



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 PM UTC

PDB ID : 6OQ5 / pdb\_00006oq5  
Title : Structure of the full-length Clostridium difficile toxin B in complex with 3 VHHs  
Authors : Chen, P.; Lam, K.; Jin, R.  
Deposited on : 2019-04-25  
Resolution : 3.87 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                                                             |

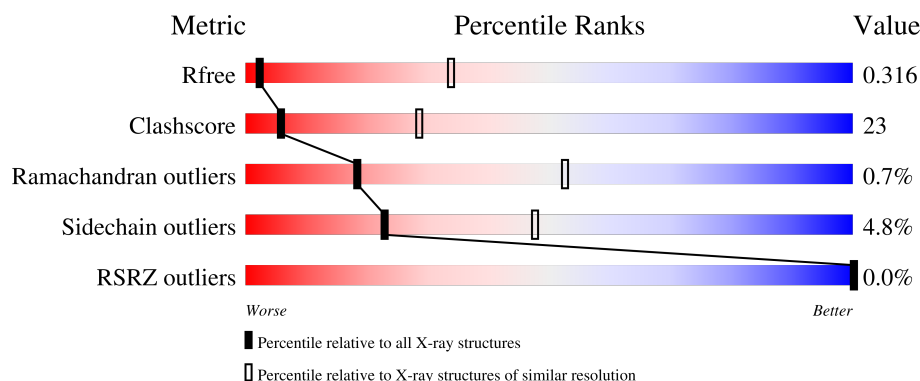
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.87 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                      | 1186 (4.06-3.70)                                      |
| Clashscore            | 190562                      | 1012 (4.04-3.72)                                      |
| Ramachandran outliers | 187476                      | 1167 (4.06-3.70)                                      |
| Sidechain outliers    | 187428                      | 1160 (4.06-3.70)                                      |
| RSRZ outliers         | 180081                      | 1185 (4.06-3.70)                                      |

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     | 2373   | <br>61% 35% . .      |
| 2   | D     | 153    | <br>52% 24% 7% 18% % |
| 3   | E     | 137    | <br>55% 23% . 22%    |
| 4   | F     | 142    | <br>51% 28% . 18%    |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21503 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 Toxin B.

| Mol | Chain | Residues | Atoms |       |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|---------|-------|
| 1   | A     | 2346     | Total | C     | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 18837 | 12009 | 2961 | 3820 | 47 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 2368    | HIS      | -      | expression tag | UNP M4NKV9 |
| A     | 2369    | HIS      | -      | expression tag | UNP M4NKV9 |
| A     | 2370    | HIS      | -      | expression tag | UNP M4NKV9 |
| A     | 2371    | HIS      | -      | expression tag | UNP M4NKV9 |
| A     | 2372    | HIS      | -      | expression tag | UNP M4NKV9 |
| A     | 2373    | HIS      | -      | expression tag | UNP M4NKV9 |

- Molecule 2 is a protein called 5D.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | D     | 126      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 986   | 617 | 179 | 187 | 3 |         |         |       |

- Molecule 3 is a protein called E3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | E     | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 802   | 498 | 141 | 159 | 4 |         |         |       |

- Molecule 4 is a protein called 7F.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | F     | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 544 | 154 | 172 | 6 |         |         |       |

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

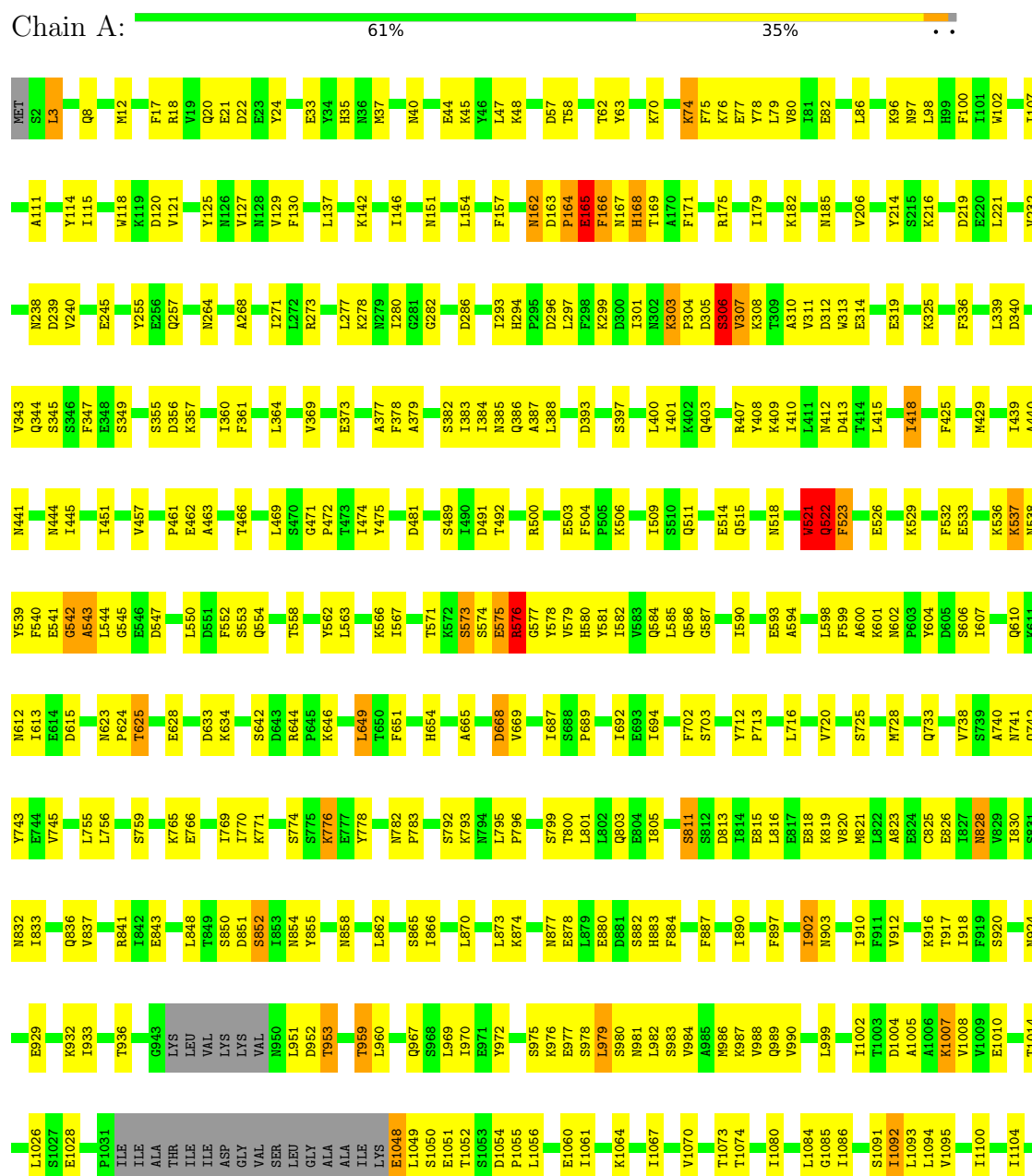
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

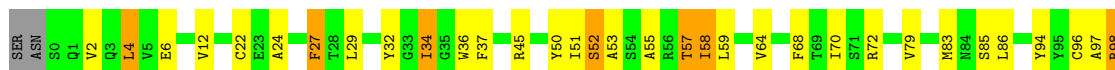
### 3 Residue-property plots

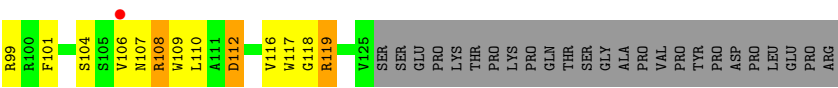
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

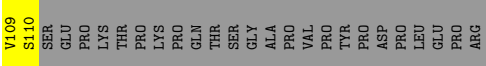


- Molecule 2: 5D

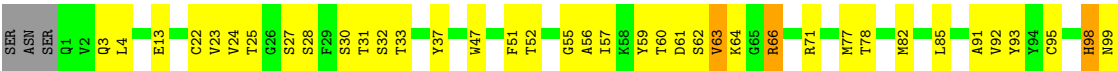




● Molecule 3: E3



● Molecule 4: 7F



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 149.62Å 168.56Å 179.92Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 48.91 – 3.87<br>48.91 – 3.87                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (48.91-3.87)<br>99.4 (48.91-3.87)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.37 (at 3.88Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0232                                             | Depositor        |
| R, $R_{free}$                                                           | 0.263 , 0.315<br>0.263 , 0.316                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2203 reflections (5.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 135.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.169                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 92.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 21503                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 169.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.42         | 0/19208     | 1.02        | 29/26012 (0.1%) |
| 2   | D     | 0.46         | 0/1006      | 0.96        | 2/1360 (0.1%)   |
| 3   | E     | 0.46         | 0/814       | 0.91        | 0/1098          |
| 4   | F     | 0.48         | 0/893       | 0.92        | 0/1206          |
| All | All   | 0.43         | 0/21921     | 1.01        | 31/29676 (0.1%) |

There are no bond length outliers.

All (31) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 2223 | TYR  | N-CA-C   | 9.68  | 124.39      | 112.59   |
| 1   | A     | 1195 | THR  | CB-CA-C  | 7.61  | 123.56      | 109.86   |
| 1   | A     | 1446 | GLN  | N-CA-C   | -6.91 | 103.44      | 110.97   |
| 1   | A     | 543  | ALA  | N-CA-C   | -6.46 | 105.03      | 113.17   |
| 2   | D     | 112  | ASP  | N-CA-C   | -6.44 | 105.58      | 113.50   |
| 1   | A     | 2122 | PHE  | CB-CA-C  | 6.19  | 119.55      | 110.26   |
| 1   | A     | 1238 | THR  | CB-CA-C  | 6.11  | 119.13      | 109.96   |
| 1   | A     | 2227 | PRO  | CB-CA-C  | -5.89 | 101.83      | 111.56   |
| 1   | A     | 575  | GLU  | CA-C-N   | 5.88  | 132.78      | 121.54   |
| 1   | A     | 575  | GLU  | C-N-CA   | 5.88  | 132.78      | 121.54   |
| 1   | A     | 2111 | TYR  | CB-CA-C  | -5.83 | 101.03      | 110.77   |
| 1   | A     | 1810 | ILE  | N-CA-C   | -5.83 | 107.60      | 113.20   |
| 2   | D     | 57   | THR  | CB-CA-C  | 5.77  | 120.54      | 111.77   |
| 1   | A     | 2109 | GLN  | CA-C-N   | 5.77  | 129.30      | 120.82   |
| 1   | A     | 2109 | GLN  | C-N-CA   | 5.77  | 129.30      | 120.82   |
| 1   | A     | 537  | LYS  | CB-CA-C  | 5.72  | 118.05      | 109.13   |
| 1   | A     | 2224 | TYR  | N-CA-C   | 5.67  | 118.03      | 109.41   |
| 1   | A     | 537  | LYS  | N-CA-C   | -5.66 | 107.37      | 114.56   |
| 1   | A     | 2112 | PHE  | CB-CA-C  | 5.61  | 118.78      | 109.53   |
| 1   | A     | 2122 | PHE  | CA-CB-CG | 5.53  | 119.33      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 1852 | ASN  | CB-CA-C  | -5.46 | 102.30      | 110.16   |
| 1   | A     | 165  | GLU  | N-CA-C   | -5.44 | 104.92      | 113.02   |
| 1   | A     | 2110 | TYR  | N-CA-C   | 5.44  | 117.31      | 110.24   |
| 1   | A     | 852  | SER  | N-CA-C   | -5.42 | 107.68      | 114.56   |
| 1   | A     | 1187 | HIS  | CB-CA-C  | -5.41 | 100.61      | 109.80   |
| 1   | A     | 2099 | TYR  | CB-CA-C  | 5.39  | 117.20      | 109.71   |
| 1   | A     | 245  | GLU  | N-CA-C   | -5.34 | 107.78      | 114.56   |
| 1   | A     | 166  | PHE  | CA-CB-CG | 5.32  | 119.12      | 113.80   |
| 1   | A     | 521  | TRP  | N-CA-C   | -5.18 | 107.09      | 113.41   |
| 1   | A     | 1639 | PHE  | CA-CB-CG | 5.14  | 118.94      | 113.80   |
| 1   | A     | 523  | PHE  | CA-CB-CG | 5.06  | 118.86      | 113.80   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 18837 | 0        | 18156    | 831     | 0            |
| 2   | D     | 986   | 0        | 959      | 90      | 0            |
| 3   | E     | 802   | 0        | 797      | 33      | 0            |
| 4   | F     | 876   | 0        | 856      | 41      | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 21503 | 0        | 20768    | 978     | 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 23.

