



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QRV  
Title : Structure of Dnmt3a-Dnmt3L C-terminal domain complex  
Authors : Jia, D.; Cheng, X.  
Deposited on : 2007-07-29  
Resolution : 2.89 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

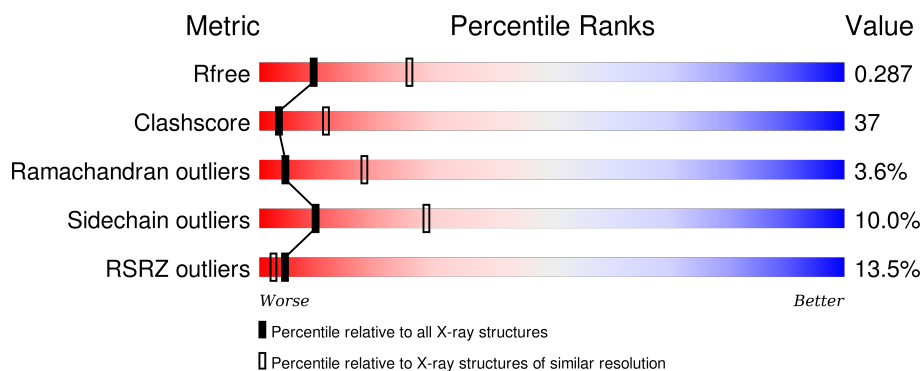
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1451 (2.90-2.90)                                      |
| Clashscore            | 102246                      | 1668 (2.90-2.90)                                      |
| Ramachandran outliers | 100387                      | 1630 (2.90-2.90)                                      |
| Sidechain outliers    | 100360                      | 1632 (2.90-2.90)                                      |
| RSRZ outliers         | 91569                       | 1456 (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. 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     | 295    | <div> <div>8%</div> <div>38% 45% 8% 8%</div> </div>   |
| 1   | D     | 295    | <div> <div>2%</div> <div>38% 44% 8% 9%</div> </div>   |
| 1   | E     | 295    | <div> <div>%</div> <div>38% 44% 8% 8%</div> </div>    |
| 1   | H     | 295    | <div> <div>8%</div> <div>35% 49% 7% 9%</div> </div>   |
| 2   | B     | 230    | <div> <div>16%</div> <div>40% 33% 8% 19%</div> </div> |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | C     | 230    | <div><div></div><div>17%</div><div>39%</div><div>38%</div><div>•</div><div>19%</div></div>  |
| 2   | F     | 230    | <div><div></div><div>17%</div><div>39%</div><div>37%</div><div>5%</div><div>19%</div></div> |
| 2   | G     | 230    | <div><div></div><div>40%</div><div>40%</div><div>37%</div><div>•</div><div>19%</div></div>  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14657 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 3A.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 272      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2143  | 1370 | 379 | 381 | 13 |         |         |       |
| 1   | D     | 267      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2111  | 1350 | 372 | 376 | 13 |         |         |       |
| 1   | E     | 270      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2128  | 1361 | 375 | 379 | 13 |         |         |       |
| 1   | H     | 267      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2111  | 1350 | 372 | 376 | 13 |         |         |       |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 614     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 615     | GLY      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 616     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 617     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 618     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 619     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 620     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 621     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| A     | 622     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 614     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 615     | GLY      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 616     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 617     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 618     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 619     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 620     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 621     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| D     | 622     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 614     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 615     | GLY      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 616     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 617     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 618     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 619     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 620     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 621     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| E     | 622     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 614     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 615     | GLY      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 616     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 617     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 618     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 619     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 620     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 621     | HIS      | -      | EXPRESSION TAG | UNP Q9Y6K1 |
| H     | 622     | MET      | -      | EXPRESSION TAG | UNP Q9Y6K1 |

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1515  | 991 | 254 | 266 | 4 |         |         |       |
| 2   | C     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1515  | 991 | 254 | 266 | 4 |         |         |       |
| 2   | F     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1515  | 991 | 254 | 266 | 4 |         |         |       |
| 2   | G     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1515  | 991 | 254 | 266 | 4 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

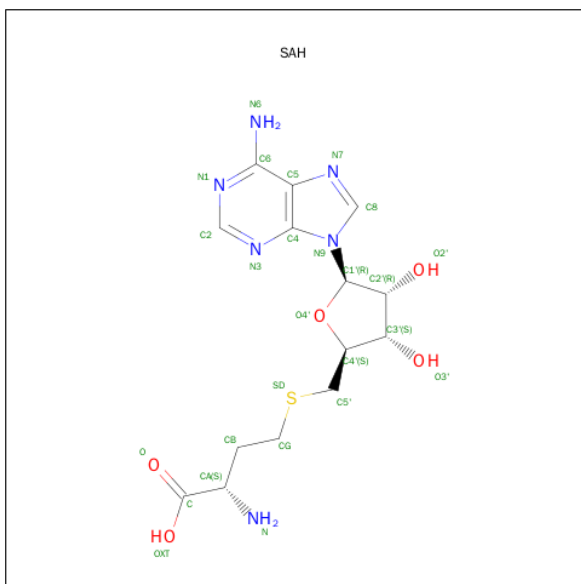
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 157     | GLY      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| B     | 158     | SER      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| B     | 159     | MET      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| C     | 157     | GLY      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| C     | 158     | SER      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| C     | 159     | MET      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| F     | 157     | GLY      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| F     | 158     | SER      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| F     | 159     | MET      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| G     | 157     | GLY      | -      | EXPRESSION TAG | UNP Q9UJW3 |
| G     | 158     | SER      | -      | EXPRESSION TAG | UNP Q9UJW3 |

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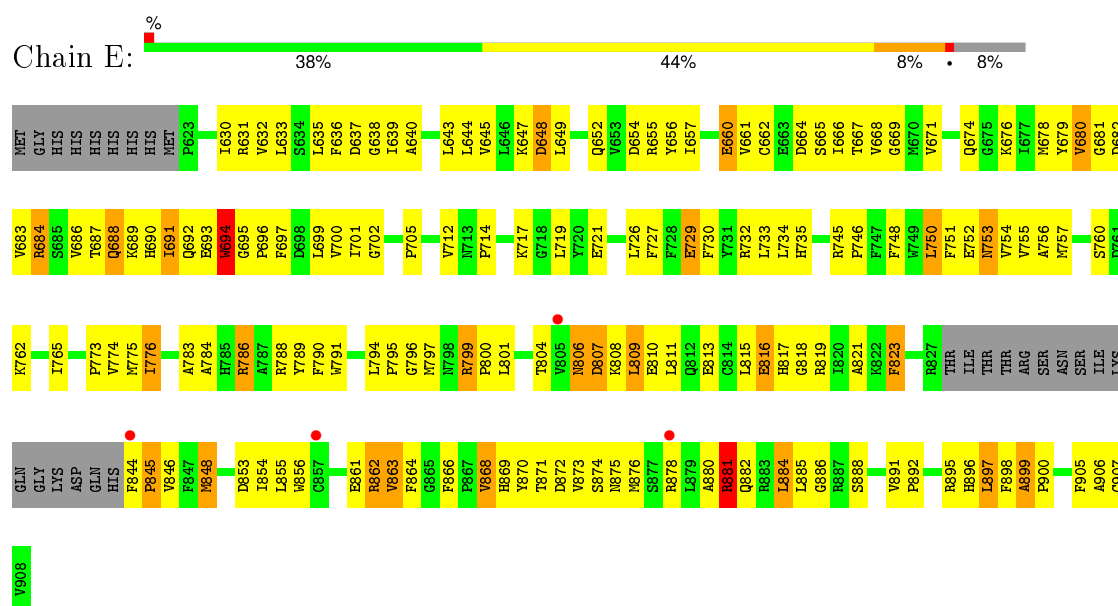
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 159     | MET      | -      | EXPRESSION TAG | UNP Q9UJW3 |

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).

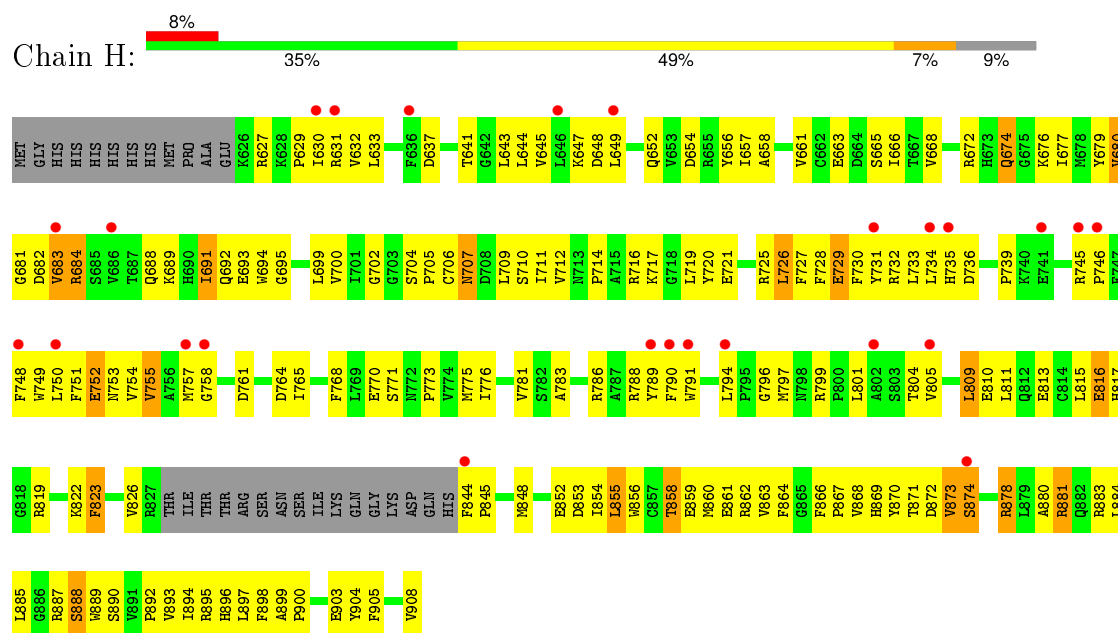


| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 3   | A     | 1        | Total<br>26 | C<br>14 | N<br>6 | O<br>5 | S<br>1 | 0       | 0       |
| 3   | D     | 1        | Total<br>26 | C<br>14 | N<br>6 | O<br>5 | S<br>1 | 0       | 0       |
| 3   | E     | 1        | Total<br>26 | C<br>14 | N<br>6 | O<br>5 | S<br>1 | 0       | 0       |
| 3   | H     | 1        | Total<br>26 | C<br>14 | N<br>6 | O<br>5 | S<br>1 | 0       | 0       |

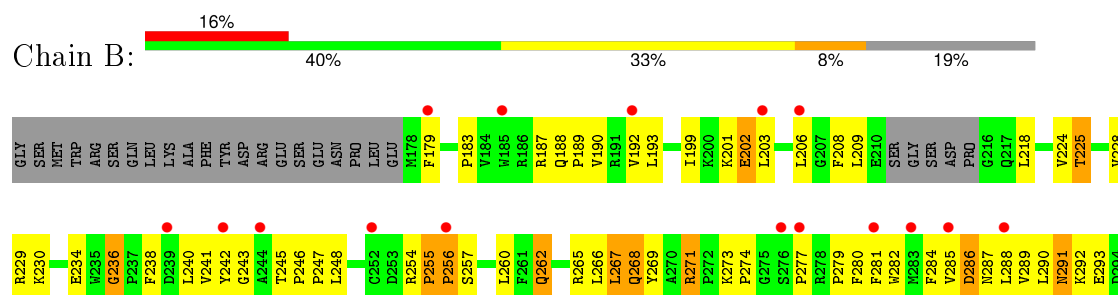




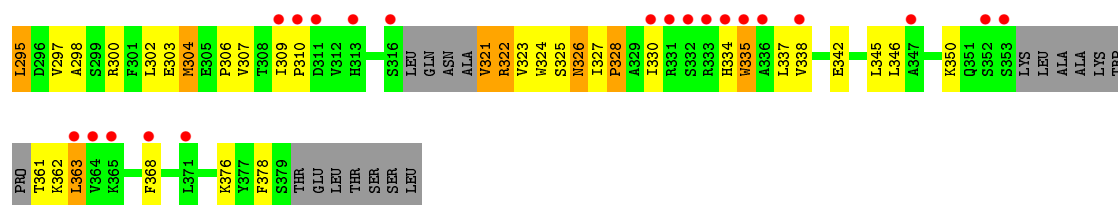
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A



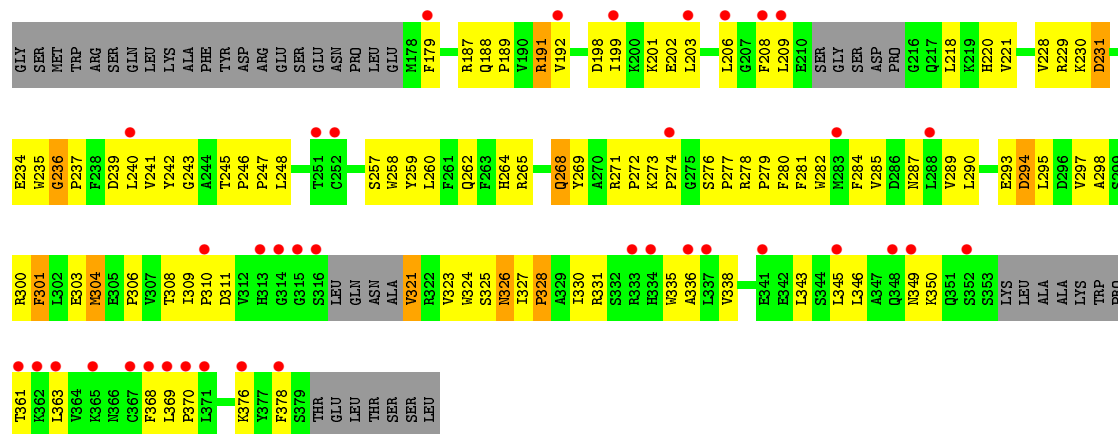
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



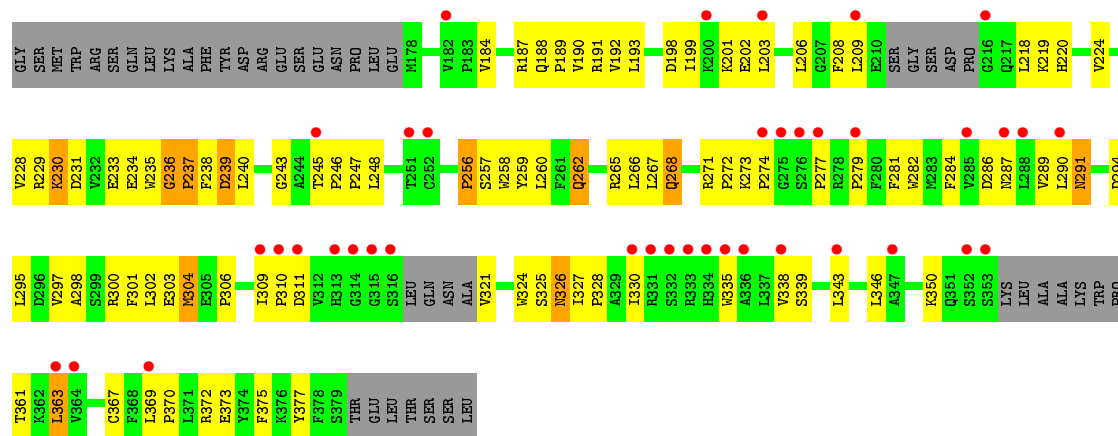




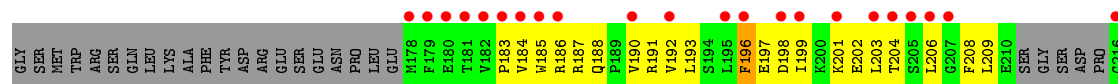
• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

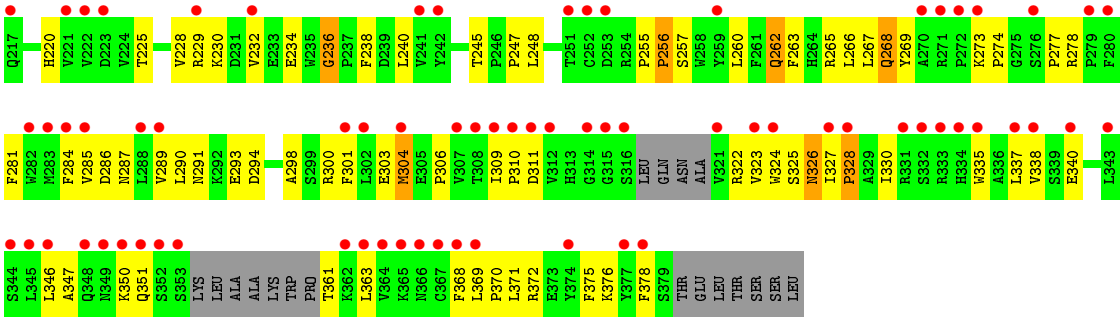


• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | H 3   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 401.88 Å   401.88 Å   49.69 Å<br>90.00°   90.00°   120.00°  | Depositor        |
| Resolution (Å)  | 38.90 – 2.89<br>43.85 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 81.9 (38.90-2.89)<br>92.7 (43.85-2.90)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.32 (at 2.90 Å)  | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.259 , 0.281<br>0.271 , 0.287                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3124 reflections (5.07%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 77.8  | Xtriage          |
| Anisotropy  | 0.423   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 79.4   | EDS              |
| Estimated twinning fraction   | 0.014 for h,-h-k,-l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 0 of 65264 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 14657   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 101.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.55         | 0/2196  | 0.83        | 2/2973 (0.1%)  |
| 1   | D     | 0.52         | 0/2162  | 0.76        | 2/2926 (0.1%)  |
| 1   | E     | 0.58         | 0/2180  | 0.78        | 1/2951 (0.0%)  |
| 1   | H     | 0.44         | 0/2162  | 0.65        | 0/2926         |
| 2   | B     | 0.41         | 0/1560  | 0.61        | 0/2120         |
| 2   | C     | 0.37         | 0/1560  | 0.59        | 0/2120         |
| 2   | F     | 0.35         | 0/1560  | 0.58        | 0/2120         |
| 2   | G     | 0.36         | 0/1560  | 0.54        | 0/2120         |
| All | All   | 0.47         | 0/14940 | 0.69        | 5/20256 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 844 | PHE  | C-N-CD    | -13.46 | 91.00       | 120.60   |
| 1   | D     | 875 | ASN  | N-CA-C    | -6.49  | 93.47       | 111.00   |
| 1   | A     | 644 | LEU  | CA-CB-CG  | 6.20   | 129.55      | 115.30   |
| 1   | D     | 872 | ASP  | CB-CG-OD2 | -5.62  | 113.24      | 118.30   |
| 1   | E     | 881 | ARG  | NE-CZ-NH1 | 5.04   | 122.82      | 120.30   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 2143  | 0        | 2076     | 174     | 0            |
| 1   | D     | 2111  | 0        | 2052     | 172     | 0            |
| 1   | E     | 2128  | 0        | 2067     | 170     | 0            |
| 1   | H     | 2111  | 0        | 2052     | 195     | 0            |
| 2   | B     | 1515  | 0        | 1484     | 122     | 0            |
| 2   | C     | 1515  | 0        | 1484     | 93      | 0            |
| 2   | F     | 1515  | 0        | 1484     | 109     | 0            |
| 2   | G     | 1515  | 0        | 1484     | 105     | 0            |
| 3   | A     | 26    | 0        | 19       | 1       | 0            |
| 3   | D     | 26    | 0        | 19       | 0       | 0            |
| 3   | E     | 26    | 0        | 19       | 1       | 0            |
| 3   | H     | 26    | 0        | 19       | 2       | 0            |
| All | All   | 14657 | 0        | 14259    | 1076    | 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 37.

