



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID : 1SUI  
Title : Alfalfa caffeoyl coenzyme A 3-O-methyltransferase  
Authors : Ferrer, J.-L.; Zubieta, C.; Dixon, R.A.; Noel, J.P.  
Deposited on : 2004-03-26  
Resolution : 2.70 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

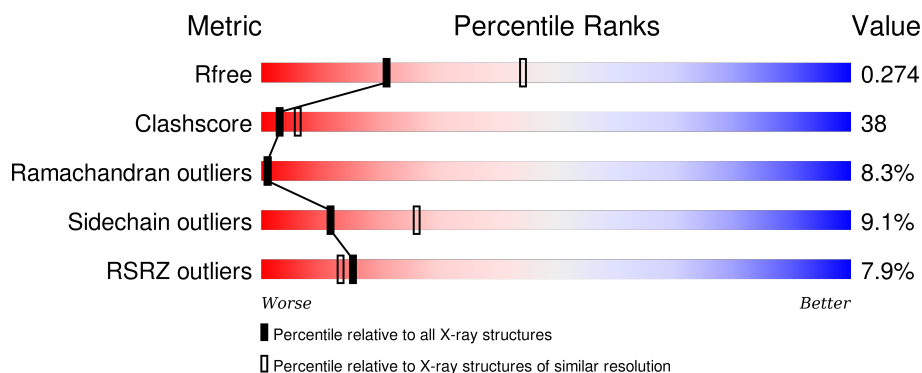
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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                       | 2103 (2.70-2.70)                                      |
| Clashscore            | 102246                      | 2422 (2.70-2.70)                                      |
| Ramachandran outliers | 100387                      | 2382 (2.70-2.70)                                      |
| Sidechain outliers    | 100360                      | 2382 (2.70-2.70)                                      |
| RSRZ outliers         | 91569                       | 2107 (2.70-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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     | 247    | <div> <div>2%</div> <div>48% 35% 9% 8%</div> </div>   |
| 1   | B     | 247    | <div> <div>4%</div> <div>47% 38% 6% 8%</div> </div>   |
| 1   | C     | 247    | <div> <div>8%</div> <div>35% 45% 12% 8%</div> </div>  |
| 1   | D     | 247    | <div> <div>16%</div> <div>25% 56% 10% 8%</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | SAH  | B     | 302 | -         | -        | -       | X                |
| 3   | SAH  | C     | 303 | -         | -        | -       | X                |
| 4   | FRE  | A     | 306 | X         | -        | -       | X                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7446 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 Caffeoyle-CoA O-methyltransferase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1807  | 1162 | 301 | 335 | 9 |         |         |       |
| 1   | B     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1807  | 1162 | 301 | 335 | 9 |         |         |       |
| 1   | C     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1807  | 1162 | 301 | 335 | 9 |         |         |       |
| 1   | D     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1789  | 1150 | 295 | 335 | 9 |         |         |       |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

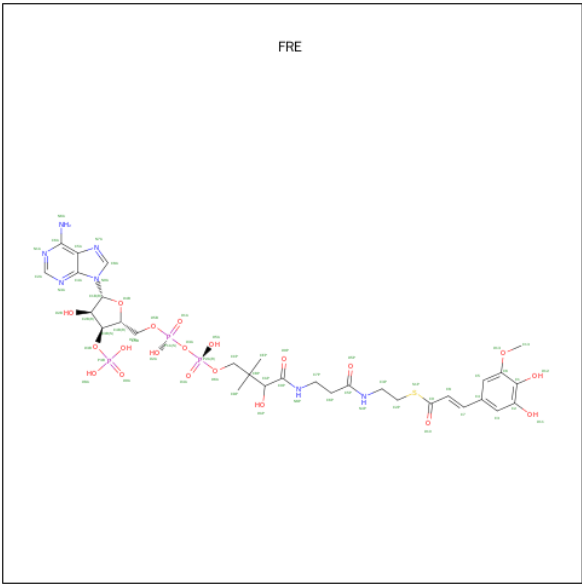
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | D     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 26    | 14 | 6 | 5 | 1 |         |         |
| 3   | B     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 26    | 14 | 6 | 5 | 1 |         |         |
| 3   | C     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 26    | 14 | 6 | 5 | 1 |         |         |
| 3   | D     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 26    | 14 | 6 | 5 | 1 |         |         |

- Molecule 4 is FERULOYL COENZYME A (three-letter code: FRE) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>7</sub>O<sub>20</sub>P<sub>3</sub>S).



| Mol | Chain | Residues | Atoms |    |   |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O  | P | S | 1       | 0       |
|     |       |          | 62    | 31 | 7 | 20 | 3 | 1 |         |         |

