



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:35 AM GMT

PDB ID : 3H2V  
Title : Human raver1 RRM1 domain in complex with human vinculin tail domain Vt  
Authors : Lee, J.H.; Rangarajan, E.S.; Yogesha, S.D.; Izard, T.  
Deposited on : 2009-04-14  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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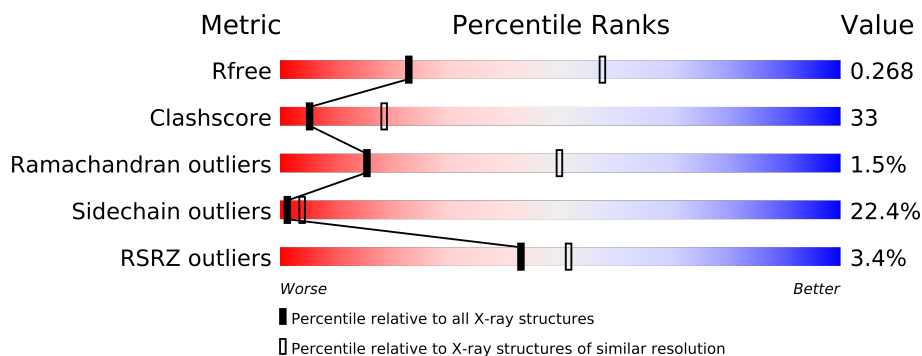
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1053 (2.90-2.90)                                      |
| Clashscore            | 79885                       | 1326 (2.90-2.90)                                      |
| Ramachandran outliers | 78287                       | 1290 (2.90-2.90)                                      |
| Sidechain outliers    | 78261                       | 1292 (2.90-2.90)                                      |
| RSRZ outliers         | 66119                       | 1054 (2.90-2.90)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 188    |                  |
| 1   | B     | 188    |                  |
| 1   | C     | 188    |                  |
| 1   | D     | 188    |                  |
| 2   | E     | 74     |                  |
| 2   | F     | 74     |                  |
| 2   | G     | 74     |                  |
| 2   | H     | 74     |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7693 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Vinculin.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 174      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1351  | 830 | 255 | 254 | 12 |         |         |       |
| 1   | B     | 167      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1299  | 796 | 243 | 248 | 12 |         |         |       |
| 1   | C     | 167      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1298  | 797 | 243 | 246 | 12 |         |         |       |
| 1   | D     | 175      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1361  | 837 | 255 | 257 | 12 |         |         |       |

- Molecule 2 is a protein called Raver-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | E     | 74       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 600   | 378 | 107 | 113 | 2 |         |         |       |
| 2   | F     | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 590   | 372 | 104 | 112 | 2 |         |         |       |
| 2   | G     | 74       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 600   | 378 | 107 | 113 | 2 |         |         |       |
| 2   | H     | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 590   | 372 | 104 | 112 | 2 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 57      | HIS      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| E     | 58      | MET      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| F     | 57      | HIS      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| F     | 58      | MET      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| G     | 57      | HIS      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| G     | 58      | MET      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| H     | 57      | HIS      | -      | CLONING ARTIFACT | UNP Q8IY67 |
| H     | 58      | MET      | -      | CLONING ARTIFACT | UNP Q8IY67 |

- Molecule 3 is water.

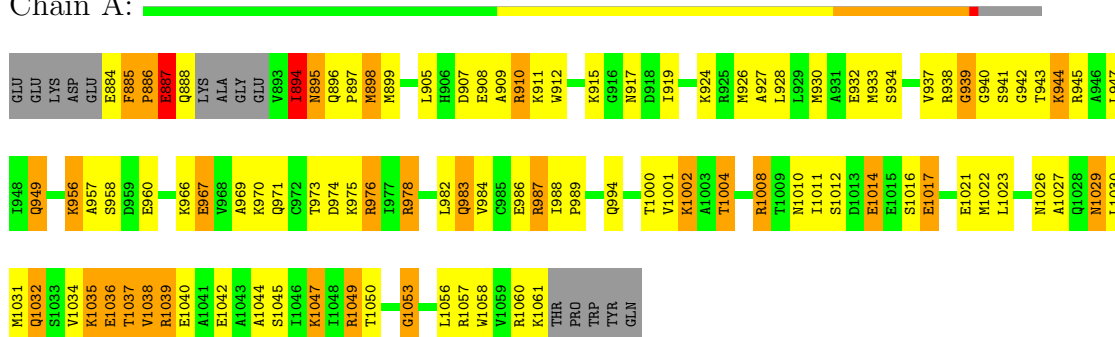
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 3   | A     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | B     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | F     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | G     | 1        | Total<br>1 | O<br>1 | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

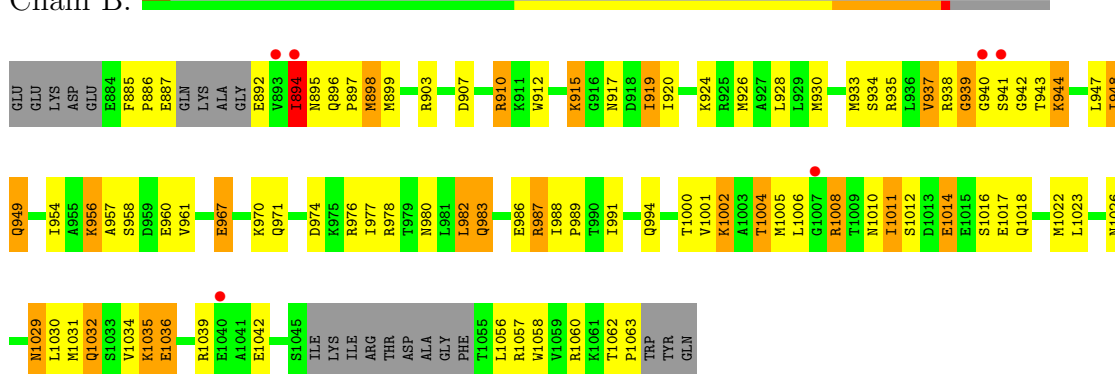
#### • Molecule 1: Vinculin

Chain A:



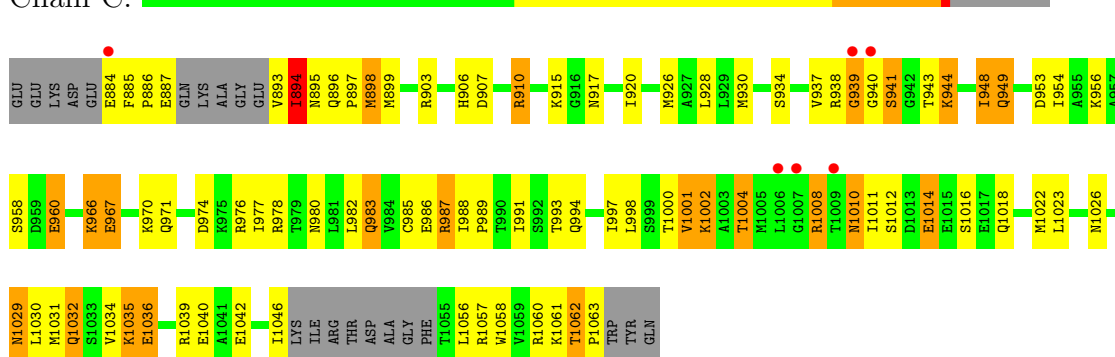
#### • Molecule 1: Vinculin

Chain B:



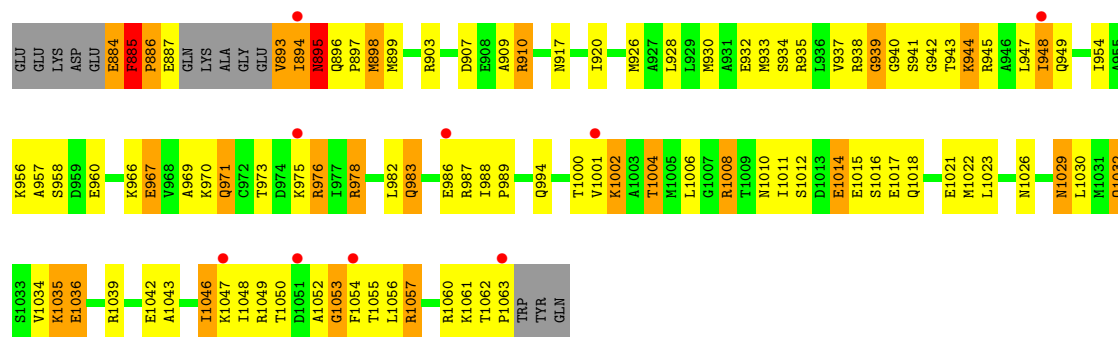
#### • Molecule 1: Vinculin

Chain C:



- Molecule 1: Vinculin

Chain D: 



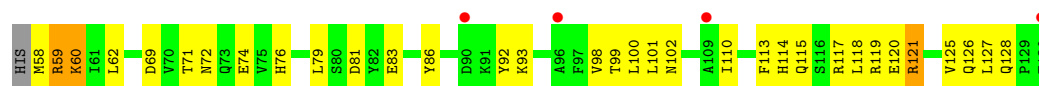
- Molecule 2: Raver-1

Chain E: 



- Molecule 2: Raver-1

Chain F: 



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 41.82Å 70.92Å 99.34Å<br>89.77° 90.04° 104.04°               | Depositor        |
| Resolution (Å)  | 20.00 – 2.90<br>40.57 – 2.89                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.0 (20.00-2.90)<br>93.2 (40.57-2.89)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.46 (at 2.90Å)   | Xtriage          |
| Refinement program  | BUSTER-TNT 2.1.1  | Depositor        |
| R, $R_{free}$   | 0.210 , 0.277<br>0.219 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1191 reflections (5.43%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.0  | Xtriage          |
| Anisotropy  | 0.310   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 21.3   | EDS              |
| Estimated twinning fraction   | 0.429 for -h,-k,l   | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Outliers  | 0 of 23190 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 7693  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 55.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 1.41         | 26/1360 (1.9%) | 0.92        | 5/1821 (0.3%)  |
| 1   | B     | 0.76         | 1/1307 (0.1%)  | 0.79        | 1/1751 (0.1%)  |
| 1   | C     | 0.75         | 1/1306 (0.1%)  | 0.81        | 1/1750 (0.1%)  |
| 1   | D     | 0.73         | 0/1371         | 0.81        | 1/1838 (0.1%)  |
| 2   | E     | 0.97         | 4/610 (0.7%)   | 0.75        | 1/821 (0.1%)   |
| 2   | F     | 0.63         | 0/599          | 0.68        | 0/806          |
| 2   | G     | 0.65         | 0/610          | 0.70        | 0/821          |
| 2   | H     | 0.65         | 0/599          | 0.68        | 0/806          |
| All | All   | 0.90         | 32/7762 (0.4%) | 0.80        | 9/10414 (0.1%) |