All (978) 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:2107:ASP:CB  | 1:A:2137:ILE:HG22 | 1.73                     | 1.19              |
| 1:A:1847:LYS:HG3 | 1:A:1848:PRO:HD2  | 1.27                     | 1.16              |
| 1:A:2025:GLU:O   | 1:A:2026:MET:HG2  | 1.44                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:120:ASP:HB3   | 1:A:357:LYS:HD2   | 1.18                     | 1.14              |
| 1:A:625:THR:HB    | 1:A:628:GLU:HG2   | 1.25                     | 1.14              |
| 3:E:86:LYS:HB2    | 3:E:87:PRO:HD2    | 1.30                     | 1.13              |
| 2:D:37:PHE:CD2    | 2:D:117:TRP:HH2   | 1.68                     | 1.10              |
| 2:D:4:LEU:HD13    | 2:D:116:VAL:HG22  | 1.32                     | 1.07              |
| 1:A:1442:ASN:HA   | 1:A:1445:GLN:HE22 | 1.12                     | 1.07              |
| 2:D:53:ALA:HA     | 2:D:72:ARG:NH1    | 1.70                     | 1.05              |
| 1:A:743:TYR:HB3   | 1:A:755:LEU:HD11  | 1.38                     | 1.05              |
| 1:A:2315:ASN:HD22 | 1:A:2321:ILE:HG21 | 1.22                     | 1.01              |
| 1:A:2109:GLN:HG2  | 1:A:2132:PHE:CZ   | 1.95                     | 1.01              |
| 1:A:2107:ASP:HB2  | 1:A:2137:ILE:CG2  | 1.92                     | 0.99              |
| 2:D:37:PHE:HD2    | 2:D:117:TRP:CH2   | 1.82                     | 0.97              |
| 2:D:4:LEU:HD23    | 2:D:96:CYS:O      | 1.64                     | 0.96              |
| 2:D:4:LEU:HD22    | 2:D:117:TRP:CA    | 1.95                     | 0.96              |
| 1:A:1171:TRP:CZ2  | 1:A:1195:THR:HG21 | 2.01                     | 0.96              |
| 1:A:2107:ASP:HB2  | 1:A:2137:ILE:HG22 | 0.97                     | 0.96              |
| 2:D:64:VAL:HG11   | 2:D:68:PHE:CG     | 1.99                     | 0.96              |
| 1:A:165:GLU:O     | 1:A:165:GLU:HG3   | 1.63                     | 0.96              |
| 1:A:1074:THR:HG23 | 1:A:1416:ILE:HD11 | 1.46                     | 0.96              |
| 1:A:625:THR:HB    | 1:A:628:GLU:CG    | 1.94                     | 0.95              |
| 1:A:2193:VAL:HG23 | 1:A:2200:TYR:H    | 1.30                     | 0.95              |
| 3:E:85:LEU:HB2    | 3:E:86:LYS:HB3    | 1.45                     | 0.95              |
| 1:A:743:TYR:HB3   | 1:A:755:LEU:CD1   | 1.96                     | 0.94              |
| 1:A:1444:ILE:O    | 1:A:1448:ILE:HG13 | 1.69                     | 0.93              |
| 1:A:1026:LEU:HD22 | 1:A:1623:GLU:OE2  | 1.68                     | 0.93              |
| 1:A:1174:GLU:O    | 1:A:1192:PRO:HD2  | 1.68                     | 0.93              |
| 2:D:37:PHE:CD2    | 2:D:117:TRP:CH2   | 2.57                     | 0.93              |
| 1:A:2112:PHE:HB2  | 1:A:2116:GLY:HA3  | 1.50                     | 0.92              |
| 1:A:1178:GLY:O    | 1:A:1188:PHE:HB3  | 1.68                     | 0.92              |
| 2:D:64:VAL:HG11   | 2:D:68:PHE:CD2    | 2.04                     | 0.91              |
| 1:A:578:TYR:HD1   | 1:A:644:ARG:HE    | 1.13                     | 0.91              |
| 2:D:37:PHE:HD2    | 2:D:117:TRP:HH2   | 0.99                     | 0.91              |
| 1:A:2199:VAL:HG23 | 1:A:2232:ALA:HB3  | 1.52                     | 0.90              |
| 1:A:1848:PRO:CD   | 1:A:1849:PRO:HD3  | 2.01                     | 0.90              |
| 2:D:53:ALA:HA     | 2:D:72:ARG:HH12   | 1.35                     | 0.89              |
| 3:E:86:LYS:HB2    | 3:E:87:PRO:CD     | 2.01                     | 0.89              |
| 1:A:979:LEU:HD13  | 1:A:980:SER:H     | 1.37                     | 0.89              |
| 1:A:576:ARG:HG3   | 1:A:577:GLY:H     | 1.38                     | 0.88              |
| 1:A:1739:ILE:HG22 | 1:A:1844:TYR:OH   | 1.72                     | 0.88              |
| 1:A:1842:SER:HB2  | 1:A:1844:TYR:HE1  | 1.38                     | 0.88              |
| 1:A:1238:THR:HG22 | 1:A:1239:PRO:HD2  | 1.55                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:4:LEU:HD22    | 2:D:117:TRP:C     | 2.00                     | 0.86              |
| 1:A:1848:PRO:CG   | 1:A:1849:PRO:HD3  | 2.05                     | 0.86              |
| 1:A:2104:LEU:HA   | 1:A:2108:GLY:HA2  | 1.58                     | 0.85              |
| 1:A:2100:ILE:HG13 | 1:A:2114:ASP:HA   | 1.58                     | 0.85              |
| 1:A:1639:PHE:HB2  | 1:A:1646:TYR:HB2  | 1.59                     | 0.85              |
| 1:A:2099:TYR:O    | 1:A:2112:PHE:CE2  | 2.30                     | 0.84              |
| 2:D:37:PHE:HE1    | 2:D:109:TRP:CD1   | 1.95                     | 0.84              |
| 1:A:2087:SER:H    | 1:A:2117:ILE:HG23 | 1.43                     | 0.84              |
| 2:D:24:ALA:HB3    | 2:D:29:LEU:CD2    | 2.07                     | 0.84              |
| 1:A:125:TYR:HE2   | 1:A:364:LEU:HD12  | 1.39                     | 0.84              |
| 1:A:1494:LEU:HB3  | 1:A:1511:SER:HB3  | 1.59                     | 0.83              |
| 2:D:4:LEU:CD2     | 2:D:96:CYS:O      | 2.26                     | 0.83              |
| 1:A:268:ALA:HA    | 1:A:271:ILE:HD12  | 1.61                     | 0.82              |
| 1:A:2107:ASP:CB   | 1:A:2137:ILE:CG2  | 2.53                     | 0.82              |
| 1:A:1442:ASN:HA   | 1:A:1445:GLN:NE2  | 1.93                     | 0.82              |
| 1:A:1489:LEU:H    | 1:A:1493:VAL:HG12 | 1.45                     | 0.81              |
| 1:A:1848:PRO:HG2  | 1:A:1849:PRO:HD3  | 1.63                     | 0.81              |
| 1:A:1107:LEU:HB3  | 1:A:1112:LEU:HD23 | 1.61                     | 0.81              |
| 1:A:668:ASP:CG    | 1:A:669:VAL:N     | 2.39                     | 0.80              |
| 2:D:4:LEU:HB3     | 2:D:118:GLY:CA    | 2.12                     | 0.80              |
| 1:A:2107:ASP:OD1  | 1:A:2109:GLN:HG3  | 1.81                     | 0.80              |
| 1:A:1510:TYR:HE2  | 1:A:1545:LEU:HD11 | 1.45                     | 0.80              |
| 1:A:2105:ILE:HD13 | 1:A:2105:ILE:O    | 1.81                     | 0.80              |
| 2:D:4:LEU:HB3     | 2:D:118:GLY:HA2   | 1.63                     | 0.80              |
| 4:F:82:MET:HB3    | 4:F:85:LEU:HD21   | 1.63                     | 0.80              |
| 1:A:538:ASN:HB3   | 4:F:100:ALA:O     | 1.80                     | 0.80              |
| 1:A:2026:MET:C    | 1:A:2027:GLN:HE21 | 1.90                     | 0.80              |
| 1:A:2303:PHE:HD2  | 1:A:2361:ALA:HB2  | 1.47                     | 0.80              |
| 2:D:4:LEU:HD21    | 2:D:97:ALA:HA     | 1.62                     | 0.80              |
| 1:A:74:LYS:NZ     | 1:A:74:LYS:HA     | 1.97                     | 0.79              |
| 1:A:538:ASN:CB    | 4:F:100:ALA:O     | 2.30                     | 0.79              |
| 2:D:4:LEU:HD13    | 2:D:116:VAL:CG2   | 2.12                     | 0.79              |
| 1:A:2033:THR:HG21 | 1:A:2038:LYS:HE2  | 1.64                     | 0.79              |
| 1:A:977:GLU:HG3   | 1:A:1663:ASP:OD1  | 1.81                     | 0.79              |
| 1:A:1056:LEU:HD12 | 1:A:1056:LEU:O    | 1.83                     | 0.79              |
| 1:A:2120:VAL:HG12 | 1:A:2132:PHE:O    | 1.82                     | 0.79              |
| 1:A:576:ARG:HG2   | 1:A:1807:ASP:OD2  | 1.83                     | 0.79              |
| 1:A:770:ILE:HD12  | 1:A:805:ILE:HD11  | 1.64                     | 0.79              |
| 1:A:1174:GLU:O    | 1:A:1192:PRO:CD   | 2.32                     | 0.78              |
| 4:F:23:VAL:HG12   | 4:F:77:MET:HG3    | 1.65                     | 0.78              |
| 1:A:1859:THR:HA   | 1:A:1863:ASP:O    | 1.84                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2199:VAL:HG23 | 1:A:2232:ALA:CB   | 2.14                     | 0.78              |
| 1:A:120:ASP:HB3   | 1:A:357:LYS:CD    | 2.07                     | 0.78              |
| 1:A:2025:GLU:O    | 1:A:2026:MET:CG   | 2.31                     | 0.78              |
| 1:A:792:SER:HB3   | 1:A:843:GLU:HB3   | 1.66                     | 0.78              |
| 2:D:34:ILE:HG21   | 2:D:79:VAL:HG11   | 1.65                     | 0.78              |
| 1:A:255:TYR:HA    | 1:A:271:ILE:HD13  | 1.64                     | 0.77              |
| 4:F:32:SER:HB3    | 4:F:99:ASN:HB3    | 1.64                     | 0.77              |
| 1:A:2101:GLY:HA2  | 1:A:2111:TYR:CD1  | 2.18                     | 0.77              |
| 1:A:2102:LEU:H    | 1:A:2102:LEU:HD23 | 1.49                     | 0.77              |
| 1:A:571:THR:HG22  | 1:A:573:SER:OG    | 1.84                     | 0.77              |
| 1:A:1178:GLY:C    | 1:A:1188:PHE:HB3  | 2.10                     | 0.76              |
| 1:A:1842:SER:HB2  | 1:A:1844:TYR:CE1  | 2.20                     | 0.76              |
| 1:A:1178:GLY:O    | 1:A:1188:PHE:CB   | 2.33                     | 0.76              |
| 4:F:63:VAL:HG12   | 4:F:66:ARG:HH21   | 1.48                     | 0.76              |
| 2:D:6:GLU:OE2     | 2:D:118:GLY:HA3   | 1.86                     | 0.76              |
| 1:A:2109:GLN:HG2  | 1:A:2132:PHE:HZ   | 1.51                     | 0.76              |
| 1:A:356:ASP:CG    | 1:A:357:LYS:H     | 1.92                     | 0.76              |
| 1:A:1232:ALA:HB3  | 1:A:1280:LYS:HB2  | 1.67                     | 0.76              |
| 1:A:2245:TYR:HB3  | 1:A:2266:PHE:HE2  | 1.51                     | 0.76              |
| 1:A:792:SER:HB2   | 1:A:841:ARG:O     | 1.86                     | 0.75              |
| 3:E:85:LEU:HD23   | 3:E:85:LEU:H      | 1.52                     | 0.75              |
| 1:A:2201:TYR:CD2  | 1:A:2201:TYR:O    | 2.40                     | 0.74              |
| 1:A:2303:PHE:CD2  | 1:A:2361:ALA:HB2  | 2.22                     | 0.74              |
| 1:A:1196:TYR:HD1  | 1:A:1197:ARG:H    | 1.34                     | 0.74              |
| 3:E:9:GLY:HA3     | 3:E:18:LEU:HD22   | 1.70                     | 0.74              |
| 1:A:1751:ILE:CG2  | 1:A:1753:MET:HE2  | 2.17                     | 0.74              |
| 2:D:24:ALA:HB3    | 2:D:29:LEU:HD22   | 1.70                     | 0.74              |
| 1:A:403:GLN:O     | 1:A:407:ARG:HG3   | 1.87                     | 0.74              |
| 1:A:694:ILE:HB    | 1:A:738:VAL:HG23  | 1.70                     | 0.74              |
| 1:A:1678:SER:HB2  | 1:A:1706:THR:HG23 | 1.68                     | 0.74              |
| 1:A:1092:ILE:HG22 | 1:A:1093:LEU:N    | 2.01                     | 0.73              |
| 1:A:1092:ILE:CG2  | 1:A:1093:LEU:H    | 2.01                     | 0.73              |
| 1:A:1739:ILE:HG21 | 1:A:1844:TYR:HE2  | 1.53                     | 0.73              |
| 2:D:50:TYR:HE2    | 2:D:99:ARG:HD2    | 1.53                     | 0.73              |
| 1:A:668:ASP:CG    | 1:A:669:VAL:H     | 1.95                     | 0.73              |
| 1:A:1487:SER:HB3  | 1:A:1494:LEU:HD12 | 1.71                     | 0.73              |
| 3:E:7:SER:N       | 3:E:21:SER:O      | 2.22                     | 0.73              |
| 1:A:1171:TRP:CE2  | 1:A:1195:THR:HG21 | 2.24                     | 0.72              |
| 1:A:462:GLU:HG3   | 1:A:771:LYS:HE3   | 1.70                     | 0.72              |
| 1:A:1310:ARG:NH1  | 1:A:1331:TYR:HB3  | 2.04                     | 0.72              |
| 1:A:415:LEU:O     | 1:A:418:ILE:HG22  | 1.88                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1670:ILE:HD12 | 1:A:1671:SER:H    | 1.55                     | 0.72              |
| 3:E:9:GLY:O       | 3:E:107:VAL:HG22  | 1.88                     | 0.72              |
| 1:A:8:GLN:HG3     | 1:A:878:GLU:HB3   | 1.70                     | 0.72              |
| 2:D:37:PHE:CE1    | 2:D:109:TRP:CD1   | 2.78                     | 0.72              |
| 1:A:2298:ASN:HA   | 1:A:2303:PHE:CD1  | 2.24                     | 0.72              |
| 2:D:53:ALA:CA     | 2:D:72:ARG:HH12   | 2.03                     | 0.72              |
| 1:A:1209:VAL:HB   | 1:A:1211:LYS:HG3  | 1.71                     | 0.72              |
| 2:D:4:LEU:HD22    | 2:D:117:TRP:HA    | 1.70                     | 0.72              |
| 2:D:4:LEU:HD23    | 2:D:118:GLY:N     | 2.05                     | 0.72              |
| 1:A:216:LYS:HE2   | 1:A:221:LEU:HD21  | 1.72                     | 0.72              |
| 3:E:85:LEU:H      | 3:E:85:LEU:CD2    | 2.02                     | 0.72              |
| 1:A:578:TYR:HB2   | 1:A:646:LYS:HB3   | 1.70                     | 0.71              |
| 1:A:587:GLY:HA3   | 1:A:612:ASN:HD22  | 1.53                     | 0.71              |
| 1:A:114:TYR:OH    | 1:A:514:GLU:HB3   | 1.89                     | 0.71              |
| 1:A:2193:VAL:HG22 | 1:A:2201:TYR:H    | 1.55                     | 0.71              |
| 1:A:969:LEU:HD21  | 1:A:983:SER:HA    | 1.72                     | 0.71              |
| 2:D:50:TYR:CE2    | 2:D:99:ARG:HD2    | 2.25                     | 0.71              |
| 1:A:1706:THR:HB   | 1:A:1735:ASN:HD22 | 1.54                     | 0.71              |
| 2:D:4:LEU:CD2     | 2:D:118:GLY:N     | 2.54                     | 0.71              |
| 2:D:53:ALA:CA     | 2:D:72:ARG:NH1    | 2.50                     | 0.71              |
| 1:A:1070:VAL:HB   | 1:A:1416:ILE:HD13 | 1.73                     | 0.71              |
| 1:A:765:LYS:O     | 1:A:769:ILE:HG13  | 1.90                     | 0.71              |
| 1:A:1816:LEU:HD21 | 1:A:1823:LYS:HB3  | 1.71                     | 0.71              |
| 1:A:2109:GLN:HG2  | 1:A:2132:PHE:CE1  | 2.25                     | 0.71              |
| 1:A:294:HIS:HB3   | 1:A:297:LEU:HB2   | 1.73                     | 0.70              |
| 1:A:1950:LYS:HG3  | 1:A:1951:GLU:H    | 1.54                     | 0.70              |
| 1:A:2200:TYR:HD1  | 1:A:2230:LYS:O    | 1.73                     | 0.70              |
| 1:A:2245:TYR:CB   | 1:A:2266:PHE:HE2  | 2.05                     | 0.70              |
| 1:A:1858:VAL:CG2  | 1:A:1867:PHE:HE2  | 2.04                     | 0.70              |
| 4:F:33:THR:HG22   | 4:F:52:THR:HA     | 1.73                     | 0.70              |
| 1:A:793:LYS:H     | 1:A:836:GLN:HE22  | 1.40                     | 0.70              |
| 3:E:40:ALA:HB3    | 3:E:43:LYS:HD2    | 1.73                     | 0.69              |
| 1:A:1092:ILE:CG2  | 1:A:1093:LEU:N    | 2.56                     | 0.69              |
| 1:A:1650:VAL:HG23 | 1:A:1654:GLN:HE21 | 1.57                     | 0.69              |
| 1:A:1739:ILE:CD1  | 1:A:1740:ARG:HG3  | 2.23                     | 0.69              |
| 1:A:2295:GLY:HA2  | 1:A:2329:LEU:HD21 | 1.72                     | 0.69              |
| 1:A:803:GLN:NE2   | 1:A:1798:LEU:O    | 2.25                     | 0.69              |
| 1:A:2298:ASN:HA   | 1:A:2303:PHE:HD1  | 1.58                     | 0.69              |
| 1:A:1793:VAL:HA   | 1:A:1796:ILE:HD12 | 1.73                     | 0.69              |
| 1:A:1848:PRO:HD2  | 1:A:1849:PRO:HD3  | 1.73                     | 0.69              |
| 4:F:22:CYS:SG     | 4:F:78:THR:HG22   | 2.32                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2101:GLY:HA2  | 1:A:2111:TYR:CE1  | 2.28                     | 0.68              |
| 1:A:1486:VAL:HA   | 1:A:1495:ILE:HD12 | 1.75                     | 0.68              |
| 1:A:2102:LEU:HD23 | 1:A:2102:LEU:N    | 2.08                     | 0.68              |
| 1:A:576:ARG:NE    | 1:A:576:ARG:HA    | 2.09                     | 0.68              |
| 1:A:2309:GLN:HG3  | 1:A:2317:GLU:HB2  | 1.74                     | 0.68              |
| 1:A:578:TYR:H     | 1:A:646:LYS:HD3   | 1.57                     | 0.68              |
| 1:A:409:LYS:O     | 1:A:413:ASP:HB2   | 1.94                     | 0.68              |
| 1:A:1094:LEU:HD12 | 1:A:1094:LEU:O    | 1.93                     | 0.67              |
| 1:A:1150:ASP:OD1  | 1:A:1229:ARG:NH1  | 2.26                     | 0.67              |
| 1:A:1856:GLY:HA2  | 1:A:1866:TYR:CE1  | 2.29                     | 0.67              |
| 1:A:1942:ASN:O    | 1:A:1944:ARG:NE   | 2.25                     | 0.67              |
| 1:A:2033:THR:HG22 | 1:A:2034:GLU:N    | 2.09                     | 0.67              |
| 1:A:120:ASP:CB    | 1:A:357:LYS:HD2   | 2.12                     | 0.67              |
| 1:A:2199:VAL:CG2  | 1:A:2232:ALA:HB3  | 2.22                     | 0.67              |
| 1:A:1706:THR:HB   | 1:A:1735:ASN:ND2  | 2.09                     | 0.67              |
| 1:A:2193:VAL:CG2  | 1:A:2201:TYR:H    | 2.08                     | 0.67              |
| 1:A:1918:ASN:HD22 | 1:A:1924:ILE:HG21 | 1.60                     | 0.67              |
| 1:A:264:ASN:ND2   | 1:A:466:THR:HG21  | 2.10                     | 0.66              |
| 1:A:848:LEU:HD11  | 1:A:1805:TYR:CD1  | 2.31                     | 0.66              |
| 1:A:2090:TYR:HD2  | 1:A:2099:TYR:HD2  | 1.42                     | 0.66              |
| 1:A:2104:LEU:HG   | 1:A:2108:GLY:HA3  | 1.78                     | 0.66              |
| 1:A:1178:GLY:C    | 1:A:1188:PHE:CB   | 2.68                     | 0.66              |
| 1:A:1187:HIS:C    | 1:A:1188:PHE:CD1  | 2.74                     | 0.66              |
| 1:A:1152:VAL:HG12 | 1:A:1166:GLY:HA3  | 1.76                     | 0.66              |
| 1:A:1846:PHE:HB3  | 1:A:1851:ASN:HB2  | 1.77                     | 0.65              |
| 2:D:83:MET:HE1    | 2:D:94:TYR:CE2    | 2.31                     | 0.65              |
| 1:A:2109:GLN:CG   | 1:A:2132:PHE:CZ   | 2.78                     | 0.65              |
| 1:A:1489:LEU:HB2  | 1:A:1490:PRO:CD   | 2.27                     | 0.65              |
| 1:A:310:ALA:C     | 1:A:312:ASP:H     | 2.03                     | 0.65              |
| 1:A:162:ASN:OD1   | 1:A:162:ASN:N     | 2.26                     | 0.65              |
| 1:A:532:PHE:CZ    | 1:A:536:LYS:HD2   | 2.32                     | 0.65              |
| 1:A:1107:LEU:HB2  | 1:A:1111:GLU:O    | 1.97                     | 0.65              |
| 1:A:1187:HIS:C    | 1:A:1188:PHE:HD1  | 2.05                     | 0.65              |
| 1:A:1406:THR:HG22 | 1:A:1416:ILE:HG12 | 1.78                     | 0.65              |
| 1:A:2122:PHE:HB3  | 1:A:2131:TYR:CE1  | 2.32                     | 0.65              |
| 1:A:800:THR:OG1   | 1:A:1828:ASN:ND2  | 2.29                     | 0.65              |
| 1:A:1510:TYR:CE2  | 1:A:1545:LEU:HD11 | 2.30                     | 0.64              |
| 1:A:1310:ARG:HH12 | 1:A:1331:TYR:CB   | 2.10                     | 0.64              |
| 1:A:1358:ILE:HD11 | 2:D:104:SER:O     | 1.97                     | 0.64              |
| 1:A:1845:TYR:CE1  | 1:A:1860:VAL:CG2  | 2.80                     | 0.64              |
| 2:D:2:VAL:HG12    | 2:D:116:VAL:HG21  | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1489:LEU:HB2  | 1:A:1490:PRO:HD2  | 1.80                     | 0.64              |
| 2:D:64:VAL:CG1    | 2:D:68:PHE:CG     | 2.81                     | 0.63              |
| 1:A:1310:ARG:NH1  | 1:A:1331:TYR:CG   | 2.56                     | 0.63              |
| 1:A:2110:TYR:CD2  | 1:A:2132:PHE:CE2  | 2.87                     | 0.63              |
| 1:A:2226:ASP:OD1  | 1:A:2232:ALA:HB2  | 1.99                     | 0.63              |
| 3:E:51:MET:HE3    | 3:E:69:ILE:HG23   | 1.80                     | 0.63              |
| 1:A:1358:ILE:HG22 | 1:A:1362:LYS:O    | 1.99                     | 0.63              |
| 1:A:2193:VAL:HG21 | 1:A:2200:TYR:HB2  | 1.79                     | 0.63              |
| 1:A:576:ARG:HG3   | 1:A:577:GLY:N     | 2.09                     | 0.63              |
| 1:A:1131:VAL:HG22 | 1:A:1148:GLN:HG3  | 1.80                     | 0.63              |
| 1:A:2109:GLN:HA   | 1:A:2132:PHE:CE1  | 2.34                     | 0.63              |
| 1:A:2137:ILE:HD12 | 1:A:2138:ILE:O    | 1.98                     | 0.63              |
| 2:D:36:TRP:HD1    | 2:D:70:ILE:HD11   | 1.64                     | 0.63              |
| 2:D:37:PHE:CE1    | 2:D:109:TRP:HD1   | 2.17                     | 0.63              |
| 1:A:296:ASP:HA    | 1:A:299:LYS:HB2   | 1.80                     | 0.63              |
| 1:A:1094:LEU:O    | 1:A:1095:VAL:HG23 | 1.98                     | 0.63              |
| 1:A:2033:THR:HB   | 1:A:2036:GLY:O    | 1.99                     | 0.63              |
| 1:A:2110:TYR:HD1  | 1:A:2112:PHE:CD1  | 2.16                     | 0.63              |
| 4:F:3:GLN:HB2     | 4:F:25:THR:HB     | 1.80                     | 0.63              |
| 4:F:63:VAL:HG12   | 4:F:66:ARG:HD3    | 1.81                     | 0.63              |
| 1:A:451:ILE:HD12  | 1:A:451:ILE:O     | 1.98                     | 0.62              |
| 2:D:29:LEU:HD12   | 2:D:72:ARG:HH21   | 1.64                     | 0.62              |
| 4:F:37:TYR:OH     | 4:F:98:HIS:NE2    | 2.25                     | 0.62              |
| 1:A:2018:PHE:HE1  | 1:A:2053:GLU:HA   | 1.64                     | 0.62              |
| 1:A:1813:ASP:C    | 1:A:1826:ILE:HD11 | 2.24                     | 0.62              |
| 1:A:1171:TRP:CG   | 1:A:1195:THR:HG1  | 2.16                     | 0.62              |
| 1:A:1743:TRP:CH2  | 1:A:1797:ILE:HG23 | 2.34                     | 0.62              |
| 2:D:24:ALA:CB     | 2:D:29:LEU:HD22   | 2.29                     | 0.62              |
| 1:A:57:ASP:CG     | 1:A:76:LYS:NZ     | 2.57                     | 0.62              |
| 1:A:1516:ASP:OD1  | 1:A:1531:TYR:HE1  | 1.83                     | 0.62              |
| 4:F:63:VAL:HG12   | 4:F:66:ARG:HG3    | 1.80                     | 0.62              |
| 1:A:578:TYR:CD1   | 1:A:644:ARG:NE    | 2.64                     | 0.62              |
| 1:A:1846:PHE:CE2  | 1:A:1853:LEU:HB3  | 2.35                     | 0.62              |
| 1:A:1070:VAL:HB   | 1:A:1416:ILE:CD1  | 2.28                     | 0.62              |
| 1:A:1842:SER:CB   | 1:A:1844:TYR:HE1  | 2.10                     | 0.62              |
| 1:A:2033:THR:HG21 | 1:A:2038:LYS:CE   | 2.29                     | 0.62              |
| 1:A:2042:HIS:CD2  | 1:A:2051:GLU:OE2  | 2.52                     | 0.62              |
| 1:A:969:LEU:HD13  | 1:A:969:LEU:O     | 2.00                     | 0.62              |
| 1:A:1739:ILE:HD13 | 1:A:1740:ARG:HG3  | 1.82                     | 0.61              |
| 1:A:541:GLU:O     | 1:A:542:GLY:C     | 2.44                     | 0.61              |