All (1076) 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:E:786:ARG:HG3  | 1:E:786:ARG:HH11 | 1.19                     | 1.06              |
| 1:E:655:ARG:HH12 | 1:E:695:GLY:HA3  | 1.20                     | 1.05              |
| 2:B:271:ARG:HH11 | 2:B:271:ARG:HG3  | 1.13                     | 1.05              |
| 1:E:854:ILE:HG22 | 1:E:855:LEU:H    | 1.18                     | 1.05              |
| 1:A:843:HIS:O    | 1:A:845:PRO:HD3  | 1.59                     | 1.02              |
| 1:D:655:ARG:HH12 | 1:D:695:GLY:HA3  | 1.25                     | 1.01              |
| 1:E:873:VAL:HG23 | 1:E:874:SER:H    | 1.22                     | 1.01              |
| 1:A:811:LEU:HD13 | 1:A:826:VAL:HG13 | 1.43                     | 1.00              |
| 1:D:874:SER:HB2  | 1:D:876:MET:HB2  | 1.40                     | 0.99              |
| 2:F:262:GLN:HA   | 2:F:262:GLN:HE21 | 1.26                     | 0.97              |
| 2:F:363:LEU:H    | 2:F:363:LEU:HD22 | 1.29                     | 0.97              |
| 1:E:662:CYS:O    | 1:E:666:ILE:HG13 | 1.65                     | 0.96              |
| 1:H:871:THR:OG1  | 1:H:881:ARG:HD3  | 1.65                     | 0.95              |
| 2:B:260:LEU:HD21 | 2:B:298:ALA:HA   | 1.49                     | 0.94              |
| 1:D:680:VAL:HG12 | 1:D:681:GLY:H    | 1.33                     | 0.93              |
| 1:A:655:ARG:HH12 | 1:A:695:GLY:HA3  | 1.33                     | 0.92              |
| 1:A:725:ARG:HH12 | 2:B:297:VAL:HG21 | 1.32                     | 0.92              |
| 2:B:363:LEU:H    | 2:B:363:LEU:HD22 | 1.34                     | 0.92              |
| 2:B:248:LEU:H    | 2:B:287:ASN:HD21 | 1.17                     | 0.91              |
| 1:A:632:VAL:HG22 | 1:A:699:LEU:HB3  | 1.51                     | 0.91              |
| 1:E:680:VAL:HG12 | 1:E:681:GLY:H    | 1.36                     | 0.89              |
| 1:A:858:THR:HG22 | 1:A:868:VAL:HG12 | 1.51                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:326:ASN:HD22 | 2:C:326:ASN:H    | 1.19                     | 0.89              |
| 1:A:878:ARG:HH11 | 1:A:878:ARG:HG2  | 1.36                     | 0.88              |
| 2:G:300:ARG:HH11 | 1:H:732:ARG:NH1  | 1.71                     | 0.88              |
| 2:G:262:GLN:HE21 | 2:G:262:GLN:HA   | 1.40                     | 0.87              |
| 1:A:686:VAL:O    | 1:A:732:ARG:NH2  | 2.07                     | 0.87              |
| 2:G:300:ARG:HH11 | 1:H:732:ARG:HH12 | 1.18                     | 0.86              |
| 1:H:815:LEU:HA   | 1:H:859:GLU:HG2  | 1.55                     | 0.86              |
| 1:E:776:ILE:HD11 | 1:E:801:LEU:HD21 | 1.57                     | 0.86              |
| 2:B:201:LYS:HB3  | 2:B:202:GLU:OE1  | 1.76                     | 0.86              |
| 2:G:300:ARG:CZ   | 1:H:684:ARG:HB2  | 2.06                     | 0.86              |
| 2:G:273:LYS:HB3  | 2:G:274:PRO:HD2  | 1.56                     | 0.85              |
| 2:F:326:ASN:H    | 2:F:326:ASN:HD22 | 1.18                     | 0.85              |
| 1:D:648:ASP:HB3  | 1:D:895:ARG:HH12 | 1.40                     | 0.85              |
| 1:H:732:ARG:HH21 | 1:H:733:LEU:HD21 | 1.41                     | 0.84              |
| 1:E:752:GLU:HG2  | 1:E:753:ASN:H    | 1.43                     | 0.84              |
| 1:H:773:PRO:HD3  | 1:H:791:TRP:NE1  | 1.93                     | 0.84              |
| 2:G:311:ASP:HB2  | 2:G:363:LEU:HD11 | 1.59                     | 0.84              |
| 2:C:310:PRO:HG2  | 2:C:338:VAL:HG21 | 1.60                     | 0.83              |
| 1:A:667:THR:O    | 1:A:671:VAL:HG23 | 1.78                     | 0.83              |
| 2:F:273:LYS:HB3  | 2:F:274:PRO:HD2  | 1.60                     | 0.83              |
| 1:A:843:HIS:C    | 1:A:845:PRO:HD3  | 1.99                     | 0.82              |
| 1:D:680:VAL:HG12 | 1:D:681:GLY:N    | 1.89                     | 0.82              |
| 1:D:786:ARG:HG3  | 1:D:786:ARG:HH11 | 1.42                     | 0.82              |
| 2:F:202:GLU:HG2  | 2:F:361:THR:HG23 | 1.62                     | 0.81              |
| 1:E:655:ARG:NH1  | 1:E:695:GLY:HA3  | 1.95                     | 0.81              |
| 2:G:256:PRO:HB3  | 2:G:290:LEU:HD23 | 1.61                     | 0.81              |
| 1:D:631:ARG:HH11 | 1:D:631:ARG:HB2  | 1.45                     | 0.81              |
| 1:H:860:MET:HG2  | 1:H:864:PHE:HE1  | 1.42                     | 0.81              |
| 1:H:873:VAL:HG23 | 1:H:874:SER:H    | 1.45                     | 0.81              |
| 1:A:739:PRO:HG3  | 1:A:745:ARG:NH2  | 1.94                     | 0.81              |
| 1:A:643:LEU:HG   | 1:A:647:LYS:HE3  | 1.61                     | 0.81              |
| 2:B:271:ARG:NH1  | 2:B:271:ARG:HG3  | 1.84                     | 0.81              |
| 1:A:725:ARG:NH1  | 2:B:297:VAL:HG21 | 1.95                     | 0.80              |
| 2:C:202:GLU:HG2  | 2:C:361:THR:HG23 | 1.64                     | 0.80              |
| 1:E:691:ILE:HD11 | 1:E:733:LEU:HD12 | 1.62                     | 0.80              |
| 2:C:285:VAL:HG22 | 2:C:323:VAL:HG22 | 1.63                     | 0.80              |
| 1:A:809:LEU:HD12 | 1:A:809:LEU:H    | 1.47                     | 0.80              |
| 1:A:750:LEU:HD12 | 1:A:791:TRP:O    | 1.82                     | 0.79              |
| 1:A:874:SER:HA   | 1:D:856:TRP:CE2  | 2.18                     | 0.79              |
| 2:B:273:LYS:HB3  | 2:B:274:PRO:HD2  | 1.65                     | 0.79              |
| 2:C:294:ASP:CG   | 1:D:725:ARG:HH22 | 1.86                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:648:ASP:HB3  | 1:D:895:ARG:NH1  | 1.97                     | 0.79              |
| 1:H:682:ASP:OD2  | 1:H:684:ARG:HD3  | 1.83                     | 0.79              |
| 2:B:188:GLN:HB3  | 2:B:189:PRO:HD2  | 1.64                     | 0.79              |
| 1:D:684:ARG:H    | 1:D:684:ARG:HD3  | 1.47                     | 0.79              |
| 1:E:786:ARG:NH1  | 1:E:786:ARG:HG3  | 1.96                     | 0.78              |
| 1:E:854:ILE:HG22 | 1:E:855:LEU:N    | 1.98                     | 0.78              |
| 2:C:247:PRO:HA   | 2:C:287:ASN:HD22 | 1.46                     | 0.78              |
| 1:A:858:THR:HG22 | 1:A:868:VAL:CG1  | 2.12                     | 0.78              |
| 1:H:732:ARG:HE   | 1:H:733:LEU:CD2  | 1.96                     | 0.78              |
| 2:C:188:GLN:HB3  | 2:C:189:PRO:HD2  | 1.65                     | 0.78              |
| 1:D:655:ARG:NH1  | 1:D:695:GLY:HA3  | 1.97                     | 0.78              |
| 1:A:655:ARG:NH1  | 1:A:695:GLY:HA3  | 1.99                     | 0.78              |
| 1:H:773:PRO:HD3  | 1:H:791:TRP:HE1  | 1.45                     | 0.78              |
| 1:H:858:THR:HG22 | 1:H:868:VAL:CG1  | 2.13                     | 0.78              |
| 1:D:755:VAL:HA   | 1:D:789:TYR:CD2  | 2.19                     | 0.78              |
| 1:H:897:LEU:O    | 1:H:900:PRO:HD2  | 1.82                     | 0.77              |
| 2:B:326:ASN:HD22 | 2:B:326:ASN:H    | 1.31                     | 0.77              |
| 1:D:801:LEU:HD12 | 1:D:801:LEU:H    | 1.48                     | 0.77              |
| 1:A:672:ARG:HG3  | 1:A:870:TYR:CE1  | 2.19                     | 0.77              |
| 1:H:873:VAL:HG23 | 1:H:874:SER:N    | 2.00                     | 0.77              |
| 1:E:861:GLU:OE1  | 1:E:869:HIS:N    | 2.18                     | 0.77              |
| 2:G:187:ARG:O    | 2:G:376:LYS:HB2  | 1.85                     | 0.77              |
| 1:E:873:VAL:HG23 | 1:E:874:SER:N    | 2.00                     | 0.77              |
| 1:D:871:THR:OG1  | 1:D:881:ARG:HD3  | 1.85                     | 0.76              |
| 2:C:260:LEU:HD21 | 2:C:298:ALA:HA   | 1.64                     | 0.76              |
| 1:E:732:ARG:NH2  | 1:E:733:LEU:HD21 | 2.00                     | 0.76              |
| 1:E:776:ILE:CD1  | 1:E:801:LEU:HD21 | 2.15                     | 0.76              |
| 1:D:664:ASP:O    | 1:D:668:VAL:HG23 | 1.85                     | 0.76              |
| 2:G:232:VAL:HG21 | 2:G:266:LEU:HD22 | 1.68                     | 0.76              |
| 1:E:680:VAL:HG12 | 1:E:681:GLY:N    | 2.02                     | 0.75              |
| 1:H:880:ALA:O    | 1:H:884:LEU:HD13 | 1.86                     | 0.75              |
| 1:A:649:LEU:O    | 1:A:902:LYS:HE2  | 1.87                     | 0.75              |
| 2:B:202:GLU:HG2  | 2:B:361:THR:HG23 | 1.67                     | 0.75              |
| 1:H:683:VAL:HG22 | 3:H:8:SAH:N1     | 2.00                     | 0.75              |
| 1:A:843:HIS:O    | 1:A:845:PRO:CD   | 2.35                     | 0.75              |
| 2:F:202:GLU:HG2  | 2:F:361:THR:CG2  | 2.17                     | 0.74              |
| 1:E:683:VAL:HG23 | 1:E:684:ARG:HD3  | 1.68                     | 0.74              |
| 1:D:857:CYS:O    | 1:D:861:GLU:HG3  | 1.88                     | 0.74              |
| 2:F:193:LEU:HB2  | 2:F:238:PHE:CE2  | 2.23                     | 0.74              |
| 1:A:723:THR:HB   | 1:A:726:LEU:HD12 | 1.69                     | 0.74              |
| 2:C:273:LYS:HB3  | 2:C:274:PRO:HD2  | 1.67                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:193:LEU:HB2  | 2:F:238:PHE:CD2  | 2.23                     | 0.73              |
| 1:A:794:LEU:O    | 1:A:797:MET:HG3  | 1.88                     | 0.73              |
| 1:H:691:ILE:HG22 | 1:H:692:GLN:N    | 2.01                     | 0.73              |
| 2:C:310:PRO:CG   | 2:C:338:VAL:HG21 | 2.19                     | 0.73              |
| 1:D:652:GLN:HB2  | 1:D:906:ALA:HB3  | 1.69                     | 0.73              |
| 2:G:192:VAL:HG22 | 2:G:240:LEU:HB3  | 1.70                     | 0.73              |
| 1:A:804:THR:HG22 | 1:A:806:ASN:H    | 1.52                     | 0.73              |
| 2:F:248:LEU:H    | 2:F:287:ASN:ND2  | 1.86                     | 0.73              |
| 1:A:878:ARG:NH1  | 1:A:878:ARG:HG2  | 1.99                     | 0.73              |
| 1:E:788:ARG:HH11 | 1:E:788:ARG:HG2  | 1.54                     | 0.72              |
| 2:C:228:VAL:HG12 | 2:C:229:ARG:N    | 2.02                     | 0.72              |
| 1:E:752:GLU:HG2  | 1:E:753:ASN:N    | 2.02                     | 0.72              |
| 2:B:262:GLN:NE2  | 2:B:265:ARG:HE   | 1.88                     | 0.72              |
| 1:A:684:ARG:H    | 1:A:684:ARG:HD3  | 1.54                     | 0.72              |
| 1:E:801:LEU:HD12 | 1:E:801:LEU:H    | 1.55                     | 0.72              |
| 2:C:192:VAL:HG21 | 2:C:203:LEU:HD21 | 1.71                     | 0.71              |
| 2:B:248:LEU:H    | 2:B:287:ASN:ND2  | 1.87                     | 0.71              |
| 2:F:240:LEU:HA   | 2:F:281:PHE:O    | 1.91                     | 0.71              |
| 1:A:823:PHE:CZ   | 1:A:842:GLN:HA   | 2.26                     | 0.71              |
| 1:H:732:ARG:HE   | 1:H:733:LEU:HD22 | 1.54                     | 0.71              |
| 1:A:680:VAL:HG12 | 1:A:681:GLY:N    | 2.04                     | 0.71              |
| 2:B:248:LEU:N    | 2:B:287:ASN:HD21 | 1.87                     | 0.71              |
| 1:D:648:ASP:CB   | 1:D:895:ARG:HH12 | 2.04                     | 0.71              |
| 2:G:281:PHE:HE2  | 2:G:328:PRO:HD3  | 1.55                     | 0.71              |
| 2:B:267:LEU:HD13 | 2:B:268:GLN:NE2  | 2.06                     | 0.71              |
| 2:G:248:LEU:H    | 2:G:287:ASN:ND2  | 1.89                     | 0.71              |
| 2:B:268:GLN:HE21 | 2:B:268:GLN:N    | 1.89                     | 0.71              |
| 2:G:247:PRO:HA   | 2:G:287:ASN:ND2  | 2.06                     | 0.70              |
| 2:F:192:VAL:HG21 | 2:F:203:LEU:HD21 | 1.72                     | 0.70              |
| 1:H:755:VAL:HG21 | 1:H:775:MET:SD   | 2.31                     | 0.70              |
| 2:B:248:LEU:N    | 2:B:287:ASN:ND2  | 2.38                     | 0.70              |
| 2:F:191:ARG:HH21 | 2:F:237:PRO:HB2  | 1.56                     | 0.70              |
| 1:H:704:SER:HG   | 1:H:751:PHE:HZ   | 1.39                     | 0.70              |
| 1:H:786:ARG:HG3  | 1:H:786:ARG:HH11 | 1.56                     | 0.70              |
| 1:H:871:THR:CB   | 1:H:881:ARG:HD3  | 2.22                     | 0.70              |
| 1:D:801:LEU:HD12 | 1:D:801:LEU:N    | 2.07                     | 0.70              |
| 1:E:866:PHE:HE2  | 1:E:888:SER:HG   | 1.40                     | 0.70              |
| 2:F:363:LEU:CD2  | 2:F:363:LEU:H    | 2.03                     | 0.70              |
| 1:H:844:PHE:HB3  | 1:H:852:GLU:HG2  | 1.72                     | 0.70              |
| 1:E:891:VAL:HB   | 1:E:892:PRO:HD3  | 1.74                     | 0.70              |
| 2:C:260:LEU:CD2  | 2:C:298:ALA:HA   | 2.21                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:376:LYS:HD3  | 2:C:378:PHE:CE2  | 2.26                     | 0.69              |
| 1:A:680:VAL:HG12 | 1:A:681:GLY:H    | 1.57                     | 0.69              |
| 1:H:823:PHE:CD1  | 1:H:823:PHE:N    | 2.57                     | 0.69              |
| 2:B:292:LYS:HA   | 2:B:295:LEU:HD22 | 1.73                     | 0.69              |
| 1:H:666:ILE:HA   | 1:H:679:TYR:HE2  | 1.56                     | 0.69              |
| 1:E:810:GLU:N    | 1:E:810:GLU:OE2  | 2.24                     | 0.69              |
| 1:A:881:ARG:O    | 1:A:884:LEU:HB2  | 1.93                     | 0.69              |
| 2:B:260:LEU:HD21 | 2:B:298:ALA:CA   | 2.21                     | 0.69              |
| 2:B:240:LEU:HA   | 2:B:281:PHE:O    | 1.93                     | 0.69              |
| 1:E:753:ASN:ND2  | 1:E:754:VAL:HG22 | 2.08                     | 0.69              |
| 1:D:686:VAL:O    | 1:D:732:ARG:NH2  | 2.26                     | 0.68              |
| 1:A:856:TRP:HB2  | 1:A:859:GLU:HG3  | 1.75                     | 0.68              |
| 2:F:262:GLN:HA   | 2:F:262:GLN:NE2  | 2.05                     | 0.68              |
| 2:G:199:ILE:HG22 | 2:G:203:LEU:HB2  | 1.75                     | 0.68              |
| 1:D:680:VAL:CG1  | 1:D:681:GLY:H    | 2.07                     | 0.68              |
| 1:H:732:ARG:NH2  | 1:H:733:LEU:HD21 | 2.08                     | 0.68              |
| 2:B:267:LEU:HD13 | 2:B:268:GLN:HE22 | 1.57                     | 0.68              |
| 2:G:262:GLN:NE2  | 2:G:262:GLN:HA   | 2.09                     | 0.68              |
| 2:G:369:LEU:HB2  | 2:G:370:PRO:HD3  | 1.75                     | 0.68              |
| 1:H:861:GLU:OE1  | 1:H:869:HIS:N    | 2.27                     | 0.67              |
| 1:D:683:VAL:HG23 | 1:D:684:ARG:N    | 2.09                     | 0.67              |
| 1:D:752:GLU:HG2  | 1:D:753:ASN:N    | 2.08                     | 0.67              |
| 1:E:854:ILE:CG2  | 1:E:855:LEU:H    | 2.00                     | 0.67              |
| 1:E:705:PRO:HG2  | 1:E:726:LEU:HD12 | 1.77                     | 0.67              |
| 1:A:853:ASP:OD2  | 1:A:854:ILE:N    | 2.27                     | 0.67              |
| 1:A:729:GLU:OE2  | 1:A:732:ARG:NH1  | 2.26                     | 0.67              |
| 2:G:306:PRO:HB3  | 2:G:324:TRP:CZ2  | 2.30                     | 0.67              |
| 1:A:683:VAL:HG22 | 3:A:1:SAH:N1     | 2.10                     | 0.67              |
| 2:B:229:ARG:HA   | 2:B:269:TYR:CD1  | 2.30                     | 0.67              |
| 1:A:859:GLU:O    | 1:A:863:VAL:HG23 | 1.95                     | 0.67              |
| 1:H:712:VAL:O    | 1:H:714:PRO:HD3  | 1.93                     | 0.67              |
| 2:G:363:LEU:HD22 | 2:G:363:LEU:H    | 1.60                     | 0.66              |
| 2:F:187:ARG:HH12 | 2:F:373:GLU:HA   | 1.59                     | 0.66              |
| 1:E:630:ILE:HG22 | 1:E:652:GLN:O    | 1.95                     | 0.66              |
| 1:D:855:LEU:HD23 | 1:D:856:TRP:H    | 1.60                     | 0.66              |
| 1:H:730:PHE:CE2  | 1:H:734:LEU:HD12 | 2.30                     | 0.66              |
| 1:E:667:THR:O    | 1:E:671:VAL:HG23 | 1.96                     | 0.66              |
| 1:E:750:LEU:HD11 | 1:E:897:LEU:HD13 | 1.78                     | 0.66              |
| 1:H:729:GLU:O    | 1:H:733:LEU:HD23 | 1.95                     | 0.66              |
| 2:F:228:VAL:HG12 | 2:F:229:ARG:H    | 1.60                     | 0.66              |
| 1:A:786:ARG:HH21 | 1:A:788:ARG:NH2  | 1.93                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:717:LYS:HB3  | 1:E:721:GLU:HB2  | 1.78                     | 0.66              |
| 2:F:282:TRP:H    | 2:F:326:ASN:HD21 | 1.44                     | 0.66              |
| 2:B:262:GLN:HE22 | 2:B:265:ARG:HE   | 1.40                     | 0.66              |
| 2:B:256:PRO:HB3  | 2:B:290:LEU:HD23 | 1.76                     | 0.66              |
| 2:G:262:GLN:HE22 | 2:G:265:ARG:HE   | 1.44                     | 0.66              |
| 2:B:291:ASN:O    | 2:B:295:LEU:HD13 | 1.96                     | 0.66              |
| 1:D:691:ILE:HD11 | 1:D:733:LEU:HD12 | 1.78                     | 0.65              |
| 2:F:363:LEU:N    | 2:F:363:LEU:HD22 | 2.08                     | 0.65              |
| 2:G:260:LEU:HD21 | 2:G:298:ALA:HA   | 1.77                     | 0.65              |
| 1:E:815:LEU:HD11 | 1:E:846:VAL:CG1  | 2.26                     | 0.65              |
| 2:G:202:GLU:HG2  | 2:G:361:THR:CG2  | 2.26                     | 0.65              |
| 1:H:860:MET:HG2  | 1:H:864:PHE:CE1  | 2.28                     | 0.65              |
| 2:C:202:GLU:O    | 2:C:206:LEU:HD23 | 1.96                     | 0.65              |
| 2:C:376:LYS:HD3  | 2:C:378:PHE:HE2  | 1.62                     | 0.65              |
| 2:B:285:VAL:HG13 | 2:B:323:VAL:HG22 | 1.77                     | 0.65              |
| 1:H:719:LEU:HB2  | 1:H:761:ASP:OD2  | 1.96                     | 0.65              |
| 2:C:268:GLN:HG2  | 1:D:735:HIS:CE1  | 2.32                     | 0.65              |
| 1:A:631:ARG:HD2  | 1:A:698:ASP:OD1  | 1.96                     | 0.65              |
| 1:A:869:HIS:CE1  | 1:D:872:ASP:HB3  | 2.32                     | 0.64              |
| 1:D:786:ARG:HG3  | 1:D:786:ARG:NH1  | 2.12                     | 0.64              |
| 2:C:247:PRO:HA   | 2:C:287:ASN:ND2  | 2.11                     | 0.64              |
| 1:H:890:SER:OG   | 1:H:892:PRO:HD2  | 1.97                     | 0.64              |
| 1:H:895:ARG:O    | 1:H:899:ALA:HB2  | 1.97                     | 0.64              |
| 2:F:248:LEU:H    | 2:F:287:ASN:HD21 | 1.44                     | 0.64              |
| 1:H:755:VAL:HG21 | 1:H:775:MET:CE   | 2.28                     | 0.64              |
| 2:F:193:LEU:HD13 | 2:F:238:PHE:CZ   | 2.31                     | 0.64              |
| 2:G:228:VAL:HG12 | 2:G:229:ARG:H    | 1.60                     | 0.64              |
| 2:F:228:VAL:HG12 | 2:F:229:ARG:N    | 2.12                     | 0.64              |
| 2:G:310:PRO:HG2  | 2:G:338:VAL:HG21 | 1.80                     | 0.64              |
| 1:D:672:ARG:HD2  | 1:D:870:TYR:CD1  | 2.33                     | 0.64              |
| 1:E:872:ASP:HB3  | 1:H:869:HIS:CE1  | 2.33                     | 0.63              |
| 2:G:228:VAL:HG12 | 2:G:229:ARG:N    | 2.13                     | 0.63              |
| 2:F:230:LYS:N    | 2:F:230:LYS:HD2  | 2.12                     | 0.63              |
| 2:G:262:GLN:CA   | 2:G:262:GLN:HE21 | 2.10                     | 0.63              |
| 2:B:199:ILE:HD11 | 2:B:242:TYR:CE2  | 2.33                     | 0.63              |
| 1:D:709:LEU:HD13 | 1:D:757:MET:HE1  | 1.80                     | 0.63              |
| 1:E:815:LEU:HD11 | 1:E:846:VAL:HG11 | 1.80                     | 0.63              |
| 1:E:801:LEU:HD12 | 1:E:801:LEU:N    | 2.12                     | 0.63              |
| 1:D:794:LEU:O    | 1:D:797:MET:HG3  | 1.98                     | 0.63              |
| 1:A:684:ARG:HB2  | 2:B:300:ARG:CZ   | 2.29                     | 0.63              |
| 2:G:202:GLU:O    | 2:G:206:LEU:HD23 | 1.99                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:202:GLU:HG2  | 2:G:361:THR:HG23 | 1.79                     | 0.63              |
| 1:D:748:PHE:HB3  | 1:D:794:LEU:CD2  | 2.28                     | 0.63              |
| 1:E:649:LEU:HD22 | 1:E:899:ALA:HA   | 1.79                     | 0.63              |
| 2:B:245:THR:HB   | 2:B:289:VAL:HG11 | 1.81                     | 0.62              |
| 1:H:867:PRO:O    | 1:H:870:TYR:HB2  | 1.99                     | 0.62              |
| 2:F:230:LYS:H    | 2:F:230:LYS:HD2  | 1.64                     | 0.62              |
| 2:C:311:ASP:HB2  | 2:C:363:LEU:HD11 | 1.82                     | 0.62              |
| 1:A:682:ASP:OD2  | 1:A:684:ARG:HD3  | 1.99                     | 0.62              |
| 2:B:293:GLU:N    | 2:B:293:GLU:OE2  | 2.33                     | 0.62              |
| 2:B:363:LEU:CD2  | 2:B:363:LEU:H    | 2.11                     | 0.62              |
| 2:B:267:LEU:CD1  | 2:B:268:GLN:HE22 | 2.12                     | 0.62              |
| 1:H:819:ARG:HD2  | 1:H:848:MET:SD   | 2.40                     | 0.62              |
| 1:H:716:ARG:HG2  | 1:H:716:ARG:HH11 | 1.64                     | 0.62              |
| 2:B:247:PRO:HA   | 2:B:287:ASN:ND2  | 2.15                     | 0.61              |
| 1:H:860:MET:O    | 1:H:863:VAL:HB   | 2.00                     | 0.61              |
| 1:H:810:GLU:H    | 1:H:810:GLU:CD   | 2.04                     | 0.61              |
| 2:B:199:ILE:HG22 | 2:B:203:LEU:HB2  | 1.81                     | 0.61              |
| 2:B:376:LYS:HD3  | 2:B:378:PHE:CE2  | 2.35                     | 0.61              |
| 1:H:691:ILE:HG21 | 1:H:736:ASP:O    | 2.00                     | 0.61              |
| 2:C:198:ASP:HB3  | 2:C:220:HIS:ND1  | 2.15                     | 0.61              |
| 1:E:875:ASN:HB3  | 1:H:878:ARG:HD2  | 1.82                     | 0.61              |
| 1:D:717:LYS:HB3  | 1:D:721:GLU:HB2  | 1.83                     | 0.61              |
| 1:H:711:ILE:HD11 | 1:H:758:GLY:N    | 2.16                     | 0.61              |
| 2:B:287:ASN:HA   | 2:B:321:VAL:HG23 | 1.83                     | 0.61              |
| 1:H:796:GLY:O    | 1:H:799:ARG:HG3  | 1.99                     | 0.61              |
| 2:B:282:TRP:CZ3  | 2:B:302:LEU:HD22 | 2.35                     | 0.61              |
| 1:H:801:LEU:N    | 1:H:801:LEU:HD12 | 2.16                     | 0.61              |
| 1:A:824:SER:O    | 1:A:825:LYS:HG2  | 2.00                     | 0.61              |
| 2:G:193:LEU:HB2  | 2:G:238:PHE:CD2  | 2.35                     | 0.61              |
| 1:H:649:LEU:HD21 | 1:H:895:ARG:HG2  | 1.81                     | 0.61              |
| 1:H:717:LYS:O    | 1:H:721:GLU:HB2  | 2.00                     | 0.61              |
| 1:D:683:VAL:HG23 | 1:D:729:GLU:HG2  | 1.83                     | 0.61              |
| 2:B:268:GLN:HE21 | 2:B:268:GLN:CA   | 2.11                     | 0.61              |
| 1:D:730:PHE:CE2  | 1:D:751:PHE:HB2  | 2.35                     | 0.61              |
| 2:G:248:LEU:H    | 2:G:287:ASN:HD21 | 1.49                     | 0.61              |
| 1:D:749:TRP:CZ3  | 1:D:769:LEU:HD13 | 2.36                     | 0.60              |
| 1:E:816:GLU:O    | 1:E:819:ARG:HG3  | 2.01                     | 0.60              |
| 1:H:815:LEU:HA   | 1:H:859:GLU:CG   | 2.29                     | 0.60              |
| 1:D:786:ARG:NH1  | 1:D:864:PHE:HE2  | 1.98                     | 0.60              |
| 1:E:729:GLU:OE2  | 2:F:301:PHE:HE1  | 1.84                     | 0.60              |
| 2:C:228:VAL:HG12 | 2:C:229:ARG:H    | 1.64                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:844:PHE:N    | 1:H:845:PRO:HD3  | 2.17                     | 0.60              |
| 1:E:655:ARG:HH12 | 1:E:695:GLY:CA   | 2.06                     | 0.60              |
