEU  |
| 1   | A     | 294 | THR  |
| 1   | A     | 296 | THR  |
| 1   | A     | 298 | LYS  |
| 1   | A     | 301 | ARG  |
| 1   | A     | 307 | GLU  |
| 1   | A     | 310 | ILE  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 333 | LEU  |
| 1   | A     | 334 | VAL  |
| 1   | A     | 352 | THR  |
| 1   | A     | 360 | VAL  |
| 1   | A     | 372 | GLN  |
| 1   | A     | 374 | GLN  |
| 1   | A     | 383 | LYS  |
| 1   | A     | 390 | ILE  |
| 1   | A     | 392 | ASN  |
| 1   | A     | 396 | ILE  |
| 1   | A     | 401 | SER  |
| 1   | A     | 410 | LEU  |
| 1   | A     | 415 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 418 | ASN  |
| 1   | A     | 421 | THR  |
| 1   | A     | 427 | LEU  |
| 1   | A     | 429 | PHE  |
| 1   | A     | 438 | LEU  |
| 1   | A     | 441 | GLU  |
| 1   | A     | 443 | VAL  |
| 1   | A     | 445 | GLU  |
| 1   | A     | 449 | MET  |
| 1   | A     | 452 | VAL  |
| 1   | A     | 460 | CYS  |
| 1   | A     | 465 | HIS  |
| 1   | A     | 467 | GLN  |
| 1   | A     | 469 | ILE  |
| 1   | A     | 476 | VAL  |
| 1   | A     | 502 | SER  |
| 1   | A     | 504 | ASN  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 518 | TYR  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 521 | ILE  |
| 1   | A     | 525 | GLU  |
| 1   | A     | 526 | LEU  |
| 1   | A     | 529 | ILE  |
| 1   | A     | 530 | SER  |
| 1   | A     | 534 | MET  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 543 | ILE  |
| 1   | A     | 544 | THR  |
| 1   | A     | 548 | ASP  |
| 1   | A     | 552 | LEU  |
| 1   | A     | 560 | LEU  |
| 1   | A     | 567 | ARG  |
| 1   | A     | 579 | LYS  |
| 1   | A     | 582 | LEU  |
| 1   | A     | 587 | ILE  |
| 1   | A     | 589 | ARG  |
| 1   | A     | 597 | GLU  |
| 1   | A     | 602 | LEU  |
| 1   | A     | 613 | TYR  |
| 1   | A     | 618 | ILE  |
| 1   | A     | 620 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 622 | LEU  |
| 1   | A     | 623 | LEU  |
| 1   | A     | 625 | ASP  |
| 1   | A     | 638 | LEU  |
| 1   | A     | 640 | THR  |
| 1   | A     | 653 | SER  |
| 1   | A     | 655 | ARG  |
| 1   | A     | 659 | ILE  |
| 1   | A     | 679 | MET  |
| 1   | A     | 691 | LEU  |
| 1   | A     | 693 | LEU  |
| 1   | A     | 698 | THR  |
| 1   | A     | 700 | THR  |
| 1   | A     | 701 | ILE  |
| 1   | A     | 713 | ARG  |
| 1   | A     | 728 | GLU  |
| 1   | A     | 730 | SER  |
| 1   | A     | 738 | SER  |
| 1   | A     | 742 | VAL  |
| 1   | A     | 755 | SER  |
| 1   | A     | 765 | VAL  |
| 1   | A     | 766 | SER  |
| 1   | A     | 772 | SER  |
| 1   | A     | 773 | SER  |
| 1   | A     | 794 | ILE  |
| 1   | A     | 815 | SER  |
| 1   | A     | 844 | LYS  |
| 1   | A     | 854 | SER  |
| 1   | A     | 855 | ASP  |
| 1   | A     | 857 | LYS  |
| 1   | A     | 858 | LEU  |
| 1   | A     | 870 | VAL  |
| 1   | A     | 873 | MET  |
| 1   | A     | 874 | VAL  |
| 1   | A     | 884 | ILE  |
| 1   | A     | 896 | GLU  |
| 1   | A     | 899 | VAL  |
| 1   | A     | 900 | ARG  |
| 1   | A     | 904 | ASN  |
| 1   | A     | 909 | ILE  |
| 1   | A     | 917 | LYS  |
| 1   | A     | 922 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 926  | LEU  |
| 1   | A     | 930  | VAL  |
| 1   | A     | 931  | LEU  |
| 1   | A     | 957  | VAL  |
| 1   | A     | 960  | LEU  |
| 1   | A     | 966  | LEU  |
| 1   | A     | 969  | GLU  |
| 1   | A     | 979  | LYS  |