| 1:A:1187:HIS:CD2  | 1:A:1268:PHE:HB2  | 2.35                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2266:PHE:CD1  | 1:A:2272:MET:HA   | 2.35                     | 0.61              |
| 1:A:1494:LEU:HB3  | 1:A:1511:SER:CB   | 2.29                     | 0.61              |
| 1:A:1739:ILE:HG21 | 1:A:1844:TYR:CE2  | 2.33                     | 0.61              |
| 1:A:1834:SER:HB2  | 1:A:1851:ASN:HD22 | 1.65                     | 0.61              |
| 1:A:1838:TYR:HE1  | 1:A:1843:LEU:HD12 | 1.66                     | 0.61              |
| 1:A:1409:ILE:HD11 | 1:A:1415:ALA:HB2  | 1.83                     | 0.61              |
| 1:A:2010:TYR:CG   | 1:A:2033:THR:HG23 | 2.36                     | 0.61              |
| 1:A:306:SER:O     | 1:A:308:LYS:N     | 2.33                     | 0.61              |
| 1:A:307:VAL:HG12  | 1:A:307:VAL:O     | 2.00                     | 0.61              |
| 1:A:855:TYR:HA    | 1:A:858:ASN:HD22  | 1.65                     | 0.61              |
| 1:A:1719:ILE:HA   | 1:A:1767:ARG:HB3  | 1.82                     | 0.61              |
| 1:A:1845:TYR:HB2  | 1:A:1867:PHE:CZ   | 2.36                     | 0.61              |
| 1:A:533:GLU:OE2   | 1:A:545:GLY:HA3   | 2.00                     | 0.61              |
| 1:A:951:LEU:HB3   | 1:A:1610:ASN:HD22 | 1.66                     | 0.60              |
| 1:A:1948:GLU:HA   | 1:A:1958:TYR:CE1  | 2.36                     | 0.60              |
| 1:A:2193:VAL:HG23 | 1:A:2200:TYR:N    | 2.10                     | 0.60              |
| 3:E:85:LEU:HB2    | 3:E:86:LYS:CB     | 2.25                     | 0.60              |
| 1:A:2266:PHE:HD1  | 1:A:2272:MET:HA   | 1.66                     | 0.60              |
| 1:A:532:PHE:CE2   | 1:A:536:LYS:HD2   | 2.36                     | 0.60              |
| 1:A:1373:LEU:HD11 | 1:A:1451:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:2112:PHE:HB2  | 1:A:2116:GLY:CA   | 2.27                     | 0.60              |
| 1:A:2112:PHE:CB   | 1:A:2116:GLY:HA3  | 2.28                     | 0.60              |
| 2:D:55:ALA:C      | 2:D:57:THR:H      | 2.09                     | 0.60              |
| 2:D:99:ARG:NH1    | 2:D:108:ARG:HG3   | 2.16                     | 0.60              |
| 1:A:356:ASP:CG    | 1:A:357:LYS:N     | 2.58                     | 0.60              |
| 1:A:1092:ILE:HG22 | 1:A:1093:LEU:H    | 1.64                     | 0.60              |
| 1:A:601:LYS:NZ    | 1:A:745:VAL:O     | 2.27                     | 0.60              |
| 1:A:1487:SER:HB3  | 1:A:1494:LEU:CD1  | 2.32                     | 0.60              |
| 1:A:2104:LEU:HG   | 1:A:2108:GLY:CA   | 2.32                     | 0.60              |
| 2:D:29:LEU:HD12   | 2:D:29:LEU:O      | 2.01                     | 0.60              |
| 1:A:586:GLN:HE21  | 1:A:665:ALA:HA    | 1.66                     | 0.60              |
| 1:A:37:MET:HG2    | 1:A:45:LYS:HZ3    | 1.67                     | 0.59              |
| 1:A:137:LEU:HB3   | 1:A:206:VAL:HG11  | 1.83                     | 0.59              |
| 1:A:1956:MET:HB2  | 1:A:1986:MET:HB3  | 1.82                     | 0.59              |
| 1:A:2098:ALA:O    | 1:A:2099:TYR:C    | 2.45                     | 0.59              |
| 1:A:2315:ASN:ND2  | 1:A:2321:ILE:HG21 | 2.05                     | 0.59              |
| 3:E:87:PRO:HA     | 3:E:109:VAL:HB    | 1.84                     | 0.59              |
| 1:A:70:LYS:HZ2    | 1:A:979:LEU:H     | 1.50                     | 0.59              |
| 1:A:1056:LEU:HD12 | 1:A:1056:LEU:C    | 2.27                     | 0.59              |
| 1:A:1453:PHE:CZ   | 1:A:1461:ILE:HD11 | 2.37                     | 0.59              |
| 1:A:820:VAL:HA    | 1:A:823:ALA:HB3   | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:17:PHE:HB2    | 1:A:1668:GLY:HA3  | 1.84                     | 0.59              |
| 1:A:874:LYS:HA    | 1:A:877:ASN:HB3   | 1.85                     | 0.59              |
| 1:A:325:LYS:HE3   | 1:A:360:ILE:HD11  | 1.84                     | 0.59              |
| 1:A:1238:THR:HG22 | 1:A:1239:PRO:CD   | 2.30                     | 0.59              |
| 1:A:100:PHE:HB2   | 1:A:129:VAL:HG22  | 1.84                     | 0.59              |
| 1:A:1751:ILE:HG22 | 1:A:1753:MET:HE2  | 1.83                     | 0.59              |
| 1:A:1678:SER:CB   | 1:A:1706:THR:HG23 | 2.33                     | 0.59              |
| 1:A:457:VAL:HA    | 1:A:463:ALA:HB1   | 1.84                     | 0.58              |
| 1:A:471:GLY:O     | 1:A:474:ILE:HG12  | 2.02                     | 0.58              |
| 1:A:2211:GLY:CA   | 1:A:2225:PHE:O    | 2.51                     | 0.58              |
| 2:D:45:ARG:NH1    | 2:D:117:TRP:CZ3   | 2.71                     | 0.58              |
| 1:A:310:ALA:O     | 1:A:313:TRP:HD1   | 1.86                     | 0.58              |
| 4:F:22:CYS:SG     | 4:F:78:THR:CG2    | 2.91                     | 0.58              |
| 1:A:571:THR:CG2   | 1:A:573:SER:OG    | 2.51                     | 0.58              |
| 1:A:2099:TYR:O    | 1:A:2112:PHE:HE2  | 1.86                     | 0.58              |
| 1:A:1512:ASN:O    | 1:A:1514:LEU:HD22 | 2.02                     | 0.58              |
| 1:A:1515:LYS:HE3  | 1:A:1531:TYR:CE2  | 2.39                     | 0.58              |
| 3:E:63:VAL:HA     | 3:E:66:ARG:HD2    | 1.85                     | 0.58              |
| 1:A:1843:LEU:C    | 1:A:1844:TYR:CD1  | 2.81                     | 0.58              |
| 1:A:2026:MET:O    | 1:A:2027:GLN:NE2  | 2.34                     | 0.58              |
| 3:E:66:ARG:HE     | 3:E:85:LEU:HD21   | 1.69                     | 0.58              |
| 1:A:1245:GLU:HB2  | 1:A:1249:THR:OG1  | 2.03                     | 0.58              |
| 1:A:1251:LEU:HA   | 1:A:1254:ARG:HD3  | 1.84                     | 0.58              |
| 1:A:2100:ILE:CG1  | 1:A:2114:ASP:HA   | 2.33                     | 0.58              |
| 1:A:278:LYS:HG3   | 1:A:393:ASP:HA    | 1.85                     | 0.58              |
| 1:A:21:GLU:HB3    | 1:A:63:TYR:HE2    | 1.69                     | 0.58              |
| 1:A:1155:GLU:HB3  | 1:A:1164:VAL:HG22 | 1.86                     | 0.58              |
| 1:A:1158:PHE:HD1  | 1:A:1216:LEU:HD13 | 1.69                     | 0.58              |
| 1:A:1742:VAL:HG23 | 1:A:1801:THR:HG22 | 1.85                     | 0.58              |
| 1:A:2311:THR:HB   | 1:A:2315:ASN:HD21 | 1.68                     | 0.58              |
| 2:D:50:TYR:CE1    | 2:D:51:ILE:O      | 2.56                     | 0.57              |
| 1:A:310:ALA:HB3   | 1:A:312:ASP:CG    | 2.29                     | 0.57              |
| 1:A:1858:VAL:HG21 | 1:A:1867:PHE:HE2  | 1.69                     | 0.57              |
| 1:A:2122:PHE:HB3  | 1:A:2131:TYR:HE1  | 1.69                     | 0.57              |
| 1:A:439:ILE:O     | 1:A:444:ASN:ND2   | 2.35                     | 0.57              |
| 1:A:1472:GLU:HG2  | 1:A:1487:SER:HA   | 1.85                     | 0.57              |
| 1:A:1908:TYR:HB2  | 1:A:1939:PHE:CZ   | 2.39                     | 0.57              |
| 1:A:2202:PHE:HD1  | 1:A:2208:ILE:HA   | 1.69                     | 0.57              |
| 1:A:1109:ASN:OD1  | 1:A:1110:ASN:N    | 2.37                     | 0.57              |
| 1:A:1462:PRO:HA   | 1:A:1475:PHE:HD1  | 1.69                     | 0.57              |
| 1:A:1918:ASN:ND2  | 1:A:1924:ILE:HG21 | 2.18                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2107:ASP:HB3  | 1:A:2137:ILE:CG2  | 2.32                     | 0.57              |
| 1:A:1563:VAL:O    | 1:A:1566:ILE:HG22 | 2.05                     | 0.57              |
| 1:A:2028:ILE:HD13 | 1:A:2042:HIS:CD2  | 2.39                     | 0.57              |
| 1:A:2090:TYR:HD2  | 1:A:2099:TYR:CD2  | 2.20                     | 0.57              |
| 1:A:325:LYS:HE3   | 1:A:360:ILE:CD1   | 2.35                     | 0.57              |
| 1:A:472:PRO:HA    | 1:A:475:TYR:HD2   | 1.70                     | 0.57              |
| 1:A:743:TYR:CB    | 1:A:755:LEU:HD11  | 2.25                     | 0.57              |
| 1:A:1907:LYS:HE3  | 1:A:1943:TYR:O    | 2.04                     | 0.57              |
| 3:E:7:SER:OG      | 3:E:21:SER:HB3    | 2.04                     | 0.57              |
| 1:A:1170:ILE:HB   | 1:A:1203:ILE:HD11 | 1.85                     | 0.57              |
| 1:A:883:HIS:HB2   | 1:A:981:ASN:HB3   | 1.87                     | 0.57              |
| 1:A:1152:VAL:HB   | 1:A:1204:TYR:HE2  | 1.70                     | 0.57              |
| 1:A:1180:THR:HG22 | 1:A:1187:HIS:O    | 2.05                     | 0.57              |
| 1:A:403:GLN:HE21  | 1:A:407:ARG:HE    | 1.52                     | 0.57              |
| 1:A:1203:ILE:O    | 1:A:1206:VAL:HG22 | 2.05                     | 0.57              |
| 2:D:36:TRP:CD1    | 2:D:70:ILE:HD11   | 2.40                     | 0.57              |
| 2:D:99:ARG:NH1    | 2:D:108:ARG:CG    | 2.68                     | 0.57              |
| 1:A:576:ARG:CG    | 1:A:1807:ASP:OD2  | 2.52                     | 0.56              |
| 1:A:2202:PHE:HE1  | 1:A:2208:ILE:HD12 | 1.70                     | 0.56              |
| 2:D:4:LEU:CD2     | 2:D:117:TRP:C     | 2.73                     | 0.56              |
| 1:A:582:ILE:HG12  | 1:A:598:LEU:HD23  | 1.87                     | 0.56              |
| 1:A:1981:ASN:HB2  | 1:A:1987:GLN:HE21 | 1.70                     | 0.56              |
| 1:A:303:LYS:HB2   | 1:A:303:LYS:NZ    | 2.20                     | 0.56              |
| 1:A:848:LEU:CD1   | 1:A:1805:TYR:CD1  | 2.87                     | 0.56              |
| 1:A:1788:LYS:HD2  | 1:A:1842:SER:OG   | 2.05                     | 0.56              |
| 1:A:1796:ILE:O    | 1:A:1800:PHE:HB2  | 2.04                     | 0.56              |
| 1:A:1698:ILE:O    | 1:A:1726:ILE:HG12 | 2.05                     | 0.56              |
| 1:A:2100:ILE:HD13 | 1:A:2100:ILE:C    | 2.31                     | 0.56              |
| 1:A:378:PHE:HB2   | 1:A:503:GLU:HB2   | 1.88                     | 0.56              |
| 1:A:986:MET:O     | 1:A:990:VAL:HG23  | 2.05                     | 0.56              |
| 1:A:1091:SER:O    | 1:A:1092:ILE:HG12 | 2.05                     | 0.56              |
| 1:A:1977:LYS:HE3  | 1:A:2023:ASN:OD1  | 2.05                     | 0.56              |
| 2:D:4:LEU:CD2     | 2:D:117:TRP:HA    | 2.35                     | 0.56              |
| 1:A:625:THR:CB    | 1:A:628:GLU:CG    | 2.76                     | 0.56              |
| 1:A:799:SER:HB3   | 1:A:1802:PRO:HG3  | 1.88                     | 0.56              |
| 1:A:1563:VAL:HG11 | 1:A:1622:PHE:CD2  | 2.41                     | 0.56              |
| 1:A:1698:ILE:HD12 | 1:A:1726:ILE:CG2  | 2.36                     | 0.56              |
| 1:A:1223:LEU:HB2  | 1:A:1302:PRO:HD3  | 1.87                     | 0.56              |
| 1:A:18:ARG:HD2    | 1:A:1669:ASP:HB3  | 1.88                     | 0.56              |
| 1:A:2032:ASN:HA   | 1:A:2037:PHE:HD1  | 1.71                     | 0.56              |
| 1:A:310:ALA:O     | 1:A:313:TRP:CD1   | 2.59                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:32:SER:CB     | 4:F:99:ASN:HB3    | 2.36                     | 0.55              |
| 1:A:1453:PHE:CE1  | 1:A:1461:ILE:HD11 | 2.41                     | 0.55              |
| 1:A:2194:ARG:HG2  | 1:A:2199:VAL:HG12 | 1.88                     | 0.55              |
| 1:A:1876:SER:HB2  | 1:A:1889:PHE:CD2  | 2.41                     | 0.55              |
| 1:A:1080:ILE:HG12 | 1:A:1220:LEU:HD21 | 1.86                     | 0.55              |
| 1:A:2193:VAL:O    | 1:A:2199:VAL:HA   | 2.06                     | 0.55              |
| 1:A:111:ALA:O     | 1:A:115:ILE:HG13  | 2.07                     | 0.55              |
| 1:A:1064:LYS:HA   | 1:A:1067:ILE:HD12 | 1.88                     | 0.55              |
| 2:D:50:TYR:CD1    | 2:D:51:ILE:N      | 2.74                     | 0.55              |
| 1:A:1510:TYR:HE2  | 1:A:1545:LEU:CD1  | 2.17                     | 0.55              |
| 1:A:2233:CYS:SG   | 1:A:2237:ASN:ND2  | 2.79                     | 0.55              |
| 2:D:37:PHE:CE2    | 2:D:117:TRP:HH2   | 2.23                     | 0.55              |
| 4:F:51:PHE:HD1    | 4:F:71:ARG:HD3    | 1.72                     | 0.55              |
| 1:A:96:LYS:HA     | 1:A:125:TYR:CD1   | 2.42                     | 0.55              |
| 1:A:1671:SER:OG   | 1:A:1672:SER:N    | 2.40                     | 0.55              |
| 1:A:1751:ILE:HG21 | 1:A:1753:MET:HE2  | 1.86                     | 0.55              |
| 1:A:2213:ILE:N    | 1:A:2224:TYR:O    | 2.39                     | 0.55              |
| 2:D:52:SER:HB3    | 2:D:57:THR:HB     | 1.88                     | 0.55              |
| 1:A:522:GLN:OE1   | 1:A:523:PHE:N     | 2.33                     | 0.55              |
| 1:A:1612:ILE:HG12 | 1:A:1625:ILE:HG22 | 1.89                     | 0.55              |
| 1:A:1998:HIS:CD2  | 1:A:2025:GLU:HA   | 2.42                     | 0.55              |
| 1:A:2356:PHE:HE1  | 1:A:2363:LEU:HD13 | 1.70                     | 0.55              |
| 1:A:378:PHE:CD1   | 1:A:382:SER:O     | 2.59                     | 0.55              |
| 1:A:1739:ILE:HD11 | 1:A:1740:ARG:HG3  | 1.88                     | 0.55              |
| 1:A:1743:TRP:CZ2  | 1:A:1797:ILE:HG23 | 2.42                     | 0.55              |
| 1:A:766:GLU:O     | 1:A:770:ILE:HG12  | 2.07                     | 0.54              |
| 1:A:379:ALA:HB2   | 1:A:384:ILE:HG22  | 1.90                     | 0.54              |
| 2:D:107:ASN:HB3   | 2:D:110:LEU:HG    | 1.88                     | 0.54              |
| 1:A:818:GLU:HA    | 1:A:821:MET:HB3   | 1.88                     | 0.54              |
| 1:A:1739:ILE:CG2  | 1:A:1844:TYR:CE2  | 2.91                     | 0.54              |
| 4:F:37:TYR:HD1    | 4:F:47:TRP:HA     | 1.73                     | 0.54              |
| 1:A:1951:GLU:OE2  | 1:A:1954:GLY:HA2  | 2.08                     | 0.54              |
| 1:A:2032:ASN:HB2  | 1:A:2037:PHE:HE1  | 1.72                     | 0.54              |
| 1:A:538:ASN:HB2   | 4:F:100:ALA:O     | 2.08                     | 0.54              |
| 1:A:1345:TRP:HB2  | 1:A:1403:VAL:HG12 | 1.90                     | 0.54              |
| 1:A:1515:LYS:HB3  | 1:A:1531:TYR:CE1  | 2.43                     | 0.54              |
| 4:F:63:VAL:HG12   | 4:F:66:ARG:CD     | 2.37                     | 0.54              |
| 1:A:884:PHE:CD2   | 1:A:902:ILE:HG22  | 2.43                     | 0.54              |
| 1:A:1901:SER:HB2  | 1:A:1906:PHE:CE1  | 2.42                     | 0.54              |
| 4:F:13:GLU:HA     | 4:F:115:SER:HB3   | 1.90                     | 0.54              |
| 1:A:17:PHE:HB2    | 1:A:1668:GLY:CA   | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:623:ASN:CG    | 1:A:624:PRO:HD2   | 2.33                     | 0.54              |
| 1:A:969:LEU:HD13  | 1:A:969:LEU:C     | 2.32                     | 0.54              |
| 1:A:1196:TYR:C    | 1:A:1198:GLU:N    | 2.62                     | 0.54              |
| 1:A:1373:LEU:HD21 | 1:A:1417:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:58:THR:HG23   | 3:E:33:THR:HG21   | 1.90                     | 0.54              |
| 1:A:1158:PHE:CD1  | 1:A:1216:LEU:HD13 | 2.43                     | 0.54              |
| 1:A:2102:LEU:H    | 1:A:2111:TYR:HD1  | 1.56                     | 0.54              |
| 1:A:537:LYS:HE3   | 1:A:542:GLY:HA2   | 1.89                     | 0.53              |
| 1:A:1308:TYR:HB2  | 2:D:101:PHE:CE2   | 2.43                     | 0.53              |
| 1:A:1358:ILE:HD11 | 2:D:104:SER:HB2   | 1.90                     | 0.53              |
| 1:A:1521:THR:HG22 | 1:A:1526:ASN:OD1  | 2.08                     | 0.53              |
| 1:A:1579:SER:HA   | 1:A:1631:ASN:HD21 | 1.72                     | 0.53              |
| 1:A:1740:ARG:NH2  | 1:A:1757:GLU:OE2  | 2.41                     | 0.53              |
| 1:A:57:ASP:CG     | 1:A:76:LYS:HZ1    | 2.16                     | 0.53              |
| 1:A:2153:ASP:OD1  | 1:A:2157:ILE:N    | 2.41                     | 0.53              |
| 1:A:2211:GLY:HA2  | 1:A:2225:PHE:O    | 2.08                     | 0.53              |
| 1:A:310:ALA:C     | 1:A:312:ASP:N     | 2.66                     | 0.53              |
| 1:A:506:LYS:HE2   | 1:A:511:GLN:HE22  | 1.73                     | 0.53              |
| 1:A:1048:GLU:HG3  | 1:A:1049:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:1155:GLU:HB3  | 1:A:1164:VAL:CG2  | 2.39                     | 0.53              |
| 1:A:1188:PHE:CD1  | 1:A:1188:PHE:N    | 2.76                     | 0.53              |
| 1:A:2212:TRP:HA   | 1:A:2212:TRP:CE3  | 2.44                     | 0.53              |
| 1:A:74:LYS:HA     | 1:A:74:LYS:CE     | 2.37                     | 0.53              |
| 1:A:277:LEU:HD11  | 1:A:388:LEU:HB3   | 1.90                     | 0.53              |
| 1:A:409:LYS:O     | 1:A:413:ASP:CB    | 2.56                     | 0.53              |
| 1:A:2033:THR:CG2  | 1:A:2034:GLU:N    | 2.71                     | 0.53              |
| 1:A:2202:PHE:CD1  | 1:A:2208:ILE:HA   | 2.43                     | 0.53              |
| 1:A:2112:PHE:CD1  | 1:A:2112:PHE:N    | 2.77                     | 0.53              |
| 1:A:2181:ASN:HD22 | 1:A:2187:VAL:HG11 | 1.74                     | 0.53              |
| 1:A:1187:HIS:HD2  | 1:A:1268:PHE:HB2  | 1.72                     | 0.53              |
| 1:A:1310:ARG:HG3  | 1:A:1311:GLU:HG2  | 1.90                     | 0.53              |
| 1:A:1701:ASP:HB3  | 1:A:1727:ASN:ND2  | 2.24                     | 0.53              |
| 4:F:63:VAL:CG1    | 4:F:66:ARG:HH21   | 2.18                     | 0.53              |
| 1:A:1515:LYS:HE2  | 1:A:1533:LEU:HG   | 1.91                     | 0.53              |
| 1:A:1522:LYS:O    | 1:A:1525:VAL:HG12 | 2.09                     | 0.53              |
| 4:F:63:VAL:HA     | 4:F:66:ARG:HD3    | 1.91                     | 0.53              |
| 1:A:70:LYS:NZ     | 1:A:979:LEU:H     | 2.07                     | 0.52              |
| 1:A:1379:GLU:HB2  | 1:A:1382:LYS:HB2  | 1.90                     | 0.52              |
| 1:A:1835:GLY:O    | 1:A:1846:PHE:HB2  | 2.09                     | 0.52              |
| 4:F:59:TYR:HB2    | 4:F:64:LYS:HD2    | 1.90                     | 0.52              |
| 1:A:541:GLU:O     | 1:A:543:ALA:N     | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:586:GLN:NE2   | 1:A:665:ALA:HA    | 2.23                     | 0.52              |
| 1:A:1194:ILE:HG12 | 1:A:1195:THR:H    | 1.73                     | 0.52              |
| 1:A:1310:ARG:NH1  | 1:A:1331:TYR:CB   | 2.69                     | 0.52              |
| 1:A:1994:ASN:O    | 1:A:1995:ASP:HB2  | 2.09                     | 0.52              |
| 3:E:85:LEU:HD23   | 3:E:85:LEU:N      | 2.23                     | 0.52              |
| 1:A:770:ILE:HG21  | 1:A:825:CYS:HB3   | 1.91                     | 0.52              |
| 1:A:1796:ILE:HG23 | 1:A:1800:PHE:CD2  | 2.44                     | 0.52              |
| 1:A:2102:LEU:H    | 1:A:2102:LEU:CD2  | 2.20                     | 0.52              |
| 1:A:154:LEU:O     | 1:A:157:PHE:HB2   | 2.09                     | 0.52              |
| 1:A:1950:LYS:CG   | 1:A:1951:GLU:H    | 2.21                     | 0.52              |
| 1:A:703:SER:HB2   | 1:A:740:ALA:HB3   | 1.90                     | 0.52              |
| 1:A:852:SER:O     | 1:A:855:TYR:N     | 2.43                     | 0.52              |
| 1:A:2336:PHE:CE1  | 1:A:2342:ALA:HB2  | 2.44                     | 0.52              |
| 2:D:4:LEU:HD23    | 2:D:118:GLY:H     | 1.74                     | 0.52              |
| 2:D:4:LEU:O       | 2:D:6:GLU:CD      | 2.53                     | 0.52              |
| 1:A:1049:LEU:O    | 1:A:1051:GLU:N    | 2.42                     | 0.52              |
| 1:A:1827:ASN:OD1  | 1:A:1831:MET:N    | 2.40                     | 0.52              |
| 1:A:1251:LEU:O    | 1:A:1255:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:576:ARG:CD    | 1:A:1807:ASP:OD2  | 2.58                     | 0.52              |
| 3:E:7:SER:OG      | 3:E:21:SER:CB     | 2.58                     | 0.52              |
| 4:F:82:MET:CB     | 4:F:85:LEU:HD21   | 2.38                     | 0.52              |
| 1:A:952:ASP:O     | 1:A:953:THR:HG23  | 2.11                     | 0.51              |
| 1:A:1130:LEU:O    | 1:A:1134:GLU:HB3  | 2.09                     | 0.51              |
| 1:A:1827:ASN:OD1  | 1:A:1830:GLY:N    | 2.41                     | 0.51              |
| 2:D:36:TRP:HD1    | 2:D:70:ILE:CD1    | 2.23                     | 0.51              |
| 1:A:1814:LEU:HA   | 1:A:1826:ILE:HD11 | 1.91                     | 0.51              |
| 1:A:1060:GLU:CD   | 1:A:1061:ILE:H    | 2.19                     | 0.51              |
| 1:A:1876:SER:HB2  | 1:A:1889:PHE:HD2  | 1.76                     | 0.51              |
| 2:D:107:ASN:O     | 2:D:108:ARG:HB2   | 2.10                     | 0.51              |
| 1:A:576:ARG:HD2   | 1:A:1807:ASP:CG   | 2.36                     | 0.51              |
| 1:A:1441:SER:O    | 1:A:1445:GLN:OE1  | 2.29                     | 0.51              |
| 1:A:2212:TRP:H    | 1:A:2225:PHE:HD1  | 1.58                     | 0.51              |
| 1:A:2286:PHE:HD1  | 1:A:2292:MET:HA   | 1.74                     | 0.51              |
| 2:D:52:SER:O      | 2:D:72:ARG:NH1    | 2.42                     | 0.51              |
| 1:A:2111:TYR:O    | 1:A:2119:GLN:HB2  | 2.11                     | 0.51              |
| 3:E:39:GLN:HB2    | 3:E:45:LEU:HD23   | 1.93                     | 0.51              |
| 1:A:795:LEU:N     | 1:A:796:PRO:CD    | 2.74                     | 0.51              |
| 1:A:1172:ARG:HD3  | 1:A:1198:GLU:HB3  | 1.90                     | 0.51              |
| 2:D:34:ILE:O      | 2:D:51:ILE:HG22   | 2.10                     | 0.51              |
| 1:A:547:ASP:OD1   | 1:A:547:ASP:N     | 2.44                     | 0.51              |
| 1:A:378:PHE:CD2   | 1:A:503:GLU:OE1   | 2.64                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1382:LYS:HG2  | 1:A:1391:ASN:OD1  | 2.11                     | 0.51              |