| 2:F:191:ARG:HB2  | 2:F:239:ASP:OD1  | 2.01                     | 0.60              |
| 2:B:271:ARG:NH1  | 2:B:271:ARG:CG   | 2.60                     | 0.60              |
| 1:D:820:ILE:O    | 1:D:847:PHE:N    | 2.30                     | 0.60              |
| 1:E:688:GLN:HE21 | 1:E:692:GLN:NE2  | 2.00                     | 0.60              |
| 1:A:811:LEU:CD1  | 1:A:826:VAL:HG13 | 2.27                     | 0.60              |
| 2:B:202:GLU:OE1  | 2:B:202:GLU:N    | 2.35                     | 0.60              |
| 2:B:248:LEU:HD21 | 2:B:288:LEU:O    | 2.01                     | 0.60              |
| 1:H:641:THR:O    | 1:H:645:VAL:HG23 | 2.02                     | 0.60              |
| 2:G:327:ILE:O    | 2:G:330:ILE:HB   | 2.01                     | 0.60              |
| 1:A:633:LEU:HD13 | 1:A:697:PHE:CZ   | 2.37                     | 0.59              |
| 2:F:190:VAL:HB   | 2:F:375:PHE:CD1  | 2.37                     | 0.59              |
| 2:C:240:LEU:HA   | 2:C:281:PHE:O    | 2.01                     | 0.59              |
| 1:E:786:ARG:NH1  | 1:E:864:PHE:CE2  | 2.70                     | 0.59              |
| 1:D:635:LEU:HD12 | 1:D:730:PHE:HD1  | 1.67                     | 0.59              |
| 1:H:668:VAL:HG22 | 1:H:873:VAL:HG21 | 1.83                     | 0.59              |
| 2:G:260:LEU:CD2  | 2:G:298:ALA:HA   | 2.33                     | 0.59              |
| 2:B:346:LEU:O    | 2:B:350:LYS:HG2  | 2.02                     | 0.59              |
| 1:H:883:ARG:HD3  | 1:H:887:ARG:NH2  | 2.18                     | 0.59              |
| 1:D:855:LEU:HD23 | 1:D:856:TRP:N    | 2.18                     | 0.59              |
| 1:H:799:ARG:HH22 | 1:H:899:ALA:HB3  | 1.68                     | 0.59              |
| 2:B:285:VAL:HG22 | 2:B:323:VAL:HG22 | 1.85                     | 0.59              |
| 1:E:635:LEU:HD12 | 1:E:730:PHE:CD1  | 2.38                     | 0.59              |
| 1:E:874:SER:HA   | 1:H:856:TRP:CE2  | 2.38                     | 0.59              |
| 1:H:732:ARG:HE   | 1:H:733:LEU:HD21 | 1.68                     | 0.59              |
| 2:F:198:ASP:HB3  | 2:F:220:HIS:ND1  | 2.18                     | 0.59              |
| 1:E:872:ASP:OD1  | 1:H:869:HIS:ND1  | 2.32                     | 0.59              |
| 1:H:811:LEU:HD13 | 1:H:811:LEU:O    | 2.03                     | 0.59              |
| 1:E:643:LEU:O    | 1:E:647:LYS:HG3  | 2.02                     | 0.59              |
| 1:A:809:LEU:HD12 | 1:A:809:LEU:N    | 2.15                     | 0.58              |
| 2:C:228:VAL:CG1  | 2:C:229:ARG:N    | 2.65                     | 0.58              |
| 1:H:680:VAL:HG12 | 1:H:681:GLY:H    | 1.68                     | 0.58              |
| 1:A:635:LEU:HD12 | 1:A:730:PHE:CD1  | 2.38                     | 0.58              |
| 1:E:729:GLU:O    | 1:E:733:LEU:HD23 | 2.03                     | 0.58              |
| 2:C:187:ARG:O    | 2:C:376:LYS:HB2  | 2.02                     | 0.58              |
| 2:F:248:LEU:N    | 2:F:287:ASN:ND2  | 2.50                     | 0.58              |
| 2:B:192:VAL:HG22 | 2:B:240:LEU:HB3  | 1.84                     | 0.58              |
| 2:C:245:THR:HB   | 2:C:289:VAL:HG11 | 1.85                     | 0.58              |
| 1:H:754:VAL:HA   | 1:H:788:ARG:HD3  | 1.85                     | 0.58              |
| 1:H:786:ARG:HG3  | 1:H:786:ARG:NH1  | 2.19                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:843:HIS:N    | 1:A:843:HIS:ND1  | 2.51                     | 0.58              |
| 2:G:300:ARG:NH1  | 1:H:732:ARG:NH1  | 2.49                     | 0.58              |
| 2:G:310:PRO:CG   | 2:G:338:VAL:HG21 | 2.33                     | 0.58              |
| 1:A:874:SER:HA   | 1:D:856:TRP:NE1  | 2.18                     | 0.58              |
| 2:B:203:LEU:HD13 | 2:B:368:PHE:CD1  | 2.39                     | 0.58              |
| 2:C:202:GLU:HG2  | 2:C:361:THR:CG2  | 2.32                     | 0.58              |
| 1:E:671:VAL:HG11 | 1:H:816:GLU:HG2  | 1.86                     | 0.58              |
| 2:B:179:PHE:HE2  | 2:B:280:PHE:H    | 1.52                     | 0.58              |
| 1:D:649:LEU:HD22 | 1:D:899:ALA:HA   | 1.86                     | 0.58              |
| 1:A:811:LEU:O    | 1:A:811:LEU:HG   | 2.02                     | 0.58              |
| 2:B:203:LEU:HG   | 2:B:209:LEU:HD11 | 1.86                     | 0.58              |
| 2:G:306:PRO:HB3  | 2:G:324:TRP:CE2  | 2.39                     | 0.58              |
| 2:F:372:ARG:HH11 | 2:F:372:ARG:HG2  | 1.69                     | 0.58              |
| 2:C:346:LEU:O    | 2:C:350:LYS:HG2  | 2.04                     | 0.58              |
| 2:F:291:ASN:O    | 2:F:295:LEU:HD13 | 2.04                     | 0.57              |
| 2:G:300:ARG:NH1  | 1:H:732:ARG:HH12 | 1.96                     | 0.57              |
| 1:D:855:LEU:CD2  | 1:D:859:GLU:HB2  | 2.35                     | 0.57              |
| 2:C:228:VAL:CG1  | 2:C:229:ARG:H    | 2.17                     | 0.57              |
| 2:F:310:PRO:HG2  | 2:F:338:VAL:HG21 | 1.85                     | 0.57              |
| 1:H:858:THR:HG22 | 1:H:868:VAL:HG12 | 1.87                     | 0.57              |
| 1:E:752:GLU:HB2  | 1:E:790:PHE:CE2  | 2.39                     | 0.57              |
| 1:E:688:GLN:NE2  | 1:E:692:GLN:NE2  | 2.52                     | 0.57              |
| 1:E:669:GLY:HA3  | 1:E:679:TYR:OH   | 2.05                     | 0.57              |
| 2:G:248:LEU:N    | 2:G:287:ASN:ND2  | 2.52                     | 0.57              |
| 1:D:673:HIS:C    | 1:D:674:GLN:HG2  | 2.24                     | 0.57              |
| 1:E:752:GLU:O    | 1:E:753:ASN:HB2  | 2.05                     | 0.57              |
| 1:A:786:ARG:NH1  | 1:A:864:PHE:CE2  | 2.73                     | 0.57              |
| 2:F:290:LEU:HB2  | 2:F:295:LEU:CD1  | 2.35                     | 0.57              |
| 1:E:688:GLN:HE21 | 1:E:692:GLN:HE22 | 1.53                     | 0.57              |
| 1:E:755:VAL:HA   | 1:E:789:TYR:CD2  | 2.40                     | 0.57              |
| 1:A:776:ILE:HD11 | 1:A:801:LEU:HD21 | 1.86                     | 0.57              |
| 1:A:656:TYR:HD2  | 1:A:677:ILE:HG12 | 1.69                     | 0.57              |
| 1:H:755:VAL:HA   | 1:H:789:TYR:CD2  | 2.39                     | 0.56              |
| 1:D:702:GLY:O    | 1:D:751:PHE:HA   | 2.05                     | 0.56              |
| 1:H:868:VAL:O    | 1:H:869:HIS:HB2  | 2.06                     | 0.56              |
| 1:D:633:LEU:HB2  | 1:D:697:PHE:CD2  | 2.40                     | 0.56              |
| 1:H:734:LEU:HD11 | 1:H:749:TRP:CE3  | 2.39                     | 0.56              |
| 2:C:271:ARG:HG3  | 2:C:271:ARG:HH11 | 1.69                     | 0.56              |
| 1:A:872:ASP:HB3  | 1:D:869:HIS:CE1  | 2.41                     | 0.56              |
| 2:C:248:LEU:H    | 2:C:287:ASN:ND2  | 2.03                     | 0.56              |
| 1:H:810:GLU:OE2  | 1:H:810:GLU:N    | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:286:ASP:OD2  | 2:F:290:LEU:HG   | 2.05                     | 0.56              |
| 2:C:246:PRO:HG2  | 2:C:259:TYR:OH   | 2.05                     | 0.56              |
| 1:E:823:PHE:CD1  | 1:E:823:PHE:N    | 2.72                     | 0.56              |
| 2:C:230:LYS:HD2  | 2:C:230:LYS:H    | 1.70                     | 0.56              |
| 2:C:309:ILE:HG13 | 2:C:321:VAL:HG12 | 1.88                     | 0.56              |
| 1:E:801:LEU:HA   | 1:E:896:HIS:CE1  | 2.41                     | 0.56              |
| 1:A:786:ARG:NH1  | 1:A:864:PHE:HE2  | 2.03                     | 0.56              |
| 1:D:635:LEU:HD12 | 1:D:730:PHE:CD1  | 2.40                     | 0.56              |
| 2:C:230:LYS:N    | 2:C:230:LYS:HD2  | 2.20                     | 0.56              |
| 2:B:361:THR:N    | 2:B:363:LEU:CD2  | 2.69                     | 0.56              |
| 1:A:680:VAL:CG1  | 1:A:681:GLY:H    | 2.19                     | 0.56              |
| 1:D:752:GLU:O    | 1:D:753:ASN:HB2  | 2.05                     | 0.56              |
| 2:B:260:LEU:CD2  | 2:B:298:ALA:HA   | 2.29                     | 0.56              |
| 1:H:691:ILE:CG2  | 1:H:692:GLN:N    | 2.69                     | 0.56              |
| 2:C:201:LYS:HB3  | 2:C:202:GLU:OE1  | 2.05                     | 0.56              |
| 1:H:726:LEU:O    | 1:H:729:GLU:HB2  | 2.05                     | 0.56              |
| 1:A:770:GLU:OE2  | 2:B:229:ARG:NH1  | 2.39                     | 0.56              |
| 1:H:632:VAL:HG12 | 1:H:633:LEU:N    | 2.21                     | 0.56              |
| 2:C:310:PRO:HG2  | 2:C:338:VAL:CG2  | 2.35                     | 0.56              |
| 1:E:632:VAL:HG13 | 1:E:699:LEU:HG   | 1.88                     | 0.56              |
| 1:E:652:GLN:HB2  | 1:E:906:ALA:HB3  | 1.86                     | 0.56              |
| 1:D:861:GLU:OE1  | 1:D:869:HIS:N    | 2.39                     | 0.56              |
| 1:A:691:ILE:HG22 | 1:A:692:GLN:N    | 2.21                     | 0.56              |
| 1:D:732:ARG:NH2  | 1:D:733:LEU:HD21 | 2.21                     | 0.55              |
| 2:B:262:GLN:HA   | 2:B:262:GLN:HE21 | 1.70                     | 0.55              |
| 1:A:680:VAL:CG1  | 1:A:681:GLY:N    | 2.70                     | 0.55              |
| 2:B:326:ASN:ND2  | 2:B:326:ASN:H    | 2.03                     | 0.55              |
| 1:H:666:ILE:HA   | 1:H:679:TYR:CE2  | 2.40                     | 0.55              |
| 1:A:878:ARG:HH12 | 1:A:879:LEU:HD23 | 1.71                     | 0.55              |
| 1:H:684:ARG:HA   | 1:H:732:ARG:HH22 | 1.70                     | 0.55              |
| 2:B:291:ASN:HB3  | 2:B:293:GLU:OE2  | 2.06                     | 0.55              |
| 1:D:752:GLU:HG2  | 1:D:753:ASN:H    | 1.69                     | 0.55              |
| 1:A:853:ASP:CG   | 1:A:854:ILE:N    | 2.59                     | 0.55              |
| 1:A:671:VAL:HG11 | 1:D:816:GLU:HG2  | 1.89                     | 0.55              |
| 1:H:799:ARG:NH2  | 1:H:900:PRO:HD3  | 2.21                     | 0.55              |
| 2:C:199:ILE:HD11 | 2:C:242:TYR:CE2  | 2.42                     | 0.55              |
| 2:B:285:VAL:HG13 | 2:B:323:VAL:CG2  | 2.36                     | 0.55              |
| 1:H:699:LEU:HA   | 1:H:748:PHE:O    | 2.07                     | 0.55              |
| 1:D:748:PHE:HA   | 1:D:793:ASN:HD21 | 1.70                     | 0.55              |
| 2:B:203:LEU:HG   | 2:B:209:LEU:CD1  | 2.37                     | 0.55              |
| 1:D:700:VAL:O    | 1:D:749:TRP:HA   | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:739:PRO:HB3  | 1:D:743:ASP:OD2  | 2.06                     | 0.55              |
| 1:E:660:GLU:HB3  | 1:E:666:ILE:HG12 | 1.89                     | 0.55              |
| 1:E:752:GLU:CG   | 1:E:753:ASN:N    | 2.69                     | 0.55              |
| 1:E:732:ARG:NH2  | 1:E:733:LEU:CD2  | 2.68                     | 0.55              |
| 2:G:230:LYS:H    | 2:G:230:LYS:HD2  | 1.72                     | 0.55              |
| 2:B:306:PRO:HB3  | 2:B:324:TRP:CE2  | 2.42                     | 0.55              |
| 1:A:748:PHE:HB3  | 1:A:794:LEU:HD23 | 1.88                     | 0.55              |
| 1:A:704:SER:HG   | 1:A:751:PHE:HZ   | 1.54                     | 0.55              |
| 1:H:750:LEU:HD12 | 1:H:791:TRP:O    | 2.07                     | 0.55              |
| 1:H:710:SER:O    | 1:H:716:ARG:HD3  | 2.06                     | 0.55              |
| 2:G:372:ARG:HH11 | 2:G:372:ARG:HG2  | 1.71                     | 0.55              |
| 2:B:228:VAL:HG12 | 2:B:229:ARG:N    | 2.20                     | 0.55              |
| 1:A:816:GLU:HG2  | 1:D:671:VAL:HG11 | 1.88                     | 0.55              |
| 1:H:656:TYR:HD2  | 1:H:677:ILE:HG23 | 1.71                     | 0.55              |
| 2:C:282:TRP:H    | 2:C:326:ASN:HD21 | 1.55                     | 0.55              |
| 2:C:326:ASN:HD22 | 2:C:326:ASN:N    | 1.91                     | 0.55              |
| 1:E:874:SER:C    | 1:E:876:MET:H    | 2.10                     | 0.54              |
| 1:A:643:LEU:HD23 | 1:A:673:HIS:ND1  | 2.22                     | 0.54              |
| 1:E:748:PHE:HB3  | 1:E:794:LEU:HD23 | 1.89                     | 0.54              |
| 1:A:635:LEU:HD12 | 1:A:730:PHE:HD1  | 1.70                     | 0.54              |
| 1:D:819:ARG:NH1  | 1:D:853:ASP:OD1  | 2.40                     | 0.54              |
| 1:A:716:ARG:HG2  | 1:A:716:ARG:HH11 | 1.70                     | 0.54              |
| 2:F:208:PHE:C    | 2:F:209:LEU:HD12 | 2.27                     | 0.54              |
| 2:B:266:LEU:N    | 2:B:266:LEU:HD23 | 2.22                     | 0.54              |
| 1:E:683:VAL:HG23 | 1:E:684:ARG:H    | 1.72                     | 0.54              |
| 2:G:240:LEU:HA   | 2:G:281:PHE:O    | 2.07                     | 0.54              |
| 2:F:324:TRP:O    | 2:F:325:SER:HB2  | 2.08                     | 0.54              |
| 2:C:324:TRP:O    | 2:C:325:SER:HB2  | 2.07                     | 0.54              |
| 2:B:199:ILE:HG21 | 2:B:368:PHE:HE1  | 1.71                     | 0.54              |
| 2:G:326:ASN:HD22 | 2:G:326:ASN:H    | 1.56                     | 0.54              |
| 2:C:303:GLU:O    | 2:C:304:MET:HB3  | 2.08                     | 0.54              |
| 1:E:726:LEU:O    | 1:E:729:GLU:HB2  | 2.08                     | 0.54              |
| 2:G:183:PRO:O    | 2:G:187:ARG:HG3  | 2.08                     | 0.54              |
| 1:A:844:PHE:O    | 1:A:853:ASP:O    | 2.25                     | 0.54              |
| 1:H:688:GLN:NE2  | 1:H:692:GLN:NE2  | 2.56                     | 0.54              |
| 2:G:199:ILE:HG22 | 2:G:199:ILE:O    | 2.08                     | 0.54              |
| 1:A:660:GLU:OE2  | 1:A:661:VAL:N    | 2.41                     | 0.54              |
| 2:B:203:LEU:HD11 | 2:B:208:PHE:HD1  | 1.72                     | 0.53              |
| 1:D:752:GLU:HB2  | 1:D:790:PHE:CE2  | 2.43                     | 0.53              |
| 2:F:187:ARG:NH1  | 2:F:373:GLU:HA   | 2.21                     | 0.53              |
| 1:H:739:PRO:HG3  | 1:H:745:ARG:NH2  | 2.23                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:849:ASN:O    | 1:A:850:GLU:HB2  | 2.08                     | 0.53              |
| 2:B:303:GLU:O    | 2:B:304:MET:HB3  | 2.07                     | 0.53              |
| 1:H:733:LEU:N    | 1:H:733:LEU:HD22 | 2.24                     | 0.53              |
| 1:H:889:TRP:NE1  | 3:H:8:SAH:N      | 2.56                     | 0.53              |
| 1:D:711:ILE:HD11 | 1:D:758:GLY:N    | 2.24                     | 0.53              |
| 2:G:192:VAL:HG21 | 2:G:203:LEU:HD21 | 1.89                     | 0.53              |
| 1:D:739:PRO:HG3  | 1:D:745:ARG:NH2  | 2.23                     | 0.53              |
| 2:B:286:ASP:O    | 2:B:321:VAL:HG22 | 2.08                     | 0.53              |
| 1:D:858:THR:HG23 | 1:D:868:VAL:CG1  | 2.39                     | 0.53              |
| 1:A:869:HIS:HE1  | 1:D:872:ASP:HB3  | 1.73                     | 0.53              |
| 1:H:873:VAL:O    | 1:H:874:SER:O    | 2.26                     | 0.53              |
| 1:H:716:ARG:HG2  | 1:H:716:ARG:NH1  | 2.23                     | 0.53              |
| 1:H:810:GLU:HG2  | 1:H:813:GLU:CB   | 2.38                     | 0.53              |
| 1:E:694:TRP:HA   | 1:E:694:TRP:HE3  | 1.73                     | 0.53              |
| 1:H:704:SER:OG   | 1:H:751:PHE:HZ   | 1.90                     | 0.53              |
| 1:E:866:PHE:HE2  | 1:E:888:SER:OG   | 1.91                     | 0.53              |
| 2:C:293:GLU:OE2  | 2:C:293:GLU:N    | 2.38                     | 0.53              |
| 1:H:817:HIS:C    | 1:H:817:HIS:CD2  | 2.82                     | 0.53              |
| 2:G:190:VAL:HB   | 2:G:375:PHE:CD1  | 2.43                     | 0.53              |
| 2:C:264:HIS:CD2  | 1:D:731:TYR:HE2  | 2.25                     | 0.53              |
| 1:E:815:LEU:CD1  | 1:E:846:VAL:HG11 | 2.39                     | 0.53              |
| 2:B:193:LEU:HD22 | 2:B:238:PHE:CE1  | 2.44                     | 0.53              |
| 1:A:875:ASN:CG   | 1:D:878:ARG:HD2  | 2.29                     | 0.53              |
| 1:E:699:LEU:HD11 | 1:E:701:ILE:CG2  | 2.39                     | 0.53              |
| 2:G:232:VAL:CG2  | 2:G:266:LEU:HD22 | 2.37                     | 0.52              |
| 1:E:694:TRP:HA   | 1:E:694:TRP:CE3  | 2.44                     | 0.52              |
| 1:E:666:ILE:HG23 | 1:E:679:TYR:CD2  | 2.43                     | 0.52              |
| 1:A:861:GLU:OE1  | 1:A:869:HIS:N    | 2.42                     | 0.52              |
| 1:H:682:ASP:OD2  | 1:H:682:ASP:C    | 2.48                     | 0.52              |
| 1:D:848:MET:O    | 1:D:851:LYS:N    | 2.35                     | 0.52              |
| 2:C:363:LEU:HD22 | 2:C:363:LEU:H    | 1.75                     | 0.52              |
| 1:H:652:GLN:HG2  | 1:H:908:VAL:CB   | 2.39                     | 0.52              |
| 1:E:898:PHE:C    | 1:E:900:PRO:HD2  | 2.30                     | 0.52              |
| 2:G:363:LEU:N    | 2:G:363:LEU:HD22 | 2.22                     | 0.52              |
| 1:A:643:LEU:HD23 | 1:A:673:HIS:CG   | 2.45                     | 0.52              |
| 1:E:712:VAL:O    | 1:E:714:PRO:HD3  | 2.09                     | 0.52              |
| 1:E:873:VAL:CG2  | 1:E:874:SER:H    | 2.04                     | 0.52              |
| 2:G:281:PHE:CE2  | 2:G:328:PRO:HD3  | 2.40                     | 0.52              |
| 2:F:191:ARG:NH2  | 2:F:237:PRO:HB2  | 2.23                     | 0.52              |
| 2:G:268:GLN:HG2  | 1:H:735:HIS:NE2  | 2.25                     | 0.52              |
| 2:C:290:LEU:HB2  | 2:C:295:LEU:CD1  | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:311:ASP:CB   | 2:G:363:LEU:HD11 | 2.36                     | 0.52              |
| 1:A:649:LEU:HD22 | 1:A:902:LYS:HE3  | 1.91                     | 0.52              |
| 1:E:794:LEU:O    | 1:E:797:MET:HG3  | 2.10                     | 0.52              |
| 2:F:303:GLU:O    | 2:F:304:MET:HB3  | 2.08                     | 0.52              |
| 1:A:799:ARG:NH2  | 1:A:900:PRO:HD3  | 2.24                     | 0.52              |
| 1:D:874:SER:HB2  | 1:D:876:MET:CB   | 2.27                     | 0.52              |
| 1:H:799:ARG:NH2  | 1:H:896:HIS:O    | 2.43                     | 0.52              |
| 1:H:700:VAL:O    | 1:H:749:TRP:HA   | 2.10                     | 0.52              |
| 2:B:346:LEU:HD23 | 2:B:346:LEU:O    | 2.09                     | 0.52              |
| 1:E:636:PHE:HE2  | 1:E:726:LEU:HD13 | 1.75                     | 0.52              |
| 1:E:686:VAL:O    | 1:E:732:ARG:NH2  | 2.43                     | 0.52              |
| 2:B:192:VAL:HG21 | 2:B:203:LEU:HD21 | 1.91                     | 0.52              |
| 1:D:643:LEU:HD23 | 1:D:673:HIS:CD2  | 2.45                     | 0.52              |
| 2:C:262:GLN:HA   | 2:C:262:GLN:NE2  | 2.24                     | 0.52              |
| 1:H:693:GLU:C    | 1:H:695:GLY:H    | 2.12                     | 0.52              |
| 1:D:753:ASN:ND2  | 1:D:754:VAL:HG22 | 2.25                     | 0.52              |
| 2:C:209:LEU:HD12 | 2:C:209:LEU:N    | 2.25                     | 0.52              |
| 1:E:753:ASN:HD22 | 1:E:754:VAL:N    | 2.08                     | 0.52              |
| 1:E:633:LEU:HB3  | 1:E:700:VAL:HG22 | 1.92                     | 0.52              |
| 2:C:304:MET:HB2  | 2:C:331:ARG:NH2  | 2.25                     | 0.52              |
| 2:G:198:ASP:HB3  | 2:G:220:HIS:CG   | 2.45                     | 0.52              |
| 1:H:706:CYS:HB2  | 1:H:754:VAL:HG13 | 1.92                     | 0.52              |
| 2:C:346:LEU:O    | 2:C:346:LEU:HD23 | 2.10                     | 0.52              |
| 1:E:817:HIS:CE1  | 1:H:674:GLN:HB3  | 2.45                     | 0.52              |
| 1:H:750:LEU:HD11 | 1:H:790:PHE:HD2  | 1.75                     | 0.51              |
| 1:H:788:ARG:HH11 | 1:H:788:ARG:HG2  | 1.75                     | 0.51              |
| 1:A:868:VAL:O    | 1:A:869:HIS:HB2  | 2.10                     | 0.51              |
| 1:H:776:ILE:HD11 | 1:H:801:LEU:HD21 | 1.93                     | 0.51              |
| 1:D:810:GLU:HG2  | 1:D:813:GLU:CB   | 2.40                     | 0.51              |
| 2:F:260:LEU:CD2  | 2:F:298:ALA:HA   | 2.40                     | 0.51              |
| 1:A:872:ASP:HB3  | 1:D:869:HIS:HE1  | 1.74                     | 0.51              |
| 2:F:327:ILE:O    | 2:F:330:ILE:HB   | 2.10                     | 0.51              |
| 1:D:645:VAL:HG11 | 1:D:895:ARG:HA   | 1.92                     | 0.51              |
| 1:A:643:LEU:CG   | 1:A:647:LYS:HE3  | 2.38                     | 0.51              |
| 2:B:203:LEU:HD13 | 2:B:368:PHE:HD1  | 1.75                     | 0.51              |
| 1:E:786:ARG:NH1  | 1:E:864:PHE:HE2  | 2.07                     | 0.51              |
| 2:G:324:TRP:O    | 2:G:325:SER:HB2  | 2.10                     | 0.51              |
| 2:F:306:PRO:HB3  | 2:F:324:TRP:CE2  | 2.45                     | 0.51              |
| 1:A:799:ARG:NH2  | 1:A:896:HIS:O    | 2.43                     | 0.51              |
| 2:G:184:VAL:C    | 2:G:186:ARG:H    | 2.14                     | 0.51              |
| 1:E:871:THR:HB   | 1:E:881:ARG:HG2  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:748:PHE:HB3  | 1:E:794:LEU:CD2  | 2.41                     | 0.51              |
| 1:A:671:VAL:CG1  | 1:D:816:GLU:HG2  | 2.41                     | 0.51              |
| 1:D:747:PHE:O    | 1:D:793:ASN:ND2  | 2.39                     | 0.51              |
| 2:B:286:ASP:OD1  | 2:B:322:ARG:HG3  | 2.11                     | 0.51              |
| 1:A:633:LEU:HD13 | 1:A:697:PHE:CE1  | 2.46                     | 0.51              |
| 1:A:854:ILE:HG22 | 1:A:855:LEU:N    | 2.25                     | 0.51              |
| 1:H:801:LEU:HD12 | 1:H:801:LEU:H    | 1.76                     | 0.51              |
| 1:D:749:TRP:HZ3  | 1:D:769:LEU:HD13 | 1.75                     | 0.51              |
| 1:E:687:THR:O    | 1:E:690:HIS:HB2  | 2.11                     | 0.51              |
| 1:D:783:ALA:O    | 1:D:826:VAL:HG22 | 2.10                     | 0.51              |
| 2:G:322:ARG:HH22 | 2:G:340:GLU:CD   | 2.12                     | 0.51              |
| 1:D:633:LEU:HB2  | 1:D:697:PHE:CE2  | 2.46                     | 0.51              |
| 2:B:201:LYS:HE3  | 2:B:202:GLU:OE1  | 2.11                     | 0.51              |
| 1:D:711:ILE:HD11 | 1:D:757:MET:C    | 2.31                     | 0.51              |
| 1:H:629:PRO:HB2  | 1:H:654:ASP:HB2  | 1.92                     | 0.51              |
| 1:E:693:GLU:C    | 1:E:695:GLY:H    | 2.14                     | 0.50              |
| 1:E:730:PHE:CE2  | 1:E:751:PHE:HB2  | 2.46                     | 0.50              |
| 2:F:234:GLU:C    | 2:F:236:GLY:H    | 2.14                     | 0.50              |
| 1:E:788:ARG:NH1  | 1:E:788:ARG:HG2  | 2.21                     | 0.50              |
| 2:B:271:ARG:CG   | 2:B:271:ARG:HH11 | 2.00                     | 0.50              |
| 1:H:856:TRP:HB2  | 1:H:859:GLU:OE1  | 2.11                     | 0.50              |
| 1:E:684:ARG:HD3  | 1:E:684:ARG:H    | 1.76                     | 0.50              |
| 2:B:282:TRP:HZ3  | 2:B:302:LEU:HD22 | 1.76                     | 0.50              |
| 1:A:858:THR:CG2  | 1:A:868:VAL:HG12 | 2.33                     | 0.50              |
| 1:D:683:VAL:CG2  | 1:D:684:ARG:N    | 2.74                     | 0.50              |
| 1:E:635:LEU:HD12 | 1:E:730:PHE:HD1  | 1.76                     | 0.50              |
| 2:F:256:PRO:HB3  | 2:F:290:LEU:HD23 | 1.93                     | 0.50              |