| 1   | A     | 985  | THR  |
| 1   | A     | 992  | LEU  |
| 1   | A     | 1000 | LEU  |
| 1   | A     | 1006 | VAL  |
| 1   | A     | 1045 | GLU  |
| 1   | A     | 1050 | LEU  |
| 1   | A     | 1052 | LEU  |
| 1   | A     | 1063 | LYS  |
| 1   | A     | 1064 | SER  |
| 1   | A     | 1089 | ILE  |
| 1   | A     | 1090 | ASP  |
| 1   | A     | 1093 | LEU  |
| 1   | A     | 1100 | ILE  |
| 1   | A     | 1129 | LEU  |
| 1   | A     | 1130 | ILE  |
| 1   | A     | 1131 | LYS  |
| 1   | A     | 1132 | VAL  |
| 2   | B     | 9    | HIS  |
| 2   | B     | 13   | ASP  |
| 2   | B     | 15   | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | ASN  |
| 1   | A     | 30  | ASN  |
| 1   | A     | 105 | HIS  |
| 1   | A     | 109 | GLN  |
| 1   | A     | 189 | HIS  |
| 1   | A     | 240 | HIS  |
| 1   | A     | 261 | HIS  |
| 1   | A     | 332 | GLN  |
| 1   | A     | 370 | GLN  |
| 1   | A     | 372 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 397  | HIS  |
| 1   | A     | 418  | ASN  |
| 1   | A     | 439  | ASN  |
| 1   | A     | 456  | GLN  |
| 1   | A     | 504  | ASN  |
| 1   | A     | 520  | GLN  |
| 1   | A     | 522  | HIS  |
| 1   | A     | 600  | HIS  |
| 1   | A     | 648  | ASN  |
| 1   | A     | 672  | ASN  |
| 1   | A     | 790  | ASN  |
| 1   | A     | 796  | GLN  |
| 1   | A     | 797  | HIS  |
| 1   | A     | 803  | HIS  |
| 1   | A     | 809  | GLN  |
| 1   | A     | 826  | ASN  |
| 1   | A     | 845  | GLN  |
| 1   | A     | 905  | HIS  |
| 1   | A     | 907  | ASN  |
| 1   | A     | 908  | ASN  |
| 1   | A     | 941  | ASN  |
| 1   | A     | 950  | ASN  |
| 1   | A     | 1055 | GLN  |
| 1   | A     | 1056 | ASN  |
| 1   | A     | 1059 | ASN  |
| 1   | A     | 1070 | HIS  |
| 1   | A     | 1140 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|------------------------------|-----------------------|-------|
| 1   | A     | 1114/1143 (97%) | 0.65   | 117 (10%) <b>11</b> <b>8</b> | 21, 70, 163, 211      | 0     |
| 2   | B     | 13/13 (100%)    | 1.16   | 2 (15%) <b>5</b> <b>4</b>    | 32, 34, 34, 50        | 0     |
| All | All   | 1127/1156 (97%) | 0.65   | 119 (10%) <b>11</b> <b>8</b> | 21, 70, 162, 211      | 0     |

All (119) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 366  | ASP  | 8.6  |
| 1   | A     | 508  | VAL  | 6.3  |
| 2   | B     | 21   | LEU  | 4.9  |
| 1   | A     | 751  | ALA  | 4.6  |
| 1   | A     | 425  | LEU  | 4.5  |
| 1   | A     | 462  | ASN  | 4.5  |
| 1   | A     | 616  | LEU  | 4.3  |
| 1   | A     | 708  | GLN  | 4.1  |
| 1   | A     | 613  | TYR  | 4.1  |
| 1   | A     | 460  | CYS  | 4.1  |
| 1   | A     | 682  | LEU  | 4.0  |
| 1   | A     | 842  | GLU  | 4.0  |
| 1   | A     | 1079 | GLU  | 4.0  |
| 1   | A     | 367  | LEU  | 3.9  |
| 1   | A     | 519  | LEU  | 3.9  |
| 1   | A     | 621  | GLY  | 3.8  |
| 1   | A     | 925  | ASP  | 3.8  |
| 1   | A     | 413  | LEU  | 3.8  |
| 1   | A     | 970  | ASN  | 3.7  |
| 1   | A     | 568  | ILE  | 3.7  |
| 1   | A     | 692  | ALA  | 3.7  |
| 1   | A     | 468  | LEU  | 3.5  |
| 1   | A     | 903  | CYS  | 3.5  |
| 1   | A     | 554  | PRO  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 924  | GLY  | 3.4  |
| 1   | A     | 426  | VAL  | 3.3  |
| 1   | A     | 690  | SER  | 3.3  |
| 1   | A     | 1096 | SER  | 3.3  |
| 1   | A     | 2    | SER  | 3.3  |
| 1   | A     | 29   | LEU  | 3.3  |