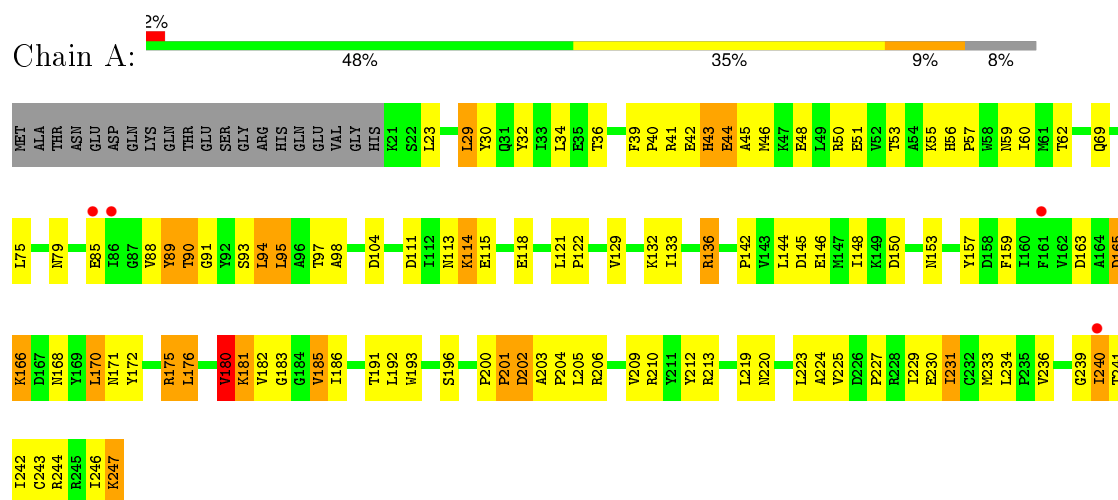
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 5   | B     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 5   | C     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 5   | D     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |

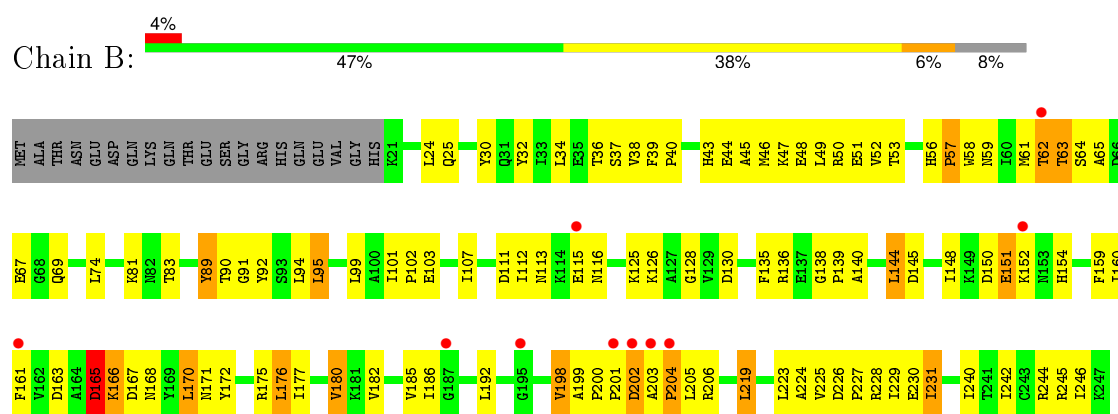
### 3 Residue-property plots

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

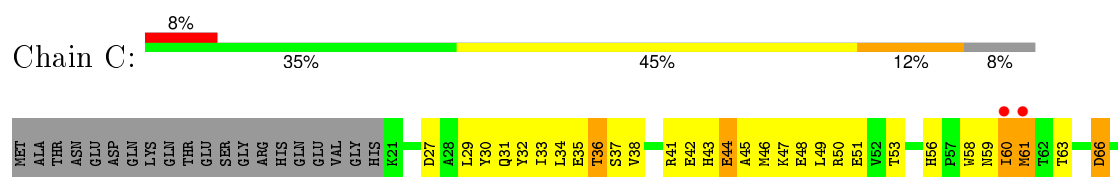
#### • Molecule 1: Caffeoyl-CoA O-methyltransferase