| 1:E:689:LYS:O    | 1:E:693:GLU:HB2  | 2.12                     | 0.50              |
| 2:F:229:ARG:O    | 2:F:233:GLU:HG3  | 2.11                     | 0.50              |
| 1:H:809:LEU:HD12 | 1:H:809:LEU:H    | 1.75                     | 0.50              |
| 2:C:300:ARG:NH1  | 1:D:684:ARG:HB2  | 2.27                     | 0.50              |
| 2:G:209:LEU:N    | 2:G:209:LEU:HD12 | 2.26                     | 0.50              |
| 1:A:796:GLY:O    | 1:A:799:ARG:CG   | 2.59                     | 0.50              |
| 1:D:680:VAL:HG11 | 1:D:686:VAL:HG22 | 1.92                     | 0.50              |
| 2:F:310:PRO:CG   | 2:F:338:VAL:HG21 | 2.41                     | 0.50              |
| 2:C:246:PRO:HG2  | 2:C:259:TYR:CZ   | 2.47                     | 0.50              |
| 2:G:291:ASN:HB3  | 2:G:293:GLU:OE2  | 2.11                     | 0.50              |
| 2:B:202:GLU:O    | 2:B:206:LEU:HD23 | 2.11                     | 0.50              |
| 1:D:630:ILE:HG22 | 1:D:652:GLN:O    | 2.11                     | 0.50              |
| 1:H:645:VAL:HG21 | 1:H:894:ILE:HB   | 1.93                     | 0.50              |
| 2:F:224:VAL:HG11 | 2:F:266:LEU:HD11 | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:201:LYS:HB3  | 2:F:202:GLU:OE1  | 2.12                     | 0.50              |
| 1:A:656:TYR:CD2  | 1:A:677:ILE:HG12 | 2.46                     | 0.50              |
| 1:D:874:SER:C    | 1:D:876:MET:H    | 2.06                     | 0.50              |
| 1:A:729:GLU:OE2  | 2:B:300:ARG:NH1  | 2.45                     | 0.50              |
| 1:D:708:ASP:OD2  | 1:D:717:LYS:HB2  | 2.12                     | 0.50              |
| 1:E:817:HIS:CD2  | 1:E:817:HIS:C    | 2.85                     | 0.50              |
| 1:E:807:ASP:O    | 1:E:809:LEU:HG   | 2.12                     | 0.50              |
| 1:H:684:ARG:HD3  | 1:H:684:ARG:H    | 1.77                     | 0.49              |
| 2:F:199:ILE:HG22 | 2:F:203:LEU:HB2  | 1.93                     | 0.49              |
| 1:E:745:ARG:HG3  | 1:E:746:PRO:HD2  | 1.93                     | 0.49              |
| 1:A:865:GLY:O    | 1:A:891:VAL:HB   | 2.12                     | 0.49              |
| 1:A:773:PRO:HB3  | 1:A:791:TRP:CE2  | 2.48                     | 0.49              |
| 1:E:643:LEU:HG   | 1:E:647:LYS:HE3  | 1.93                     | 0.49              |
| 1:E:643:LEU:HB2  | 1:E:656:TYR:CE1  | 2.47                     | 0.49              |
| 1:H:627:ARG:NH1  | 1:H:903:GLU:HA   | 2.26                     | 0.49              |
| 2:B:290:LEU:HB2  | 2:B:295:LEU:CD1  | 2.42                     | 0.49              |
| 1:E:753:ASN:ND2  | 1:E:754:VAL:H    | 2.10                     | 0.49              |
| 1:E:686:VAL:HG12 | 1:E:733:LEU:HD11 | 1.93                     | 0.49              |
| 2:B:310:PRO:HG3  | 2:B:338:VAL:HG21 | 1.95                     | 0.49              |
| 2:B:183:PRO:O    | 2:B:187:ARG:HG3  | 2.12                     | 0.49              |
| 1:D:632:VAL:HG21 | 1:D:646:LEU:HD11 | 1.94                     | 0.49              |
| 1:E:680:VAL:CG1  | 1:E:681:GLY:H    | 2.17                     | 0.49              |
| 2:C:191:ARG:HH21 | 2:C:237:PRO:HB2  | 1.78                     | 0.49              |
| 2:G:368:PHE:O    | 2:G:371:LEU:HB2  | 2.12                     | 0.49              |
| 1:E:668:VAL:HG22 | 1:E:873:VAL:HG21 | 1.93                     | 0.49              |
| 1:D:874:SER:HB2  | 1:D:876:MET:H    | 1.78                     | 0.49              |
| 1:E:810:GLU:HG2  | 1:E:813:GLU:CB   | 2.42                     | 0.49              |
| 1:A:700:VAL:O    | 1:A:749:TRP:HA   | 2.12                     | 0.49              |
| 2:G:346:LEU:HD23 | 2:G:346:LEU:O    | 2.13                     | 0.49              |
| 1:D:631:ARG:HH11 | 1:D:631:ARG:CB   | 2.21                     | 0.49              |
| 1:E:699:LEU:HD11 | 1:E:701:ILE:HG23 | 1.95                     | 0.49              |
| 2:F:326:ASN:N    | 2:F:326:ASN:HD22 | 1.92                     | 0.49              |
| 1:D:776:ILE:CG2  | 1:D:790:PHE:HD1  | 2.25                     | 0.49              |
| 1:H:754:VAL:HA   | 1:H:788:ARG:CD   | 2.42                     | 0.49              |
| 1:D:885:LEU:O    | 1:D:886:GLY:C    | 2.52                     | 0.49              |
| 2:B:287:ASN:HA   | 2:B:321:VAL:CG2  | 2.43                     | 0.48              |
| 1:A:716:ARG:NH1  | 1:A:716:ARG:HG2  | 2.28                     | 0.48              |
| 1:A:759:VAL:HG23 | 1:A:760:SER:N    | 2.28                     | 0.48              |
| 1:A:630:ILE:HG12 | 1:A:632:VAL:HG23 | 1.95                     | 0.48              |
| 2:F:367:CYS:O    | 2:F:370:PRO:HD2  | 2.13                     | 0.48              |
| 1:D:691:ILE:HG22 | 1:D:692:GLN:N    | 2.27                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:775:MET:SD   | 1:A:776:ILE:N    | 2.86                     | 0.48              |
| 2:G:263:PHE:CE2  | 2:G:284:PHE:HB2  | 2.48                     | 0.48              |
| 2:G:309:ILE:HG13 | 2:G:309:ILE:O    | 2.13                     | 0.48              |
| 1:E:786:ARG:CG   | 1:E:786:ARG:NH1  | 2.70                     | 0.48              |
| 1:D:858:THR:HG23 | 1:D:868:VAL:HG13 | 1.95                     | 0.48              |
| 1:A:684:ARG:HB2  | 2:B:300:ARG:NH1  | 2.28                     | 0.48              |
| 1:D:709:LEU:HD13 | 1:D:757:MET:CE   | 2.42                     | 0.48              |
| 2:F:198:ASP:HB3  | 2:F:220:HIS:CG   | 2.49                     | 0.48              |
| 1:E:817:HIS:CD2  | 1:E:818:GLY:N    | 2.82                     | 0.48              |
| 1:D:876:MET:SD   | 1:D:884:LEU:CD2  | 3.01                     | 0.48              |
| 1:A:869:HIS:HB3  | 1:D:869:HIS:CE1  | 2.48                     | 0.48              |
| 2:F:256:PRO:O    | 2:F:259:TYR:HD1  | 1.96                     | 0.48              |
| 2:C:243:GLY:O    | 2:C:284:PHE:HA   | 2.14                     | 0.48              |
| 2:G:290:LEU:HD22 | 2:G:294:ASP:HB3  | 1.95                     | 0.48              |
| 1:H:668:VAL:HG22 | 1:H:873:VAL:CG2  | 2.43                     | 0.48              |
| 1:A:874:SER:HA   | 1:D:856:TRP:CZ2  | 2.49                     | 0.48              |
| 1:A:823:PHE:HZ   | 1:A:842:GLN:HA   | 1.79                     | 0.48              |
| 2:F:243:GLY:O    | 2:F:284:PHE:HA   | 2.14                     | 0.48              |
| 1:H:861:GLU:OE2  | 1:H:881:ARG:NH1  | 2.46                     | 0.48              |
| 2:C:279:PRO:HB2  | 2:C:281:PHE:HE1  | 1.77                     | 0.48              |
| 2:B:209:LEU:N    | 2:B:209:LEU:HD12 | 2.28                     | 0.48              |
| 2:G:267:LEU:HD22 | 2:G:267:LEU:O    | 2.14                     | 0.48              |
| 1:A:869:HIS:ND1  | 1:D:869:HIS:HB3  | 2.29                     | 0.48              |
| 2:F:199:ILE:O    | 2:F:199:ILE:HG22 | 2.14                     | 0.48              |
| 1:E:794:LEU:HD13 | 1:E:897:LEU:O    | 2.14                     | 0.48              |
| 2:B:234:GLU:C    | 2:B:236:GLY:H    | 2.16                     | 0.48              |
| 1:H:691:ILE:CD1  | 1:H:733:LEU:HD12 | 2.44                     | 0.48              |
| 1:E:773:PRO:HD3  | 1:E:791:TRP:NE1  | 2.29                     | 0.48              |
| 1:H:682:ASP:OD2  | 1:H:683:VAL:N    | 2.47                     | 0.47              |
| 2:F:326:ASN:ND2  | 2:F:326:ASN:H    | 1.99                     | 0.47              |
| 1:H:717:LYS:HB3  | 1:H:721:GLU:CB   | 2.44                     | 0.47              |
| 2:F:372:ARG:HD2  | 2:F:377:TYR:HB2  | 1.96                     | 0.47              |
| 2:C:327:ILE:O    | 2:C:330:ILE:HB   | 2.14                     | 0.47              |
| 1:D:657:ILE:HD12 | 1:D:697:PHE:CZ   | 2.49                     | 0.47              |
| 1:H:773:PRO:CD   | 1:H:791:TRP:NE1  | 2.70                     | 0.47              |
| 1:A:647:LYS:HZ1  | 1:A:673:HIS:HB3  | 1.78                     | 0.47              |
| 1:E:632:VAL:HG12 | 1:E:633:LEU:N    | 2.29                     | 0.47              |
| 2:C:264:HIS:O    | 2:C:268:GLN:NE2  | 2.47                     | 0.47              |
| 1:H:885:LEU:O    | 1:H:888:SER:OG   | 2.32                     | 0.47              |
| 1:A:666:ILE:HG12 | 1:A:679:TYR:CE2  | 2.48                     | 0.47              |
| 2:C:326:ASN:ND2  | 2:C:326:ASN:H    | 1.98                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:804:THR:HG22 | 1:A:805:VAL:N    | 2.30                     | 0.47              |
| 2:G:201:LYS:HB3  | 2:G:202:GLU:OE1  | 2.13                     | 0.47              |
| 1:D:810:GLU:CD   | 1:D:810:GLU:H    | 2.17                     | 0.47              |
| 1:H:861:GLU:OE1  | 1:H:868:VAL:HA   | 2.14                     | 0.47              |
| 2:B:361:THR:N    | 2:B:363:LEU:HD23 | 2.28                     | 0.47              |
| 2:F:224:VAL:HG11 | 2:F:266:LEU:CD1  | 2.45                     | 0.47              |
| 1:E:727:PHE:CE1  | 1:E:765:ILE:HG23 | 2.49                     | 0.47              |
| 1:D:748:PHE:CE1  | 1:D:795:PRO:HD3  | 2.50                     | 0.47              |
| 1:E:686:VAL:CG1  | 1:E:733:LEU:HD11 | 2.44                     | 0.47              |
| 2:F:202:GLU:O    | 2:F:206:LEU:HD23 | 2.13                     | 0.47              |
| 1:H:732:ARG:NE   | 1:H:733:LEU:HD21 | 2.30                     | 0.47              |
| 2:G:290:LEU:HB3  | 2:G:294:ASP:HB2  | 1.96                     | 0.47              |
| 1:H:819:ARG:CD   | 1:H:848:MET:SD   | 3.02                     | 0.47              |
| 1:D:748:PHE:HB3  | 1:D:794:LEU:HD23 | 1.95                     | 0.47              |
| 1:H:786:ARG:NH1  | 1:H:864:PHE:HE2  | 2.12                     | 0.47              |
| 2:G:204:THR:OG1  | 2:G:209:LEU:HD22 | 2.15                     | 0.47              |
| 2:F:247:PRO:HA   | 2:F:287:ASN:ND2  | 2.29                     | 0.47              |
| 1:H:663:GLU:O    | 1:H:666:ILE:HB   | 2.14                     | 0.47              |
| 2:G:346:LEU:O    | 2:G:350:LYS:HG2  | 2.14                     | 0.47              |
| 1:A:623:PRO:O    | 1:A:624:ALA:HB2  | 2.14                     | 0.47              |
| 1:E:885:LEU:O    | 1:E:886:GLY:C    | 2.51                     | 0.47              |
| 1:H:720:TYR:HH   | 1:H:764:ASP:CG   | 2.17                     | 0.47              |
| 1:D:662:CYS:O    | 1:D:666:ILE:HG13 | 2.14                     | 0.47              |
| 2:G:300:ARG:NH1  | 1:H:684:ARG:HB2  | 2.29                     | 0.47              |
| 1:A:680:VAL:HG21 | 1:A:694:TRP:CH2  | 2.50                     | 0.47              |
| 1:E:702:GLY:O    | 1:E:751:PHE:HA   | 2.15                     | 0.47              |
| 2:C:290:LEU:HB2  | 2:C:295:LEU:HD13 | 1.96                     | 0.47              |
| 2:G:257:SER:OG   | 1:H:725:ARG:NH2  | 2.47                     | 0.47              |
| 2:C:300:ARG:NH1  | 1:D:729:GLU:OE2  | 2.48                     | 0.47              |
| 2:B:282:TRP:H    | 2:B:326:ASN:HD21 | 1.62                     | 0.47              |
| 1:D:752:GLU:CG   | 1:D:753:ASN:N    | 2.75                     | 0.47              |
| 2:B:376:LYS:HD3  | 2:B:378:PHE:HE2  | 1.77                     | 0.47              |
| 1:H:706:CYS:CB   | 1:H:754:VAL:HG13 | 2.45                     | 0.47              |
| 2:G:198:ASP:HB3  | 2:G:220:HIS:ND1  | 2.30                     | 0.47              |
| 2:G:293:GLU:OE2  | 2:G:293:GLU:N    | 2.46                     | 0.47              |
| 1:D:873:VAL:HG23 | 1:D:874:SER:N    | 2.29                     | 0.47              |
| 1:H:871:THR:HB   | 1:H:881:ARG:HD3  | 1.96                     | 0.47              |
| 1:E:683:VAL:HG23 | 1:E:684:ARG:N    | 2.29                     | 0.46              |
| 1:D:855:LEU:HD21 | 1:D:859:GLU:HB2  | 1.97                     | 0.46              |
| 1:E:633:LEU:HB2  | 1:E:697:PHE:CD2  | 2.50                     | 0.46              |
| 1:E:755:VAL:HG13 | 1:E:756:ALA:N    | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:699:LEU:HA   | 1:D:748:PHE:O    | 2.15                     | 0.46              |
| 1:D:871:THR:CB   | 1:D:881:ARG:HD3  | 2.46                     | 0.46              |
| 1:H:691:ILE:HD11 | 1:H:733:LEU:HD12 | 1.96                     | 0.46              |
| 1:H:691:ILE:HG22 | 1:H:692:GLN:H    | 1.80                     | 0.46              |
| 1:D:648:ASP:CG   | 1:D:895:ARG:HH12 | 2.19                     | 0.46              |
| 1:A:816:GLU:HG2  | 1:D:671:VAL:CG1  | 2.45                     | 0.46              |
| 1:D:629:PRO:HB2  | 1:D:654:ASP:HB2  | 1.97                     | 0.46              |
| 1:H:823:PHE:HD1  | 1:H:823:PHE:N    | 2.12                     | 0.46              |
| 2:F:188:GLN:N    | 2:F:188:GLN:OE1  | 2.49                     | 0.46              |
| 1:A:686:VAL:HG13 | 1:A:694:TRP:CZ3  | 2.50                     | 0.46              |
| 1:D:645:VAL:CG1  | 1:D:895:ARG:HA   | 2.45                     | 0.46              |
| 1:D:635:LEU:O    | 1:D:636:PHE:HB2  | 2.16                     | 0.46              |
| 1:D:693:GLU:C    | 1:D:695:GLY:H    | 2.18                     | 0.46              |
| 1:H:873:VAL:CG2  | 1:H:874:SER:N    | 2.71                     | 0.46              |
| 1:E:671:VAL:CG1  | 1:H:816:GLU:HG2  | 2.46                     | 0.46              |
| 2:C:346:LEU:HD23 | 2:C:346:LEU:C    | 2.36                     | 0.46              |
| 2:C:262:GLN:HE21 | 2:C:262:GLN:CA   | 2.29                     | 0.46              |
| 1:H:854:ILE:HG22 | 1:H:855:LEU:N    | 2.30                     | 0.46              |
| 1:D:819:ARG:CZ   | 1:D:846:VAL:HG21 | 2.46                     | 0.46              |
| 1:D:801:LEU:CD1  | 1:D:801:LEU:H    | 2.21                     | 0.46              |
| 2:G:208:PHE:C    | 2:G:209:LEU:HD12 | 2.36                     | 0.46              |
| 1:H:709:LEU:HD13 | 1:H:753:ASN:ND2  | 2.30                     | 0.46              |
| 1:H:661:VAL:O    | 1:H:661:VAL:HG22 | 2.16                     | 0.46              |
| 2:B:188:GLN:HB3  | 2:B:189:PRO:CD   | 2.42                     | 0.46              |
| 2:G:202:GLU:HG2  | 2:G:361:THR:HG21 | 1.97                     | 0.46              |
| 2:G:267:LEU:HD12 | 2:G:268:GLN:HE22 | 1.79                     | 0.46              |
| 1:E:631:ARG:NH1  | 1:E:696:PRO:O    | 2.48                     | 0.46              |
| 2:F:268:GLN:OE1  | 2:F:271:ARG:NH1  | 2.49                     | 0.46              |
| 1:A:869:HIS:CE1  | 1:D:869:HIS:HB3  | 2.51                     | 0.46              |
| 1:E:699:LEU:HD12 | 1:E:700:VAL:N    | 2.30                     | 0.46              |
| 1:A:755:VAL:HG23 | 1:A:789:TYR:CE1  | 2.51                     | 0.46              |
| 2:F:218:LEU:C    | 2:F:218:LEU:HD23 | 2.37                     | 0.46              |
| 1:E:810:GLU:H    | 1:E:810:GLU:CD   | 2.17                     | 0.46              |
| 2:F:369:LEU:HB2  | 2:F:370:PRO:HD3  | 1.98                     | 0.46              |
| 2:F:245:THR:HB   | 2:F:289:VAL:HG11 | 1.97                     | 0.46              |
| 2:B:309:ILE:HG13 | 2:B:309:ILE:O    | 2.15                     | 0.46              |
| 1:H:705:PRO:HG2  | 1:H:726:LEU:HD12 | 1.97                     | 0.45              |
| 2:B:203:LEU:CD1  | 2:B:208:PHE:HD1  | 2.29                     | 0.45              |
| 2:B:229:ARG:HA   | 2:B:269:TYR:HD1  | 1.79                     | 0.45              |
| 1:A:860:MET:O    | 1:A:864:PHE:HD1  | 1.98                     | 0.45              |
| 2:F:372:ARG:NH1  | 2:F:372:ARG:HG2  | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:218:LEU:C    | 2:B:218:LEU:HD23 | 2.37                     | 0.45              |
| 2:G:300:ARG:HG2  | 1:H:732:ARG:NH1  | 2.31                     | 0.45              |
| 1:H:732:ARG:NE   | 1:H:733:LEU:CD2  | 2.72                     | 0.45              |
| 2:B:268:GLN:NE2  | 2:B:268:GLN:CA   | 2.79                     | 0.45              |
| 1:H:866:PHE:O    | 1:H:867:PRO:C    | 2.55                     | 0.45              |
| 1:A:801:LEU:HD12 | 1:A:801:LEU:N    | 2.31                     | 0.45              |
| 1:H:752:GLU:CG   | 1:H:753:ASN:N    | 2.79                     | 0.45              |
| 2:F:279:PRO:CB   | 2:F:281:PHE:HE1  | 2.29                     | 0.45              |
| 2:F:184:VAL:HA   | 2:F:187:ARG:NE   | 2.31                     | 0.45              |
| 1:E:643:LEU:HD22 | 1:E:656:TYR:CG   | 2.50                     | 0.45              |
| 1:H:794:LEU:O    | 1:H:797:MET:HG3  | 2.16                     | 0.45              |
| 2:G:268:GLN:HG2  | 1:H:735:HIS:CE1  | 2.51                     | 0.45              |
| 2:G:322:ARG:NH2  | 2:G:340:GLU:OE1  | 2.33                     | 0.45              |
| 2:B:202:GLU:H    | 2:B:202:GLU:CD   | 2.20                     | 0.45              |
| 2:G:232:VAL:O    | 2:G:232:VAL:HG12 | 2.17                     | 0.45              |
| 1:H:657:ILE:CG2  | 1:H:680:VAL:CG2  | 2.95                     | 0.45              |
| 2:B:248:LEU:HG   | 2:B:287:ASN:ND2  | 2.32                     | 0.45              |
| 2:G:310:PRO:HG2  | 2:G:338:VAL:CG2  | 2.46                     | 0.45              |
| 2:G:203:LEU:HG   | 2:G:209:LEU:HD11 | 1.99                     | 0.45              |
| 2:B:228:VAL:CG1  | 2:B:229:ARG:N    | 2.79                     | 0.45              |
| 1:A:693:GLU:C    | 1:A:695:GLY:H    | 2.19                     | 0.45              |
| 1:E:753:ASN:HD22 | 1:E:754:VAL:HG22 | 1.79                     | 0.45              |
| 1:E:682:ASP:OD2  | 1:E:684:ARG:HG2  | 2.16                     | 0.45              |
| 2:F:224:VAL:CB   | 2:F:266:LEU:HD11 | 2.46                     | 0.45              |
| 2:F:188:GLN:HB3  | 2:F:189:PRO:CD   | 2.47                     | 0.45              |
| 2:C:221:VAL:HG21 | 2:C:235:TRP:CH2  | 2.52                     | 0.45              |
| 2:C:234:GLU:C    | 2:C:236:GLY:H    | 2.20                     | 0.45              |
| 1:D:691:ILE:HD11 | 1:D:733:LEU:CD1  | 2.44                     | 0.45              |
| 1:A:773:PRO:HD3  | 1:A:791:TRP:NE1  | 2.32                     | 0.45              |
| 2:F:192:VAL:HG21 | 2:F:203:LEU:CD2  | 2.42                     | 0.45              |
| 1:D:776:ILE:CG2  | 1:D:790:PHE:CD1  | 3.00                     | 0.45              |
| 1:E:817:HIS:ND1  | 1:H:674:GLN:HB3  | 2.32                     | 0.45              |
| 2:G:230:LYS:N    | 2:G:230:LYS:HD2  | 2.32                     | 0.45              |
| 1:D:812:GLN:OE1  | 1:D:821:ALA:N    | 2.34                     | 0.45              |
| 2:C:300:ARG:CZ   | 1:D:684:ARG:HB2  | 2.47                     | 0.45              |
| 2:G:372:ARG:HG2  | 2:G:372:ARG:NH1  | 2.31                     | 0.45              |
| 1:D:810:GLU:HG2  | 1:D:813:GLU:H    | 1.82                     | 0.45              |
| 1:E:796:GLY:O    | 1:E:799:ARG:HG3  | 2.17                     | 0.45              |
| 1:D:680:VAL:CG1  | 1:D:681:GLY:N    | 2.61                     | 0.45              |
| 2:B:202:GLU:HG2  | 2:B:361:THR:CG2  | 2.43                     | 0.45              |
| 1:D:819:ARG:HD2  | 1:D:848:MET:SD   | 2.56                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:199:ILE:O    | 2:B:199:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:891:VAL:N    | 1:A:892:PRO:CD   | 2.79                     | 0.45              |
| 1:E:735:HIS:NE2  | 2:F:268:GLN:CG   | 2.80                     | 0.45              |
| 2:G:188:GLN:OE1  | 2:G:188:GLN:N    | 2.50                     | 0.45              |
| 1:D:786:ARG:NH1  | 1:D:864:PHE:CE2  | 2.83                     | 0.44              |
| 2:G:255:PRO:HA   | 2:G:256:PRO:HD3  | 1.90                     | 0.44              |
| 1:E:732:ARG:HD3  | 2:F:301:PHE:CE1  | 2.52                     | 0.44              |
| 1:A:717:LYS:HD2  | 1:A:722:GLY:HA3  | 1.99                     | 0.44              |
| 2:C:369:LEU:HB2  | 2:C:370:PRO:HD3  | 1.99                     | 0.44              |
| 1:E:664:ASP:O    | 1:E:668:VAL:HG23 | 2.17                     | 0.44              |
| 1:E:875:ASN:ND2  | 1:H:856:TRP:HD1  | 2.15                     | 0.44              |
| 2:G:376:LYS:HD3  | 2:G:378:PHE:CE2  | 2.53                     | 0.44              |
| 1:H:702:GLY:O    | 1:H:751:PHE:HA   | 2.16                     | 0.44              |
| 1:E:810:GLU:HG2  | 1:E:813:GLU:H    | 1.82                     | 0.44              |
| 1:E:816:GLU:CD   | 1:E:862:ARG:HH22 | 2.21                     | 0.44              |
| 1:E:719:LEU:HG   | 1:E:719:LEU:O    | 2.16                     | 0.44              |
| 1:E:638:GLY:HA2  | 1:E:660:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:725:ARG:HH12 | 2:B:297:VAL:CG2  | 2.17                     | 0.44              |
| 1:H:781:VAL:CG1  | 1:H:892:PRO:HB2  | 2.48                     | 0.44              |
| 1:H:893:VAL:O    | 1:H:896:HIS:HB3  | 2.17                     | 0.44              |
| 2:B:326:ASN:HD22 | 2:B:326:ASN:N    | 1.98                     | 0.44              |
| 1:E:844:PHE:O    | 1:E:846:VAL:N    | 2.51                     | 0.44              |
| 1:A:875:ASN:HB3  | 1:D:878:ARG:CD   | 2.47                     | 0.44              |
| 2:C:221:VAL:HG21 | 2:C:235:TRP:CZ3  | 2.52                     | 0.44              |
| 2:B:325:SER:OG   | 2:B:327:ILE:HG13 | 2.18                     | 0.44              |
| 2:G:347:ALA:O    | 2:G:351:GLN:HG3  | 2.17                     | 0.44              |
| 1:A:808:LYS:HG2  | 1:A:808:LYS:H    | 1.56                     | 0.44              |
| 1:A:775:MET:CE   | 1:A:787:ALA:HB1  | 2.48                     | 0.44              |
| 2:C:271:ARG:HG3  | 2:C:271:ARG:NH1  | 2.33                     | 0.44              |
| 1:A:865:GLY:O    | 1:A:891:VAL:CB   | 2.66                     | 0.44              |
| 1:E:657:ILE:HG12 | 1:E:678:MET:HB3  | 2.00                     | 0.44              |
| 2:B:330:ILE:O    | 2:B:330:ILE:HG13 | 2.17                     | 0.44              |
| 2:C:231:ASP:N    | 2:C:231:ASP:OD1  | 2.49                     | 0.44              |
| 2:C:326:ASN:ND2  | 2:C:326:ASN:N    | 2.62                     | 0.44              |
| 1:D:786:ARG:HH21 | 1:D:788:ARG:NH2  | 2.16                     | 0.44              |
| 1:D:652:GLN:HG3  | 1:D:906:ALA:O    | 2.17                     | 0.44              |
| 1:E:819:ARG:HD2  | 1:E:848:MET:SD   | 2.58                     | 0.44              |
| 1:A:899:ALA:HB3  | 1:A:900:PRO:CD   | 2.48                     | 0.44              |
| 1:A:871:THR:HG1  | 1:A:881:ARG:HH11 | 1.64                     | 0.44              |
| 1:H:717:LYS:HB3  | 1:H:721:GLU:HB2  | 1.98                     | 0.44              |
| 1:A:728:PHE:HA   | 1:A:731:TYR:HB3  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:262:GLN:HE22 | 2:F:265:ARG:HE   | 1.65                     | 0.44              |
| 1:E:753:ASN:ND2  | 1:E:754:VAL:N    | 2.66                     | 0.44              |
| 1:E:691:ILE:HG22 | 1:E:692:GLN:N    | 2.32                     | 0.44              |
| 2:G:248:LEU:N    | 2:G:287:ASN:HD22 | 2.15                     | 0.44              |
| 2:C:208:PHE:C    | 2:C:209:LEU:HD12 | 2.38                     | 0.44              |
| 1:A:719:LEU:HG   | 1:A:719:LEU:O    | 2.18                     | 0.44              |
| 2:F:346:LEU:C    | 2:F:346:LEU:HD23 | 2.37                     | 0.44              |
| 1:E:872:ASP:HB3  | 1:H:869:HIS:HE1  | 1.81                     | 0.44              |
| 2:G:310:PRO:O    | 2:G:363:LEU:HD12 | 2.17                     | 0.44              |
| 1:E:699:LEU:CD1  | 1:E:701:ILE:HG23 | 2.48                     | 0.44              |
| 2:F:361:THR:N    | 2:F:363:LEU:HD23 | 2.33                     | 0.44              |
| 1:E:868:VAL:O    | 1:E:869:HIS:HB2  | 2.18                     | 0.44              |