All (32) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | A     | 1038 | VAL  | CB-CG1  | -16.49 | 1.18        | 1.52     |
| 1   | A     | 1038 | VAL  | CA-CB   | -12.68 | 1.28        | 1.54     |
| 1   | A     | 1038 | VAL  | C-O     | -10.21 | 1.03        | 1.23     |
| 1   | A     | 885  | PHE  | CE2-CZ  | -10.01 | 1.18        | 1.37     |
| 1   | A     | 1040 | GLU  | C-O     | -9.99  | 1.04        | 1.23     |
| 1   | A     | 1039 | ARG  | C-O     | -9.41  | 1.05        | 1.23     |
| 1   | A     | 885  | PHE  | CG-CD1  | -8.57  | 1.25        | 1.38     |
| 1   | A     | 1038 | VAL  | CB-CG2  | -8.43  | 1.35        | 1.52     |
| 2   | E     | 119  | ARG  | C-O     | -8.21  | 1.07        | 1.23     |
| 1   | A     | 1040 | GLU  | CD-OE2  | -8.01  | 1.16        | 1.25     |
| 2   | E     | 119  | ARG  | CZ-NH1  | -7.99  | 1.22        | 1.33     |
| 1   | A     | 885  | PHE  | CD2-CE2 | -7.84  | 1.23        | 1.39     |
| 1   | A     | 886  | PRO  | CG-CD   | -7.30  | 1.26        | 1.50     |
| 1   | A     | 1039 | ARG  | CB-CG   | -7.20  | 1.33        | 1.52     |
| 2   | E     | 119  | ARG  | CZ-NH2  | -7.08  | 1.23        | 1.33     |
| 1   | A     | 1038 | VAL  | CA-C    | -6.70  | 1.35        | 1.52     |
| 1   | A     | 1039 | ARG  | CA-C    | -6.62  | 1.35        | 1.52     |
| 1   | A     | 1039 | ARG  | CZ-NH2  | -6.47  | 1.24        | 1.33     |
| 1   | A     | 1040 | GLU  | N-CA    | -6.32  | 1.33        | 1.46     |
| 1   | A     | 885  | PHE  | C-O     | -6.14  | 1.11        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 1038 | VAL  | N-CA    | -6.10 | 1.34        | 1.46     |
| 1   | A     | 1040 | GLU  | CA-C    | -5.87 | 1.37        | 1.52     |
| 1   | B     | 1017 | GLU  | CB-CG   | 5.78  | 1.63        | 1.52     |
| 1   | A     | 1037 | THR  | C-N     | -5.77 | 1.20        | 1.34     |
| 1   | A     | 1040 | GLU  | CB-CG   | -5.76 | 1.41        | 1.52     |
| 2   | E     | 119  | ARG  | CB-CG   | -5.52 | 1.37        | 1.52     |
| 1   | A     | 1039 | ARG  | CG-CD   | -5.50 | 1.38        | 1.51     |
| 1   | A     | 887  | GLU  | C-O     | -5.38 | 1.13        | 1.23     |
| 1   | A     | 1017 | GLU  | CG-CD   | 5.24  | 1.59        | 1.51     |
| 1   | A     | 886  | PRO  | CB-CG   | -5.24 | 1.23        | 1.50     |
| 1   | A     | 885  | PHE  | CD1-CE1 | -5.11 | 1.29        | 1.39     |
| 1   | C     | 960  | GLU  | CG-CD   | 5.04  | 1.59        | 1.51     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | D     | 885  | PHE  | C-N-CD     | -11.37 | 95.59       | 120.60   |
| 1   | A     | 1040 | GLU  | OE1-CD-OE2 | -8.34  | 113.29      | 123.30   |
| 1   | A     | 1039 | ARG  | NE-CZ-NH1  | 8.31   | 124.45      | 120.30   |
| 2   | E     | 119  | ARG  | NE-CZ-NH1  | 7.86   | 124.23      | 120.30   |
| 1   | C     | 1062 | THR  | C-N-CD     | -5.90  | 107.63      | 120.60   |
| 1   | A     | 1039 | ARG  | NE-CZ-NH2  | -5.65  | 117.48      | 120.30   |
| 1   | A     | 885  | PHE  | N-CA-C     | -5.50  | 96.15       | 111.00   |
| 1   | B     | 982  | LEU  | CA-CB-CG   | -5.45  | 102.77      | 115.30   |
| 1   | A     | 942  | GLY  | N-CA-C     | -5.22  | 100.05      | 113.10   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1351  | 0        | 1412     | 98      | 0            |
| 1   | B     | 1299  | 0        | 1352     | 105     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 1298  | 0        | 1357     | 108     | 0            |
| 1   | D     | 1361  | 0        | 1423     | 115     | 0            |
| 2   | E     | 600   | 0        | 597      | 29      | 0            |
| 2   | F     | 590   | 0        | 590      | 34      | 0            |
| 2   | G     | 600   | 0        | 597      | 37      | 0            |
| 2   | H     | 590   | 0        | 590      | 33      | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 7693  | 0        | 7918     | 513     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (513) close contacts within the same asymmetric unit are listed below.

| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:939:GLY:HA3   | 1:B:943:THR:HG21  | 1.22        | 1.17     |
| 1:C:938:ARG:HH22  | 1:D:938:ARG:NH1   | 1.47        | 1.11     |
| 1:C:939:GLY:HA3   | 1:C:943:THR:HG21  | 1.22        | 1.10     |
| 1:C:896:GLN:NE2   | 1:D:896:GLN:HE22  | 1.51        | 1.09     |
| 1:D:939:GLY:HA3   | 1:D:943:THR:HG21  | 1.28        | 1.08     |
| 1:A:939:GLY:HA3   | 1:A:943:THR:HG21  | 1.37        | 1.05     |
| 1:A:973:THR:HG22  | 1:A:1049:ARG:HG3  | 1.43        | 1.00     |
| 1:B:894:ILE:HD12  | 1:B:899:MET:HG3   | 1.44        | 0.99     |
| 1:C:949:GLN:HG2   | 2:G:120:GLU:HB2   | 1.40        | 0.98     |
| 1:B:886:PRO:HG2   | 2:F:92:TYR:CE2    | 1.98        | 0.98     |
| 1:D:1047:LYS:HD2  | 1:D:1047:LYS:H    | 1.29        | 0.97     |
| 1:A:1047:LYS:HZ2  | 1:A:1047:LYS:H    | 1.11        | 0.96     |
| 1:B:949:GLN:HG2   | 2:F:120:GLU:HB2   | 1.47        | 0.95     |
| 1:A:949:GLN:HG2   | 2:E:120:GLU:HB2   | 1.50        | 0.93     |
| 1:D:1057:ARG:HH11 | 1:D:1057:ARG:HG2  | 1.32        | 0.92     |
| 1:C:896:GLN:HE22  | 1:D:896:GLN:HE22  | 1.04        | 0.92     |
| 1:A:898:MET:HB2   | 1:A:934:SER:HB3   | 1.52        | 0.91     |
| 1:B:917:ASN:HA    | 1:B:1056:LEU:HD22 | 1.53        | 0.91     |
| 1:C:894:ILE:HD12  | 1:C:899:MET:HG3   | 1.51        | 0.90     |
| 2:F:58:MET:HG3    | 2:F:59:ARG:H      | 1.38        | 0.89     |
| 1:C:917:ASN:HA    | 1:C:1056:LEU:HD22 | 1.52        | 0.89     |
| 1:A:1050:THR:HG23 | 1:A:1053:GLY:H    | 1.37        | 0.88     |
| 2:E:86:TYR:HB3    | 2:E:99:THR:HB     | 1.55        | 0.87     |
| 1:A:1038:VAL:O    | 1:A:1038:VAL:HG12 | 1.71        | 0.87     |
| 2:H:58:MET:HG3    | 2:H:59:ARG:H      | 1.41        | 0.85     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:G:92:TYR:CE2    | 2:G:93:LYS:HD3    | 2.12        | 0.84     |
| 2:G:92:TYR:CD2    | 2:G:93:LYS:HD3    | 2.11        | 0.84     |
| 1:C:917:ASN:HA    | 1:C:1056:LEU:CD2  | 2.07        | 0.84     |
| 1:C:938:ARG:HH22  | 1:D:938:ARG:HH12  | 1.22        | 0.84     |
| 1:C:938:ARG:NH2   | 1:D:938:ARG:NH1   | 2.26        | 0.84     |
| 1:C:896:GLN:NE2   | 1:D:896:GLN:NE2   | 2.25        | 0.83     |
| 1:D:949:GLN:HG2   | 2:H:120:GLU:HB2   | 1.58        | 0.83     |
| 1:A:1029:ASN:HD22 | 1:A:1029:ASN:N    | 1.75        | 0.83     |
| 1:C:949:GLN:HG2   | 2:G:120:GLU:CB    | 2.08        | 0.82     |
| 1:D:898:MET:HB2   | 1:D:934:SER:HB3   | 1.61        | 0.82     |
| 2:H:86:TYR:HB3    | 2:H:99:THR:HB     | 1.60        | 0.81     |
| 1:C:896:GLN:HE22  | 1:D:896:GLN:NE2   | 1.79        | 0.81     |
| 1:A:907:ASP:HA    | 1:A:910:ARG:HD3   | 1.61        | 0.80     |
| 1:B:907:ASP:HA    | 1:B:910:ARG:HD3   | 1.63        | 0.80     |
| 2:F:118:LEU:O     | 2:F:121:ARG:HG2   | 1.82        | 0.80     |
| 2:E:118:LEU:O     | 2:E:121:ARG:HG2   | 1.81        | 0.80     |
| 1:C:938:ARG:NH2   | 1:D:938:ARG:HH12  | 1.79        | 0.79     |
| 1:B:910:ARG:HH11  | 1:B:910:ARG:HB2   | 1.47        | 0.79     |
| 1:B:982:LEU:O     | 1:B:986:GLU:HG2   | 1.83        | 0.79     |
| 1:C:982:LEU:O     | 1:C:986:GLU:HG2   | 1.83        | 0.79     |
| 1:C:939:GLY:CA    | 1:C:943:THR:HG21  | 2.08        | 0.79     |
| 2:F:92:TYR:CE2    | 2:F:93:LYS:HD3    | 2.19        | 0.78     |
| 2:F:83:GLU:OE2    | 2:F:101:LEU:HD22  | 1.83        | 0.78     |
| 1:D:893:VAL:O     | 1:D:938:ARG:HG3   | 1.84        | 0.78     |
| 1:D:982:LEU:O     | 1:D:986:GLU:HG2   | 1.84        | 0.78     |
| 1:C:907:ASP:HA    | 1:C:910:ARG:HD3   | 1.64        | 0.77     |
| 1:C:926:MET:CE    | 1:C:1034:VAL:HG21 | 2.15        | 0.76     |
| 1:C:967:GLU:OE1   | 1:C:970:LYS:HD3   | 1.86        | 0.76     |
| 1:B:919:ILE:HG13  | 1:B:1056:LEU:HD11 | 1.67        | 0.76     |
| 2:G:86:TYR:HB3    | 2:G:99:THR:HB     | 1.68        | 0.76     |
| 1:B:949:GLN:HG2   | 2:F:120:GLU:CB    | 2.16        | 0.76     |
| 2:E:83:GLU:OE2    | 2:E:101:LEU:HD22  | 1.85        | 0.76     |
| 1:A:986:GLU:O     | 1:A:989:PRO:HD2   | 1.86        | 0.76     |
| 2:F:92:TYR:CD2    | 2:F:93:LYS:HD3    | 2.21        | 0.76     |
| 2:E:119:ARG:O     | 2:E:120:GLU:HB2   | 1.86        | 0.75     |
| 1:A:982:LEU:O     | 1:A:986:GLU:HG2   | 1.86        | 0.75     |
| 2:H:92:TYR:CE2    | 2:H:93:LYS:HD3    | 2.22        | 0.75     |
| 1:A:973:THR:CG2   | 1:A:1049:ARG:HG3  | 2.16        | 0.74     |
| 1:C:894:ILE:O     | 1:C:938:ARG:HD3   | 1.86        | 0.74     |
| 1:C:1029:ASN:N    | 1:C:1029:ASN:HD22 | 1.84        | 0.74     |
| 1:D:1029:ASN:HD22 | 1:D:1029:ASN:N    | 1.84        | 0.74     |
| 1:A:894:ILE:O     | 1:A:938:ARG:HD3   | 1.87        | 0.74     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:910:ARG:HH11  | 1:B:910:ARG:CB    | 2.00        | 0.74     |
| 2:F:86:TYR:HB3    | 2:F:99:THR:HB     | 1.69        | 0.74     |
| 2:H:83:GLU:OE2    | 2:H:101:LEU:HD22  | 1.87        | 0.74     |
| 1:C:939:GLY:HA3   | 1:C:943:THR:CG2   | 2.11        | 0.73     |
| 2:E:58:MET:HG3    | 2:E:59:ARG:H      | 1.54        | 0.73     |
| 1:C:1000:THR:O    | 1:C:1004:THR:HG23 | 1.88        | 0.73     |
| 1:D:986:GLU:O     | 1:D:989:PRO:HD2   | 1.88        | 0.73     |
| 1:D:1047:LYS:HD2  | 1:D:1047:LYS:N    | 2.03        | 0.73     |
| 1:B:939:GLY:CA    | 1:B:943:THR:HG21  | 2.10        | 0.72     |
| 1:D:939:GLY:HA3   | 1:D:943:THR:CG2   | 2.16        | 0.72     |
| 1:A:1008:ARG:HG2  | 1:A:1011:ILE:CD1  | 2.19        | 0.72     |
| 1:C:1057:ARG:HH11 | 1:C:1057:ARG:HG2  | 1.53        | 0.72     |
| 1:D:1052:ALA:HA   | 1:D:1053:GLY:O    | 1.90        | 0.71     |
| 1:A:1038:VAL:O    | 1:A:1038:VAL:CG1  | 2.27        | 0.71     |
| 2:H:119:ARG:O     | 2:H:120:GLU:HB2   | 1.91        | 0.71     |
| 1:B:1000:THR:O    | 1:B:1004:THR:HG23 | 1.90        | 0.71     |
| 1:B:967:GLU:OE1   | 1:B:970:LYS:HD3   | 1.91        | 0.71     |
| 2:H:92:TYR:CD2    | 2:H:93:LYS:HD3    | 2.25        | 0.70     |
| 1:D:1008:ARG:HG2  | 1:D:1011:ILE:CD1  | 2.21        | 0.70     |
| 1:B:895:ASN:ND2   | 1:B:898:MET:HG3   | 2.06        | 0.70     |
| 1:B:894:ILE:O     | 1:B:938:ARG:HD3   | 1.90        | 0.70     |
| 1:B:907:ASP:HA    | 1:B:910:ARG:CD    | 2.20        | 0.70     |
| 1:C:907:ASP:HA    | 1:C:910:ARG:CD    | 2.21        | 0.70     |
| 1:B:912:TRP:CH2   | 1:B:1060:ARG:HD3  | 2.27        | 0.70     |
| 1:A:949:GLN:HG2   | 2:E:120:GLU:CB    | 2.21        | 0.69     |
| 1:D:907:ASP:HA    | 1:D:910:ARG:HD3   | 1.75        | 0.69     |
| 1:C:1008:ARG:HG2  | 1:C:1011:ILE:CD1  | 2.23        | 0.69     |
| 1:C:1032:GLN:NE2  | 1:C:1036:GLU:OE2  | 2.23        | 0.69     |
| 2:F:119:ARG:O     | 2:F:120:GLU:HB2   | 1.92        | 0.69     |
| 1:B:1029:ASN:HD22 | 1:B:1029:ASN:N    | 1.90        | 0.69     |
| 1:D:1014:GLU:OE1  | 1:D:1014:GLU:HA   | 1.92        | 0.69     |
| 1:C:887:GLU:N     | 1:C:887:GLU:OE2   | 2.25        | 0.69     |
| 1:C:938:ARG:HH12  | 1:D:938:ARG:HH12  | 1.40        | 0.69     |
| 1:C:910:ARG:HH11  | 1:C:910:ARG:HB2   | 1.58        | 0.69     |
| 1:D:1057:ARG:NH1  | 1:D:1057:ARG:HG2  | 2.03        | 0.68     |
| 1:B:1008:ARG:HG2  | 1:B:1011:ILE:CD1  | 2.24        | 0.68     |
| 1:B:898:MET:HB2   | 1:B:934:SER:HB3   | 1.74        | 0.68     |
| 2:F:58:MET:HG3    | 2:F:59:ARG:N      | 2.08        | 0.68     |
| 1:C:938:ARG:NH1   | 1:D:938:ARG:HH12  | 1.91        | 0.68     |