| 1:A:1627:ASP:HB3  | 1:A:1633:GLN:HB2  | 1.93                     | 0.51              |
| 1:A:2000:PHE:HE1  | 1:A:2006:MET:HB2  | 1.76                     | 0.51              |
| 1:A:2110:TYR:CD1  | 1:A:2112:PHE:CD1  | 2.98                     | 0.51              |
| 1:A:642:SER:O     | 1:A:687:ILE:HG22  | 2.11                     | 0.50              |
| 1:A:1177:SER:OG   | 1:A:1189:PHE:HB2  | 2.10                     | 0.50              |
| 2:D:4:LEU:HD11    | 2:D:116:VAL:HG13  | 1.93                     | 0.50              |
| 2:D:4:LEU:CD1     | 2:D:116:VAL:HG13  | 2.41                     | 0.50              |
| 1:A:1112:LEU:O    | 1:A:1280:LYS:HA   | 2.11                     | 0.50              |
| 1:A:1886:ASN:HB2  | 1:A:1923:ALA:HB3  | 1.93                     | 0.50              |
| 1:A:1901:SER:HB2  | 1:A:1906:PHE:HE1  | 1.75                     | 0.50              |
| 1:A:1901:SER:CB   | 1:A:1906:PHE:CE1  | 2.94                     | 0.50              |
| 1:A:2101:GLY:O    | 1:A:2102:LEU:C    | 2.53                     | 0.50              |
| 1:A:1007:LYS:O    | 1:A:1010:GLU:HB2  | 2.12                     | 0.50              |
| 1:A:1220:LEU:HA   | 1:A:1298:SER:O    | 2.12                     | 0.50              |
| 1:A:1855:THR:HG21 | 1:A:1869:PRO:CA   | 2.41                     | 0.50              |
| 1:A:1947:VAL:HA   | 1:A:1959:PHE:HB2  | 1.92                     | 0.50              |
| 4:F:63:VAL:HG12   | 4:F:66:ARG:CG     | 2.41                     | 0.50              |
| 1:A:725:SER:HB3   | 1:A:733:GLN:HB3   | 1.93                     | 0.50              |
| 1:A:303:LYS:HB2   | 1:A:303:LYS:HZ2   | 1.76                     | 0.50              |
| 1:A:933:ILE:HD11  | 1:A:959:THR:O     | 2.12                     | 0.50              |
| 1:A:1307:GLU:OE1  | 2:D:52:SER:HB2    | 2.11                     | 0.50              |
| 1:A:1698:ILE:HD12 | 1:A:1726:ILE:HG21 | 1.93                     | 0.50              |
| 1:A:1847:LYS:HG3  | 1:A:1848:PRO:CD   | 2.18                     | 0.50              |
| 1:A:1856:GLY:HA2  | 1:A:1866:TYR:CD1  | 2.47                     | 0.50              |
| 4:F:91:ALA:HB3    | 4:F:93:TYR:HE1    | 1.76                     | 0.50              |
| 1:A:801:LEU:O     | 1:A:805:ILE:HG12  | 2.11                     | 0.50              |
| 1:A:1196:TYR:O    | 1:A:1198:GLU:HB2  | 2.11                     | 0.50              |
| 1:A:1320:SER:O    | 1:A:1320:SER:OG   | 2.26                     | 0.50              |
| 1:A:1492:VAL:HG12 | 1:A:1492:VAL:O    | 2.11                     | 0.50              |
| 1:A:1739:ILE:HG22 | 1:A:1844:TYR:CZ   | 2.45                     | 0.50              |
| 1:A:125:TYR:CE2   | 1:A:364:LEU:HD12  | 2.31                     | 0.50              |
| 1:A:164:PRO:HG3   | 1:A:759:SER:HB3   | 1.94                     | 0.50              |
| 1:A:795:LEU:N     | 1:A:796:PRO:HD2   | 2.27                     | 0.50              |
| 1:A:1308:TYR:O    | 1:A:1312:LYS:HG2  | 2.12                     | 0.50              |
| 1:A:1499:TYR:CE2  | 1:A:1504:LYS:HG3  | 2.46                     | 0.50              |
| 1:A:1665:ASP:OD1  | 1:A:1670:ILE:O    | 2.30                     | 0.50              |
| 1:A:2106:ASN:N    | 1:A:2106:ASN:ND2  | 2.60                     | 0.50              |
| 1:A:466:THR:HA    | 1:A:469:LEU:HB3   | 1.94                     | 0.49              |
| 1:A:970:ILE:HD11  | 1:A:987:LYS:HE3   | 1.94                     | 0.49              |
| 1:A:339:LEU:HB2   | 1:A:344:GLN:HE21  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:576:ARG:CG    | 1:A:577:GLY:H     | 2.19                     | 0.49              |
| 1:A:1005:ALA:O    | 1:A:1008:VAL:HG22 | 2.12                     | 0.49              |
| 1:A:1107:LEU:HD23 | 1:A:1107:LEU:H    | 1.77                     | 0.49              |
| 1:A:2022:GLU:O    | 1:A:2023:ASN:ND2  | 2.43                     | 0.49              |
| 1:A:2211:GLY:HA2  | 1:A:2225:PHE:CD1  | 2.47                     | 0.49              |
| 1:A:425:PHE:CE1   | 1:A:429:MET:HE2   | 2.47                     | 0.49              |
| 1:A:1845:TYR:HE1  | 1:A:1860:VAL:CG2  | 2.23                     | 0.49              |
| 1:A:2110:TYR:HD1  | 1:A:2112:PHE:CE1  | 2.30                     | 0.49              |
| 1:A:2129:VAL:HG22 | 1:A:2183:TYR:CE1  | 2.47                     | 0.49              |
| 1:A:2130:PHE:CD2  | 1:A:2157:ILE:HD13 | 2.48                     | 0.49              |
| 1:A:8:GLN:CG      | 1:A:878:GLU:HB3   | 2.41                     | 0.49              |
| 1:A:77:GLU:O      | 1:A:80:VAL:N      | 2.45                     | 0.49              |
| 1:A:97:ASN:HB2    | 1:A:282:GLY:HA3   | 1.94                     | 0.49              |
| 1:A:1152:VAL:O    | 1:A:1166:GLY:N    | 2.45                     | 0.49              |
| 1:A:1738:SER:HA   | 1:A:1785:PHE:CD2  | 2.47                     | 0.49              |
| 2:D:51:ILE:HG13   | 2:D:58:ILE:HG13   | 1.93                     | 0.49              |
| 1:A:74:LYS:HA     | 1:A:74:LYS:HZ3    | 1.74                     | 0.49              |
| 1:A:98:LEU:HB2    | 1:A:127:VAL:HG22  | 1.93                     | 0.49              |
| 1:A:1948:GLU:HA   | 1:A:1958:TYR:CD1  | 2.48                     | 0.49              |
| 1:A:216:LYS:HG2   | 1:A:221:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:811:SER:O     | 1:A:813:ASP:N     | 2.44                     | 0.49              |
| 1:A:1052:THR:C    | 1:A:1055:PRO:HD2  | 2.37                     | 0.49              |
| 1:A:1955:GLU:HB3  | 1:A:1985:VAL:HG13 | 1.93                     | 0.49              |
| 1:A:33:GLU:HB3    | 1:A:48:LYS:NZ     | 2.28                     | 0.49              |
| 1:A:567:ILE:HG22  | 1:A:600:ALA:HB2   | 1.95                     | 0.49              |
| 1:A:518:ASN:O     | 1:A:521:TRP:HD1   | 1.96                     | 0.49              |
| 1:A:1094:LEU:HD12 | 1:A:1094:LEU:C    | 2.37                     | 0.49              |
| 1:A:2088:LYS:CD   | 1:A:2110:TYR:OH   | 2.60                     | 0.49              |
| 1:A:2193:VAL:CG2  | 1:A:2200:TYR:H    | 2.16                     | 0.49              |
| 1:A:57:ASP:CG     | 1:A:76:LYS:HZ3    | 2.21                     | 0.49              |
| 1:A:1845:TYR:CE1  | 1:A:1860:VAL:HG21 | 2.47                     | 0.49              |
| 1:A:2236:ILE:HA   | 1:A:2244:TYR:O    | 2.13                     | 0.49              |
| 1:A:293:ILE:HG23  | 1:A:297:LEU:HD23  | 1.95                     | 0.49              |
| 1:A:613:ILE:HG22  | 1:A:615:ASP:OD1   | 2.13                     | 0.49              |
| 1:A:815:GLU:O     | 1:A:819:LYS:HB2   | 2.12                     | 0.49              |
| 1:A:1844:TYR:CD1  | 1:A:1844:TYR:N    | 2.81                     | 0.48              |
| 1:A:2090:TYR:CD2  | 1:A:2099:TYR:HD2  | 2.27                     | 0.48              |
| 1:A:2223:TYR:HD1  | 1:A:2252:MET:HB3  | 1.78                     | 0.48              |
| 2:D:50:TYR:CE1    | 2:D:51:ILE:C      | 2.91                     | 0.48              |
| 1:A:1625:ILE:HG23 | 1:A:1635:TYR:HB2  | 1.95                     | 0.48              |
| 1:A:1665:ASP:CG   | 1:A:1670:ILE:O    | 2.56                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1670:ILE:HD12 | 1:A:1671:SER:O    | 2.13                     | 0.48              |
| 1:A:848:LEU:HD11  | 1:A:1805:TYR:CG   | 2.48                     | 0.48              |
| 1:A:1643:GLU:HA   | 1:A:1661:ASN:ND2  | 2.28                     | 0.48              |
| 1:A:1970:LEU:HA   | 1:A:1979:TYR:HA   | 1.94                     | 0.48              |
| 1:A:2208:ILE:CD1  | 1:A:2230:LYS:HG2  | 2.43                     | 0.48              |
| 1:A:2285:TYR:HB2  | 1:A:2306:PHE:CE2  | 2.48                     | 0.48              |
| 1:A:425:PHE:HE1   | 1:A:429:MET:HE2   | 1.79                     | 0.48              |
| 1:A:1028:GLU:O    | 1:A:1028:GLU:HG2  | 2.14                     | 0.48              |
| 1:A:1179:HIS:HA   | 1:A:1188:PHE:HB3  | 1.95                     | 0.48              |
| 1:A:1397:ASN:HA   | 1:A:1422:LEU:HD11 | 1.96                     | 0.48              |
| 1:A:1484:LEU:HB3  | 1:A:1497:LYS:HD2  | 1.94                     | 0.48              |
| 1:A:1814:LEU:HA   | 1:A:1826:ILE:CD1  | 2.43                     | 0.48              |
| 1:A:2090:TYR:CD2  | 1:A:2099:TYR:CD2  | 3.02                     | 0.48              |
| 1:A:1373:LEU:CD1  | 1:A:1451:ILE:HD12 | 2.42                     | 0.48              |
| 2:D:6:GLU:CD      | 2:D:118:GLY:HA3   | 2.38                     | 0.48              |
| 1:A:2032:ASN:HA   | 1:A:2037:PHE:CD1  | 2.48                     | 0.48              |
| 1:A:2033:THR:CB   | 1:A:2036:GLY:O    | 2.60                     | 0.48              |
| 1:A:547:ASP:HA    | 1:A:550:LEU:HD12  | 1.96                     | 0.48              |
| 1:A:933:ILE:HD12  | 1:A:960:LEU:HD23  | 1.96                     | 0.48              |
| 1:A:1843:LEU:C    | 1:A:1844:TYR:HD1  | 2.22                     | 0.48              |
| 1:A:12:MET:HE2    | 1:A:874:LYS:HD2   | 1.96                     | 0.48              |
| 1:A:311:VAL:CG1   | 1:A:314:GLU:OE1   | 2.61                     | 0.48              |
| 1:A:799:SER:O     | 1:A:803:GLN:HG2   | 2.14                     | 0.48              |
| 1:A:1803:SER:OG   | 1:A:1804:TYR:N    | 2.46                     | 0.48              |
| 2:D:22:CYS:HB3    | 2:D:79:VAL:HG12   | 1.96                     | 0.48              |
| 1:A:369:VAL:HB    | 1:A:373:GLU:OE2   | 2.14                     | 0.48              |
| 1:A:2212:TRP:CZ2  | 1:A:2239:ILE:HG21 | 2.48                     | 0.48              |
| 2:D:32:TYR:CD2    | 2:D:98:ARG:HD2    | 2.49                     | 0.48              |
| 1:A:313:TRP:CD1   | 1:A:313:TRP:H     | 2.30                     | 0.47              |
| 1:A:771:LYS:O     | 1:A:774:SER:OG    | 2.26                     | 0.47              |
| 1:A:830:ILE:HA    | 1:A:833:ILE:HG22  | 1.96                     | 0.47              |
| 1:A:866:ILE:O     | 1:A:870:LEU:N     | 2.42                     | 0.47              |
| 1:A:1440:ASN:O    | 1:A:1444:ILE:HG12 | 2.14                     | 0.47              |
| 1:A:2256:LEU:HA   | 1:A:2264:TYR:O    | 2.14                     | 0.47              |
| 1:A:118:TRP:HH2   | 1:A:509:ILE:HG22  | 1.79                     | 0.47              |
| 1:A:130:PHE:HE1   | 1:A:238:ASN:ND2   | 2.12                     | 0.47              |
| 1:A:897:PHE:CE2   | 1:A:917:THR:HA    | 2.49                     | 0.47              |
| 1:A:1824:PHE:HE1  | 1:A:1852:ASN:HA   | 1.79                     | 0.47              |
| 1:A:2088:LYS:CB   | 1:A:2118:MET:HG3  | 2.44                     | 0.47              |
| 1:A:1814:LEU:CA   | 1:A:1826:ILE:HD11 | 2.44                     | 0.47              |
| 4:F:52:THR:OG1    | 4:F:56:ALA:N      | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:580:HIS:O     | 1:A:606:SER:HA    | 2.14                     | 0.47              |
| 1:A:975:SER:O     | 1:A:976:LYS:HB2   | 2.14                     | 0.47              |
| 1:A:1996:ASN:HB3  | 1:A:2025:GLU:HB2  | 1.97                     | 0.47              |
| 4:F:51:PHE:CD1    | 4:F:71:ARG:HD3    | 2.49                     | 0.47              |
| 1:A:1174:GLU:HB3  | 1:A:1192:PRO:HG2  | 1.95                     | 0.47              |
| 1:A:22:ASP:OD2    | 3:E:96:LYS:HG2    | 2.14                     | 0.47              |
| 1:A:121:VAL:HG21  | 1:A:361:PHE:HB2   | 1.95                     | 0.47              |
| 1:A:562:TYR:HD1   | 1:A:566:LYS:HD2   | 1.79                     | 0.47              |
| 1:A:1652:ASN:O    | 1:A:1655:ASN:ND2  | 2.48                     | 0.47              |
| 1:A:1838:TYR:CE1  | 1:A:1843:LEU:HD12 | 2.47                     | 0.47              |
| 1:A:1857:PHE:CE1  | 1:A:1882:ILE:HD13 | 2.49                     | 0.47              |
| 1:A:2209:GLU:HB3  | 1:A:2213:ILE:HD11 | 1.96                     | 0.47              |
| 2:D:32:TYR:CG     | 2:D:98:ARG:HD2    | 2.49                     | 0.47              |
| 2:D:83:MET:HE1    | 2:D:94:TYR:CD2    | 2.50                     | 0.47              |
| 1:A:308:LYS:O     | 1:A:308:LYS:HG3   | 2.13                     | 0.47              |
| 1:A:1858:VAL:HG22 | 1:A:1867:PHE:HE2  | 1.79                     | 0.47              |
| 1:A:62:THR:HB     | 3:E:98:PRO:HB3    | 1.97                     | 0.47              |
| 1:A:355:SER:OG    | 1:A:356:ASP:N     | 2.48                     | 0.47              |
| 1:A:979:LEU:CD1   | 1:A:980:SER:H     | 2.19                     | 0.47              |
| 1:A:1174:GLU:O    | 1:A:1192:PRO:CG   | 2.63                     | 0.47              |
| 1:A:1670:ILE:CD1  | 1:A:1671:SER:H    | 2.26                     | 0.47              |
| 1:A:2214:TYR:HB2  | 1:A:2222:LYS:HB2  | 1.97                     | 0.47              |
| 2:D:4:LEU:HD22    | 2:D:117:TRP:N     | 2.29                     | 0.47              |
| 1:A:167:ASN:O     | 1:A:169:THR:N     | 2.48                     | 0.47              |
| 1:A:378:PHE:HD1   | 1:A:382:SER:O     | 1.98                     | 0.47              |
| 1:A:286:ASP:OD2   | 1:A:386:GLN:HG2   | 2.14                     | 0.46              |
| 1:A:575:GLU:O     | 1:A:576:ARG:O     | 2.33                     | 0.46              |
| 1:A:2110:TYR:HD2  | 1:A:2132:PHE:CE2  | 2.32                     | 0.46              |
| 1:A:2213:ILE:HB   | 1:A:2224:TYR:HB2  | 1.97                     | 0.46              |
| 3:E:55:ASN:OD1    | 3:E:71:ARG:NH2    | 2.46                     | 0.46              |
| 1:A:311:VAL:HG12  | 1:A:314:GLU:HB3   | 1.96                     | 0.46              |
| 1:A:1010:GLU:O    | 1:A:1014:THR:HB   | 2.16                     | 0.46              |
| 1:A:1516:ASP:OD1  | 1:A:1531:TYR:CE1  | 2.67                     | 0.46              |
| 1:A:558:THR:OG1   | 1:A:610:GLN:NE2   | 2.48                     | 0.46              |
| 1:A:820:VAL:HA    | 1:A:823:ALA:CB    | 2.45                     | 0.46              |
| 1:A:887:PHE:HB2   | 1:A:989:GLN:HG2   | 1.97                     | 0.46              |
| 1:A:1185:ILE:HD13 | 1:A:1242:ARG:HD2  | 1.98                     | 0.46              |
| 1:A:1238:THR:CG2  | 1:A:1239:PRO:HD2  | 2.36                     | 0.46              |
| 1:A:1703:ILE:HB   | 1:A:1732:VAL:HG22 | 1.97                     | 0.46              |
| 1:A:74:LYS:HA     | 1:A:74:LYS:HZ2    | 1.78                     | 0.46              |
| 1:A:340:ASP:OD1   | 1:A:343:VAL:HG23  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1180:THR:CG2  | 1:A:1187:HIS:HB2  | 2.45                     | 0.46              |
| 1:A:1810:ILE:HG13 | 1:A:1810:ILE:O    | 2.15                     | 0.46              |
| 1:A:2208:ILE:HD11 | 1:A:2230:LYS:HG2  | 1.96                     | 0.46              |
| 3:E:96:LYS:NZ     | 3:E:97:GLY:O      | 2.44                     | 0.46              |
| 4:F:59:TYR:HD2    | 4:F:64:LYS:HG3    | 1.80                     | 0.46              |
| 1:A:76:LYS:O      | 1:A:79:LEU:HB2    | 2.15                     | 0.46              |
| 1:A:712:TYR:CD1   | 1:A:713:PRO:HA    | 2.51                     | 0.46              |
| 1:A:932:LYS:HB3   | 1:A:959:THR:HG21  | 1.96                     | 0.46              |
| 1:A:969:LEU:HD11  | 1:A:983:SER:O     | 2.15                     | 0.46              |
| 1:A:2046:ASP:O    | 1:A:2047:LEU:HB2  | 2.15                     | 0.46              |
| 3:E:93:TYR:O      | 3:E:104:GLY:HA2   | 2.14                     | 0.46              |
| 1:A:850:SER:HB2   | 1:A:854:ASN:HB2   | 1.96                     | 0.46              |
| 1:A:1067:ILE:O    | 1:A:1070:VAL:HG22 | 2.16                     | 0.46              |
| 1:A:2246:PHE:HD1  | 1:A:2252:MET:HA   | 1.80                     | 0.46              |
| 3:E:13:GLN:HA     | 3:E:110:SER:HB3   | 1.98                     | 0.46              |
| 1:A:594:ALA:HB2   | 1:A:756:LEU:HD23  | 1.98                     | 0.46              |
| 1:A:1850:VAL:O    | 1:A:1851:ASN:CG   | 2.59                     | 0.46              |
| 1:A:1977:LYS:HD2  | 1:A:2023:ASN:HB2  | 1.98                     | 0.46              |
| 1:A:2112:PHE:C    | 1:A:2113:ASN:O    | 2.54                     | 0.46              |
| 1:A:1663:ASP:OD1  | 1:A:1663:ASP:O    | 2.34                     | 0.46              |
| 1:A:1563:VAL:HG11 | 1:A:1622:PHE:CE2  | 2.51                     | 0.46              |
| 1:A:1647:THR:HB   | 1:A:1657:ILE:HB   | 1.97                     | 0.46              |
| 1:A:1679:GLN:HG3  | 1:A:1715:TYR:HD1  | 1.80                     | 0.46              |
| 1:A:1734:ILE:HG21 | 1:A:1741:TYR:HE2  | 1.81                     | 0.46              |
| 1:A:1814:LEU:N    | 1:A:1826:ILE:HD11 | 2.31                     | 0.46              |
| 1:A:2107:ASP:OD1  | 1:A:2107:ASP:O    | 2.33                     | 0.46              |
| 4:F:4:LEU:HG      | 4:F:24:VAL:HG22   | 1.98                     | 0.46              |
| 1:A:1646:TYR:HE2  | 1:A:1681:TYR:HB2  | 1.81                     | 0.45              |
| 1:A:1784:ASN:OD1  | 1:A:1790:ASP:N    | 2.48                     | 0.45              |
| 1:A:1832:MET:HB3  | 1:A:1851:ASN:HD21 | 1.81                     | 0.45              |
| 1:A:2303:PHE:HB2  | 1:A:2342:ALA:HB3  | 1.97                     | 0.45              |
| 1:A:175:ARG:O     | 1:A:179:ILE:HG13  | 2.16                     | 0.45              |
| 1:A:590:ILE:HG21  | 1:A:654:HIS:CE1   | 2.51                     | 0.45              |
| 1:A:1619:ILE:HG21 | 1:A:1639:PHE:HD1  | 1.82                     | 0.45              |
| 1:A:2245:TYR:HB3  | 1:A:2266:PHE:CE2  | 2.42                     | 0.45              |
| 1:A:2315:ASN:HD22 | 1:A:2321:ILE:CG2  | 2.11                     | 0.45              |
| 3:E:7:SER:O       | 3:E:21:SER:N      | 2.45                     | 0.45              |
| 4:F:27:SER:OG     | 4:F:28:SER:N      | 2.49                     | 0.45              |
| 1:A:1662:TYR:C    | 1:A:1664:LEU:H    | 2.25                     | 0.45              |
| 1:A:1993:ILE:HG13 | 1:A:1998:HIS:CE1  | 2.52                     | 0.45              |
| 1:A:2221:ASP:HB3  | 1:A:2223:TYR:HE2  | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2235:GLY:O    | 1:A:2246:PHE:N    | 2.40                     | 0.45              |
| 1:A:377:ALA:HB2   | 1:A:387:ALA:HB3   | 1.97                     | 0.45              |
| 1:A:880:GLU:O     | 1:A:883:HIS:HD2   | 1.98                     | 0.45              |
| 1:A:967:GLN:NE2   | 1:A:970:ILE:HG21  | 2.31                     | 0.45              |
| 1:A:1140:LEU:HB3  | 1:A:1144:VAL:HG13 | 1.98                     | 0.45              |
| 1:A:1240:GLY:O    | 1:A:1241:LEU:HB2  | 2.15                     | 0.45              |
| 1:A:1835:GLY:H    | 1:A:1846:PHE:HB2  | 1.81                     | 0.45              |
| 1:A:1999:TYR:HB3  | 1:A:2020:PHE:CZ   | 2.52                     | 0.45              |
| 1:A:305:ASP:O     | 1:A:306:SER:CB    | 2.65                     | 0.45              |
| 1:A:1195:THR:HA   | 1:A:1196:TYR:HA   | 1.52                     | 0.45              |
| 1:A:97:ASN:ND2    | 1:A:280:ILE:HG12  | 2.32                     | 0.45              |
| 1:A:526:GLU:OE1   | 1:A:702:PHE:HB2   | 2.17                     | 0.45              |
| 1:A:1205:ASP:OD1  | 1:A:1205:ASP:N    | 2.41                     | 0.45              |
| 1:A:2033:THR:HG22 | 1:A:2035:ASP:H    | 1.81                     | 0.45              |
| 1:A:44:GLU:HA     | 1:A:47:LEU:HD12   | 1.99                     | 0.45              |
| 1:A:175:ARG:HE    | 1:A:179:ILE:HD11  | 1.82                     | 0.45              |
| 1:A:382:SER:OG    | 1:A:383:ILE:N     | 2.49                     | 0.45              |
| 1:A:1855:THR:HG21 | 1:A:1869:PRO:HA   | 1.98                     | 0.45              |
| 1:A:301:ILE:HG21  | 1:A:347:PHE:HE1   | 1.82                     | 0.45              |
| 1:A:929:GLU:O     | 1:A:933:ILE:HG12  | 2.17                     | 0.45              |
| 1:A:936:THR:HG21  | 1:A:960:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:1067:ILE:HG23 | 1:A:1464:SER:HB2  | 1.98                     | 0.45              |
| 1:A:1378:ILE:HG12 | 1:A:1419:VAL:HG21 | 1.98                     | 0.45              |
| 1:A:1967:PHE:HB3  | 1:A:1971:ASN:HD22 | 1.82                     | 0.45              |
| 1:A:2225:PHE:CD1  | 1:A:2225:PHE:C    | 2.92                     | 0.45              |
| 1:A:2088:LYS:HB3  | 1:A:2118:MET:CG   | 2.47                     | 0.45              |
| 1:A:2196:GLY:C    | 1:A:2198:ASP:H    | 2.24                     | 0.45              |
| 2:D:119:ARG:HG2   | 2:D:119:ARG:HH11  | 1.82                     | 0.45              |
| 1:A:182:LYS:HA    | 1:A:185:ASN:HD22  | 1.82                     | 0.45              |
| 1:A:866:ILE:O     | 1:A:870:LEU:HB2   | 2.17                     | 0.45              |
| 1:A:590:ILE:HG21  | 1:A:654:HIS:HE1   | 1.82                     | 0.44              |
| 1:A:2240:ASP:O    | 1:A:2242:ILE:HD12 | 2.17                     | 0.44              |
| 1:A:539:TYR:HD1   | 1:A:540:PHE:CD2   | 2.34                     | 0.44              |
| 1:A:1708:VAL:HA   | 1:A:1715:TYR:CE1  | 2.51                     | 0.44              |
| 1:A:1760:LYS:O    | 1:A:1763:GLN:NE2  | 2.49                     | 0.44              |
| 1:A:741:ASN:OD1   | 1:A:776:LYS:HD3   | 2.16                     | 0.44              |
| 1:A:1837:ILE:HG12 | 1:A:1838:TYR:N    | 2.32                     | 0.44              |
| 1:A:1967:PHE:HB3  | 1:A:1971:ASN:ND2  | 2.32                     | 0.44              |
| 1:A:2010:TYR:CD1  | 1:A:2033:THR:HG23 | 2.51                     | 0.44              |
| 1:A:2171:TYR:HB2  | 1:A:2202:PHE:CE2  | 2.52                     | 0.44              |
| 4:F:23:VAL:CG1    | 4:F:77:MET:HG3    | 2.43                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:257:GLN:NE2   | 1:A:412:ASN:HD21  | 2.15                     | 0.44              |
| 1:A:345:SER:O     | 1:A:349:SER:OG    | 2.28                     | 0.44              |
| 1:A:984:VAL:O     | 1:A:988:VAL:HG23  | 2.16                     | 0.44              |
| 1:A:1868:ASN:O    | 1:A:1870:ILE:N    | 2.51                     | 0.44              |
| 1:A:2110:TYR:HD2  | 1:A:2132:PHE:CD2  | 2.36                     | 0.44              |