| 2:B:309:ILE:HA   | 2:B:310:PRO:HD3  | 1.78                     | 0.44              |
| 2:G:303:GLU:O    | 2:G:304:MET:HB3  | 2.18                     | 0.44              |
| 1:H:689:LYS:O    | 1:H:692:GLN:OE1  | 2.36                     | 0.43              |
| 2:G:256:PRO:CB   | 2:G:290:LEU:HD23 | 2.39                     | 0.43              |
| 1:H:873:VAL:O    | 1:H:874:SER:C    | 2.57                     | 0.43              |
| 2:F:267:LEU:HD12 | 2:F:268:GLN:HE22 | 1.83                     | 0.43              |
| 1:A:706:CYS:SG   | 1:A:707:ASN:N    | 2.90                     | 0.43              |
| 1:D:811:LEU:HD13 | 1:D:811:LEU:O    | 2.17                     | 0.43              |
| 1:E:648:ASP:OD2  | 1:E:895:ARG:NH1  | 2.46                     | 0.43              |
| 2:F:326:ASN:N    | 2:F:326:ASN:ND2  | 2.63                     | 0.43              |
| 1:H:890:SER:O    | 1:H:893:VAL:HB   | 2.17                     | 0.43              |
| 1:H:788:ARG:NH1  | 1:H:788:ARG:HG2  | 2.33                     | 0.43              |
| 2:B:289:VAL:O    | 2:B:289:VAL:HG22 | 2.19                     | 0.43              |
| 1:A:739:PRO:HG3  | 1:A:745:ARG:CZ   | 2.48                     | 0.43              |
| 1:A:738:ARG:HA   | 1:A:747:PHE:CE2  | 2.52                     | 0.43              |
| 1:A:750:LEU:HD11 | 1:A:790:PHE:HD2  | 1.83                     | 0.43              |
| 2:C:199:ILE:HG21 | 2:C:368:PHE:HE1  | 1.82                     | 0.43              |
| 2:F:228:VAL:CG1  | 2:F:229:ARG:H    | 2.29                     | 0.43              |
| 1:D:810:GLU:OE1  | 1:D:813:GLU:CB   | 2.67                     | 0.43              |
| 1:H:752:GLU:O    | 1:H:753:ASN:HB2  | 2.17                     | 0.43              |
| 2:B:335:TRP:O    | 2:B:337:LEU:N    | 2.46                     | 0.43              |
| 2:F:309:ILE:HG13 | 2:F:321:VAL:HG12 | 2.00                     | 0.43              |
| 1:H:757:MET:HE3  | 1:H:757:MET:HB2  | 1.83                     | 0.43              |
| 1:A:883:ARG:O    | 1:A:887:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:699:LEU:HG   | 1:A:701:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:869:HIS:HB3  | 1:D:869:HIS:ND1  | 2.33                     | 0.43              |
| 2:G:203:LEU:CG   | 2:G:209:LEU:HD11 | 2.47                     | 0.43              |
| 2:F:229:ARG:HG2  | 2:F:233:GLU:OE1  | 2.18                     | 0.43              |
| 2:C:262:GLN:HA   | 2:C:262:GLN:HE21 | 1.82                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:346:LEU:HD23 | 2:F:346:LEU:O    | 2.19                     | 0.43              |
| 1:D:822:LYS:NZ   | 1:D:852:GLU:OE2  | 2.49                     | 0.43              |
| 1:A:672:ARG:CG   | 1:A:870:TYR:CE1  | 2.97                     | 0.43              |
| 1:H:822:LYS:HB2  | 1:H:823:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:855:LEU:HD23 | 1:A:855:LEU:HA   | 1.84                     | 0.43              |
| 1:E:630:ILE:HD11 | 1:E:699:LEU:HD23 | 2.01                     | 0.43              |
| 2:C:363:LEU:CD2  | 2:C:363:LEU:H    | 2.31                     | 0.43              |
| 2:G:193:LEU:HB2  | 2:G:238:PHE:CE2  | 2.52                     | 0.43              |
| 1:E:881:ARG:HH22 | 1:H:872:ASP:CG   | 2.22                     | 0.43              |
| 2:F:346:LEU:O    | 2:F:350:LYS:HG2  | 2.18                     | 0.43              |
| 1:E:757:MET:HE2  | 1:E:762:LYS:N    | 2.34                     | 0.43              |
| 1:H:728:PHE:HE2  | 1:H:768:PHE:CZ   | 2.35                     | 0.43              |
| 2:C:198:ASP:HB3  | 2:C:220:HIS:CG   | 2.53                     | 0.43              |
| 1:D:687:THR:O    | 1:D:690:HIS:HB2  | 2.18                     | 0.43              |
| 1:A:646:LEU:HA   | 1:A:646:LEU:HD23 | 1.84                     | 0.43              |
| 2:G:234:GLU:C    | 2:G:236:GLY:H    | 2.20                     | 0.43              |
| 1:H:815:LEU:HA   | 1:H:859:GLU:OE2  | 2.19                     | 0.43              |
| 1:A:635:LEU:O    | 1:A:636:PHE:HB2  | 2.19                     | 0.43              |
| 2:B:255:PRO:HA   | 2:B:256:PRO:HD3  | 1.84                     | 0.43              |
| 1:A:786:ARG:HG3  | 1:A:786:ARG:HH11 | 1.83                     | 0.43              |
| 2:G:228:VAL:CG1  | 2:G:229:ARG:N    | 2.82                     | 0.43              |
| 1:E:786:ARG:HB3  | 1:E:788:ARG:HH12 | 1.84                     | 0.43              |
| 1:D:859:GLU:O    | 1:D:863:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:711:ILE:HG12 | 1:D:756:ALA:O    | 2.19                     | 0.43              |
| 1:H:899:ALA:N    | 1:H:900:PRO:HD2  | 2.34                     | 0.43              |
| 1:A:649:LEU:CD2  | 1:A:902:LYS:HE3  | 2.49                     | 0.43              |
| 2:F:246:PRO:HA   | 2:F:247:PRO:HD3  | 1.92                     | 0.43              |
| 2:C:192:VAL:HG21 | 2:C:203:LEU:CD2  | 2.45                     | 0.43              |
| 2:B:190:VAL:HG22 | 2:B:192:VAL:HG23 | 2.00                     | 0.43              |
| 1:A:749:TRP:CZ3  | 1:A:792:GLY:HA2  | 2.53                     | 0.43              |
| 1:E:735:HIS:NE2  | 2:F:268:GLN:HG2  | 2.33                     | 0.43              |
| 2:F:260:LEU:CD2  | 2:F:297:VAL:HG12 | 2.49                     | 0.43              |
| 2:F:258:TRP:CE2  | 2:F:262:GLN:HG3  | 2.53                     | 0.43              |
| 1:D:750:LEU:HD13 | 1:D:794:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:682:ASP:OD2  | 1:A:684:ARG:CD   | 2.66                     | 0.43              |
| 1:A:739:PRO:HD3  | 1:A:747:PHE:CG   | 2.53                     | 0.43              |
| 2:F:199:ILE:HG22 | 2:F:203:LEU:N    | 2.34                     | 0.43              |
| 1:A:666:ILE:HA   | 1:A:679:TYR:CE2  | 2.53                     | 0.43              |
| 2:C:218:LEU:HD23 | 2:C:218:LEU:C    | 2.40                     | 0.43              |
| 1:D:694:TRP:HA   | 1:D:694:TRP:HE3  | 1.84                     | 0.43              |
| 2:B:257:SER:O    | 2:B:260:LEU:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:286:ASP:OD2  | 2:B:289:VAL:HG12 | 2.18                     | 0.43              |
| 1:A:878:ARG:CG   | 1:A:878:ARG:HH11 | 2.15                     | 0.43              |
| 2:F:282:TRP:CZ3  | 2:F:302:LEU:HD22 | 2.54                     | 0.43              |
| 2:C:289:VAL:HG22 | 2:C:289:VAL:O    | 2.19                     | 0.43              |
| 2:C:306:PRO:HB3  | 2:C:324:TRP:CE2  | 2.54                     | 0.43              |
| 2:F:219:LYS:HE2  | 2:F:235:TRP:CD2  | 2.54                     | 0.43              |
| 2:G:269:TYR:CD2  | 2:G:269:TYR:N    | 2.87                     | 0.43              |
| 1:E:774:VAL:O    | 1:E:776:ILE:HG22 | 2.19                     | 0.42              |
| 1:D:773:PRO:HD3  | 1:D:791:TRP:NE1  | 2.34                     | 0.42              |
| 2:C:345:LEU:HD12 | 2:C:349:ASN:OD1  | 2.18                     | 0.42              |
| 1:D:876:MET:SD   | 1:D:884:LEU:HD23 | 2.59                     | 0.42              |
| 2:B:260:LEU:CD2  | 2:B:298:ALA:CA   | 2.94                     | 0.42              |
| 1:D:868:VAL:O    | 1:D:869:HIS:HB2  | 2.18                     | 0.42              |
| 1:H:730:PHE:CE2  | 1:H:751:PHE:HB2  | 2.54                     | 0.42              |
| 1:A:675:GLY:O    | 1:A:677:ILE:N    | 2.52                     | 0.42              |
| 2:B:307:VAL:HG13 | 2:B:334:HIS:ND1  | 2.35                     | 0.42              |
| 2:C:199:ILE:O    | 2:C:203:LEU:HB2  | 2.19                     | 0.42              |
| 2:F:228:VAL:CG1  | 2:F:229:ARG:N    | 2.80                     | 0.42              |
| 1:H:720:TYR:CD1  | 1:H:720:TYR:N    | 2.87                     | 0.42              |
| 2:F:267:LEU:C    | 2:F:267:LEU:HD13 | 2.39                     | 0.42              |
| 1:A:727:PHE:CE1  | 1:A:765:ILE:HG23 | 2.54                     | 0.42              |
| 1:A:783:ALA:O    | 1:A:826:VAL:HG22 | 2.20                     | 0.42              |
| 1:D:862:ARG:NH1  | 1:D:868:VAL:HG21 | 2.33                     | 0.42              |
| 1:H:730:PHE:CZ   | 1:H:734:LEU:HD12 | 2.54                     | 0.42              |
| 2:C:279:PRO:CB   | 2:C:281:PHE:HE1  | 2.32                     | 0.42              |
| 1:H:632:VAL:CG1  | 1:H:633:LEU:N    | 2.82                     | 0.42              |
| 2:G:326:ASN:ND2  | 2:G:326:ASN:H    | 2.18                     | 0.42              |
| 1:H:692:GLN:OE1  | 1:H:692:GLN:N    | 2.52                     | 0.42              |
| 1:H:786:ARG:NH1  | 1:H:864:PHE:CE2  | 2.88                     | 0.42              |
| 1:A:775:MET:HE1  | 1:A:787:ALA:HB1  | 2.01                     | 0.42              |
| 1:H:904:TYR:C    | 1:H:905:PHE:CD1  | 2.92                     | 0.42              |
| 1:E:687:THR:O    | 1:E:690:HIS:N    | 2.53                     | 0.42              |
| 2:F:257:SER:O    | 2:F:260:LEU:N    | 2.53                     | 0.42              |
| 1:A:632:VAL:CG1  | 1:A:633:LEU:N    | 2.82                     | 0.42              |
| 2:G:363:LEU:CD2  | 2:G:363:LEU:H    | 2.28                     | 0.42              |
| 1:D:819:ARG:HH21 | 1:D:859:GLU:CD   | 2.21                     | 0.42              |
| 1:A:880:ALA:O    | 1:A:881:ARG:C    | 2.58                     | 0.42              |
| 1:H:883:ARG:HD3  | 1:H:887:ARG:HH22 | 1.85                     | 0.42              |
| 2:F:372:ARG:CD   | 2:F:377:TYR:HB2  | 2.50                     | 0.42              |
| 2:B:230:LYS:N    | 2:B:230:LYS:HD2  | 2.35                     | 0.42              |
| 1:E:876:MET:CG   | 1:E:880:ALA:HB3  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:699:LEU:HG   | 1:D:701:ILE:HG23 | 2.02                     | 0.42              |
| 1:A:691:ILE:HG21 | 1:A:736:ASP:O    | 2.18                     | 0.42              |
| 2:B:342:GLU:O    | 2:B:345:LEU:HB3  | 2.19                     | 0.42              |
| 2:G:245:THR:HB   | 2:G:289:VAL:HG11 | 2.02                     | 0.42              |
| 2:G:300:ARG:NH1  | 1:H:729:GLU:OE2  | 2.48                     | 0.42              |
| 1:A:683:VAL:HG23 | 1:A:684:ARG:H    | 1.85                     | 0.42              |
| 1:D:815:LEU:CD1  | 1:D:846:VAL:HG12 | 2.50                     | 0.42              |
| 2:B:267:LEU:HD22 | 2:B:267:LEU:O    | 2.20                     | 0.42              |
| 1:H:630:ILE:HG13 | 1:H:905:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:849:ASN:O    | 1:A:850:GLU:CB   | 2.68                     | 0.42              |
| 1:E:690:HIS:O    | 1:E:694:TRP:N    | 2.49                     | 0.42              |
| 1:H:728:PHE:HA   | 1:H:731:TYR:HB3  | 2.02                     | 0.42              |
| 1:D:778:ALA:HB2  | 1:D:893:VAL:HG21 | 2.02                     | 0.42              |
| 1:E:878:ARG:O    | 1:E:882:GLN:HB2  | 2.20                     | 0.42              |
| 1:E:639:ILE:O    | 1:E:870:TYR:OH   | 2.28                     | 0.42              |
| 1:H:871:THR:HB   | 1:H:881:ARG:CG   | 2.50                     | 0.42              |
| 1:D:657:ILE:CG2  | 1:D:680:VAL:HG23 | 2.50                     | 0.42              |
| 1:A:632:VAL:HG12 | 1:A:633:LEU:N    | 2.33                     | 0.42              |
| 1:A:856:TRP:HB2  | 1:A:859:GLU:CG   | 2.47                     | 0.42              |
| 1:E:699:LEU:HA   | 1:E:748:PHE:O    | 2.20                     | 0.42              |
| 1:E:881:ARG:NH2  | 1:H:872:ASP:OD2  | 2.49                     | 0.42              |
| 1:D:687:THR:O    | 1:D:690:HIS:N    | 2.53                     | 0.42              |
| 1:E:639:ILE:O    | 1:E:640:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:779:LYS:HA   | 1:A:784:ALA:O    | 2.20                     | 0.42              |
| 1:E:786:ARG:HB3  | 1:E:788:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:730:PHE:CE2  | 1:A:751:PHE:HB2  | 2.54                     | 0.42              |
| 2:F:273:LYS:CB   | 2:F:274:PRO:HD2  | 2.42                     | 0.42              |
| 1:D:848:MET:O    | 1:D:849:ASN:C    | 2.59                     | 0.42              |
| 1:D:773:PRO:HB2  | 1:D:789:TYR:HD1  | 1.84                     | 0.42              |
| 2:F:247:PRO:HA   | 2:F:287:ASN:HD22 | 1.85                     | 0.42              |
| 2:C:368:PHE:CD2  | 2:C:368:PHE:N    | 2.86                     | 0.42              |
| 1:E:888:SER:HA   | 3:E:5:SAH:C      | 2.49                     | 0.42              |
| 2:F:187:ARG:HB3  | 2:F:375:PHE:HA   | 2.01                     | 0.42              |
| 1:A:706:CYS:HB2  | 1:A:754:VAL:HG13 | 2.00                     | 0.42              |
| 2:B:243:GLY:O    | 2:B:284:PHE:HA   | 2.20                     | 0.42              |
| 1:A:627:ARG:HH12 | 1:A:903:GLU:HA   | 1.85                     | 0.42              |
| 1:H:898:PHE:N    | 1:H:898:PHE:CD2  | 2.86                     | 0.42              |
| 2:F:260:LEU:HD21 | 2:F:298:ALA:HA   | 2.02                     | 0.41              |
| 1:H:811:LEU:CD2  | 1:H:826:VAL:HG13 | 2.50                     | 0.41              |
| 1:D:898:PHE:O    | 1:D:901:LEU:HB2  | 2.20                     | 0.41              |
| 2:G:346:LEU:HD23 | 2:G:346:LEU:C    | 2.40                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:694:TRP:CE3  | 1:D:694:TRP:HA   | 2.55                     | 0.41              |
| 2:F:282:TRP:H    | 2:F:326:ASN:ND2  | 2.15                     | 0.41              |
| 1:D:755:VAL:HG13 | 1:D:756:ALA:N    | 2.35                     | 0.41              |
| 2:C:229:ARG:HA   | 2:C:269:TYR:CD1  | 2.55                     | 0.41              |
| 2:G:184:VAL:HG13 | 2:G:185:TRP:N    | 2.34                     | 0.41              |
| 2:F:271:ARG:HG3  | 2:F:271:ARG:HH11 | 1.85                     | 0.41              |
| 2:G:196:PHE:O    | 2:G:197:GLU:HG2  | 2.20                     | 0.41              |
| 1:E:876:MET:SD   | 1:E:884:LEU:HD22 | 2.60                     | 0.41              |
| 1:D:683:VAL:HG23 | 1:D:684:ARG:H    | 1.83                     | 0.41              |
| 2:C:229:ARG:HB2  | 1:D:770:GLU:OE1  | 2.21                     | 0.41              |
| 2:B:208:PHE:C    | 2:B:209:LEU:HD12 | 2.41                     | 0.41              |
| 2:F:224:VAL:HB   | 2:F:266:LEU:HD11 | 2.01                     | 0.41              |
| 2:C:179:PHE:HE2  | 2:C:280:PHE:H    | 1.60                     | 0.41              |
| 2:C:343:LEU:HA   | 2:C:343:LEU:HD12 | 1.94                     | 0.41              |
| 2:B:224:VAL:O    | 2:B:225:THR:C    | 2.59                     | 0.41              |
| 2:B:248:LEU:HD11 | 2:B:288:LEU:HB2  | 2.02                     | 0.41              |
| 1:A:633:LEU:CD2  | 1:A:635:LEU:HD21 | 2.50                     | 0.41              |
| 2:C:363:LEU:N    | 2:C:363:LEU:HD22 | 2.33                     | 0.41              |
| 2:G:285:VAL:HG13 | 2:G:323:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:815:LEU:HD11 | 1:A:821:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:683:VAL:HG23 | 1:A:684:ARG:HD3  | 2.02                     | 0.41              |
| 1:E:898:PHE:O    | 1:E:900:PRO:N    | 2.53                     | 0.41              |
| 2:G:199:ILE:CG2  | 2:G:203:LEU:HB2  | 2.47                     | 0.41              |
| 1:A:796:GLY:O    | 1:A:799:ARG:HG2  | 2.20                     | 0.41              |
| 2:F:224:VAL:CG1  | 2:F:266:LEU:HD11 | 2.50                     | 0.41              |
| 2:B:327:ILE:HA   | 2:B:328:PRO:HD3  | 1.93                     | 0.41              |
| 1:E:874:SER:C    | 1:E:876:MET:N    | 2.74                     | 0.41              |
| 1:A:811:LEU:HD23 | 1:A:821:ALA:HB1  | 2.01                     | 0.41              |
| 2:F:311:ASP:HB2  | 2:F:363:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:702:GLY:O    | 1:A:751:PHE:HA   | 2.21                     | 0.41              |
| 1:A:872:ASP:CG   | 1:D:881:ARG:HH22 | 2.24                     | 0.41              |
| 2:G:262:GLN:NE2  | 2:G:265:ARG:HE   | 2.12                     | 0.41              |
| 1:E:896:HIS:O    | 1:E:898:PHE:N    | 2.53                     | 0.41              |
| 1:A:804:THR:CG2  | 1:A:805:VAL:N    | 2.83                     | 0.41              |
| 1:H:801:LEU:N    | 1:H:801:LEU:CD1  | 2.83                     | 0.41              |
| 1:A:691:ILE:HD12 | 1:A:691:ILE:HA   | 1.81                     | 0.41              |
| 1:A:799:ARG:NH2  | 1:A:900:PRO:CD   | 2.84                     | 0.41              |
| 1:E:645:VAL:HG11 | 1:E:895:ARG:HA   | 2.03                     | 0.41              |
| 1:E:784:ALA:HB2  | 1:E:863:VAL:HG13 | 2.02                     | 0.41              |
| 1:D:627:ARG:HG3  | 1:D:627:ARG:H    | 1.71                     | 0.41              |
| 2:C:294:ASP:OD2  | 1:D:725:ARG:NH2  | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:203:LEU:HD11 | 2:B:208:PHE:CD1  | 2.53                     | 0.41              |
| 1:A:799:ARG:HA   | 1:A:800:PRO:HD3  | 1.83                     | 0.41              |
| 1:H:672:ARG:HA   | 1:H:672:ARG:HD3  | 1.84                     | 0.41              |
| 1:E:811:LEU:HD12 | 1:E:821:ALA:HB1  | 2.02                     | 0.41              |
| 1:D:669:GLY:HA3  | 1:D:679:TYR:OH   | 2.21                     | 0.41              |
| 1:E:876:MET:HG3  | 1:E:880:ALA:CB   | 2.51                     | 0.41              |
| 2:C:241:VAL:O    | 2:C:282:TRP:HA   | 2.20                     | 0.41              |
| 2:G:203:LEU:HD23 | 2:G:209:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:898:PHE:O    | 1:A:899:ALA:C    | 2.58                     | 0.41              |
| 1:H:804:THR:HG22 | 1:H:805:VAL:N    | 2.36                     | 0.41              |
| 1:D:891:VAL:N    | 1:D:892:PRO:CD   | 2.84                     | 0.41              |
| 1:E:788:ARG:NH1  | 1:E:788:ARG:CG   | 2.84                     | 0.41              |
| 1:A:699:LEU:HA   | 1:A:748:PHE:O    | 2.20                     | 0.41              |
| 1:A:682:ASP:C    | 1:A:682:ASP:OD2  | 2.58                     | 0.41              |
| 2:B:368:PHE:CD2  | 2:B:368:PHE:N    | 2.89                     | 0.41              |
| 2:B:346:LEU:C    | 2:B:346:LEU:HD23 | 2.41                     | 0.41              |
| 1:D:899:ALA:HB3  | 1:D:900:PRO:CD   | 2.51                     | 0.41              |
| 1:D:810:GLU:OE2  | 1:D:810:GLU:N    | 2.53                     | 0.41              |
| 1:A:752:GLU:O    | 1:A:753:ASN:HB2  | 2.21                     | 0.41              |
| 2:F:339:SER:O    | 2:F:343:LEU:HB2  | 2.21                     | 0.41              |
| 1:H:727:PHE:CZ   | 1:H:765:ILE:HG23 | 2.55                     | 0.41              |
| 1:H:643:LEU:HG   | 1:H:647:LYS:HE3  | 2.02                     | 0.41              |
| 2:C:297:VAL:O    | 2:C:301:PHE:HB2  | 2.20                     | 0.41              |
| 1:H:863:VAL:HG12 | 1:H:864:PHE:N    | 2.36                     | 0.41              |
| 1:E:856:TRP:CE2  | 1:H:874:SER:HA   | 2.55                     | 0.41              |
| 1:A:873:VAL:O    | 1:A:874:SER:OG   | 2.26                     | 0.41              |
| 1:D:860:MET:O    | 1:D:863:VAL:HB   | 2.21                     | 0.41              |
| 2:B:241:VAL:O    | 2:B:282:TRP:HA   | 2.21                     | 0.41              |
| 1:D:630:ILE:HA   | 1:D:905:PHE:CD2  | 2.56                     | 0.41              |
| 1:E:905:PHE:O    | 1:E:906:ALA:C    | 2.60                     | 0.41              |
| 1:H:783:ALA:O    | 1:H:826:VAL:HG22 | 2.21                     | 0.41              |
| 1:D:898:PHE:O    | 1:D:899:ALA:C    | 2.59                     | 0.41              |
| 1:A:801:LEU:HD12 | 1:A:801:LEU:H    | 1.85                     | 0.41              |
| 1:H:752:GLU:HG2  | 1:H:753:ASN:N    | 2.36                     | 0.41              |
| 1:D:632:VAL:HG13 | 1:D:699:LEU:HB3  | 2.03                     | 0.40              |
| 2:C:189:PRO:HB3  | 2:C:378:PHE:HZ   | 1.86                     | 0.40              |
| 1:A:817:HIS:CD2  | 1:D:674:GLN:HA   | 2.56                     | 0.40              |
| 2:F:325:SER:OG   | 2:F:327:ILE:HG13 | 2.21                     | 0.40              |
| 1:H:853:ASP:CG   | 1:H:854:ILE:N    | 2.74                     | 0.40              |
| 1:A:717:LYS:HB3  | 1:A:721:GLU:HB2  | 2.02                     | 0.40              |
| 1:D:808:LYS:HG2  | 1:D:808:LYS:H    | 1.71                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:202:GLU:OE1  | 2:F:202:GLU:N    | 2.45                     | 0.40              |
| 1:H:732:ARG:CZ   | 1:H:733:LEU:HD21 | 2.51                     | 0.40              |
| 1:E:684:ARG:HB2  | 2:F:300:ARG:CZ   | 2.52                     | 0.40              |
| 1:E:729:GLU:OE2  | 2:F:300:ARG:NH1  | 2.55                     | 0.40              |
| 1:D:815:LEU:HD11 | 1:D:846:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:652:GLN:CD   | 1:D:906:ALA:HB1  | 2.41                     | 0.40              |
| 2:B:203:LEU:CG   | 2:B:209:LEU:HD11 | 2.50                     | 0.40              |
| 1:H:816:GLU:CD   | 1:H:862:ARG:NH2  | 2.75                     | 0.40              |
| 1:H:632:VAL:HG22 | 1:H:699:LEU:HB3  | 2.03                     | 0.40              |
| 1:E:794:LEU:HA   | 1:E:795:PRO:HD2  | 1.95                     | 0.40              |
| 1:H:801:LEU:CD1  | 1:H:801:LEU:H    | 2.35                     | 0.40              |
| 2:B:179:PHE:CE2  | 2:B:279:PRO:HA   | 2.56                     | 0.40              |
| 1:H:745:ARG:HA   | 1:H:746:PRO:HD3  | 1.93                     | 0.40              |
| 1:E:804:THR:HB   | 1:E:806:ASN:O    | 2.21                     | 0.40              |
| 1:H:770:GLU:O    | 1:H:771:SER:HB3  | 2.22                     | 0.40              |
| 1:D:632:VAL:HG12 | 1:D:633:LEU:N    | 2.37                     | 0.40              |
| 2:B:246:PRO:HA   | 2:B:247:PRO:HD3  | 1.91                     | 0.40              |
| 1:H:873:VAL:C    | 1:H:874:SER:O    | 2.60                     | 0.40              |
| 2:F:248:LEU:N    | 2:F:287:ASN:HD22 | 2.16                     | 0.40              |
| 1:D:706:CYS:CB   | 1:D:754:VAL:HG13 | 2.52                     | 0.40              |
| 1:H:657:ILE:HG22 | 1:H:680:VAL:HG23 | 2.03                     | 0.40              |
| 1:H:748:PHE:HB3  | 1:H:794:LEU:HD23 | 2.02                     | 0.40              |
| 1:H:637:ASP:CB   | 1:H:658:ALA:HB1  | 2.51                     | 0.40              |
| 2:F:257:SER:O    | 2:F:258:TRP:C    | 2.60                     | 0.40              |
| 2:G:203:LEU:HG   | 2:G:209:LEU:CD1  | 2.51                     | 0.40              |
| 1:H:748:PHE:HZ   | 1:H:904:TYR:CD2  | 2.38                     | 0.40              |
| 2:C:258:TRP:CE2  | 2:C:262:GLN:HG3  | 2.57                     | 0.40              |
| 1:D:799:ARG:CZ   | 1:D:896:HIS:CE1  | 3.05                     | 0.40              |
| 2:C:265:ARG:HG2  | 2:C:265:ARG:HH11 | 1.87                     | 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     | 268/295 (91%)   | 228 (85%)  | 30 (11%)  | 10 (4%)  | 4           | 17 |
| 1   | D     | 263/295 (89%)   | 221 (84%)  | 35 (13%)  | 7 (3%)   | 6           | 25 |
| 1   | E     | 266/295 (90%)   | 223 (84%)  | 34 (13%)  | 9 (3%)   | 5           | 19 |
| 1   | H     | 263/295 (89%)   | 226 (86%)  | 29 (11%)  | 8 (3%)   | 5           | 22 |
| 2   | B     | 178/230 (77%)   | 135 (76%)  | 34 (19%)  | 9 (5%)   | 2           | 9  |
| 2   | C     | 178/230 (77%)   | 138 (78%)  | 32 (18%)  | 8 (4%)   | 3           | 12 |
| 2   | F     | 178/230 (77%)   | 136 (76%)  | 36 (20%)  | 6 (3%)   | 5           | 19 |
| 2   | G     | 178/230 (77%)   | 138 (78%)  | 33 (18%)  | 7 (4%)   | 4           | 15 |
| All | All   | 1772/2100 (84%) | 1445 (82%) | 263 (15%) | 64 (4%)  | 4           | 18 |