| 2:G:83:GLU:OE2    | 2:G:101:LEU:HD22  | 1.94        | 0.67     |
| 1:D:1030:LEU:O    | 1:D:1034:VAL:HG23 | 1.94        | 0.67     |
| 1:B:899:MET:HG2   | 1:B:934:SER:OG    | 1.95        | 0.67     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C:895:ASN:HD22  | 1:C:898:MET:H     | 1.43        | 0.67     |
| 1:C:899:MET:HG2   | 1:C:934:SER:OG    | 1.94        | 0.67     |
| 2:F:69:ASP:OD1    | 2:F:119:ARG:NH2   | 2.26        | 0.67     |
| 2:E:71:THR:OG1    | 2:E:74:GLU:HG3    | 1.95        | 0.66     |
| 1:A:1014:GLU:HA   | 1:A:1014:GLU:OE1  | 1.93        | 0.66     |
| 1:D:939:GLY:CA    | 1:D:943:THR:HG21  | 2.17        | 0.66     |
| 2:G:119:ARG:O     | 2:G:120:GLU:HB2   | 1.95        | 0.66     |
| 1:D:942:GLY:CA    | 1:D:944:LYS:HE3   | 2.26        | 0.66     |
| 1:B:1018:GLN:O    | 1:B:1022:MET:HG3  | 1.96        | 0.66     |
| 2:H:71:THR:OG1    | 2:H:74:GLU:HG3    | 1.96        | 0.65     |
| 1:B:938:ARG:O     | 1:B:940:GLY:N     | 2.28        | 0.65     |
| 1:A:967:GLU:OE1   | 1:A:970:LYS:HD3   | 1.96        | 0.65     |
| 1:A:1049:ARG:HH11 | 1:A:1049:ARG:HB3  | 1.60        | 0.65     |
| 1:C:986:GLU:HA    | 1:C:986:GLU:OE2   | 1.96        | 0.65     |
| 1:C:1008:ARG:NH1  | 1:C:1008:ARG:HG2  | 2.11        | 0.65     |
| 2:H:58:MET:HG3    | 2:H:59:ARG:N      | 2.11        | 0.65     |
| 1:B:895:ASN:HD22  | 1:B:898:MET:H     | 1.44        | 0.64     |
| 1:C:910:ARG:HH11  | 1:C:910:ARG:CB    | 2.09        | 0.64     |
| 1:D:942:GLY:HA2   | 1:D:944:LYS:HE3   | 1.79        | 0.64     |
| 1:A:910:ARG:HH11  | 1:A:910:ARG:HB2   | 1.63        | 0.64     |
| 1:C:1008:ARG:HH11 | 1:C:1008:ARG:HG2  | 1.62        | 0.64     |
| 1:B:986:GLU:OE2   | 1:B:986:GLU:HA    | 1.98        | 0.64     |
| 1:C:1014:GLU:OE1  | 1:C:1014:GLU:HA   | 1.98        | 0.64     |
| 1:C:895:ASN:ND2   | 1:C:898:MET:HG3   | 2.13        | 0.64     |
| 1:A:1008:ARG:NH1  | 1:A:1008:ARG:HG2  | 2.13        | 0.64     |
| 2:G:72:ASN:O      | 2:G:76:HIS:HD2    | 1.80        | 0.64     |
| 1:C:898:MET:HB2   | 1:C:934:SER:HB3   | 1.79        | 0.63     |
| 1:C:926:MET:HE2   | 1:C:1034:VAL:HG21 | 1.79        | 0.63     |
| 2:G:58:MET:HG3    | 2:G:59:ARG:H      | 1.63        | 0.63     |
| 1:D:1008:ARG:HG2  | 1:D:1011:ILE:HD12 | 1.79        | 0.63     |
| 1:B:886:PRO:HG2   | 2:F:92:TYR:CZ     | 2.32        | 0.63     |
| 1:B:1032:GLN:NE2  | 1:B:1036:GLU:OE2  | 2.29        | 0.63     |
| 1:A:939:GLY:CA    | 1:A:943:THR:HG21  | 2.21        | 0.62     |
| 2:F:72:ASN:O      | 2:F:76:HIS:HD2    | 1.81        | 0.62     |
| 1:C:938:ARG:CZ    | 1:D:938:ARG:HH12  | 2.12        | 0.62     |
| 1:C:1008:ARG:HH11 | 1:C:1008:ARG:CG   | 2.12        | 0.62     |
| 1:C:938:ARG:HH22  | 1:D:938:ARG:CZ    | 2.12        | 0.62     |
| 1:B:926:MET:CE    | 1:B:1034:VAL:HG21 | 2.29        | 0.62     |
| 1:A:938:ARG:O     | 1:A:940:GLY:N     | 2.32        | 0.62     |
| 1:D:930:MET:HE2   | 1:D:954:ILE:CD1   | 2.30        | 0.62     |
| 1:A:1008:ARG:CG   | 1:A:1008:ARG:HH11 | 2.13        | 0.62     |
| 1:D:1000:THR:O    | 1:D:1004:THR:HG23 | 2.00        | 0.62     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1008:ARG:HG2  | 1:A:1011:ILE:HD12 | 1.81        | 0.61     |
| 1:B:1008:ARG:HH11 | 1:B:1008:ARG:CG   | 2.13        | 0.61     |
| 1:B:939:GLY:HA3   | 1:B:943:THR:CG2   | 2.15        | 0.61     |
| 1:A:1030:LEU:O    | 1:A:1034:VAL:HG23 | 2.00        | 0.61     |
| 1:D:910:ARG:HH11  | 1:D:910:ARG:HB2   | 1.65        | 0.61     |
| 1:C:1008:ARG:HG2  | 1:C:1011:ILE:HD12 | 1.81        | 0.61     |
| 1:A:907:ASP:HA    | 1:A:910:ARG:CD    | 2.30        | 0.61     |
| 2:F:92:TYR:HE2    | 2:F:93:LYS:HZ2    | 1.47        | 0.61     |
| 1:A:939:GLY:HA3   | 1:A:943:THR:CG2   | 2.23        | 0.61     |
| 1:B:917:ASN:HA    | 1:B:1056:LEU:CD2  | 2.29        | 0.61     |
| 2:H:78:LEU:O      | 2:H:113:PHE:CZ    | 2.53        | 0.61     |
| 1:A:1000:THR:O    | 1:A:1004:THR:HG23 | 2.01        | 0.61     |
| 1:A:986:GLU:OE2   | 1:A:986:GLU:HA    | 2.00        | 0.61     |
| 1:D:930:MET:HE2   | 1:D:954:ILE:HD11  | 1.80        | 0.61     |
| 2:G:110:ILE:HD11  | 2:G:127:LEU:HD23  | 1.83        | 0.61     |
| 1:D:949:GLN:HG2   | 2:H:120:GLU:CB    | 2.30        | 0.60     |
| 1:C:986:GLU:O     | 1:C:989:PRO:HD2   | 2.01        | 0.60     |
| 1:C:938:ARG:NH1   | 1:D:938:ARG:HH22  | 1.99        | 0.60     |
| 1:D:986:GLU:OE2   | 1:D:986:GLU:HA    | 1.98        | 0.60     |
| 1:A:1008:ARG:HH11 | 1:A:1008:ARG:HG2  | 1.66        | 0.60     |
| 2:E:74:GLU:OE1    | 2:E:119:ARG:NH1   | 2.35        | 0.60     |
| 1:A:899:MET:HG2   | 1:A:934:SER:OG    | 2.01        | 0.60     |
| 1:A:917:ASN:HA    | 1:A:1056:LEU:HD22 | 1.83        | 0.60     |
| 2:H:74:GLU:OE1    | 2:H:119:ARG:NH1   | 2.33        | 0.60     |
| 1:A:1029:ASN:N    | 1:A:1029:ASN:ND2  | 2.44        | 0.59     |
| 1:C:949:GLN:HG3   | 2:G:121:ARG:HH11  | 1.67        | 0.59     |
| 1:B:1014:GLU:HA   | 1:B:1014:GLU:OE1  | 2.02        | 0.59     |
| 2:F:92:TYR:HE2    | 2:F:93:LYS:NZ     | 2.00        | 0.59     |
| 1:D:895:ASN:HD22  | 1:D:898:MET:H     | 1.49        | 0.59     |
| 1:D:1008:ARG:HH11 | 1:D:1008:ARG:CG   | 2.16        | 0.59     |
| 2:G:59:ARG:HD2    | 2:G:100:LEU:O     | 2.02        | 0.58     |
| 2:E:114:HIS:O     | 2:E:115:GLN:HB2   | 2.03        | 0.58     |
| 1:D:1029:ASN:ND2  | 1:D:1029:ASN:N    | 2.50        | 0.58     |
| 1:C:938:ARG:HH12  | 1:D:938:ARG:NH1   | 2.00        | 0.58     |
| 2:F:114:HIS:O     | 2:F:115:GLN:HB2   | 2.03        | 0.58     |
| 1:C:949:GLN:CG    | 2:G:120:GLU:HB2   | 2.23        | 0.58     |
| 1:C:896:GLN:HB3   | 1:C:897:PRO:HD3   | 1.86        | 0.57     |
| 2:G:69:ASP:OD1    | 2:G:119:ARG:NH2   | 2.26        | 0.57     |
| 1:A:895:ASN:HD22  | 1:A:898:MET:H     | 1.52        | 0.57     |
| 1:B:1008:ARG:NH1  | 1:B:1008:ARG:HG2  | 2.19        | 0.57     |
| 1:B:949:GLN:CG    | 2:F:120:GLU:HB2   | 2.29        | 0.57     |
| 1:B:1030:LEU:O    | 1:B:1034:VAL:HG23 | 2.03        | 0.57     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C:941:SER:C     | 1:C:943:THR:H     | 2.07        | 0.57     |
| 1:A:1044:ALA:HA   | 1:A:1047:LYS:NZ   | 2.19        | 0.57     |
| 2:F:71:THR:OG1    | 2:F:74:GLU:HG3    | 2.05        | 0.57     |
| 1:B:1035:LYS:O    | 1:B:1039:ARG:HG3  | 2.04        | 0.57     |
| 1:C:938:ARG:CZ    | 1:D:938:ARG:HH22  | 2.18        | 0.57     |
| 1:A:894:ILE:HD12  | 1:A:899:MET:HG3   | 1.86        | 0.57     |
| 1:D:886:PRO:HA    | 1:D:887:GLU:OE1   | 2.05        | 0.57     |
| 1:A:905:LEU:HD23  | 1:A:927:ALA:HB2   | 1.85        | 0.57     |
| 1:D:896:GLN:HB3   | 1:D:897:PRO:HD3   | 1.87        | 0.56     |
| 1:D:895:ASN:CG    | 1:D:898:MET:HG3   | 2.25        | 0.56     |
| 1:C:1010:ASN:O    | 2:H:129:PRO:HB3   | 2.04        | 0.56     |
| 2:H:69:ASP:OD1    | 2:H:119:ARG:NH2   | 2.32        | 0.56     |
| 2:H:118:LEU:O     | 2:H:121:ARG:HG2   | 2.05        | 0.56     |
| 1:C:1018:GLN:O    | 1:C:1022:MET:HG3  | 2.05        | 0.56     |
| 1:A:1017:GLU:O    | 1:A:1021:GLU:HG3  | 2.06        | 0.56     |
| 1:D:1008:ARG:NH1  | 1:D:1008:ARG:HG2  | 2.20        | 0.56     |
| 1:D:1035:LYS:O    | 1:D:1039:ARG:HG3  | 2.06        | 0.56     |
| 1:C:1057:ARG:HG2  | 1:C:1057:ARG:NH1  | 2.14        | 0.56     |
| 2:G:114:HIS:CD2   | 2:G:115:GLN:HG3   | 2.40        | 0.56     |