| 1:A:2132:PHE:CE1  | 1:A:2136:GLY:O    | 2.71                     | 0.44              |
| 1:A:2171:TYR:HB2  | 1:A:2202:PHE:HE2  | 1.82                     | 0.44              |
| 1:A:37:MET:HG3    | 1:A:40:ASN:HD22   | 1.82                     | 0.44              |
| 1:A:168:HIS:O     | 1:A:171:PHE:HB3   | 2.18                     | 0.44              |
| 1:A:239:ASP:OD1   | 1:A:240:VAL:N     | 2.49                     | 0.44              |
| 1:A:576:ARG:HA    | 1:A:576:ARG:HE    | 1.79                     | 0.44              |
| 1:A:1357:THR:CG2  | 1:A:1364:LYS:HD3  | 2.48                     | 0.44              |
| 1:A:1999:TYR:HB3  | 1:A:2020:PHE:HZ   | 1.82                     | 0.44              |
| 1:A:2026:MET:CE   | 1:A:2052:GLY:HA3  | 2.47                     | 0.44              |
| 1:A:689:PRO:HD2   | 1:A:728:MET:SD    | 2.58                     | 0.44              |
| 1:A:1054:ASP:N    | 1:A:1055:PRO:HD2  | 2.33                     | 0.44              |
| 1:A:1670:ILE:HD12 | 1:A:1671:SER:N    | 2.29                     | 0.44              |
| 1:A:529:LYS:CD    | 1:A:742:GLN:HE22  | 2.31                     | 0.44              |
| 1:A:1351:ASN:OD1  | 1:A:1365:LYS:NZ   | 2.51                     | 0.44              |
| 1:A:2194:ARG:C    | 1:A:2196:GLY:H    | 2.25                     | 0.44              |
| 1:A:2216:MET:HB3  | 1:A:2219:GLU:O    | 2.17                     | 0.44              |
| 2:D:68:PHE:CD1    | 2:D:83:MET:HA     | 2.53                     | 0.44              |
| 1:A:539:TYR:O     | 1:A:540:PHE:C     | 2.61                     | 0.44              |
| 1:A:576:ARG:NE    | 1:A:576:ARG:CA    | 2.79                     | 0.44              |
| 1:A:776:LYS:HE3   | 1:A:778:TYR:OH    | 2.18                     | 0.44              |
| 1:A:2214:TYR:O    | 1:A:2222:LYS:CB   | 2.66                     | 0.44              |
| 1:A:257:GLN:CD    | 1:A:412:ASN:HD21  | 2.26                     | 0.44              |
| 1:A:880:GLU:O     | 1:A:883:HIS:CD2   | 2.71                     | 0.44              |
| 1:A:1627:ASP:OD1  | 1:A:1631:ASN:N    | 2.33                     | 0.44              |
| 1:A:1633:GLN:HG2  | 1:A:1654:GLN:HE22 | 1.82                     | 0.44              |
| 1:A:1860:VAL:N    | 1:A:1863:ASP:O    | 2.47                     | 0.44              |
| 3:E:66:ARG:HE     | 3:E:85:LEU:CD2    | 2.29                     | 0.44              |
| 1:A:999:LEU:HA    | 1:A:1002:ILE:HD12 | 1.99                     | 0.43              |
| 1:A:1109:ASN:C    | 1:A:1111:GLU:H    | 2.26                     | 0.43              |
| 1:A:1857:PHE:HE1  | 1:A:1882:ILE:HD13 | 1.82                     | 0.43              |
| 1:A:2130:PHE:HB3  | 1:A:2157:ILE:HA   | 2.00                     | 0.43              |
| 1:A:2200:TYR:CD1  | 1:A:2230:LYS:O    | 2.63                     | 0.43              |
| 1:A:264:ASN:HD21  | 1:A:466:THR:HG21  | 1.81                     | 0.43              |
| 1:A:602:ASN:C     | 1:A:604:TYR:H     | 2.25                     | 0.43              |
| 1:A:1484:LEU:HD21 | 1:A:1526:ASN:HB3  | 2.01                     | 0.43              |
| 1:A:1646:TYR:HE2  | 1:A:1681:TYR:CB   | 2.31                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2265:TYR:HB3  | 1:A:2286:PHE:CE2  | 2.52                     | 0.43              |
| 1:A:151:ASN:OD1   | 4:F:100:ALA:HB2   | 2.18                     | 0.43              |
| 1:A:377:ALA:HA    | 1:A:504:PHE:HB3   | 2.00                     | 0.43              |
| 1:A:1141:ASP:O    | 1:A:1143:LYS:HG2  | 2.18                     | 0.43              |
| 1:A:1960:SER:HB3  | 1:A:1964:GLY:H    | 1.82                     | 0.43              |
| 2:D:110:LEU:C     | 2:D:112:ASP:H     | 2.26                     | 0.43              |
| 1:A:1740:ARG:HH21 | 1:A:1756:SER:HB3  | 1.84                     | 0.43              |
| 1:A:1848:PRO:HG2  | 1:A:1849:PRO:CD   | 2.43                     | 0.43              |
| 1:A:2212:TRP:HA   | 1:A:2212:TRP:HE3  | 1.83                     | 0.43              |
| 3:E:66:ARG:NE     | 3:E:85:LEU:HD21   | 2.33                     | 0.43              |
| 1:A:378:PHE:HD2   | 1:A:503:GLU:OE1   | 2.00                     | 0.43              |
| 1:A:929:GLU:HA    | 1:A:932:LYS:HB2   | 2.00                     | 0.43              |
| 1:A:1287:ASN:HA   | 1:A:1314:SER:HB3  | 2.00                     | 0.43              |
| 1:A:2023:ASN:ND2  | 1:A:2023:ASN:C    | 2.76                     | 0.43              |
| 1:A:2031:PHE:O    | 1:A:2037:PHE:HA   | 2.18                     | 0.43              |
| 1:A:2305:TYR:HB2  | 1:A:2336:PHE:CZ   | 2.53                     | 0.43              |
| 3:E:9:GLY:HA3     | 3:E:18:LEU:CD2    | 2.46                     | 0.43              |
| 1:A:584:GLN:OE1   | 1:A:610:GLN:HG2   | 2.19                     | 0.43              |
| 1:A:1004:ASP:O    | 1:A:1008:VAL:HG13 | 2.18                     | 0.43              |
| 4:F:98:HIS:HA     | 4:F:104:SER:HB2   | 2.01                     | 0.43              |
| 1:A:33:GLU:HB3    | 1:A:48:LYS:HZ1    | 1.84                     | 0.43              |
| 1:A:716:LEU:O     | 1:A:720:VAL:HG22  | 2.18                     | 0.43              |
| 1:A:1648:LEU:HB2  | 1:A:1656:MET:SD   | 2.59                     | 0.43              |
| 1:A:2264:TYR:HE1  | 1:A:2291:VAL:HG22 | 1.84                     | 0.43              |
| 2:D:4:LEU:HD21    | 2:D:96:CYS:O      | 2.13                     | 0.43              |
| 1:A:1092:ILE:HG23 | 1:A:1093:LEU:H    | 1.78                     | 0.43              |
| 1:A:585:LEU:HD22  | 1:A:651:PHE:HB3   | 2.01                     | 0.43              |
| 1:A:884:PHE:HD2   | 1:A:902:ILE:HG22  | 1.83                     | 0.43              |
| 1:A:897:PHE:HE2   | 1:A:917:THR:HA    | 1.84                     | 0.43              |
| 3:E:5:VAL:O       | 3:E:23:ALA:N      | 2.51                     | 0.43              |
| 1:A:17:PHE:CB     | 1:A:1668:GLY:HA3  | 2.48                     | 0.43              |
| 1:A:214:TYR:O     | 4:F:30:SER:OG     | 2.32                     | 0.43              |
| 1:A:539:TYR:CE2   | 4:F:98:HIS:O      | 2.71                     | 0.43              |
| 1:A:578:TYR:O     | 1:A:579:VAL:C     | 2.62                     | 0.43              |
| 1:A:1108:VAL:HG23 | 1:A:1109:ASN:H    | 1.84                     | 0.43              |
| 1:A:1755:THR:O    | 1:A:1755:THR:HG22 | 2.17                     | 0.43              |
| 1:A:1858:VAL:HG22 | 1:A:1867:PHE:CE2  | 2.54                     | 0.43              |
| 1:A:1112:LEU:HD12 | 1:A:1283:TYR:HE2  | 1.84                     | 0.42              |
| 1:A:1800:PHE:HA   | 1:A:1840:ASN:HA   | 2.00                     | 0.42              |
| 1:A:1976:ASP:OD2  | 1:A:2005:VAL:HB   | 2.19                     | 0.42              |
| 2:D:24:ALA:HB1    | 2:D:27:PHE:CZ     | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:27:PHE:N      | 2:D:27:PHE:CD1    | 2.86                     | 0.42              |
| 1:A:77:GLU:O      | 1:A:80:VAL:HB     | 2.19                     | 0.42              |
| 1:A:1085:GLY:C    | 1:A:1086:ILE:HG13 | 2.44                     | 0.42              |
| 1:A:1104:ILE:HD12 | 1:A:1104:ILE:H    | 1.84                     | 0.42              |
| 1:A:1237:TRP:HZ3  | 1:A:1272:ALA:O    | 2.02                     | 0.42              |
| 1:A:1372:ILE:O    | 1:A:1375:THR:OG1  | 2.29                     | 0.42              |
| 1:A:1514:LEU:HD22 | 1:A:1514:LEU:N    | 2.35                     | 0.42              |
| 1:A:1674:VAL:HG12 | 1:A:1702:GLU:HB3  | 2.01                     | 0.42              |
| 1:A:2088:LYS:HB3  | 1:A:2118:MET:HG3  | 2.01                     | 0.42              |
| 1:A:2106:ASN:N    | 1:A:2106:ASN:HD22 | 2.16                     | 0.42              |
| 2:D:24:ALA:CB     | 2:D:29:LEU:CD2    | 2.86                     | 0.42              |
| 4:F:52:THR:HG1    | 4:F:56:ALA:H      | 1.63                     | 0.42              |
| 1:A:142:LYS:O     | 1:A:146:ILE:HG13  | 2.20                     | 0.42              |
| 1:A:581:TYR:CE1   | 1:A:607:ILE:HB    | 2.54                     | 0.42              |
| 1:A:978:SER:HB3   | 1:A:1662:TYR:HE2  | 1.83                     | 0.42              |
| 1:A:1409:ILE:CD1  | 1:A:1415:ALA:HB2  | 2.46                     | 0.42              |
| 1:A:1592:LYS:HG2  | 1:A:1605:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:1613:ILE:HG23 | 1:A:1624:PHE:HB2  | 2.00                     | 0.42              |
| 1:A:2110:TYR:CD1  | 1:A:2112:PHE:CE1  | 3.07                     | 0.42              |
| 1:A:2118:MET:O    | 1:A:2119:GLN:C    | 2.62                     | 0.42              |
| 2:D:64:VAL:HG11   | 2:D:68:PHE:CD1    | 2.51                     | 0.42              |
| 1:A:3:LEU:HD11    | 1:A:35:HIS:HA     | 2.01                     | 0.42              |
| 1:A:1757:GLU:HG3  | 1:A:1764:VAL:HG23 | 2.01                     | 0.42              |
| 1:A:1817:VAL:HB   | 1:A:1819:LEU:HD23 | 2.00                     | 0.42              |
| 1:A:1825:TYR:HB3  | 1:A:1833:VAL:HG11 | 2.00                     | 0.42              |
| 1:A:2102:LEU:N    | 1:A:2102:LEU:CD2  | 2.78                     | 0.42              |
| 1:A:2229:THR:O    | 1:A:2230:LYS:HB2  | 2.18                     | 0.42              |
| 1:A:20:GLN:HG3    | 1:A:24:TYR:CE2    | 2.54                     | 0.42              |
| 1:A:461:PRO:HA    | 1:A:523:PHE:CD2   | 2.55                     | 0.42              |
| 1:A:1233:TRP:CE3  | 1:A:1276:ILE:HG12 | 2.54                     | 0.42              |
| 1:A:1308:TYR:HB2  | 2:D:101:PHE:HE2   | 1.83                     | 0.42              |
| 1:A:12:MET:HE1    | 1:A:878:GLU:HG3   | 2.02                     | 0.42              |
| 1:A:441:ASN:O     | 1:A:445:ILE:HB    | 2.19                     | 0.42              |
| 1:A:1349:VAL:HB   | 1:A:1352:VAL:HG22 | 2.00                     | 0.42              |
| 1:A:1358:ILE:CD1  | 2:D:104:SER:HB2   | 2.49                     | 0.42              |
| 1:A:1563:VAL:HG11 | 1:A:1622:PHE:HD2  | 1.84                     | 0.42              |
| 1:A:1616:THR:HG22 | 1:A:1621:GLN:HB3  | 2.01                     | 0.42              |
| 1:A:1694:ILE:HG22 | 1:A:1696:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:1881:ILE:O    | 1:A:1882:ILE:HG13 | 2.19                     | 0.42              |
| 2:D:29:LEU:CD1    | 2:D:72:ARG:HH21   | 2.31                     | 0.42              |
| 1:A:522:GLN:OE1   | 1:A:522:GLN:HA    | 2.09                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:552:PHE:HB2   | 1:A:554:GLN:HG2   | 2.02                     | 0.42              |
| 1:A:593:GLU:OE1   | 1:A:593:GLU:HA    | 2.20                     | 0.42              |
| 1:A:2221:ASP:HB3  | 1:A:2223:TYR:CE2  | 2.54                     | 0.42              |
| 2:D:55:ALA:C      | 2:D:57:THR:N      | 2.76                     | 0.42              |
| 1:A:407:ARG:HA    | 1:A:410:ILE:HD12  | 2.01                     | 0.42              |
| 1:A:481:ASP:OD1   | 1:A:489:SER:HB3   | 2.19                     | 0.42              |
| 1:A:539:TYR:HD1   | 1:A:540:PHE:CE2   | 2.37                     | 0.42              |
| 1:A:916:LYS:HG3   | 1:A:918:ILE:HB    | 2.02                     | 0.42              |
| 1:A:2021:ALA:O    | 1:A:2024:GLY:N    | 2.53                     | 0.42              |
| 1:A:2233:CYS:SG   | 1:A:2237:ASN:HB2  | 2.59                     | 0.42              |
| 1:A:980:SER:C     | 1:A:982:LEU:H     | 2.28                     | 0.42              |
| 1:A:1204:TYR:HD1  | 1:A:1204:TYR:HA   | 1.72                     | 0.42              |
| 1:A:1357:THR:HG23 | 1:A:1364:LYS:HD3  | 2.01                     | 0.42              |
| 1:A:1825:TYR:O    | 1:A:1833:VAL:HG12 | 2.18                     | 0.42              |
| 1:A:1848:PRO:N    | 1:A:1849:PRO:HD3  | 2.35                     | 0.42              |
| 1:A:2211:GLY:N    | 1:A:2225:PHE:O    | 2.52                     | 0.42              |
| 2:D:4:LEU:CB      | 2:D:118:GLY:HA2   | 2.43                     | 0.42              |
| 1:A:920:SER:O     | 1:A:924:ASN:ND2   | 2.53                     | 0.42              |
| 1:A:1373:LEU:CD2  | 1:A:1417:ILE:HD11 | 2.50                     | 0.42              |
| 1:A:1738:SER:H    | 1:A:1787:ASP:CG   | 2.28                     | 0.42              |
| 1:A:1866:TYR:CG   | 1:A:1882:ILE:HD11 | 2.55                     | 0.42              |
| 1:A:1894:VAL:CG2  | 1:A:1896:GLN:HE21 | 2.33                     | 0.42              |
| 1:A:1938:TYR:HB3  | 1:A:1959:PHE:HE2  | 1.85                     | 0.42              |
| 2:D:12:VAL:HG21   | 2:D:86:LEU:CD1    | 2.50                     | 0.42              |
| 4:F:60:THR:HG23   | 4:F:62:SER:O      | 2.20                     | 0.42              |
| 1:A:77:GLU:O      | 1:A:78:TYR:C      | 2.61                     | 0.41              |
| 1:A:151:ASN:ND2   | 4:F:31:THR:O      | 2.53                     | 0.41              |
| 1:A:743:TYR:HB3   | 1:A:755:LEU:HD13  | 1.92                     | 0.41              |
| 1:A:862:LEU:O     | 1:A:865:SER:HB2   | 2.20                     | 0.41              |
| 1:A:1049:LEU:O    | 1:A:1050:SER:C    | 2.63                     | 0.41              |
| 1:A:1173:MET:HB2  | 1:A:1262:GLU:O    | 2.20                     | 0.41              |
| 1:A:1178:GLY:O    | 1:A:1188:PHE:CA   | 2.68                     | 0.41              |
| 1:A:1847:LYS:CG   | 1:A:1848:PRO:HD2  | 2.20                     | 0.41              |
| 1:A:408:TYR:HE1   | 1:A:469:LEU:HD21  | 1.85                     | 0.41              |
| 1:A:440:ALA:HB1   | 1:A:445:ILE:HD13  | 2.01                     | 0.41              |
| 1:A:515:GLN:HA    | 1:A:518:ASN:HB2   | 2.01                     | 0.41              |
| 1:A:1358:ILE:H    | 1:A:1358:ILE:HG12 | 1.70                     | 0.41              |
| 1:A:2033:THR:CG2  | 1:A:2034:GLU:H    | 2.33                     | 0.41              |
| 1:A:62:THR:CG2    | 3:E:98:PRO:HB3    | 2.51                     | 0.41              |
| 1:A:273:ARG:NH1   | 1:A:385:ASN:O     | 2.49                     | 0.41              |
| 1:A:1223:LEU:HB3  | 1:A:1315:TYR:CE1  | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1950:LYS:HG3  | 1:A:1951:GLU:N    | 2.28                     | 0.41              |
| 2:D:22:CYS:HB3    | 2:D:79:VAL:CG1    | 2.50                     | 0.41              |
| 1:A:539:TYR:CD1   | 1:A:540:PHE:CE2   | 3.08                     | 0.41              |
| 1:A:563:LEU:HD21  | 1:A:599:PHE:CD2   | 2.56                     | 0.41              |
| 1:A:976:LYS:HD3   | 1:A:976:LYS:HA    | 1.89                     | 0.41              |
| 1:A:1373:LEU:HD11 | 1:A:1451:ILE:CD1  | 2.49                     | 0.41              |
| 3:E:50:SER:O      | 3:E:58:ILE:CG2    | 2.68                     | 0.41              |
| 4:F:52:THR:HG1    | 4:F:55:GLY:H      | 1.63                     | 0.41              |
| 1:A:581:TYR:HB3   | 1:A:649:LEU:HG    | 2.02                     | 0.41              |
| 1:A:2080:TRP:CH2  | 1:A:2109:GLN:OE1  | 2.74                     | 0.41              |
| 4:F:92:VAL:HG22   | 4:F:111:GLN:HA    | 2.02                     | 0.41              |
| 1:A:107:ILE:CD1   | 1:A:232:VAL:HB    | 2.50                     | 0.41              |
| 1:A:668:ASP:OD2   | 1:A:669:VAL:HG23  | 2.20                     | 0.41              |
| 1:A:910:ILE:HG22  | 1:A:912:VAL:HG23  | 2.02                     | 0.41              |
| 1:A:1061:ILE:HD12 | 1:A:1061:ILE:O    | 2.21                     | 0.41              |
| 1:A:1115:ARG:HH11 | 1:A:1120:LYS:HB3  | 1.86                     | 0.41              |
| 1:A:1265:TRP:O    | 1:A:1275:LEU:HG   | 2.21                     | 0.41              |
| 1:A:1513:ASN:OD1  | 1:A:1514:LEU:N    | 2.54                     | 0.41              |
| 1:A:1757:GLU:HB2  | 1:A:1763:GLN:HG2  | 2.02                     | 0.41              |
| 1:A:823:ALA:O     | 1:A:826:GLU:HB3   | 2.21                     | 0.41              |
| 1:A:1836:LEU:HD21 | 1:A:1843:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:1886:ASN:HB2  | 1:A:1923:ALA:CB   | 2.50                     | 0.41              |
| 1:A:2037:PHE:HB2  | 1:A:2076:ALA:HB3  | 2.03                     | 0.41              |
| 1:A:102:TRP:CD1   | 1:A:107:ILE:HG12  | 2.55                     | 0.41              |
| 1:A:882:SER:HA    | 1:A:903:ASN:HA    | 2.02                     | 0.41              |
| 1:A:1073:THR:CG2  | 1:A:1346:ILE:HD12 | 2.51                     | 0.41              |
| 1:A:1720:VAL:HB   | 1:A:1768:PHE:HD1  | 1.85                     | 0.41              |
| 1:A:2118:MET:O    | 1:A:2120:VAL:HG22 | 2.21                     | 0.41              |
| 2:D:27:PHE:N      | 2:D:27:PHE:HD1    | 2.19                     | 0.41              |
| 1:A:378:PHE:CZ    | 1:A:500:ARG:HG2   | 2.56                     | 0.41              |
| 1:A:397:SER:O     | 1:A:401:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:818:GLU:OE1   | 1:A:818:GLU:N     | 2.35                     | 0.41              |
| 1:A:1310:ARG:HG3  | 1:A:1311:GLU:N    | 2.35                     | 0.41              |
| 1:A:1698:ILE:HD12 | 1:A:1726:ILE:HG23 | 2.03                     | 0.41              |
| 1:A:1973:ILE:O    | 1:A:1976:ASP:O    | 2.38                     | 0.41              |
| 1:A:2113:ASN:O    | 1:A:2114:ASP:C    | 2.64                     | 0.41              |
| 1:A:82:GLU:O      | 1:A:86:LEU:HB2    | 2.21                     | 0.41              |
| 1:A:633:ASP:O     | 1:A:634:LYS:HB2   | 2.21                     | 0.41              |
| 1:A:883:HIS:HB2   | 1:A:981:ASN:CG    | 2.46                     | 0.41              |
| 1:A:1227:PRO:HD2  | 1:A:1229:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:1930:LEU:HD22 | 1:A:1939:PHE:HE2  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2025:GLU:H    | 1:A:2025:GLU:HG2  | 1.67                     | 0.41              |
| 2:D:51:ILE:HD12   | 2:D:70:ILE:HG23   | 2.02                     | 0.41              |
| 4:F:66:ARG:CZ     | 4:F:66:ARG:HB3    | 2.51                     | 0.41              |
| 1:A:167:ASN:O     | 1:A:168:HIS:C     | 2.65                     | 0.40              |
| 1:A:1477:ASN:HB3  | 1:A:1480:THR:OG1  | 2.21                     | 0.40              |
| 1:A:2033:THR:HG22 | 1:A:2034:GLU:H    | 1.84                     | 0.40              |
| 1:A:2080:TRP:CZ3  | 1:A:2110:TYR:OH   | 2.74                     | 0.40              |
| 1:A:2223:TYR:CD1  | 1:A:2252:MET:HB3  | 2.56                     | 0.40              |
| 2:D:4:LEU:CD2     | 2:D:117:TRP:CA    | 2.82                     | 0.40              |
| 1:A:319:GLU:OE1   | 1:A:336:PHE:N     | 2.54                     | 0.40              |
| 1:A:407:ARG:O     | 1:A:410:ILE:HB    | 2.20                     | 0.40              |
| 1:A:491:ASP:OD1   | 1:A:492:THR:N     | 2.54                     | 0.40              |
| 1:A:1979:TYR:HB3  | 1:A:2000:PHE:CE2  | 2.57                     | 0.40              |
| 1:A:2131:TYR:CE2  | 1:A:2145:ILE:HD13 | 2.57                     | 0.40              |
| 1:A:2201:TYR:O    | 1:A:2201:TYR:CG   | 2.74                     | 0.40              |
| 1:A:2254:THR:OG1  | 1:A:2267:ASN:O    | 2.38                     | 0.40              |
| 1:A:793:LYS:H     | 1:A:836:GLN:NE2   | 2.13                     | 0.40              |
| 1:A:828:ASN:O     | 1:A:832:ASN:HB2   | 2.20                     | 0.40              |
| 1:A:1484:LEU:HD22 | 1:A:1497:LYS:NZ   | 2.36                     | 0.40              |
| 1:A:1663:ASP:OD1  | 1:A:1663:ASP:C    | 2.64                     | 0.40              |
| 1:A:782:ASN:HD22  | 1:A:783:PRO:HD2   | 1.86                     | 0.40              |
| 1:A:816:LEU:HA    | 1:A:819:LYS:NZ    | 2.36                     | 0.40              |
| 1:A:2107:ASP:OD1  | 1:A:2107:ASP:C    | 2.65                     | 0.40              |
| 1:A:2130:PHE:HD2  | 1:A:2157:ILE:HD13 | 1.84                     | 0.40              |
| 1:A:2194:ARG:HG2  | 1:A:2199:VAL:CG1  | 2.51                     | 0.40              |
| 2:D:12:VAL:HG21   | 2:D:86:LEU:HD13   | 2.04                     | 0.40              |
| 2:D:55:ALA:O      | 2:D:57:THR:N      | 2.49                     | 0.40              |
| 1:A:972:TYR:O     | 1:A:977:GLU:OE1   | 2.39                     | 0.40              |
| 1:A:1321:GLY:HA2  | 1:A:1343:ASP:HB3  | 2.03                     | 0.40              |
| 1:A:1850:VAL:O    | 1:A:1851:ASN:OD1  | 2.38                     | 0.40              |
| 1:A:1915:LEU:H    | 1:A:1918:ASN:ND2  | 2.20                     | 0.40              |
| 3:E:9:GLY:C       | 3:E:18:LEU:HD13   | 2.47                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 2340/2373 (99%) | 2001 (86%) | 319 (14%) | 20 (1%)  | 14          | 47  |
| 2   | D     | 124/153 (81%)   | 112 (90%)  | 12 (10%)  | 0        | 100         | 100 |
| 3   | E     | 105/137 (77%)   | 94 (90%)   | 11 (10%)  | 0        | 100         | 100 |
| 4   | F     | 114/142 (80%)   | 98 (86%)   | 16 (14%)  | 0        | 100         | 100 |
| All | All   | 2683/2805 (96%) | 2305 (86%) | 358 (13%) | 20 (1%)  | 18          | 52  |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 164  | PRO  |
| 1   | A     | 306  | SER  |
| 1   | A     | 307  | VAL  |
| 1   | A     | 574  | SER  |
| 1   | A     | 576  | ARG  |
| 1   | A     | 168  | HIS  |
| 1   | A     | 522  | GLN  |
| 1   | A     | 542  | GLY  |
| 1   | A     | 1510 | TYR  |
| 1   | A     | 1949 | TRP  |
| 1   | A     | 1512 | ASN  |
| 1   | A     | 1849 | PRO  |
| 1   | A     | 2222 | LYS  |
| 1   | A     | 166  | PHE  |
| 1   | A     | 1670 | ILE  |
| 1   | A     | 1505 | PRO  |
| 1   | A     | 2228 | GLU  |
| 1   | A     | 1092 | ILE  |
| 1   | A     | 2125 | ILE  |
| 1   | A     | 304  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 2113/2142 (99%) | 2017 (96%) | 96 (4%)  | 24          | 49 |
| 2   | D     | 102/127 (80%)   | 91 (89%)   | 11 (11%) | 6           | 24 |
| 3   | E     | 89/117 (76%)    | 87 (98%)   | 2 (2%)   | 45          | 64 |
| 4   | F     | 95/119 (80%)    | 88 (93%)   | 7 (7%)   | 13          | 38 |
| All | All   | 2399/2505 (96%) | 2283 (95%) | 116 (5%) | 23          | 48 |