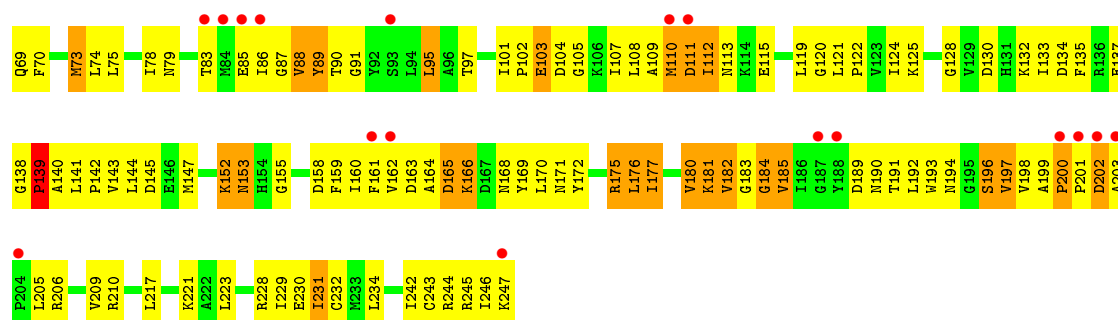


#### • Molecule 1: Caffeoyl-CoA O-methyltransferase

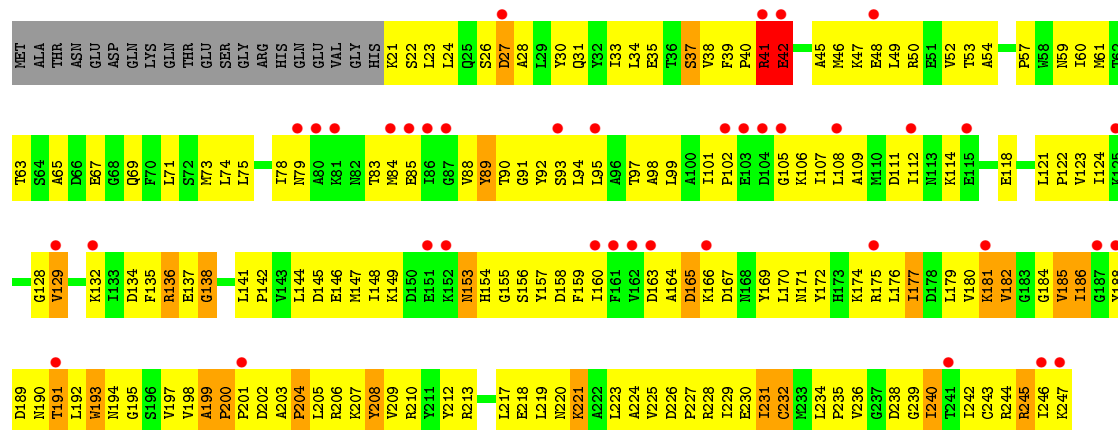


#### • Molecule 1: Caffeoyl-CoA O-methyltransferase





• Molecule 1: Caffeoyl-CoA O-methyltransferase





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 60.85Å 136.49Å 332.78Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 25.00 – 2.70<br>25.08 – 2.67                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (25.00-2.70)<br>87.8 (25.08-2.67)           | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.06  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.13 (at 2.68Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.235 , 0.285<br>0.229 , 0.274                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1761 reflections (5.07%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 78.4  | Xtriage          |
| Anisotropy  | 0.327   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 54.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 0 of 34905 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 7446  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 81.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: CA, SAH, FRE

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     | 0.46         | 0/1844      | 0.73        | 1/2496 (0.0%) |
| 1   | B     | 0.45         | 0/1844      | 0.71        | 1/2496 (0.0%) |
| 1   | C     | 0.37         | 0/1844      | 0.66        | 0/2496        |
| 1   | D     | 0.30         | 0/1824      | 0.57        | 0/2472        |
| All | All   | 0.40         | 0/7356      | 0.67        | 2/9960 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 64  | SER  | N-CA-C  | -5.83 | 95.27       | 111.00   |
| 1   | A     | 180 | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |

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     | 1807  | 0        | 1831     | 106     | 0            |
| 1   | B     | 1807  | 0        | 1831     | 90      | 0            |
| 1   | C     | 1807  | 0        | 1831     | 166     | 0            |
| 1   | D     | 1789  | 0        | 1799     | 215     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 26    | 0        | 19       | 3       | 0            |
| 3   | B     | 26    | 0        | 19       | 2       | 0            |
| 3   | C     | 26    | 0        | 19       | 6       | 0            |
| 3   | D     | 26    | 0        | 19       | 4       | 0            |
| 4   | A     | 62    | 0        | 38       | 6       | 0            |
| 5   | A     | 19    | 0        | 0        | 0       | 0            |
| 5   | B     | 31    | 0        | 0        | 0       | 0            |
| 5   | C     | 11    | 0        | 0        | 0       | 0            |
| 5   | D     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 7446  | 0        | 7406     | 566     | 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 38.