All (64) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 845 | PRO  |
| 1   | D     | 849 | ASN  |
| 1   | E     | 845 | PRO  |
| 1   | H     | 874 | SER  |
| 1   | H     | 888 | SER  |
| 1   | A     | 676 | LYS  |
| 1   | A     | 707 | ASN  |
| 1   | A     | 884 | LEU  |
| 1   | E     | 897 | LEU  |
| 2   | G     | 328 | PRO  |
| 1   | A     | 624 | ALA  |
| 2   | B     | 277 | PRO  |
| 2   | B     | 291 | ASN  |
| 2   | B     | 328 | PRO  |
| 2   | C     | 277 | PRO  |
| 2   | C     | 328 | PRO  |
| 1   | D     | 845 | PRO  |
| 2   | F     | 277 | PRO  |
| 2   | F     | 328 | PRO  |
| 2   | G     | 277 | PRO  |
| 1   | H     | 707 | ASN  |
| 1   | H     | 726 | LEU  |
| 1   | A     | 684 | ARG  |
| 1   | A     | 708 | ASP  |
| 1   | A     | 726 | LEU  |
| 1   | A     | 783 | ALA  |
| 1   | A     | 844 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 225 | THR  |
| 2   | B     | 304 | MET  |
| 2   | B     | 362 | LYS  |
| 2   | C     | 236 | GLY  |
| 2   | C     | 304 | MET  |
| 1   | D     | 676 | LYS  |
| 1   | D     | 783 | ALA  |
| 1   | D     | 855 | LEU  |
| 1   | D     | 874 | SER  |
| 1   | E     | 808 | LYS  |
| 1   | E     | 899 | ALA  |
| 2   | F     | 304 | MET  |
| 2   | G     | 225 | THR  |
| 2   | G     | 236 | GLY  |
| 1   | H     | 676 | LYS  |
| 1   | H     | 873 | VAL  |
| 2   | B     | 256 | PRO  |
| 1   | E     | 637 | ASP  |
| 1   | E     | 676 | LYS  |
| 1   | E     | 694 | TRP  |
| 1   | E     | 783 | ALA  |
| 2   | F     | 236 | GLY  |
| 2   | C     | 336 | ALA  |
| 2   | G     | 304 | MET  |
| 1   | E     | 680 | VAL  |
| 2   | B     | 236 | GLY  |
| 2   | C     | 278 | ARG  |
| 2   | G     | 256 | PRO  |
| 2   | B     | 254 | ARG  |
| 2   | F     | 256 | PRO  |
| 1   | H     | 680 | VAL  |
| 1   | H     | 691 | ILE  |
| 2   | C     | 272 | PRO  |
| 2   | C     | 276 | SER  |
| 1   | D     | 680 | VAL  |
| 2   | F     | 272 | PRO  |
| 2   | G     | 278 | ARG  |