| 2:G:114:HIS:O     | 2:G:115:GLN:HB2   | 2.06        | 0.56     |
| 1:C:938:ARG:O     | 1:C:940:GLY:N     | 2.39        | 0.56     |
| 1:D:894:ILE:HG12  | 1:D:894:ILE:O     | 2.04        | 0.55     |
| 1:D:899:MET:HG2   | 1:D:934:SER:OG    | 2.06        | 0.55     |
| 2:G:118:LEU:O     | 2:G:121:ARG:HG2   | 2.07        | 0.55     |
| 1:B:941:SER:C     | 1:B:943:THR:H     | 2.10        | 0.55     |
| 1:B:896:GLN:HB3   | 1:B:897:PRO:HD3   | 1.88        | 0.55     |
| 1:A:988:ILE:HB    | 1:A:989:PRO:HD3   | 1.87        | 0.55     |
| 1:D:1032:GLN:NE2  | 1:D:1036:GLU:OE2  | 2.34        | 0.55     |
| 1:D:967:GLU:OE1   | 1:D:970:LYS:HD3   | 2.07        | 0.55     |
| 1:C:895:ASN:CG    | 1:C:898:MET:HG3   | 2.27        | 0.55     |
| 1:B:988:ILE:HB    | 1:B:989:PRO:HD3   | 1.87        | 0.55     |
| 1:B:974:ASP:OD2   | 1:B:977:ILE:HG12  | 2.07        | 0.55     |
| 2:G:86:TYR:HB3    | 2:G:99:THR:CB     | 2.36        | 0.54     |
| 1:B:930:MET:HE3   | 1:B:1031:MET:CE   | 2.38        | 0.54     |
| 1:A:915:LYS:O     | 1:A:1057:ARG:NH1  | 2.40        | 0.54     |
| 1:A:895:ASN:ND2   | 1:A:898:MET:HG3   | 2.22        | 0.54     |
| 1:B:894:ILE:CD1   | 1:B:899:MET:HG3   | 2.29        | 0.54     |
| 1:A:926:MET:CE    | 1:A:1034:VAL:HG21 | 2.38        | 0.54     |
| 1:B:1008:ARG:HH11 | 1:B:1008:ARG:HG2  | 1.71        | 0.54     |
| 1:C:896:GLN:CB    | 1:C:897:PRO:HD3   | 2.38        | 0.53     |
| 1:A:895:ASN:ND2   | 1:A:897:PRO:HD2   | 2.22        | 0.53     |
| 1:A:910:ARG:HH11  | 1:A:910:ARG:CB    | 2.21        | 0.53     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:E:58:MET:HG3    | 2:E:59:ARG:N      | 2.21        | 0.53     |
| 1:B:895:ASN:CG    | 1:B:898:MET:HG3   | 2.29        | 0.53     |
| 1:A:1001:VAL:HG22 | 1:A:1002:LYS:N    | 2.22        | 0.53     |
| 1:D:1008:ARG:CG   | 1:D:1011:ILE:HD12 | 2.38        | 0.53     |
| 1:A:941:SER:C     | 1:A:943:THR:H     | 2.12        | 0.52     |
| 1:B:894:ILE:HG22  | 1:B:935:ARG:HG2   | 1.90        | 0.52     |
| 1:D:1062:THR:CG2  | 1:D:1063:PRO:HD2  | 2.38        | 0.52     |
| 1:C:1008:ARG:CG   | 1:C:1011:ILE:HD12 | 2.38        | 0.52     |
| 1:A:1032:GLN:NE2  | 1:A:1036:GLU:OE2  | 2.42        | 0.52     |
| 1:D:976:ARG:C     | 1:D:976:ARG:HD2   | 2.27        | 0.52     |
| 1:D:894:ILE:HG13  | 1:D:899:MET:HG3   | 1.91        | 0.52     |
| 1:D:896:GLN:CB    | 1:D:897:PRO:HD3   | 2.39        | 0.52     |
| 1:B:920:ILE:HD11  | 1:B:1058:TRP:CZ3  | 2.45        | 0.52     |
| 1:B:910:ARG:NH1   | 1:B:910:ARG:HB2   | 2.22        | 0.52     |
| 1:C:988:ILE:HB    | 1:C:989:PRO:HD3   | 1.91        | 0.52     |
| 2:E:86:TYR:HB3    | 2:E:99:THR:CB     | 2.33        | 0.52     |
| 2:E:101:LEU:O     | 2:E:101:LEU:HD12  | 2.10        | 0.52     |
| 1:B:1001:VAL:HG22 | 1:B:1002:LYS:N    | 2.25        | 0.52     |
| 1:C:884:GLU:HG2   | 1:C:910:ARG:NH1   | 2.25        | 0.52     |
| 1:C:1029:ASN:N    | 1:C:1029:ASN:ND2  | 2.54        | 0.52     |
| 1:C:987:ARG:O     | 1:C:991:ILE:HD12  | 2.10        | 0.52     |
| 1:D:1054:PHE:CD1  | 1:D:1055:THR:N    | 2.78        | 0.52     |
| 1:D:926:MET:CE    | 1:D:1034:VAL:HG21 | 2.39        | 0.52     |
| 1:D:1001:VAL:HG22 | 1:D:1002:LYS:N    | 2.25        | 0.51     |
| 1:C:993:THR:O     | 1:C:997:ILE:HG13  | 2.11        | 0.51     |
| 2:G:86:TYR:CB     | 2:G:99:THR:HB     | 2.39        | 0.51     |
| 1:D:1062:THR:CG2  | 1:D:1063:PRO:CD   | 2.88        | 0.51     |
| 1:D:884:GLU:O     | 1:D:885:PHE:HB2   | 2.08        | 0.51     |
| 2:E:92:TYR:HE2    | 2:E:93:LYS:HZ2    | 1.56        | 0.51     |
| 1:A:994:GLN:CB    | 1:A:1026:ASN:HD21 | 2.23        | 0.51     |
| 1:D:886:PRO:O     | 1:D:903:ARG:NH1   | 2.43        | 0.51     |
| 1:A:930:MET:HE2   | 1:A:930:MET:HA    | 1.92        | 0.51     |
| 1:A:1037:THR:O    | 1:A:1039:ARG:N    | 2.43        | 0.51     |
| 2:H:86:TYR:CB     | 2:H:99:THR:HB     | 2.36        | 0.51     |
| 1:A:1027:ALA:O    | 1:A:1031:MET:HG2  | 2.10        | 0.51     |
| 1:C:1035:LYS:O    | 1:C:1039:ARG:HG3  | 2.11        | 0.51     |
| 1:B:933:MET:CE    | 1:B:947:LEU:HD12  | 2.41        | 0.51     |
| 1:C:886:PRO:O     | 1:C:903:ARG:NH1   | 2.43        | 0.51     |
| 2:G:101:LEU:O     | 2:G:101:LEU:HD12  | 2.10        | 0.51     |
| 1:C:886:PRO:HG2   | 2:G:92:TYR:CE2    | 2.45        | 0.51     |
| 1:A:886:PRO:O     | 1:A:887:GLU:O     | 2.28        | 0.51     |
| 1:D:932:GLU:OE2   | 2:H:68:GLY:N      | 2.44        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:D:938:ARG:O     | 1:D:940:GLY:N     | 2.44        | 0.51     |
| 1:D:944:LYS:HZ2   | 1:D:945:ARG:H     | 1.59        | 0.51     |
| 1:B:1008:ARG:NH1  | 1:B:1008:ARG:CG   | 2.74        | 0.50     |
| 1:B:1008:ARG:HG2  | 1:B:1011:ILE:HD12 | 1.90        | 0.50     |
| 2:E:75:VAL:HG21   | 2:E:89:VAL:CG2    | 2.40        | 0.50     |
| 2:F:59:ARG:HD2    | 2:F:100:LEU:O     | 2.11        | 0.50     |
| 1:A:1008:ARG:CG   | 1:A:1011:ILE:HD12 | 2.41        | 0.50     |
| 1:A:910:ARG:HB2   | 1:A:910:ARG:NH1   | 2.25        | 0.50     |
| 1:C:910:ARG:CG    | 1:C:910:ARG:HH11  | 2.25        | 0.50     |
| 1:B:976:ARG:HD2   | 1:B:976:ARG:C     | 2.29        | 0.50     |
| 1:B:949:GLN:HE21  | 2:F:120:GLU:HG3   | 1.76        | 0.50     |
| 1:B:910:ARG:CG    | 1:B:910:ARG:HH11  | 2.24        | 0.50     |
| 2:F:86:TYR:HB3    | 2:F:99:THR:CB     | 2.38        | 0.50     |
| 1:B:930:MET:HE3   | 1:B:1031:MET:HE1  | 1.94        | 0.50     |
| 2:H:58:MET:CG     | 2:H:59:ARG:H      | 2.20        | 0.50     |
| 1:D:907:ASP:HA    | 1:D:910:ARG:CD    | 2.40        | 0.50     |
| 2:F:114:HIS:CD2   | 2:F:115:GLN:HG3   | 2.47        | 0.50     |
| 2:H:59:ARG:HD2    | 2:H:100:LEU:O     | 2.12        | 0.50     |
| 1:D:969:ALA:O     | 1:D:978:ARG:HG3   | 2.12        | 0.50     |
| 1:B:942:GLY:HA2   | 1:B:944:LYS:HE3   | 1.94        | 0.49     |
| 2:H:92:TYR:HE2    | 2:H:93:LYS:HZ2    | 1.57        | 0.49     |
| 2:H:86:TYR:HB3    | 2:H:99:THR:CB     | 2.37        | 0.49     |
| 1:C:1030:LEU:O    | 1:C:1034:VAL:HG23 | 2.13        | 0.49     |
| 1:A:944:LYS:HZ2   | 1:A:945:ARG:H     | 1.60        | 0.49     |
| 1:D:1057:ARG:CG   | 1:D:1057:ARG:HH11 | 2.15        | 0.49     |
| 2:H:59:ARG:HB3    | 2:H:102:ASN:O     | 2.12        | 0.49     |
| 1:C:974:ASP:OD2   | 1:C:977:ILE:HG12  | 2.12        | 0.49     |
| 1:A:896:GLN:HB3   | 1:A:897:PRO:HD3   | 1.95        | 0.49     |
| 1:C:920:ILE:HD11  | 1:C:1058:TRP:CZ3  | 2.48        | 0.49     |
| 1:B:1002:LYS:HE3  | 1:B:1006:LEU:HD21 | 1.95        | 0.49     |
| 2:F:113:PHE:O     | 2:F:125:VAL:HG23  | 2.13        | 0.49     |
| 1:C:949:GLN:HG2   | 2:G:120:GLU:CG    | 2.43        | 0.49     |
| 1:A:969:ALA:O     | 1:A:978:ARG:HG3   | 2.13        | 0.49     |
| 1:C:944:LYS:HZ1   | 2:G:117:ARG:HH22  | 1.61        | 0.49     |
| 1:D:895:ASN:ND2   | 1:D:897:PRO:HD2   | 2.28        | 0.48     |
| 2:G:59:ARG:HB3    | 2:G:102:ASN:C     | 2.34        | 0.48     |
| 2:E:101:LEU:HB3   | 2:E:105:GLN:OE1   | 2.13        | 0.48     |
| 1:C:1062:THR:HG22 | 1:C:1063:PRO:N    | 2.29        | 0.48     |
| 1:D:942:GLY:HA3   | 1:D:944:LYS:HE3   | 1.96        | 0.48     |
| 1:D:917:ASN:HA    | 1:D:1056:LEU:HD22 | 1.96        | 0.48     |
| 1:A:994:GLN:HB3   | 1:A:1026:ASN:HD21 | 1.77        | 0.48     |