All (566) 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) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:306:FRE:O9P  | 4:A:306:FRE:H62  | 1.45                     | 1.12              |
| 1:D:185:VAL:HG13 | 1:D:186:ILE:H    | 1.12                     | 1.11              |
| 1:C:182:VAL:HG13 | 1:C:183:GLY:H    | 1.24                     | 1.03              |
| 1:B:165:ASP:O    | 1:B:166:LYS:HB2  | 1.64                     | 0.97              |
| 1:B:53:THR:OG1   | 1:B:90:THR:HG21  | 1.65                     | 0.97              |
| 1:C:141:LEU:H    | 1:C:141:LEU:HD12 | 1.30                     | 0.97              |
| 1:A:165:ASP:O    | 1:A:166:LYS:HB2  | 1.62                     | 0.95              |
| 1:C:185:VAL:HA   | 1:C:243:CYS:O    | 1.69                     | 0.91              |
| 1:C:60:ILE:HG13  | 1:C:61:MET:HG3   | 1.52                     | 0.91              |
| 4:A:306:FRE:C6P  | 4:A:306:FRE:O9P  | 2.20                     | 0.90              |
| 1:D:38:VAL:HG23  | 1:D:39:PHE:H     | 1.37                     | 0.90              |
| 1:A:180:VAL:HG21 | 1:A:186:ILE:HD11 | 1.55                     | 0.87              |
| 1:D:185:VAL:HG13 | 1:D:186:ILE:N    | 1.89                     | 0.86              |
| 1:D:21:LYS:HG2   | 1:D:22:SER:H     | 1.37                     | 0.86              |
| 1:D:199:ALA:HB3  | 1:D:203:ALA:HB2  | 1.57                     | 0.86              |
| 1:D:182:VAL:H    | 1:D:245:ARG:HH11 | 1.22                     | 0.86              |
| 1:D:141:LEU:HD21 | 1:D:175:ARG:HH21 | 1.40                     | 0.85              |
| 1:C:143:VAL:O    | 1:C:147:MET:HG3  | 1.75                     | 0.84              |
| 1:C:60:ILE:HG23  | 1:C:61:MET:HE2   | 1.59                     | 0.84              |
| 1:D:146:GLU:HG3  | 1:D:147:MET:HG3  | 1.60                     | 0.84              |
| 1:C:46:MET:HE1   | 1:C:95:LEU:HB3   | 1.59                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:42:GLU:HG3   | 1:A:42:GLU:O     | 1.77                     | 0.83              |
| 1:B:67:GLU:HG2   | 1:B:240:ILE:HD11 | 1.60                     | 0.83              |
| 1:A:180:VAL:CG2  | 1:A:186:ILE:HD11 | 2.10                     | 0.82              |
| 1:C:95:LEU:HG    | 1:C:124:ILE:HG12 | 1.61                     | 0.81              |
| 1:A:136:ARG:HG2  | 1:A:136:ARG:HH11 | 1.45                     | 0.81              |
| 1:C:177:ILE:HD13 | 1:C:177:ILE:O    | 1.81                     | 0.79              |
| 1:C:87:GLY:HA2   | 3:C:303:SAH:H2   | 1.65                     | 0.79              |
| 1:A:55:LYS:O     | 1:A:55:LYS:HD3   | 1.83                     | 0.78              |
| 1:D:129:VAL:HG22 | 1:D:132:LYS:HD2  | 1.66                     | 0.78              |
| 1:B:198:VAL:HG11 | 1:B:205:LEU:HD11 | 1.65                     | 0.77              |
| 1:C:86:ILE:HG12  | 1:C:110:MET:HG2  | 1.64                     | 0.77              |
| 1:C:181:LYS:HG3  | 1:C:182:VAL:H    | 1.49                     | 0.77              |
| 1:C:110:MET:HG3  | 1:C:111:ASP:OD1  | 1.84                     | 0.77              |
| 1:C:43:HIS:HD2   | 1:C:46:MET:HG3   | 1.50                     | 0.77              |
| 1:A:163:ASP:OD1  | 4:A:306:FRE:C13  | 2.33                     | 0.76              |
| 1:A:46:MET:SD    | 1:A:95:LEU:HD13  | 2.25                     | 0.76              |
| 1:D:46:MET:SD    | 1:D:95:LEU:HD22  | 2.25                     | 0.76              |
| 1:D:185:VAL:CG1  | 1:D:186:ILE:H    | 1.93                     | 0.76              |
| 1:D:205:LEU:CD1  | 1:D:213:ARG:HH21 | 1.98                     | 0.76              |