All (116) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3    | LEU  |
| 1   | A     | 74   | LYS  |
| 1   | A     | 75   | PHE  |
| 1   | A     | 162  | ASN  |
| 1   | A     | 163  | ASP  |
| 1   | A     | 165  | GLU  |
| 1   | A     | 219  | ASP  |
| 1   | A     | 303  | LYS  |
| 1   | A     | 306  | SER  |
| 1   | A     | 400  | LEU  |
| 1   | A     | 418  | ILE  |
| 1   | A     | 521  | TRP  |
| 1   | A     | 522  | GLN  |
| 1   | A     | 544  | LEU  |
| 1   | A     | 553  | SER  |
| 1   | A     | 573  | SER  |
| 1   | A     | 576  | ARG  |
| 1   | A     | 625  | THR  |
| 1   | A     | 649  | LEU  |
| 1   | A     | 668  | ASP  |
| 1   | A     | 692  | ILE  |
| 1   | A     | 776  | LYS  |
| 1   | A     | 811  | SER  |
| 1   | A     | 828  | ASN  |
| 1   | A     | 837  | VAL  |
| 1   | A     | 851  | ASP  |
| 1   | A     | 873  | LEU  |
| 1   | A     | 890  | ILE  |
| 1   | A     | 902  | ILE  |
| 1   | A     | 953  | THR  |
| 1   | A     | 959  | THR  |
| 1   | A     | 979  | LEU  |
| 1   | A     | 1007 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1048 | GLU  |
| 1   | A     | 1084 | LEU  |
| 1   | A     | 1100 | ILE  |
| 1   | A     | 1144 | VAL  |
| 1   | A     | 1195 | THR  |
| 1   | A     | 1196 | TYR  |
| 1   | A     | 1205 | ASP  |
| 1   | A     | 1300 | ILE  |
| 1   | A     | 1358 | ILE  |
| 1   | A     | 1396 | VAL  |
| 1   | A     | 1430 | ILE  |
| 1   | A     | 1489 | LEU  |
| 1   | A     | 1529 | THR  |
| 1   | A     | 1628 | GLU  |
| 1   | A     | 1662 | TYR  |
| 1   | A     | 1667 | SER  |
| 1   | A     | 1680 | LYS  |
| 1   | A     | 1698 | ILE  |
| 1   | A     | 1706 | THR  |
| 1   | A     | 1708 | VAL  |
| 1   | A     | 1724 | ASN  |
| 1   | A     | 1729 | LYS  |
| 1   | A     | 1739 | ILE  |
| 1   | A     | 1816 | LEU  |
| 1   | A     | 1817 | VAL  |
| 1   | A     | 1839 | ILE  |
| 1   | A     | 1844 | TYR  |
| 1   | A     | 1850 | VAL  |
| 1   | A     | 1853 | LEU  |
| 1   | A     | 1855 | THR  |
| 1   | A     | 1864 | LYS  |
| 1   | A     | 1870 | ILE  |
| 1   | A     | 1881 | ILE  |
| 1   | A     | 1933 | ASP  |
| 1   | A     | 1940 | GLU  |
| 1   | A     | 1973 | ILE  |
| 1   | A     | 1975 | ASP  |
| 1   | A     | 2023 | ASN  |
| 1   | A     | 2025 | GLU  |
| 1   | A     | 2027 | GLN  |
| 1   | A     | 2030 | VAL  |
| 1   | A     | 2042 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2100 | ILE  |
| 1   | A     | 2102 | LEU  |
| 1   | A     | 2104 | LEU  |
| 1   | A     | 2105 | ILE  |
| 1   | A     | 2106 | ASN  |
| 1   | A     | 2112 | PHE  |
| 1   | A     | 2114 | ASP  |
| 1   | A     | 2115 | ASP  |
| 1   | A     | 2120 | VAL  |
| 1   | A     | 2137 | ILE  |
| 1   | A     | 2142 | VAL  |
| 1   | A     | 2192 | LEU  |
| 1   | A     | 2193 | VAL  |
| 1   | A     | 2213 | ILE  |
| 1   | A     | 2228 | GLU  |
| 1   | A     | 2243 | LYS  |
| 1   | A     | 2257 | ILE  |
| 1   | A     | 2262 | ASN  |
| 1   | A     | 2330 | ASP  |
| 1   | A     | 2347 | VAL  |
| 1   | A     | 2365 | ILE  |
| 2   | D     | 4    | LEU  |
| 2   | D     | 27   | PHE  |
| 2   | D     | 34   | ILE  |
| 2   | D     | 52   | SER  |
| 2   | D     | 58   | ILE  |
| 2   | D     | 59   | LEU  |
| 2   | D     | 85   | SER  |
| 2   | D     | 98   | ARG  |
| 2   | D     | 106  | VAL  |
| 2   | D     | 108  | ARG  |
| 2   | D     | 119  | ARG  |
| 3   | E     | 57   | GLU  |
| 3   | E     | 85   | LEU  |
| 4   | F     | 57   | ILE  |
| 4   | F     | 61   | ASP  |
| 4   | F     | 63   | VAL  |
| 4   | F     | 66   | ARG  |
| 4   | F     | 95   | CYS  |
| 4   | F     | 98   | HIS  |
| 4   | F     | 101  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60)