| 1   | A     | 502  | SER  | 3.2  |
| 1   | A     | 518  | TYR  | 3.2  |
| 1   | A     | 510  | VAL  | 3.1  |
| 1   | A     | 929  | SER  | 3.1  |
| 1   | A     | 703  | THR  | 3.1  |
| 1   | A     | 572  | PRO  | 3.0  |
| 1   | A     | 602  | LEU  | 3.0  |
| 1   | A     | 412  | PRO  | 3.0  |
| 1   | A     | 513  | GLY  | 3.0  |
| 1   | A     | 752  | LEU  | 3.0  |
| 1   | A     | 557  | ALA  | 3.0  |
| 1   | A     | 469  | ILE  | 2.9  |
| 1   | A     | 461  | GLY  | 2.9  |
| 1   | A     | 750  | THR  | 2.9  |
| 1   | A     | 689  | ASP  | 2.9  |
| 1   | A     | 295  | VAL  | 2.9  |
| 1   | A     | 430  | VAL  | 2.9  |
| 1   | A     | 680  | CYS  | 2.9  |
| 2   | B     | 12   | TRP  | 2.8  |
| 1   | A     | 745  | THR  | 2.8  |
| 1   | A     | 555  | LEU  | 2.8  |
| 1   | A     | 693  | LEU  | 2.8  |
| 1   | A     | 313  | CYS  | 2.7  |
| 1   | A     | 515  | ALA  | 2.7  |
| 1   | A     | 632  | GLY  | 2.7  |
| 1   | A     | 365  | VAL  | 2.7  |
| 1   | A     | 441  | GLU  | 2.7  |
| 1   | A     | 639  | ARG  | 2.7  |
| 1   | A     | 1059 | ASN  | 2.7  |
| 1   | A     | 1108 | VAL  | 2.7  |
| 1   | A     | 599  | SER  | 2.7  |
| 1   | A     | 623  | LEU  | 2.7  |
| 1   | A     | 773  | SER  | 2.7  |
| 1   | A     | 844  | LYS  | 2.6  |
| 1   | A     | 940  | GLY  | 2.6  |
| 1   | A     | 746  | SER  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 841  | ALA  | 2.6  |
| 1   | A     | 660  | TYR  | 2.6  |
| 1   | A     | 861  | VAL  | 2.6  |
| 1   | A     | 436  | LEU  | 2.6  |
| 1   | A     | 577  | LEU  | 2.6  |
| 1   | A     | 643  | SER  | 2.5  |
| 1   | A     | 840  | GLU  | 2.5  |
| 1   | A     | 28   | ASP  | 2.5  |
| 1   | A     | 357  | GLY  | 2.5  |
| 1   | A     | 629  | VAL  | 2.4  |
| 1   | A     | 1    | MET  | 2.4  |
| 1   | A     | 569  | LEU  | 2.4  |
| 1   | A     | 509  | VAL  | 2.4  |
| 1   | A     | 501  | ALA  | 2.4  |
| 1   | A     | 917  | LYS  | 2.4  |
| 1   | A     | 411  | TRP  | 2.3  |
| 1   | A     | 581  | MET  | 2.3  |
| 1   | A     | 294  | THR  | 2.3  |
| 1   | A     | 648  | ASN  | 2.3  |
| 1   | A     | 706  | GLU  | 2.3  |
| 1   | A     | 1124 | ALA  | 2.3  |
| 1   | A     | 859  | GLN  | 2.3  |
| 1   | A     | 571  | LEU  | 2.3  |
| 1   | A     | 598  | SER  | 2.3  |
| 1   | A     | 628  | LYS  | 2.3  |
| 1   | A     | 346  | TYR  | 2.3  |
| 1   | A     | 614  | PHE  | 2.3  |
| 1   | A     | 288  | GLU  | 2.3  |
| 1   | A     | 919  | ASP  | 2.3  |
| 1   | A     | 574  | PHE  | 2.2  |
| 1   | A     | 422  | TYR  | 2.2  |
| 1   | A     | 618  | ILE  | 2.2  |
| 1   | A     | 684  | SER  | 2.2  |
| 1   | A     | 592  | LEU  | 2.2  |
| 1   | A     | 843  | PRO  | 2.2  |
| 1   | A     | 18   | CYS  | 2.2  |
| 1   | A     | 556  | CYS  | 2.2  |
| 1   | A     | 297  | LEU  | 2.2  |
| 1   | A     | 983  | ALA  | 2.2  |
| 1   | A     | 552  | LEU  | 2.2  |
| 1   | A     | 634  | GLN  | 2.1  |
| 1   | A     | 483  | PRO  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 226  | PHE  | 2.1  |
| 1   | A     | 495  | ALA  | 2.1  |
| 1   | A     | 435  | VAL  | 2.1  |
| 1   | A     | 443  | VAL  | 2.1  |
| 1   | A     | 458  | PHE  | 2.1  |
| 1   | A     | 838  | PRO  | 2.1  |
| 1   | A     | 1110 | ALA  | 2.1  |
| 1   | A     | 397  | HIS  | 2.0  |
| 1   | A     | 507  | GLN  | 2.0  |
| 1   | A     | 222  | VAL  | 2.0  |
| 1   | A     | 1130 | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.