| 1:C:130:ASP:HA   | 1:C:133:ILE:HD13 | 1.66                     | 0.76              |
| 1:A:30:TYR:CE2   | 1:A:34:LEU:HD11  | 2.20                     | 0.76              |
| 1:A:53:THR:OG1   | 1:A:90:THR:HG21  | 1.86                     | 0.76              |
| 1:C:32:TYR:O     | 1:C:36:THR:HG23  | 1.86                     | 0.75              |
| 1:C:58:TRP:C     | 1:C:60:ILE:H     | 1.89                     | 0.75              |
| 1:C:43:HIS:CD2   | 1:C:46:MET:HG3   | 2.22                     | 0.74              |
| 1:D:181:LYS:HD2  | 1:D:245:ARG:HH12 | 1.50                     | 0.74              |
| 1:C:141:LEU:HB2  | 1:C:142:PRO:HD3  | 1.69                     | 0.74              |
| 1:A:163:ASP:OD1  | 4:A:306:FRE:H131 | 1.88                     | 0.74              |
| 1:C:198:VAL:HG12 | 1:C:199:ALA:H    | 1.52                     | 0.73              |
| 1:C:165:ASP:O    | 1:C:166:LYS:HB2  | 1.88                     | 0.73              |
| 1:D:159:PHE:HD1  | 1:D:185:VAL:HG21 | 1.54                     | 0.73              |
| 1:C:205:LEU:H    | 1:C:205:LEU:HD23 | 1.54                     | 0.72              |
| 1:D:160:ILE:HD13 | 1:D:176:LEU:HD11 | 1.71                     | 0.72              |
| 1:D:166:LYS:HB2  | 1:D:212:TYR:CD1  | 2.24                     | 0.72              |
| 1:B:230:GLU:O    | 1:B:231:ILE:HG12 | 1.91                     | 0.71              |
| 1:A:231:ILE:HD11 | 1:C:41:ARG:HD3   | 1.72                     | 0.71              |
| 1:C:31:GLN:O     | 1:C:35:GLU:HG2   | 1.91                     | 0.71              |
| 1:B:200:PRO:N    | 1:B:201:PRO:HD2  | 2.06                     | 0.71              |
| 1:D:38:VAL:HG23  | 1:D:39:PHE:N     | 2.04                     | 0.70              |
| 1:D:141:LEU:HD21 | 1:D:175:ARG:NH2  | 2.04                     | 0.70              |
| 1:A:191:THR:HG21 | 1:A:241:THR:OG1  | 1.91                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:37:SER:O     | 1:B:69:GLN:NE2   | 2.24                     | 0.70              |
| 1:D:135:PHE:O    | 1:D:136:ARG:HD2  | 1.91                     | 0.70              |
| 1:C:53:THR:OG1   | 1:C:90:THR:HG21  | 1.91                     | 0.70              |
| 1:A:43:HIS:O     | 1:A:44:GLU:HB3   | 1.92                     | 0.70              |
| 1:D:192:LEU:HB2  | 1:D:238:ASP:O    | 1.91                     | 0.70              |
| 1:B:145:ASP:O    | 1:B:148:ILE:HG22 | 1.92                     | 0.70              |
| 1:C:88:VAL:O     | 1:C:89:TYR:HB3   | 1.92                     | 0.70              |
| 1:C:44:GLU:OE1   | 1:C:44:GLU:N     | 2.24                     | 0.69              |
| 1:C:133:ILE:N    | 1:C:133:ILE:HD12 | 2.06                     | 0.69              |
| 1:A:225:VAL:HG12 | 1:A:225:VAL:O    | 1.93                     | 0.69              |
| 1:C:182:VAL:HG13 | 1:C:183:GLY:N    | 2.03                     | 0.69              |
| 1:B:34:LEU:HD22  | 1:B:65:ALA:HB3   | 1.75                     | 0.69              |
| 1:C:152:LYS:O    | 1:C:152:LYS:HE3  | 1.92                     | 0.69              |
| 1:D:231:ILE:HA   | 1:D:242:ILE:O    | 1.92                     | 0.69              |
| 1:A:172:TYR:HB3  | 1:A:176:LEU:HD22 | 1.74                     | 0.69              |
| 1:D:47:LYS:HD3   | 1:D:50:ARG:HH21  | 1.58                     | 0.68              |
| 1:A:142:PRO:O    | 1:A:146:GLU:HG3  | 1.93                     | 0.68              |
| 1:C:120:GLY:C    | 1:C:122:PRO:HD2  | 2.13                     | 0.68              |
| 1:C:200:PRO:O    | 1:C:202:ASP:N    | 2.25                     | 0.68              |