| 1:B:980:ASN:N     | 1:B:980:ASN:HD22  | 2.11        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:D:1043:ALA:O    | 1:D:1046:ILE:HG13 | 2.14        | 0.48     |
| 1:D:940:GLY:O     | 1:D:1006:LEU:HB3  | 2.14        | 0.48     |
| 1:B:988:ILE:N     | 1:B:989:PRO:HD2   | 2.29        | 0.48     |
| 1:D:1008:ARG:HH11 | 1:D:1008:ARG:HG2  | 1.76        | 0.48     |
| 2:E:92:TYR:CE2    | 2:E:93:LYS:HD3    | 2.49        | 0.48     |
| 2:E:106:ALA:O     | 2:E:110:ILE:HG13  | 2.14        | 0.48     |
| 2:F:86:TYR:CB     | 2:F:99:THR:HB     | 2.40        | 0.47     |
| 1:B:1029:ASN:ND2  | 1:B:1029:ASN:N    | 2.61        | 0.47     |
| 1:D:1001:VAL:CG2  | 1:D:1002:LYS:N    | 2.76        | 0.47     |
| 1:C:949:GLN:HE21  | 2:G:120:GLU:HG3   | 1.79        | 0.47     |
| 1:A:895:ASN:CG    | 1:A:898:MET:HG3   | 2.33        | 0.47     |
| 2:E:86:TYR:CB     | 2:E:99:THR:HB     | 2.34        | 0.47     |
| 2:F:110:ILE:HD11  | 2:F:127:LEU:HD23  | 1.95        | 0.47     |
| 1:D:983:GLN:HB3   | 1:D:983:GLN:HE21  | 1.56        | 0.47     |
| 1:B:1062:THR:HA   | 1:B:1063:PRO:HD3  | 1.68        | 0.47     |
| 1:B:896:GLN:CB    | 1:B:897:PRO:HD3   | 2.45        | 0.47     |
| 1:B:886:PRO:HG2   | 2:F:92:TYR:CD2    | 2.47        | 0.47     |
| 1:A:926:MET:HG3   | 1:A:957:ALA:HB1   | 1.96        | 0.47     |
| 1:C:988:ILE:N     | 1:C:989:PRO:CD    | 2.77        | 0.47     |
| 1:C:1001:VAL:CG2  | 1:C:1002:LYS:N    | 2.77        | 0.47     |
| 1:C:930:MET:HE3   | 1:C:1031:MET:HE1  | 1.97        | 0.47     |
| 2:H:115:GLN:HG2   | 2:H:122:GLU:OE1   | 2.15        | 0.47     |
| 1:C:894:ILE:HG13  | 1:C:895:ASN:N     | 2.29        | 0.47     |
| 1:D:933:MET:CE    | 1:D:947:LEU:HD12  | 2.45        | 0.47     |
| 1:A:1037:THR:C    | 1:A:1039:ARG:H    | 2.18        | 0.47     |
| 1:B:1008:ARG:CG   | 1:B:1011:ILE:HD12 | 2.45        | 0.47     |
| 1:B:980:ASN:N     | 1:B:980:ASN:ND2   | 2.61        | 0.47     |
| 1:D:1017:GLU:O    | 1:D:1021:GLU:HG3  | 2.15        | 0.47     |
| 1:C:953:ASP:OD2   | 2:G:121:ARG:NH1   | 2.33        | 0.47     |
| 1:B:949:GLN:HG2   | 2:F:120:GLU:CG    | 2.44        | 0.47     |
| 1:A:898:MET:CB    | 1:A:934:SER:HB3   | 2.37        | 0.47     |
| 1:B:944:LYS:HZ1   | 2:F:117:ARG:HH22  | 1.62        | 0.47     |
| 1:D:1062:THR:HG23 | 1:D:1063:PRO:HD2  | 1.97        | 0.47     |
| 2:H:92:TYR:HE2    | 2:H:93:LYS:NZ     | 2.14        | 0.46     |
| 2:G:64:ARG:HB2    | 2:G:124:SER:OG    | 2.16        | 0.46     |
| 2:F:117:ARG:HA    | 2:F:121:ARG:O     | 2.15        | 0.46     |
| 1:B:920:ILE:HG22  | 1:B:924:LYS:HE3   | 1.96        | 0.46     |
| 1:C:926:MET:HE1   | 1:C:1034:VAL:HG21 | 1.92        | 0.46     |
| 1:A:930:MET:HA    | 1:A:930:MET:CE    | 2.46        | 0.46     |
| 1:C:917:ASN:CA    | 1:C:1056:LEU:HD22 | 2.37        | 0.46     |
| 1:A:932:GLU:OE2   | 2:E:68:GLY:N      | 2.47        | 0.46     |
| 1:A:956:LYS:HB2   | 1:A:956:LYS:HE2   | 1.79        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:C:938:ARG:NH2   | 1:D:938:ARG:CZ    | 2.76        | 0.46     |
| 1:D:926:MET:HG3   | 1:D:957:ALA:HB1   | 1.96        | 0.46     |
| 1:C:1062:THR:HG23 | 1:C:1063:PRO:HD2  | 1.98        | 0.46     |
| 1:A:949:GLN:HE21  | 2:E:120:GLU:HG3   | 1.81        | 0.46     |
| 2:E:114:HIS:CD2   | 2:E:115:GLN:HG3   | 2.51        | 0.46     |
| 1:B:944:LYS:H     | 1:B:944:LYS:HG3   | 1.52        | 0.46     |
| 1:A:988:ILE:N     | 1:A:989:PRO:CD    | 2.79        | 0.46     |
| 2:H:101:LEU:HD12  | 2:H:101:LEU:O     | 2.16        | 0.46     |
| 1:B:920:ILE:CG2   | 1:B:924:LYS:HE3   | 2.46        | 0.45     |
| 1:B:910:ARG:CG    | 1:B:910:ARG:NH1   | 2.78        | 0.45     |
| 1:C:977:ILE:HG23  | 1:C:1040:GLU:OE2  | 2.17        | 0.45     |
| 1:C:1001:VAL:HG22 | 1:C:1002:LYS:N    | 2.31        | 0.45     |
| 1:D:1018:GLN:O    | 1:D:1022:MET:HG3  | 2.15        | 0.45     |
| 1:D:910:ARG:HH11  | 1:D:910:ARG:CB    | 2.29        | 0.45     |
| 1:B:988:ILE:N     | 1:B:989:PRO:CD    | 2.79        | 0.45     |
| 1:D:941:SER:HA    | 1:D:943:THR:H     | 1.82        | 0.45     |
| 1:A:915:LYS:HB3   | 1:A:1057:ARG:NH1  | 2.32        | 0.45     |
| 1:B:933:MET:HE2   | 1:B:947:LEU:HD12  | 1.98        | 0.45     |
| 1:C:1057:ARG:CG   | 1:C:1057:ARG:HH11 | 2.27        | 0.45     |
| 1:B:956:LYS:HB2   | 1:B:956:LYS:HE2   | 1.79        | 0.45     |
| 1:C:948:ILE:HG22  | 1:C:949:GLN:N     | 2.31        | 0.45     |
| 1:C:980:ASN:N     | 1:C:980:ASN:HD22  | 2.15        | 0.45     |
| 1:B:894:ILE:CG1   | 1:B:895:ASN:N     | 2.78        | 0.45     |
| 1:D:1062:THR:HG23 | 1:D:1063:PRO:CD   | 2.47        | 0.45     |
| 1:C:930:MET:HE2   | 1:C:954:ILE:CD1   | 2.47        | 0.45     |
| 2:F:72:ASN:O      | 2:F:76:HIS:CD2    | 2.67        | 0.45     |
| 1:B:1001:VAL:CG2  | 1:B:1002:LYS:N    | 2.76        | 0.45     |
| 2:G:118:LEU:O     | 2:G:121:ARG:CG    | 2.64        | 0.45     |
| 1:D:930:MET:CE    | 1:D:954:ILE:HD13  | 2.48        | 0.45     |
| 2:H:78:LEU:O      | 2:H:113:PHE:HZ    | 1.96        | 0.45     |
| 1:A:1044:ALA:HA   | 1:A:1047:LYS:HZ3  | 1.82        | 0.44     |
| 1:A:974:ASP:HB2   | 1:A:1047:LYS:HG3  | 1.99        | 0.44     |
| 2:E:85:LYS:HE3    | 2:E:101:LEU:HD13  | 1.99        | 0.44     |
| 1:D:930:MET:HE2   | 1:D:930:MET:HA    | 1.99        | 0.44     |
| 1:B:930:MET:HB2   | 1:B:930:MET:HE3   | 1.66        | 0.44     |
| 1:C:886:PRO:HG2   | 2:G:92:TYR:CD2    | 2.52        | 0.44     |
| 1:D:949:GLN:HE21  | 2:H:120:GLU:HG3   | 1.82        | 0.44     |
| 1:C:980:ASN:N     | 1:C:980:ASN:ND2   | 2.65        | 0.44     |
| 1:A:930:MET:CA    | 1:A:930:MET:CE    | 2.95        | 0.44     |
| 1:A:930:MET:HB2   | 1:A:930:MET:HE3   | 1.79        | 0.44     |
| 1:C:953:ASP:CG    | 2:G:121:ARG:HH12  | 2.18        | 0.44     |
| 1:B:948:ILE:HG22  | 1:B:949:GLN:N     | 2.30        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:H:114:HIS:O    | 2:H:115:GLN:C     | 2.56        | 0.44     |
| 1:A:975:LYS:HA   | 1:A:978:ARG:NH2   | 2.33        | 0.44     |
| 1:B:983:GLN:HE21 | 1:B:983:GLN:HB3   | 1.64        | 0.44     |
| 2:G:113:PHE:O    | 2:G:125:VAL:HG23  | 2.18        | 0.44     |
| 1:C:910:ARG:NH1  | 1:C:910:ARG:CG    | 2.80        | 0.44     |
| 1:B:895:ASN:H    | 1:B:934:SER:HB2   | 1.83        | 0.44     |
| 1:B:894:ILE:HG13 | 1:B:895:ASN:N     | 2.33        | 0.43     |
| 1:A:1034:VAL:O   | 1:A:1038:VAL:HG23 | 2.17        | 0.43     |
| 1:C:886:PRO:HD2  | 2:G:92:TYR:CG     | 2.52        | 0.43     |
| 1:A:1001:VAL:CG2 | 1:A:1002:LYS:N    | 2.78        | 0.43     |
| 1:D:973:THR:HG21 | 1:D:1049:ARG:HA   | 1.99        | 0.43     |
| 1:D:930:MET:HB2  | 1:D:930:MET:HE3   | 1.65        | 0.43     |
| 2:E:92:TYR:CD2   | 2:E:93:LYS:HD3    | 2.54        | 0.43     |
| 1:D:895:ASN:ND2  | 1:D:898:MET:HG3   | 2.33        | 0.43     |
| 1:A:894:ILE:CG1  | 1:A:895:ASN:N     | 2.79        | 0.43     |
| 1:A:895:ASN:H    | 1:A:934:SER:HB2   | 1.81        | 0.43     |
| 2:G:93:LYS:O     | 2:G:95:THR:HG23   | 2.19        | 0.43     |
| 1:B:930:MET:HE2  | 1:B:954:ILE:HD11  | 2.01        | 0.43     |
| 1:A:930:MET:HE2  | 1:A:930:MET:CA    | 2.48        | 0.43     |
| 1:A:983:GLN:HE21 | 1:A:983:GLN:HB3   | 1.57        | 0.43     |
| 1:C:895:ASN:H    | 1:C:934:SER:HB2   | 1.82        | 0.43     |
| 1:B:895:ASN:ND2  | 1:B:895:ASN:O     | 2.50        | 0.43     |