### 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     | 224/259 (86%)   | 196 (88%)  | 28 (12%)  | 6           | 17 |
| 1   | D     | 222/259 (86%)   | 194 (87%)  | 28 (13%)  | 5           | 16 |
| 1   | E     | 223/259 (86%)   | 188 (84%)  | 35 (16%)  | 3           | 9  |
| 1   | H     | 222/259 (86%)   | 203 (91%)  | 19 (9%)   | 13          | 36 |
| 2   | B     | 166/210 (79%)   | 153 (92%)  | 13 (8%)   | 16          | 41 |
| 2   | C     | 166/210 (79%)   | 154 (93%)  | 12 (7%)   | 18          | 46 |
| 2   | F     | 166/210 (79%)   | 155 (93%)  | 11 (7%)   | 21          | 51 |
| 2   | G     | 166/210 (79%)   | 157 (95%)  | 9 (5%)    | 27          | 62 |
| All | All   | 1555/1876 (83%) | 1400 (90%) | 155 (10%) | 9           | 28 |

All (155) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 631 | ARG  |
| 1   | A     | 644 | LEU  |
| 1   | A     | 648 | ASP  |
| 1   | A     | 660 | GLU  |
| 1   | A     | 671 | VAL  |
| 1   | A     | 674 | GLN  |
| 1   | A     | 683 | VAL  |
| 1   | A     | 684 | ARG  |
| 1   | A     | 688 | GLN  |
| 1   | A     | 691 | ILE  |
| 1   | A     | 701 | ILE  |
| 1   | A     | 706 | CYS  |
| 1   | A     | 760 | SER  |
| 1   | A     | 775 | MET  |
| 1   | A     | 798 | ASN  |
| 1   | A     | 807 | ASP  |
| 1   | A     | 809 | LEU  |
| 1   | A     | 816 | GLU  |
| 1   | A     | 843 | HIS  |
| 1   | A     | 845 | PRO  |
| 1   | A     | 848 | MET  |
| 1   | A     | 858 | THR  |
| 1   | A     | 860 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 878 | ARG  |
| 1   | A     | 881 | ARG  |
| 1   | A     | 891 | VAL  |
| 1   | A     | 904 | TYR  |
| 1   | A     | 907 | CYS  |
| 2   | B     | 202 | GLU  |
| 2   | B     | 255 | PRO  |
| 2   | B     | 262 | GLN  |
| 2   | B     | 267 | LEU  |
| 2   | B     | 268 | GLN  |
| 2   | B     | 271 | ARG  |
| 2   | B     | 286 | ASP  |
| 2   | B     | 295 | LEU  |
| 2   | B     | 321 | VAL  |
| 2   | B     | 322 | ARG  |
| 2   | B     | 326 | ASN  |
| 2   | B     | 335 | TRP  |
| 2   | B     | 363 | LEU  |
| 2   | C     | 191 | ARG  |
| 2   | C     | 231 | ASP  |
| 2   | C     | 239 | ASP  |
| 2   | C     | 257 | SER  |
| 2   | C     | 268 | GLN  |
| 2   | C     | 294 | ASP  |
| 2   | C     | 301 | PHE  |
| 2   | C     | 308 | THR  |
| 2   | C     | 321 | VAL  |
| 2   | C     | 326 | ASN  |
| 2   | C     | 328 | PRO  |
| 2   | C     | 335 | TRP  |
| 1   | D     | 631 | ARG  |
| 1   | D     | 644 | LEU  |
| 1   | D     | 648 | ASP  |
| 1   | D     | 660 | GLU  |
| 1   | D     | 665 | SER  |
| 1   | D     | 674 | GLN  |
| 1   | D     | 684 | ARG  |
| 1   | D     | 692 | GLN  |
| 1   | D     | 694 | TRP  |
| 1   | D     | 707 | ASN  |
| 1   | D     | 729 | GLU  |
| 1   | D     | 734 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 752 | GLU  |
| 1   | D     | 775 | MET  |
| 1   | D     | 776 | ILE  |
| 1   | D     | 799 | ARG  |
| 1   | D     | 801 | LEU  |
| 1   | D     | 807 | ASP  |
| 1   | D     | 809 | LEU  |
| 1   | D     | 816 | GLU  |
| 1   | D     | 823 | PHE  |
| 1   | D     | 826 | VAL  |
| 1   | D     | 845 | PRO  |
| 1   | D     | 851 | LYS  |
| 1   | D     | 853 | ASP  |
| 1   | D     | 855 | LEU  |
| 1   | D     | 881 | ARG  |
| 1   | D     | 884 | LEU  |
| 1   | E     | 644 | LEU  |
| 1   | E     | 648 | ASP  |
| 1   | E     | 654 | ASP  |
| 1   | E     | 660 | GLU  |
| 1   | E     | 661 | VAL  |
| 1   | E     | 665 | SER  |
| 1   | E     | 674 | GLN  |
| 1   | E     | 684 | ARG  |
| 1   | E     | 688 | GLN  |
| 1   | E     | 691 | ILE  |
| 1   | E     | 694 | TRP  |
| 1   | E     | 729 | GLU  |
| 1   | E     | 734 | LEU  |
| 1   | E     | 750 | LEU  |
| 1   | E     | 753 | ASN  |
| 1   | E     | 760 | SER  |
| 1   | E     | 775 | MET  |
| 1   | E     | 776 | ILE  |
| 1   | E     | 786 | ARG  |
| 1   | E     | 799 | ARG  |
| 1   | E     | 800 | PRO  |
| 1   | E     | 806 | ASN  |
| 1   | E     | 807 | ASP  |
| 1   | E     | 809 | LEU  |
| 1   | E     | 816 | GLU  |
| 1   | E     | 823 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 845 | PRO  |
| 1   | E     | 848 | MET  |
| 1   | E     | 853 | ASP  |
| 1   | E     | 862 | ARG  |
| 1   | E     | 863 | VAL  |
| 1   | E     | 868 | VAL  |
| 1   | E     | 881 | ARG  |
| 1   | E     | 884 | LEU  |
| 1   | E     | 907 | CYS  |
| 2   | F     | 230 | LYS  |
| 2   | F     | 231 | ASP  |
| 2   | F     | 237 | PRO  |
| 2   | F     | 239 | ASP  |
| 2   | F     | 262 | GLN  |
| 2   | F     | 268 | GLN  |
| 2   | F     | 291 | ASN  |
| 2   | F     | 294 | ASP  |
| 2   | F     | 326 | ASN  |
| 2   | F     | 335 | TRP  |
| 2   | F     | 363 | LEU  |
| 2   | G     | 191 | ARG  |
| 2   | G     | 196 | PHE  |
| 2   | G     | 262 | GLN  |
| 2   | G     | 268 | GLN  |
| 2   | G     | 286 | ASP  |
| 2   | G     | 301 | PHE  |
| 2   | G     | 326 | ASN  |
| 2   | G     | 335 | TRP  |
| 2   | G     | 337 | LEU  |
| 1   | H     | 631 | ARG  |
| 1   | H     | 644 | LEU  |
| 1   | H     | 648 | ASP  |
| 1   | H     | 665 | SER  |
| 1   | H     | 674 | GLN  |
| 1   | H     | 683 | VAL  |
| 1   | H     | 684 | ARG  |
| 1   | H     | 694 | TRP  |
| 1   | H     | 707 | ASN  |
| 1   | H     | 729 | GLU  |
| 1   | H     | 752 | GLU  |
| 1   | H     | 755 | VAL  |
| 1   | H     | 809 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 816 | GLU  |
| 1   | H     | 823 | PHE  |
| 1   | H     | 855 | LEU  |
| 1   | H     | 858 | THR  |
| 1   | H     | 878 | ARG  |
| 1   | H     | 881 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 688 | GLN  |
| 1   | A     | 753 | ASN  |
| 2   | B     | 262 | GLN  |
| 2   | B     | 264 | HIS  |
| 2   | B     | 268 | GLN  |
| 2   | B     | 287 | ASN  |
| 2   | B     | 313 | HIS  |
| 2   | B     | 326 | ASN  |
| 2   | C     | 262 | GLN  |
| 2   | C     | 264 | HIS  |
| 2   | C     | 268 | GLN  |
| 2   | C     | 287 | ASN  |
| 2   | C     | 326 | ASN  |
| 1   | D     | 707 | ASN  |
| 1   | D     | 753 | ASN  |
| 1   | D     | 896 | HIS  |
| 1   | E     | 688 | GLN  |
| 1   | E     | 753 | ASN  |
| 1   | E     | 817 | HIS  |
| 1   | E     | 896 | HIS  |
| 2   | F     | 262 | GLN  |
| 2   | F     | 264 | HIS  |
| 2   | F     | 287 | ASN  |
| 2   | F     | 313 | HIS  |
| 2   | F     | 326 | ASN  |
| 2   | G     | 262 | GLN  |
| 2   | G     | 268 | GLN  |
| 2   | G     | 287 | ASN  |
| 2   | G     | 326 | ASN  |
| 1   | H     | 688 | GLN  |
| 1   | H     | 753 | ASN  |
| 1   | H     | 817 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 882 | GLN  |
| 1   | H     | 896 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SAH  | A     | 1   | -    | 20,28,28     | 1.96 | 6 (30%)     | 19,40,40    | 2.79 | 6 (31%)     |
| 3   | SAH  | D     | 4   | -    | 20,28,28     | 1.72 | 5 (25%)     | 19,40,40    | 3.07 | 6 (31%)     |
| 3   | SAH  | E     | 5   | -    | 20,28,28     | 1.97 | 6 (30%)     | 19,40,40    | 2.88 | 6 (31%)     |
| 3   | SAH  | H     | 8   | -    | 20,28,28     | 1.91 | 4 (20%)     | 19,40,40    | 3.20 | 8 (42%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | SAH  | A     | 1   | -    | -       | 0/7/31/31 | 0/3/3/3 |
| 3   | SAH  | D     | 4   | -    | -       | 0/7/31/31 | 0/3/3/3 |
| 3   | SAH  | E     | 5   | -    | -       | 0/7/31/31 | 0/3/3/3 |
| 3   | SAH  | H     | 8   | -    | -       | 0/7/31/31 | 0/3/3/3 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | H     | 8   | SAH  | C5'-SD  | -3.94 | 1.73        | 1.81     |
| 3   | D     | 4   | SAH  | C5'-SD  | -3.92 | 1.73        | 1.81     |
| 3   | E     | 5   | SAH  | C5'-SD  | -2.70 | 1.75        | 1.81     |
| 3   | E     | 5   | SAH  | C8-N7   | -2.54 | 1.29        | 1.34     |
| 3   | A     | 1   | SAH  | C8-N7   | -2.34 | 1.30        | 1.34     |
| 3   | A     | 1   | SAH  | C5'-SD  | -2.26 | 1.76        | 1.81     |
| 3   | H     | 8   | SAH  | C8-N7   | -2.07 | 1.30        | 1.34     |
| 3   | D     | 4   | SAH  | C2'-C3' | 2.03  | 1.58        | 1.53     |
| 3   | D     | 4   | SAH  | O4'-C1' | 2.17  | 1.43        | 1.41     |
| 3   | E     | 5   | SAH  | C2-N1   | 2.35  | 1.38        | 1.33     |
| 3   | D     | 4   | SAH  | C5'-C4' | 2.41  | 1.59        | 1.52     |
| 3   | A     | 1   | SAH  | C2'-C3' | 2.48  | 1.60        | 1.53     |
| 3   | A     | 1   | SAH  | C5'-C4' | 2.51  | 1.59        | 1.52     |
| 3   | E     | 5   | SAH  | C5'-C4' | 2.55  | 1.59        | 1.52     |
| 3   | H     | 8   | SAH  | C2-N3   | 3.36  | 1.38        | 1.32     |
| 3   | A     | 1   | SAH  | C2-N3   | 3.63  | 1.38        | 1.32     |
| 3   | D     | 4   | SAH  | C2-N3   | 3.64  | 1.38        | 1.32     |
| 3   | E     | 5   | SAH  | C2-N3   | 4.23  | 1.39        | 1.32     |
| 3   | E     | 5   | SAH  | O4'-C1' | 4.70  | 1.47        | 1.41     |
| 3   | H     | 8   | SAH  | O4'-C1' | 5.02  | 1.47        | 1.41     |
| 3   | A     | 1   | SAH  | O4'-C1' | 5.07  | 1.47        | 1.41     |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | E     | 5   | SAH  | N3-C2-N1    | -9.38 | 121.71      | 128.89   |
| 3   | A     | 1   | SAH  | N3-C2-N1    | -8.59 | 122.31      | 128.89   |
| 3   | H     | 8   | SAH  | N3-C2-N1    | -8.49 | 122.39      | 128.89   |
| 3   | D     | 4   | SAH  | N3-C2-N1    | -7.93 | 122.82      | 128.89   |
| 3   | H     | 8   | SAH  | CB-CG-SD    | -6.52 | 100.99      | 113.57   |
| 3   | D     | 4   | SAH  | O4'-C4'-C5' | -6.16 | 92.07       | 108.85   |
| 3   | E     | 5   | SAH  | C1'-N9-C4   | -4.73 | 119.81      | 126.94   |
| 3   | H     | 8   | SAH  | C4'-O4'-C1' | -4.59 | 104.68      | 109.72   |
| 3   | D     | 4   | SAH  | C1'-N9-C4   | -4.58 | 120.03      | 126.94   |
| 3   | D     | 4   | SAH  | C4'-O4'-C1' | -4.57 | 104.69      | 109.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 1   | SAH  | CB-CG-SD    | -4.35 | 105.18      | 113.57   |
| 3   | A     | 1   | SAH  | C1'-N9-C4   | -4.28 | 120.48      | 126.94   |
| 3   | H     | 8   | SAH  | C1'-N9-C4   | -4.24 | 120.54      | 126.94   |
| 3   | D     | 4   | SAH  | CB-CG-SD    | -3.97 | 105.91      | 113.57   |
| 3   | E     | 5   | SAH  | CB-CG-SD    | -3.91 | 106.03      | 113.57   |
| 3   | E     | 5   | SAH  | C4'-C5'-SD  | -2.42 | 106.08      | 113.53   |
| 3   | H     | 8   | SAH  | C4'-C5'-SD  | -2.03 | 107.27      | 113.53   |
| 3   | E     | 5   | SAH  | C2'-C1'-N9  | 2.08  | 117.46      | 114.29   |
| 3   | H     | 8   | SAH  | O4'-C4'-C3' | 2.46  | 110.10      | 105.15   |
| 3   | D     | 4   | SAH  | C2-N1-C6    | 2.48  | 123.20      | 118.77   |
| 3   | A     | 1   | SAH  | C2-N1-C6    | 2.50  | 123.24      | 118.77   |
| 3   | A     | 1   | SAH  | CB-CA-N     | 2.71  | 118.24      | 110.52   |
| 3   | H     | 8   | SAH  | C2-N1-C6    | 2.83  | 123.83      | 118.77   |
| 3   | E     | 5   | SAH  | C2-N1-C6    | 2.94  | 124.01      | 118.77   |
| 3   | A     | 1   | SAH  | C2'-C1'-N9  | 3.38  | 119.45      | 114.29   |
| 3   | H     | 8   | SAH  | O4'-C1'-N9  | 3.91  | 116.28      | 108.10   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 1   | SAH  | 1       | 0            |
| 3   | E     | 5   | SAH  | 1       | 0            |
| 3   | H     | 8   | SAH  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 272/295 (92%)   | 0.21   | 4 (1%) 76 74  | 30, 64, 106, 146      | 0     |
| 1   | D     | 267/295 (90%)   | 0.16   | 5 (1%) 70 66  | 37, 75, 122, 157      | 0     |
| 1   | E     | 270/295 (91%)   | 0.23   | 4 (1%) 76 74  | 27, 67, 111, 132      | 0     |
| 1   | H     | 267/295 (90%)   | 0.57   | 25 (9%) 11 6  | 51, 101, 138, 170     | 0     |
| 2   | B     | 186/230 (80%)   | 1.08   | 37 (19%) 1 1  | 55, 121, 187, 207     | 0     |
| 2   | C     | 186/230 (80%)   | 1.06   | 38 (20%) 1 1  | 61, 118, 189, 206     | 0     |
| 2   | F     | 186/230 (80%)   | 1.20   | 39 (20%) 1 1  | 66, 121, 189, 210     | 0     |
| 2   | G     | 186/230 (80%)   | 2.83   | 93 (50%) 0 0  | 109, 163, 201, 210    | 0     |
| All | All   | 1820/2100 (86%) | 0.80   | 245 (13%) 4 2 | 27, 93, 181, 210      | 0     |