| 1:C:198:VAL:HG12 | 1:C:199:ALA:N    | 2.07                     | 0.68              |
| 1:D:177:ILE:O    | 1:D:177:ILE:HD13 | 1.92                     | 0.68              |
| 1:D:31:GLN:O     | 1:D:35:GLU:HG2   | 1.92                     | 0.68              |
| 1:B:30:TYR:CE1   | 1:B:34:LEU:HD11  | 2.29                     | 0.68              |
| 1:D:181:LYS:HA   | 1:D:245:ARG:NH1  | 2.09                     | 0.68              |
| 1:B:230:GLU:HG3  | 1:B:244:ARG:NH2  | 2.09                     | 0.68              |
| 1:C:60:ILE:HG23  | 1:C:61:MET:H     | 1.57                     | 0.68              |
| 1:D:21:LYS:CG    | 1:D:22:SER:H     | 2.06                     | 0.68              |
| 1:D:141:LEU:HB3  | 1:D:142:PRO:HD3  | 1.75                     | 0.68              |
| 1:D:193:TRP:HE1  | 1:D:209:VAL:HA   | 1.59                     | 0.67              |
| 1:D:159:PHE:HA   | 1:D:185:VAL:HG11 | 1.76                     | 0.67              |
| 1:C:121:LEU:N    | 1:C:122:PRO:HD2  | 2.08                     | 0.67              |
| 1:A:136:ARG:HG2  | 1:A:136:ARG:NH1  | 2.09                     | 0.67              |
| 1:B:170:LEU:HD22 | 1:B:219:LEU:HD23 | 1.75                     | 0.67              |
| 1:D:170:LEU:HD12 | 1:D:218:GLU:HG2  | 1.77                     | 0.66              |
| 1:D:159:PHE:CD1  | 1:D:185:VAL:HG21 | 2.31                     | 0.66              |
| 1:C:228:ARG:HH21 | 1:C:245:ARG:HH21 | 1.42                     | 0.66              |
| 1:D:205:LEU:H    | 1:D:205:LEU:HD23 | 1.61                     | 0.65              |
| 1:C:47:LYS:O     | 1:C:51:GLU:HG3   | 1.97                     | 0.65              |
| 1:D:27:ASP:O     | 1:D:31:GLN:HB2   | 1.97                     | 0.65              |
| 1:A:231:ILE:HA   | 1:A:242:ILE:O    | 1.97                     | 0.65              |
| 1:D:229:ILE:HA   | 1:D:244:ARG:O    | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:163:ASP:OD2  | 3:B:302:SAH:HG1  | 1.97                     | 0.65              |
| 1:C:163:ASP:OD2  | 3:C:303:SAH:HG2  | 1.97                     | 0.64              |
| 1:C:60:ILE:CG2   | 1:C:61:MET:HE2   | 2.28                     | 0.64              |
| 1:C:103:GLU:HA   | 1:C:132:LYS:HE2  | 1.78                     | 0.64              |
| 1:B:32:TYR:O     | 1:B:36:THR:HG23  | 1.97                     | 0.64              |
| 1:D:146:GLU:HG3  | 1:D:147:MET:N    | 2.13                     | 0.64              |
| 1:C:203:ALA:O    | 1:C:205:LEU:HD23 | 1.97                     | 0.64              |
| 1:A:113:ASN:O    | 1:A:114:LYS:HB3  | 1.98                     | 0.64              |
| 1:B:176:LEU:O    | 1:B:180:VAL:HG22 | 1.98                     | 0.64              |
| 1:D:159:PHE:HA   | 1:D:185:VAL:HG21 | 1.80                     | 0.64              |
| 1:D:205:LEU:HD11 | 1:D:213:ARG:HH21 | 1.62                     | 0.64              |
| 1:C:231:ILE:HA   | 1:C:242:ILE:O    | 1.98                     | 0.64              |
| 1:B:230:GLU:HG3  | 1:B:244:ARG:CZ   | 2.27                     | 0.63              |
| 1:B:199:ALA:O    | 1:B:202:ASP:HB3  | 1.98                     | 0.63              |
| 1:A:233:MET:CE   | 1:C:37:SER:HB2   | 2.27                     | 0.63              |
| 1:B:151:GLU:HA   | 1:B:154:HIS:CD2  | 2.33                     | 0.63              |
| 1:C:115:GLU:OE1  | 1:C:115:GLU:HA   | 1.98                     | 0.63              |
| 1:D:38:VAL:HG23  | 1:D:39:PHE:HD1   | 1.64                     | 0.63              |
| 1:D:202:ASP:O    | 1:D:204:PRO:HD3  | 1.99                     | 0.63              |
| 1:C:73:MET:HA    | 1:C:73:MET:HE3   | 1.80                     | 0.63              |