| 1:C:1062:THR:CG2 | 1:C:1063:PRO:N    | 2.82        | 0.43     |
| 1:B:917:ASN:ND2  | 1:B:920:ILE:HG12  | 2.33        | 0.43     |
| 1:D:910:ARG:HB2  | 1:D:910:ARG:NH1   | 2.32        | 0.43     |
| 1:D:976:ARG:HD2  | 1:D:976:ARG:O     | 2.18        | 0.43     |
| 1:A:944:LYS:HG3  | 1:A:944:LYS:H     | 1.43        | 0.43     |
| 1:B:926:MET:HE1  | 1:B:1034:VAL:HG21 | 1.99        | 0.43     |
| 1:A:984:VAL:HG12 | 1:A:987:ARG:NH2   | 2.34        | 0.43     |
| 1:D:1055:THR:CG2 | 1:D:1056:LEU:N    | 2.79        | 0.43     |
| 2:E:93:LYS:O     | 2:E:95:THR:HG23   | 2.19        | 0.43     |
| 1:A:1037:THR:C   | 1:A:1039:ARG:N    | 2.66        | 0.43     |
| 1:B:1005:MET:O   | 1:B:1008:ARG:HB2  | 2.19        | 0.43     |
| 1:C:994:GLN:CB   | 1:C:1026:ASN:HD21 | 2.31        | 0.43     |
| 1:D:994:GLN:CB   | 1:D:1026:ASN:HD21 | 2.32        | 0.43     |
| 1:A:976:ARG:HD2  | 1:A:976:ARG:HA    | 1.48        | 0.43     |
| 1:A:917:ASN:OD1  | 1:A:1056:LEU:HD13 | 2.18        | 0.43     |
| 1:B:930:MET:HE2  | 1:B:954:ILE:CD1   | 2.49        | 0.43     |
| 1:C:894:ILE:CG1  | 1:C:895:ASN:N     | 2.79        | 0.42     |
| 1:C:895:ASN:ND2  | 1:C:897:PRO:HD2   | 2.33        | 0.42     |
| 1:B:895:ASN:ND2  | 1:B:898:MET:CG    | 2.79        | 0.42     |
| 2:G:58:MET:HG3   | 2:G:59:ARG:N      | 2.33        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:D:930:MET:CE    | 1:D:930:MET:CA    | 2.96        | 0.42     |
| 1:D:944:LYS:O     | 1:D:948:ILE:HD12  | 2.18        | 0.42     |
| 1:B:982:LEU:HA    | 1:B:982:LEU:HD23  | 1.51        | 0.42     |
| 1:D:971:GLN:O     | 1:D:1049:ARG:HB2  | 2.19        | 0.42     |
| 1:D:926:MET:HE1   | 1:D:1034:VAL:HG21 | 2.01        | 0.42     |
| 1:D:1056:LEU:HD23 | 1:D:1056:LEU:HA   | 1.78        | 0.42     |
| 1:B:886:PRO:O     | 1:B:903:ARG:NH1   | 2.53        | 0.42     |
| 2:E:73:GLN:HA     | 2:E:73:GLN:NE2    | 2.35        | 0.42     |
| 1:A:1035:LYS:O    | 1:A:1039:ARG:HG3  | 2.20        | 0.42     |
| 1:A:1044:ALA:HA   | 1:A:1047:LYS:HZ1  | 1.84        | 0.42     |
| 1:D:930:MET:CE    | 1:D:930:MET:HA    | 2.50        | 0.42     |
| 1:B:976:ARG:HD2   | 1:B:976:ARG:O     | 2.20        | 0.42     |
| 1:B:939:GLY:O     | 1:B:941:SER:N     | 2.53        | 0.42     |
| 1:B:957:ALA:O     | 1:B:961:VAL:HG23  | 2.19        | 0.42     |
| 1:A:944:LYS:NZ    | 1:A:945:ARG:H     | 2.16        | 0.42     |
| 1:C:930:MET:HE3   | 1:C:1031:MET:CE   | 2.48        | 0.42     |
| 2:H:75:VAL:HG21   | 2:H:89:VAL:CG2    | 2.49        | 0.42     |
| 1:A:926:MET:HG3   | 1:A:957:ALA:CB    | 2.50        | 0.41     |
| 2:H:59:ARG:HB3    | 2:H:102:ASN:C     | 2.40        | 0.41     |
| 1:D:988:ILE:N     | 1:D:989:PRO:CD    | 2.82        | 0.41     |
| 1:D:1062:THR:HG22 | 1:D:1063:PRO:HD2  | 2.02        | 0.41     |
| 2:F:60:LYS:HG2    | 2:F:60:LYS:HZ2    | 1.69        | 0.41     |
| 1:D:944:LYS:H     | 1:D:944:LYS:HG3   | 1.48        | 0.41     |
| 1:B:892:GLU:HB3   | 1:B:894:ILE:HD13  | 2.02        | 0.41     |
| 1:B:895:ASN:ND2   | 1:B:897:PRO:HD2   | 2.35        | 0.41     |
| 1:B:926:MET:HE2   | 1:B:1034:VAL:HG21 | 1.99        | 0.41     |
| 1:D:988:ILE:HB    | 1:D:989:PRO:HD3   | 2.02        | 0.41     |
| 1:B:926:MET:HG3   | 1:B:957:ALA:HB1   | 2.02        | 0.41     |
| 1:C:998:LEU:HD13  | 1:C:1022:MET:O    | 2.20        | 0.41     |
| 1:D:932:GLU:HA    | 1:D:935:ARG:CZ    | 2.50        | 0.41     |
| 1:A:909:ALA:O     | 1:A:924:LYS:HE3   | 2.21        | 0.41     |
| 1:B:987:ARG:O     | 1:B:991:ILE:HD12  | 2.19        | 0.41     |
| 1:A:896:GLN:CB    | 1:A:897:PRO:HD3   | 2.50        | 0.41     |
| 1:C:884:GLU:HG3   | 1:C:906:HIS:HE1   | 1.85        | 0.41     |
| 1:B:930:MET:CE    | 1:B:1031:MET:HE3  | 2.50        | 0.41     |
| 2:E:63:ILE:O      | 2:E:95:THR:HA     | 2.21        | 0.41     |
| 1:D:994:GLN:OE1   | 1:D:1026:ASN:ND2  | 2.54        | 0.41     |
| 1:B:994:GLN:OE1   | 1:B:1026:ASN:ND2  | 2.53        | 0.41     |
| 1:D:1062:THR:HA   | 1:D:1063:PRO:HD3  | 1.90        | 0.41     |
| 2:F:59:ARG:HB3    | 2:F:102:ASN:C     | 2.41        | 0.41     |
| 2:G:92:TYR:HE2    | 2:G:93:LYS:HZ2    | 1.64        | 0.41     |
| 2:E:67:PRO:HG3    | 2:E:121:ARG:HG3   | 2.03        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:985:CYS:HA   | 1:C:988:ILE:HG13 | 2.03        | 0.41     |
| 1:D:982:LEU:HD23 | 1:D:982:LEU:HA   | 1.79        | 0.41     |
| 1:B:930:MET:CE   | 1:B:1031:MET:CE  | 2.99        | 0.41     |
| 2:F:113:PHE:O    | 2:F:125:VAL:CG2  | 2.68        | 0.41     |
| 1:C:983:GLN:HE21 | 1:C:983:GLN:HB3  | 1.59        | 0.41     |
| 1:A:1045:SER:OG  | 1:A:1058:TRP:NE1 | 2.53        | 0.41     |
| 2:G:71:THR:OG1   | 2:G:74:GLU:HG3   | 2.21        | 0.41     |
| 1:D:1047:LYS:H   | 1:D:1047:LYS:CD  | 2.14        | 0.40     |
| 1:A:1037:THR:O   | 1:A:1038:VAL:C   | 2.57        | 0.40     |
| 1:D:948:ILE:HG22 | 1:D:949:GLN:N    | 2.37        | 0.40     |
| 1:A:912:TRP:CH2  | 1:A:1060:ARG:HD3 | 2.56        | 0.40     |
| 1:B:986:GLU:O    | 1:B:989:PRO:HD2  | 2.21        | 0.40     |
| 1:A:908:GLU:O    | 1:A:911:LYS:HB2  | 2.21        | 0.40     |
| 1:A:894:ILE:HG13 | 1:A:895:ASN:N    | 2.36        | 0.40     |
| 1:C:982:LEU:HA   | 1:C:982:LEU:HD23 | 1.60        | 0.40     |
| 2:E:57:HIS:HB3   | 2:E:58:MET:H     | 1.48        | 0.40     |
| 1:C:966:LYS:HZ3  | 1:C:966:LYS:HG3  | 1.50        | 0.40     |
| 1:D:909:ALA:HB1  | 1:D:920:ILE:HG23 | 2.03        | 0.40     |
| 2:H:79:LEU:HD23  | 2:H:113:PHE:CE2  | 2.56        | 0.40     |
| 1:B:915:LYS:O    | 1:B:1057:ARG:HD3 | 2.22        | 0.40     |
| 1:A:933:MET:HE3  | 1:A:947:LEU:HD12 | 2.04        | 0.40     |
| 1:A:966:LYS:HZ3  | 1:A:966:LYS:HG3  | 1.69        | 0.40     |
| 2:G:60:LYS:HZ2   | 2:G:60:LYS:HG2   | 1.58        | 0.40     |
| 1:B:937:VAL:HG12 | 1:B:938:ARG:HD2  | 2.03        | 0.40     |
| 2:H:61:ILE:O     | 2:H:128:GLN:OE1  | 2.40        | 0.40     |
| 2:H:73:GLN:NE2   | 2:H:73:GLN:HA    | 2.35        | 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     | 170/188 (90%) | 157 (92%) | 9 (5%)  | 4 (2%)   | 9           | 35 |
| 1   | B     | 161/188 (86%) | 148 (92%) | 10 (6%) | 3 (2%)   | 12          | 42 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | C     | 161/188 (86%)  | 149 (92%) | 10 (6%) | 2 (1%)   | 19          | 57  |
| 1   | D     | 171/188 (91%)  | 156 (91%) | 10 (6%) | 5 (3%)   | 7           | 28  |
| 2   | E     | 72/74 (97%)    | 66 (92%)  | 6 (8%)  | 0        | 100         | 100 |
| 2   | F     | 71/74 (96%)    | 67 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| 2   | G     | 72/74 (97%)    | 67 (93%)  | 5 (7%)  | 0        | 100         | 100 |
| 2   | H     | 71/74 (96%)    | 67 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| All | All   | 949/1048 (91%) | 877 (92%) | 58 (6%) | 14 (2%)  | 15          | 50  |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 887  | GLU  |
| 1   | A     | 939  | GLY  |
| 1   | B     | 939  | GLY  |
| 1   | C     | 939  | GLY  |
| 1   | D     | 939  | GLY  |
| 1   | D     | 885  | PHE  |
| 1   | D     | 1053 | GLY  |
| 1   | D     | 895  | ASN  |
| 1   | B     | 915  | LYS  |
| 1   | D     | 886  | PRO  |
| 1   | A     | 1053 | GLY  |
| 1   | A     | 894  | ILE  |
| 1   | B     | 894  | ILE  |
| 1   | C     | 894  | ILE  |