such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 8    | GLN  |
| 1   | A     | 36   | ASN  |
| 1   | A     | 40   | ASN  |
| 1   | A     | 126  | ASN  |
| 1   | A     | 139  | ASN  |
| 1   | A     | 167  | ASN  |
| 1   | A     | 168  | HIS  |
| 1   | A     | 185  | ASN  |
| 1   | A     | 235  | ASN  |
| 1   | A     | 257  | GLN  |
| 1   | A     | 324  | HIS  |
| 1   | A     | 344  | GLN  |
| 1   | A     | 403  | GLN  |
| 1   | A     | 412  | ASN  |
| 1   | A     | 511  | GLN  |
| 1   | A     | 515  | GLN  |
| 1   | A     | 597  | ASN  |
| 1   | A     | 602  | ASN  |
| 1   | A     | 610  | GLN  |
| 1   | A     | 742  | GLN  |
| 1   | A     | 782  | ASN  |
| 1   | A     | 786  | ASN  |
| 1   | A     | 828  | ASN  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 924  | ASN  |
| 1   | A     | 967  | GLN  |
| 1   | A     | 981  | ASN  |
| 1   | A     | 989  | GLN  |
| 1   | A     | 1210 | GLN  |
| 1   | A     | 1291 | ASN  |
| 1   | A     | 1388 | HIS  |
| 1   | A     | 1445 | GLN  |
| 1   | A     | 1571 | ASN  |
| 1   | A     | 1610 | ASN  |
| 1   | A     | 1640 | ASN  |
| 1   | A     | 1645 | ASN  |
| 1   | A     | 1654 | GLN  |
| 1   | A     | 1735 | ASN  |
| 1   | A     | 1770 | ASN  |
| 1   | A     | 1828 | ASN  |
| 1   | A     | 1851 | ASN  |
| 1   | A     | 1852 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1871 | ASN  |
| 1   | A     | 1886 | ASN  |
| 1   | A     | 1896 | GLN  |
| 1   | A     | 1935 | ASN  |
| 1   | A     | 1971 | ASN  |
| 1   | A     | 1987 | GLN  |
| 1   | A     | 1998 | HIS  |
| 1   | A     | 2027 | GLN  |
| 1   | A     | 2042 | HIS  |
| 1   | A     | 2106 | ASN  |
| 1   | A     | 2119 | GLN  |
| 1   | A     | 2237 | ASN  |
| 1   | A     | 2310 | ASN  |
| 1   | A     | 2322 | ASN  |
| 1   | A     | 2369 | HIS  |
| 2   | D     | 3    | GLN  |
| 2   | D     | 13   | GLN  |
| 2   | D     | 74   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 2346/2373 (98%) | -0.55  | 0 100 100      | 80, 160, 233, 324     | 0     |
| 2   | D     | 126/153 (82%)   | -0.46  | 1 (0%) 82 63   | 147, 200, 255, 290    | 0     |
| 3   | E     | 107/137 (78%)   | -0.53  | 0 100 100      | 213, 260, 307, 341    | 0     |
| 4   | F     | 116/142 (81%)   | -0.72  | 0 100 100      | 117, 166, 214, 240    | 0     |
| All | All   | 2695/2805 (96%) | -0.56  | 1 (0%) 100 100 | 80, 165, 249, 341     | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 106 | VAL  | 2.6  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