| 1:D:200:PRO:C    | 1:D:202:ASP:H    | 2.00                     | 0.62              |
| 1:C:125:LYS:HA   | 1:C:130:ASP:OD1  | 1.98                     | 0.62              |
| 1:A:43:HIS:O     | 1:A:44:GLU:CB    | 2.48                     | 0.62              |
| 1:B:160:ILE:HD12 | 1:B:180:VAL:HG13 | 1.82                     | 0.62              |
| 1:C:44:GLU:O     | 1:C:45:ALA:HB3   | 1.99                     | 0.62              |
| 1:A:185:VAL:HA   | 1:A:243:CYS:O    | 1.98                     | 0.62              |
| 1:A:129:VAL:HG23 | 1:A:132:LYS:HE3  | 1.82                     | 0.62              |
| 1:D:184:GLY:O    | 1:D:185:VAL:HB   | 2.00                     | 0.61              |
| 1:C:34:LEU:HD23  | 1:C:38:VAL:HG21  | 1.80                     | 0.61              |
| 1:A:163:ASP:OD2  | 3:A:301:SAH:HB1  | 2.00                     | 0.61              |
| 1:A:42:GLU:OE2   | 1:A:50:ARG:NH2   | 2.33                     | 0.61              |
| 1:C:60:ILE:HG23  | 1:C:61:MET:CE    | 2.29                     | 0.61              |
| 1:B:170:LEU:CD2  | 1:B:219:LEU:HA   | 2.31                     | 0.61              |
| 1:D:33:ILE:O     | 1:D:37:SER:HB3   | 2.00                     | 0.61              |
| 1:A:85:GLU:OE2   | 1:A:93:SER:HB2   | 2.00                     | 0.61              |
| 1:D:123:VAL:O    | 1:D:123:VAL:HG12 | 2.01                     | 0.61              |
| 1:C:172:TYR:O    | 1:C:176:LEU:HB2  | 2.01                     | 0.60              |
| 1:C:141:LEU:CD1  | 1:C:141:LEU:H    | 2.08                     | 0.60              |
| 1:C:139:PRO:HB3  | 1:C:141:LEU:HD13 | 1.82                     | 0.60              |
| 1:D:49:LEU:HD11  | 1:D:90:THR:HG23  | 1.84                     | 0.60              |
| 1:D:141:LEU:HD11 | 1:D:175:ARG:HH21 | 1.67                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:95:LEU:HD23  | 1:D:95:LEU:O     | 2.01                     | 0.60              |
| 1:C:172:TYR:HB3  | 1:C:176:LEU:HD22 | 1.83                     | 0.59              |
| 1:B:203:ALA:N    | 1:B:204:PRO:CD   | 2.66                     | 0.59              |
| 1:D:197:VAL:O    | 1:D:197:VAL:HG13 | 2.03                     | 0.59              |
| 1:A:236:VAL:HG23 | 1:A:240:ILE:HD11 | 1.82                     | 0.59              |
| 1:C:209:VAL:HG23 | 1:C:210:ARG:N    | 2.18                     | 0.59              |
| 1:A:163:ASP:OD1  | 4:A:306:FRE:H133 | 2.02                     | 0.59              |
| 1:D:200:PRO:O    | 1:D:202:ASP:N    | 2.35                     | 0.59              |
| 1:C:196:SER:O    | 1:C:198:VAL:HG23 | 2.03                     | 0.59              |
| 1:D:159:PHE:HD1  | 1:D:185:VAL:CG2  | 2.16                     | 0.58              |
| 1:D:200:PRO:C    | 1:D:202:ASP:N    | 2.56                     | 0.58              |
| 1:A:191:THR:HG23 | 1:A:220:ASN:OD1  | 2.03                     | 0.58              |
| 1:B:160:ILE:HG21 | 1:B:176:LEU:HG   | 1.85                     | 0.58              |
| 1:B:50:ARG:HG2   | 1:B:63:THR:HG21  | 1.83                     | 0.58              |
| 1:D:205:LEU:HD13 | 1:D:213:ARG:HH21 | 1.68                     | 0.58              |
| 1:D:232:CYS:HB3  | 1:D:242:ILE:HG13 | 1.86                     | 0.58              |
| 1:D:141:LEU:CD2  | 1:D:175:ARG:HH21 | 2.14                     | 0.58              |
| 1:C:56:HIS:HE1   | 1:C:58:TRP:HB2   | 1.68                     | 0.58              |
| 1:D:34:LEU:HA    | 1:D:38:VAL:HG22  | 1.84                     | 0.58              |
| 1:C:144:LEU:HD21 | 1:C:176:LEU:HD13 | 1.85                     | 0.58              |