All (245) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 321 | VAL  | 28.1 |
| 2   | G     | 309 | ILE  | 17.9 |
| 2   | G     | 334 | HIS  | 17.1 |
| 2   | F     | 334 | HIS  | 14.3 |
| 2   | F     | 310 | PRO  | 11.8 |
| 2   | G     | 308 | THR  | 11.6 |
| 2   | G     | 353 | SER  | 11.6 |
| 2   | G     | 331 | ARG  | 11.5 |
| 2   | F     | 315 | GLY  | 11.5 |
| 2   | F     | 331 | ARG  | 10.6 |
| 2   | G     | 344 | SER  | 10.0 |
| 2   | C     | 361 | THR  | 8.6  |
| 2   | G     | 310 | PRO  | 8.5  |
| 2   | F     | 314 | GLY  | 8.1  |
| 2   | B     | 352 | SER  | 8.1  |
| 2   | G     | 335 | TRP  | 7.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 334 | HIS  | 7.8  |
| 2   | F     | 316 | SER  | 7.4  |
| 2   | G     | 222 | VAL  | 7.2  |
| 2   | C     | 316 | SER  | 7.1  |
| 2   | C     | 315 | GLY  | 7.0  |
| 2   | G     | 280 | PHE  | 6.9  |
| 2   | B     | 336 | ALA  | 6.8  |
| 2   | G     | 196 | PHE  | 6.7  |
| 2   | G     | 206 | LEU  | 6.5  |
| 2   | G     | 362 | LYS  | 6.5  |
| 2   | G     | 185 | TRP  | 6.4  |
| 2   | G     | 279 | PRO  | 6.3  |
| 2   | G     | 182 | VAL  | 6.2  |
| 2   | F     | 336 | ALA  | 6.2  |
| 2   | G     | 311 | ASP  | 6.1  |
| 2   | F     | 276 | SER  | 6.0  |
| 2   | B     | 364 | VAL  | 6.0  |
| 2   | G     | 348 | GLN  | 5.9  |
| 2   | C     | 313 | HIS  | 5.9  |
| 2   | F     | 363 | LEU  | 5.9  |
| 2   | G     | 192 | VAL  | 5.9  |
| 2   | G     | 350 | LYS  | 5.8  |
| 2   | C     | 336 | ALA  | 5.8  |
| 2   | B     | 203 | LEU  | 5.7  |
| 2   | G     | 203 | LEU  | 5.7  |
| 2   | G     | 312 | VAL  | 5.7  |
| 2   | G     | 377 | TYR  | 5.6  |
| 2   | B     | 242 | TYR  | 5.4  |
| 2   | G     | 252 | CYS  | 5.4  |
| 2   | G     | 183 | PRO  | 5.4  |
| 2   | G     | 324 | TRP  | 5.4  |
| 2   | G     | 216 | GLY  | 5.2  |
| 2   | C     | 349 | ASN  | 5.2  |
| 2   | G     | 199 | ILE  | 5.2  |
| 2   | C     | 365 | LYS  | 5.2  |
| 2   | G     | 364 | VAL  | 5.2  |
| 1   | H     | 731 | TYR  | 5.2  |
| 2   | G     | 217 | GLN  | 5.1  |
| 2   | G     | 307 | VAL  | 5.0  |
| 2   | G     | 316 | SER  | 5.0  |
| 2   | G     | 343 | LEU  | 4.9  |
| 2   | G     | 241 | VAL  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 310 | PRO  | 4.9  |
| 2   | F     | 251 | THR  | 4.8  |
| 2   | C     | 192 | VAL  | 4.8  |
| 2   | C     | 314 | GLY  | 4.7  |
| 2   | G     | 270 | ALA  | 4.7  |
| 2   | F     | 364 | VAL  | 4.7  |
| 2   | C     | 341 | GLU  | 4.7  |
| 2   | G     | 186 | ARG  | 4.7  |
| 2   | G     | 328 | PRO  | 4.6  |
| 2   | G     | 302 | LEU  | 4.5  |
| 2   | F     | 333 | ARG  | 4.5  |
| 2   | G     | 184 | VAL  | 4.5  |
| 2   | F     | 353 | SER  | 4.4  |
| 2   | G     | 205 | SER  | 4.4  |
| 2   | G     | 284 | PHE  | 4.4  |
| 2   | G     | 363 | LEU  | 4.4  |
| 2   | G     | 282 | TRP  | 4.4  |
| 2   | C     | 334 | HIS  | 4.3  |
| 1   | D     | 740 | LYS  | 4.2  |
| 2   | G     | 289 | VAL  | 4.2  |
| 1   | H     | 735 | HIS  | 4.1  |
| 2   | F     | 343 | LEU  | 4.1  |
| 2   | G     | 349 | ASN  | 4.1  |
| 2   | G     | 366 | ASN  | 4.1  |
| 2   | B     | 192 | VAL  | 4.1  |
| 2   | C     | 348 | GLN  | 4.1  |
| 2   | B     | 310 | PRO  | 4.1  |
| 2   | B     | 332 | SER  | 4.1  |
| 1   | H     | 686 | VAL  | 4.0  |
| 2   | G     | 340 | GLU  | 3.9  |
| 2   | G     | 201 | LYS  | 3.9  |
| 2   | G     | 288 | LEU  | 3.9  |
| 1   | A     | 806 | ASN  | 3.9  |
| 2   | G     | 374 | TYR  | 3.9  |
| 2   | F     | 313 | HIS  | 3.9  |
| 2   | C     | 376 | LYS  | 3.9  |
| 2   | G     | 323 | VAL  | 3.8  |
| 2   | G     | 327 | ILE  | 3.8  |
| 1   | E     | 805 | VAL  | 3.8  |
| 2   | B     | 309 | ILE  | 3.8  |
| 2   | C     | 208 | PHE  | 3.8  |
| 2   | G     | 285 | VAL  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 346 | LEU  | 3.8  |
| 2   | F     | 309 | ILE  | 3.8  |
| 2   | G     | 315 | GLY  | 3.8  |
| 2   | G     | 229 | ARG  | 3.7  |
| 2   | C     | 206 | LEU  | 3.7  |
| 2   | G     | 180 | GLU  | 3.7  |
| 2   | B     | 353 | SER  | 3.7  |
| 2   | C     | 274 | PRO  | 3.7  |
| 2   | G     | 378 | PHE  | 3.6  |
| 2   | C     | 370 | PRO  | 3.6  |
| 2   | G     | 251 | THR  | 3.6  |
| 1   | H     | 794 | LEU  | 3.6  |
| 2   | G     | 367 | CYS  | 3.6  |
| 2   | F     | 330 | ILE  | 3.5  |
| 1   | H     | 630 | ILE  | 3.5  |
| 1   | H     | 734 | LEU  | 3.5  |
| 2   | C     | 352 | SER  | 3.5  |
| 2   | G     | 273 | LYS  | 3.5  |
| 2   | F     | 279 | PRO  | 3.4  |
| 2   | B     | 285 | VAL  | 3.4  |
| 2   | B     | 244 | ALA  | 3.4  |
| 2   | C     | 369 | LEU  | 3.4  |
| 1   | H     | 805 | VAL  | 3.4  |
| 2   | F     | 335 | TRP  | 3.4  |
| 1   | H     | 844 | PHE  | 3.4  |
| 2   | G     | 178 | MET  | 3.4  |
| 2   | F     | 252 | CYS  | 3.3  |
| 2   | F     | 332 | SER  | 3.3  |
| 2   | B     | 335 | TRP  | 3.3  |
| 2   | G     | 232 | VAL  | 3.3  |
| 1   | H     | 745 | ARG  | 3.3  |
| 2   | F     | 182 | VAL  | 3.3  |
| 1   | H     | 790 | PHE  | 3.3  |
| 2   | F     | 203 | LEU  | 3.2  |
| 2   | F     | 311 | ASP  | 3.2  |
| 2   | G     | 190 | VAL  | 3.2  |
| 2   | C     | 333 | ARG  | 3.2  |
| 2   | F     | 352 | SER  | 3.2  |
| 2   | B     | 252 | CYS  | 3.2  |
| 1   | H     | 683 | VAL  | 3.2  |
| 2   | G     | 368 | PHE  | 3.2  |
| 2   | G     | 272 | PRO  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 259 | TYR  | 3.1  |
| 2   | C     | 251 | THR  | 3.1  |
| 2   | C     | 240 | LEU  | 3.1  |
| 2   | C     | 368 | PHE  | 3.1  |
| 2   | G     | 314 | GLY  | 3.1  |
| 2   | F     | 277 | PRO  | 3.1  |
| 2   | G     | 271 | ARG  | 3.1  |
| 2   | B     | 371 | LEU  | 3.1  |
| 2   | G     | 195 | LEU  | 3.0  |
| 2   | B     | 179 | PHE  | 3.0  |
| 1   | H     | 748 | PHE  | 3.0  |
| 2   | B     | 277 | PRO  | 3.0  |
| 2   | B     | 365 | LYS  | 3.0  |
| 2   | F     | 274 | PRO  | 2.9  |
| 1   | A     | 805 | VAL  | 2.9  |
| 2   | G     | 198 | ASP  | 2.9  |
| 2   | G     | 283 | MET  | 2.9  |
| 1   | H     | 636 | PHE  | 2.9  |
| 2   | C     | 367 | CYS  | 2.9  |
| 2   | G     | 338 | VAL  | 2.9  |
| 2   | F     | 209 | LEU  | 2.8  |
| 2   | C     | 288 | LEU  | 2.8  |
| 2   | G     | 276 | SER  | 2.8  |
| 2   | B     | 330 | ILE  | 2.8  |
| 2   | B     | 363 | LEU  | 2.8  |
| 2   | F     | 369 | LEU  | 2.8  |
| 2   | G     | 179 | PHE  | 2.8  |
| 1   | H     | 631 | ARG  | 2.8  |
| 2   | B     | 331 | ARG  | 2.8  |
| 1   | D     | 741 | GLU  | 2.8  |
| 2   | C     | 378 | PHE  | 2.8  |
| 2   | F     | 216 | GLY  | 2.7  |
| 2   | C     | 179 | PHE  | 2.7  |
| 2   | G     | 304 | MET  | 2.7  |
| 2   | C     | 209 | LEU  | 2.7  |
| 2   | G     | 369 | LEU  | 2.7  |
| 2   | G     | 365 | LYS  | 2.7  |
| 2   | B     | 368 | PHE  | 2.7  |
| 2   | C     | 363 | LEU  | 2.6  |
| 2   | F     | 347 | ALA  | 2.6  |
| 1   | H     | 789 | TYR  | 2.6  |
| 1   | D     | 739 | PRO  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 207 | GLY  | 2.6  |
| 2   | B     | 338 | VAL  | 2.6  |
| 2   | C     | 203 | LEU  | 2.6  |
| 2   | F     | 285 | VAL  | 2.5  |
| 2   | C     | 345 | LEU  | 2.5  |
| 2   | C     | 252 | CYS  | 2.5  |
| 1   | H     | 802 | ALA  | 2.5  |
| 2   | G     | 352 | SER  | 2.5  |
| 2   | G     | 181 | THR  | 2.5  |
| 2   | B     | 185 | TRP  | 2.5  |
| 2   | B     | 316 | SER  | 2.5  |
| 1   | H     | 646 | LEU  | 2.5  |
| 1   | H     | 649 | LEU  | 2.5  |
| 2   | F     | 290 | LEU  | 2.5  |
| 2   | G     | 351 | GLN  | 2.5  |
| 2   | F     | 275 | GLY  | 2.5  |
| 1   | H     | 746 | PRO  | 2.4  |
| 1   | H     | 750 | LEU  | 2.4  |
| 1   | E     | 844 | PHE  | 2.4  |
| 2   | B     | 347 | ALA  | 2.4  |
| 2   | G     | 345 | LEU  | 2.4  |
| 2   | F     | 338 | VAL  | 2.3  |
| 1   | H     | 757 | MET  | 2.3  |
| 2   | B     | 281 | PHE  | 2.3  |
| 2   | C     | 362 | LYS  | 2.3  |
| 1   | E     | 878 | ARG  | 2.3  |
| 2   | G     | 221 | VAL  | 2.3  |
| 2   | G     | 204 | THR  | 2.3  |
| 1   | D     | 852 | GLU  | 2.3  |
| 2   | G     | 242 | TYR  | 2.3  |
| 2   | G     | 333 | ARG  | 2.3  |
| 2   | B     | 333 | ARG  | 2.3  |
| 2   | B     | 239 | ASP  | 2.3  |
| 1   | H     | 791 | TRP  | 2.3  |
| 2   | B     | 256 | PRO  | 2.2  |
| 2   | B     | 206 | LEU  | 2.2  |
| 2   | F     | 288 | LEU  | 2.2  |
| 2   | C     | 283 | MET  | 2.2  |
| 2   | F     | 287 | ASN  | 2.2  |
| 2   | B     | 313 | HIS  | 2.2  |
| 2   | G     | 301 | PHE  | 2.2  |
| 2   | C     | 371 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 337 | LEU  | 2.2  |
| 2   | B     | 311 | ASP  | 2.1  |
| 1   | A     | 854 | ILE  | 2.1  |
| 2   | B     | 288 | LEU  | 2.1  |
| 2   | C     | 337 | LEU  | 2.1  |
| 2   | G     | 223 | ASP  | 2.1  |
| 2   | G     | 253 | ASP  | 2.1  |
| 2   | B     | 283 | MET  | 2.1  |
| 1   | H     | 741 | GLU  | 2.1  |
| 1   | H     | 758 | GLY  | 2.1  |
| 1   | A     | 811 | LEU  | 2.1  |
| 2   | B     | 276 | SER  | 2.1  |
| 2   | F     | 245 | THR  | 2.1  |
| 1   | H     | 874 | SER  | 2.0  |
| 2   | C     | 199 | ILE  | 2.0  |
| 1   | E     | 857 | CYS  | 2.0  |
| 2   | G     | 332 | SER  | 2.0  |
| 2   | F     | 200 | LYS  | 2.0  |
| 1   | D     | 697 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3   | SAH  | A     | 1   | 26/26 | 0.94 | 0.23 | 0.05  | 38,67,84,95                | 0     |
| 3   | SAH  | D     | 4   | 26/26 | 0.91 | 0.20 | -0.32 | 40,59,71,73                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 3   | SAH  | E     | 5   | 26/26 | 0.96 | 0.19 | -0.54 | 31,56,66,69                 | 0     |
| 3   | SAH  | H     | 8   | 26/26 | 0.90 | 0.18 | -0.59 | 49,104,112,114              | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.