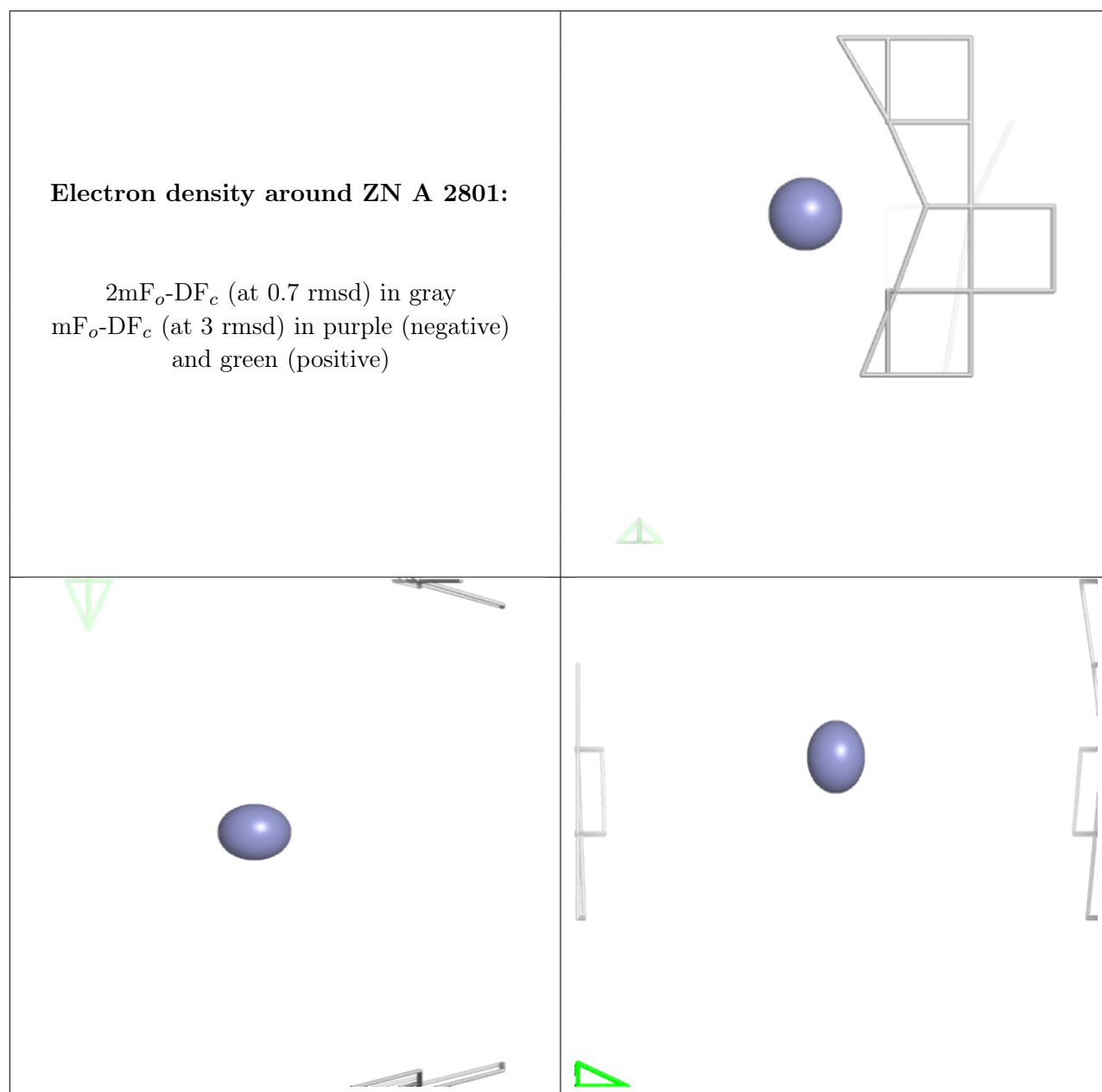
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 6   | MG   | A     | 2802 | 1/1   | 0.89 | 0.12 | 119,119,119,119            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | ZN   | A     | 2801 | 1/1   | 1.00 | 0.02 | 120,120,120,120             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.