### 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     | 146/159 (92%) | 108 (74%) | 38 (26%) | 1           | 2 |
| 1   | B     | 142/159 (89%) | 109 (77%) | 33 (23%) | 1           | 3 |
| 1   | C     | 142/159 (89%) | 103 (72%) | 39 (28%) | 0           | 2 |
| 1   | D     | 148/159 (93%) | 106 (72%) | 42 (28%) | 0           | 2 |

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| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |    |
|-----|-------|---------------|-----------|-----------|-------------|----|
| 2   | E     | 65/65 (100%)  | 56 (86%)  | 9 (14%)   | 5           | 14 |
| 2   | F     | 64/65 (98%)   | 55 (86%)  | 9 (14%)   | 5           | 14 |
| 2   | G     | 65/65 (100%)  | 56 (86%)  | 9 (14%)   | 5           | 14 |
| 2   | H     | 64/65 (98%)   | 56 (88%)  | 8 (12%)   | 7           | 19 |
| All | All   | 836/896 (93%) | 649 (78%) | 187 (22%) | 1           | 4  |

All (187) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 884  | GLU  |
| 1   | A     | 885  | PHE  |
| 1   | A     | 888  | GLN  |
| 1   | A     | 894  | ILE  |
| 1   | A     | 895  | ASN  |
| 1   | A     | 898  | MET  |
| 1   | A     | 910  | ARG  |
| 1   | A     | 919  | ILE  |
| 1   | A     | 928  | LEU  |
| 1   | A     | 937  | VAL  |
| 1   | A     | 944  | LYS  |
| 1   | A     | 949  | GLN  |
| 1   | A     | 956  | LYS  |
| 1   | A     | 958  | SER  |
| 1   | A     | 960  | GLU  |
| 1   | A     | 967  | GLU  |
| 1   | A     | 971  | GLN  |
| 1   | A     | 976  | ARG  |
| 1   | A     | 978  | ARG  |
| 1   | A     | 983  | GLN  |
| 1   | A     | 987  | ARG  |
| 1   | A     | 1002 | LYS  |
| 1   | A     | 1004 | THR  |
| 1   | A     | 1008 | ARG  |
| 1   | A     | 1010 | ASN  |
| 1   | A     | 1012 | SER  |
| 1   | A     | 1014 | GLU  |
| 1   | A     | 1016 | SER  |
| 1   | A     | 1022 | MET  |
| 1   | A     | 1023 | LEU  |
| 1   | A     | 1029 | ASN  |
| 1   | A     | 1032 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1035 | LYS  |
| 1   | A     | 1036 | GLU  |
| 1   | A     | 1042 | GLU  |
| 1   | A     | 1047 | LYS  |
| 1   | A     | 1049 | ARG  |
| 1   | A     | 1061 | LYS  |
| 1   | B     | 885  | PHE  |
| 1   | B     | 887  | GLU  |
| 1   | B     | 894  | ILE  |
| 1   | B     | 898  | MET  |
| 1   | B     | 910  | ARG  |
| 1   | B     | 919  | ILE  |
| 1   | B     | 928  | LEU  |
| 1   | B     | 937  | VAL  |
| 1   | B     | 944  | LYS  |
| 1   | B     | 948  | ILE  |
| 1   | B     | 949  | GLN  |
| 1   | B     | 956  | LYS  |
| 1   | B     | 958  | SER  |
| 1   | B     | 960  | GLU  |
| 1   | B     | 967  | GLU  |
| 1   | B     | 971  | GLN  |
| 1   | B     | 978  | ARG  |
| 1   | B     | 983  | GLN  |
| 1   | B     | 987  | ARG  |
| 1   | B     | 1002 | LYS  |
| 1   | B     | 1004 | THR  |
| 1   | B     | 1008 | ARG  |
| 1   | B     | 1010 | ASN  |
| 1   | B     | 1011 | ILE  |
| 1   | B     | 1012 | SER  |
| 1   | B     | 1014 | GLU  |
| 1   | B     | 1016 | SER  |
| 1   | B     | 1023 | LEU  |
| 1   | B     | 1029 | ASN  |
| 1   | B     | 1032 | GLN  |
| 1   | B     | 1035 | LYS  |
| 1   | B     | 1036 | GLU  |
| 1   | B     | 1042 | GLU  |
| 1   | C     | 885  | PHE  |
| 1   | C     | 893  | VAL  |
| 1   | C     | 894  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 898  | MET  |
| 1   | C     | 910  | ARG  |
| 1   | C     | 915  | LYS  |
| 1   | C     | 928  | LEU  |
| 1   | C     | 937  | VAL  |
| 1   | C     | 941  | SER  |
| 1   | C     | 944  | LYS  |
| 1   | C     | 948  | ILE  |
| 1   | C     | 949  | GLN  |
| 1   | C     | 956  | LYS  |
| 1   | C     | 958  | SER  |
| 1   | C     | 960  | GLU  |
| 1   | C     | 966  | LYS  |
| 1   | C     | 967  | GLU  |
| 1   | C     | 971  | GLN  |
| 1   | C     | 976  | ARG  |
| 1   | C     | 978  | ARG  |
| 1   | C     | 983  | GLN  |
| 1   | C     | 987  | ARG  |
| 1   | C     | 1001 | VAL  |
| 1   | C     | 1002 | LYS  |
| 1   | C     | 1004 | THR  |
| 1   | C     | 1008 | ARG  |
| 1   | C     | 1010 | ASN  |
| 1   | C     | 1012 | SER  |
| 1   | C     | 1014 | GLU  |
| 1   | C     | 1016 | SER  |
| 1   | C     | 1023 | LEU  |
| 1   | C     | 1029 | ASN  |
| 1   | C     | 1032 | GLN  |
| 1   | C     | 1035 | LYS  |
| 1   | C     | 1036 | GLU  |
| 1   | C     | 1042 | GLU  |
| 1   | C     | 1046 | ILE  |
| 1   | C     | 1060 | ARG  |
| 1   | C     | 1061 | LYS  |
| 1   | D     | 884  | GLU  |
| 1   | D     | 885  | PHE  |
| 1   | D     | 893  | VAL  |
| 1   | D     | 894  | ILE  |
| 1   | D     | 895  | ASN  |
| 1   | D     | 898  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 910  | ARG  |
| 1   | D     | 928  | LEU  |
| 1   | D     | 937  | VAL  |
| 1   | D     | 944  | LYS  |
| 1   | D     | 948  | ILE  |
| 1   | D     | 956  | LYS  |
| 1   | D     | 958  | SER  |
| 1   | D     | 960  | GLU  |
| 1   | D     | 966  | LYS  |
| 1   | D     | 967  | GLU  |
| 1   | D     | 971  | GLN  |
| 1   | D     | 975  | LYS  |
| 1   | D     | 976  | ARG  |
| 1   | D     | 978  | ARG  |
| 1   | D     | 983  | GLN  |
| 1   | D     | 987  | ARG  |
| 1   | D     | 1002 | LYS  |
| 1   | D     | 1004 | THR  |
| 1   | D     | 1008 | ARG  |
| 1   | D     | 1010 | ASN  |
| 1   | D     | 1012 | SER  |
| 1   | D     | 1014 | GLU  |
| 1   | D     | 1015 | GLU  |
| 1   | D     | 1016 | SER  |
| 1   | D     | 1023 | LEU  |
| 1   | D     | 1029 | ASN  |
| 1   | D     | 1032 | GLN  |
| 1   | D     | 1035 | LYS  |
| 1   | D     | 1036 | GLU  |
| 1   | D     | 1042 | GLU  |
| 1   | D     | 1046 | ILE  |
| 1   | D     | 1048 | ILE  |
| 1   | D     | 1050 | THR  |
| 1   | D     | 1057 | ARG  |
| 1   | D     | 1060 | ARG  |
| 1   | D     | 1061 | LYS  |
| 2   | E     | 57   | HIS  |
| 2   | E     | 59   | ARG  |
| 2   | E     | 62   | LEU  |
| 2   | E     | 79   | LEU  |
| 2   | E     | 81   | ASP  |
| 2   | E     | 98   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 121 | ARG  |
| 2   | E     | 124 | SER  |
| 2   | E     | 128 | GLN  |
| 2   | F     | 59  | ARG  |
| 2   | F     | 60  | LYS  |
| 2   | F     | 62  | LEU  |
| 2   | F     | 79  | LEU  |
| 2   | F     | 81  | ASP  |
| 2   | F     | 98  | VAL  |
| 2   | F     | 121 | ARG  |
| 2   | F     | 126 | GLN  |
| 2   | F     | 128 | GLN  |
| 2   | G     | 59  | ARG  |
| 2   | G     | 60  | LYS  |
| 2   | G     | 62  | LEU  |
| 2   | G     | 79  | LEU  |
| 2   | G     | 81  | ASP  |
| 2   | G     | 98  | VAL  |
| 2   | G     | 121 | ARG  |
| 2   | G     | 126 | GLN  |
| 2   | G     | 128 | GLN  |
| 2   | H     | 59  | ARG  |
| 2   | H     | 62  | LEU  |
| 2   | H     | 79  | LEU  |
| 2   | H     | 81  | ASP  |
| 2   | H     | 91  | LYS  |
| 2   | H     | 98  | VAL  |
| 2   | H     | 121 | ARG  |
| 2   | H     | 128 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 888  | GLN  |
| 1   | A     | 895  | ASN  |
| 1   | A     | 949  | GLN  |
| 1   | A     | 980  | ASN  |
| 1   | A     | 983  | GLN  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 1018 | GLN  |
| 1   | A     | 1026 | ASN  |
| 1   | A     | 1029 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 895  | ASN  |
| 1   | B     | 949  | GLN  |
| 1   | B     | 980  | ASN  |
| 1   | B     | 983  | GLN  |
| 1   | B     | 994  | GLN  |
| 1   | B     | 1018 | GLN  |
| 1   | B     | 1026 | ASN  |
| 1   | B     | 1029 | ASN  |
| 1   | C     | 895  | ASN  |
| 1   | C     | 896  | GLN  |
| 1   | C     | 906  | HIS  |
| 1   | C     | 949  | GLN  |
| 1   | C     | 980  | ASN  |
| 1   | C     | 983  | GLN  |
| 1   | C     | 1026 | ASN  |
| 1   | C     | 1029 | ASN  |
| 1   | D     | 895  | ASN  |
| 1   | D     | 949  | GLN  |
| 1   | D     | 980  | ASN  |
| 1   | D     | 983  | GLN  |
| 1   | D     | 994  | GLN  |
| 1   | D     | 1018 | GLN  |
| 1   | D     | 1026 | ASN  |
| 1   | D     | 1029 | ASN  |
| 2   | E     | 76   | HIS  |
| 2   | E     | 128  | GLN  |
| 2   | F     | 76   | HIS  |
| 2   | F     | 128  | GLN  |
| 2   | G     | 72   | ASN  |
| 2   | G     | 76   | HIS  |
| 2   | G     | 128  | GLN  |
| 2   | H     | 73   | GLN  |
| 2   | H     | 76   | HIS  |
| 2   | H     | 128  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 174/188 (92%)  | -0.05  | 0 100 100     | 31, 51, 81, 95        | 0     |
| 1   | B     | 167/188 (88%)  | 0.15   | 6 (3%) 41 48  | 34, 54, 86, 104       | 0     |
| 1   | C     | 167/188 (88%)  | 0.21   | 6 (3%) 41 48  | 34, 54, 86, 102       | 0     |
| 1   | D     | 175/188 (93%)  | 0.12   | 9 (5%) 27 33  | 30, 51, 82, 95        | 0     |
| 2   | E     | 74/74 (100%)   | 0.06   | 0 100 100     | 42, 54, 73, 95        | 0     |
| 2   | F     | 73/74 (98%)    | 0.20   | 4 (5%) 24 29  | 44, 55, 71, 90        | 0     |
| 2   | G     | 74/74 (100%)   | 0.18   | 1 (1%) 72 80  | 43, 55, 74, 95        | 0     |
| 2   | H     | 73/74 (98%)    | 0.13   | 7 (9%) 8 11   | 42, 54, 69, 87        | 0     |
| All | All   | 977/1048 (93%) | 0.11   | 33 (3%) 43 51 | 30, 54, 83, 104       | 0     |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1009 | THR  | 5.0  |
| 2   | F     | 130  | THR  | 4.6  |
| 2   | H     | 130  | THR  | 4.5  |
| 2   | G     | 130  | THR  | 4.0  |
| 1   | C     | 940  | GLY  | 3.9  |
| 1   | B     | 1007 | GLY  | 3.7  |
| 1   | C     | 1007 | GLY  | 3.7  |
| 1   | D     | 1063 | PRO  | 3.6  |
| 1   | C     | 939  | GLY  | 3.1  |
| 1   | B     | 1040 | GLU  | 3.1  |
| 1   | D     | 986  | GLU  | 3.1  |
| 1   | B     | 894  | ILE  | 3.0  |
| 1   | D     | 894  | ILE  | 2.9  |
| 2   | H     | 86   | TYR  | 2.8  |
| 2   | H     | 96   | ALA  | 2.8  |
| 1   | C     | 1006 | LEU  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 1051 | ASP  | 2.6  |
| 1   | B     | 940  | GLY  | 2.5  |
| 2   | F     | 109  | ALA  | 2.5  |
| 1   | D     | 1001 | VAL  | 2.5  |
| 1   | B     | 941  | SER  | 2.3  |
| 2   | F     | 90   | ASP  | 2.3  |
| 2   | H     | 113  | PHE  | 2.3  |
| 1   | C     | 884  | GLU  | 2.3  |
| 1   | B     | 893  | VAL  | 2.3  |
| 2   | F     | 96   | ALA  | 2.3  |
| 2   | H     | 98   | VAL  | 2.3  |
| 1   | D     | 1047 | LYS  | 2.2  |
| 1   | D     | 1054 | PHE  | 2.1  |
| 2   | H     | 62   | LEU  | 2.1  |
| 1   | D     | 948  | ILE  | 2.1  |
| 1   | D     | 975  | LYS  | 2.1  |
| 2   | H     | 61   | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.