| 1:B:227:PRO:O    | 1:B:246:ILE:HD11 | 2.03                     | 0.58              |
| 1:C:206:ARG:O    | 1:C:209:VAL:HG22 | 2.03                     | 0.58              |
| 1:D:63:THR:HG21  | 1:D:93:SER:HB3   | 1.85                     | 0.57              |
| 1:A:42:GLU:CD    | 1:A:50:ARG:HH22  | 2.07                     | 0.57              |
| 1:A:88:VAL:O     | 1:A:89:TYR:O     | 2.22                     | 0.57              |
| 1:C:112:ILE:HG12 | 1:C:113:ASN:N    | 2.19                     | 0.57              |
| 1:C:56:HIS:CE1   | 1:C:58:TRP:HB2   | 2.39                     | 0.57              |
| 1:D:71:LEU:O     | 1:D:75:LEU:HD13  | 2.05                     | 0.57              |
| 1:D:42:GLU:OE2   | 1:D:47:LYS:HE3   | 2.04                     | 0.57              |
| 1:D:141:LEU:HD11 | 1:D:175:ARG:NH2  | 2.20                     | 0.57              |
| 1:D:180:VAL:HG23 | 1:D:181:LYS:N    | 2.20                     | 0.57              |
| 1:C:75:LEU:HD21  | 1:C:159:PHE:CD2  | 2.40                     | 0.57              |
| 1:B:53:THR:HG21  | 1:B:62:THR:HG21  | 1.86                     | 0.57              |
| 1:D:128:GLY:O    | 1:D:129:VAL:HG12 | 2.05                     | 0.57              |
| 1:C:189:ASP:OD1  | 1:C:190:ASN:N    | 2.38                     | 0.57              |
| 1:A:163:ASP:O    | 3:A:301:SAH:H5'1 | 2.06                     | 0.56              |
| 1:B:165:ASP:OD1  | 1:B:168:ASN:HB2  | 2.04                     | 0.56              |
| 1:C:166:LYS:HD3  | 1:C:169:TYR:CE2  | 2.40                     | 0.56              |
| 1:B:39:PHE:N     | 1:B:40:PRO:HD2   | 2.20                     | 0.56              |
| 1:C:61:MET:HE3   | 1:C:61:MET:O     | 2.04                     | 0.56              |
| 1:A:39:PHE:HB2   | 1:A:40:PRO:HD3   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:94:LEU:HD13  | 1:A:133:ILE:HD13 | 1.88                     | 0.56              |
| 1:C:58:TRP:C     | 1:C:60:ILE:N     | 2.58                     | 0.56              |
| 1:C:58:TRP:O     | 1:C:60:ILE:N     | 2.39                     | 0.56              |
| 1:D:28:ALA:HA    | 1:D:31:GLN:HB3   | 1.87                     | 0.56              |
| 1:D:246:ILE:HG13 | 1:D:247:LYS:N    | 2.20                     | 0.56              |
| 1:B:101:ILE:HB   | 1:B:102:PRO:HD2  | 1.88                     | 0.56              |
| 1:D:155:GLY:C    | 1:D:157:TYR:H    | 2.10                     | 0.56              |
| 1:B:231:ILE:HA   | 1:B:242:ILE:O    | 2.06                     | 0.56              |
| 1:D:114:LYS:HG3  | 1:D:135:PHE:HE2  | 1.71                     | 0.56              |
| 1:A:42:GLU:O     | 1:A:44:GLU:N     | 2.39                     | 0.56              |
| 1:A:196:SER:O    | 1:A:213:ARG:HD2  | 2.05                     | 0.56              |
| 1:D:198:VAL:HG22 | 1:D:199:ALA:H    | 1.72                     | 0.55              |
| 1:D:74:LEU:O     | 1:D:78:ILE:HG12  | 2.06                     | 0.55              |
| 1:D:184:GLY:HA2  | 1:D:245:ARG:HB2  | 1.88                     | 0.55              |
| 1:D:38:VAL:HG12  | 1:D:69:GLN:NE2   | 2.21                     | 0.55              |
| 1:B:49:LEU:HD23  | 1:B:92:TYR:HA    | 1.87                     | 0.55              |
| 1:C:229:ILE:HA   | 1:C:244:ARG:O    | 2.07                     | 0.55              |
| 1:A:233:MET:HE3  | 1:C:37:SER:HB2   | 1.89                     | 0.55              |
| 1:C:155:GLY:O    | 1:C:181:LYS:HD2  | 2.06                     | 0.55              |
| 1:D:94:LEU:HD21  | 1:D:107:ILE:HG21 | 1.87                     | 0.55              |
| 1:D:141:LEU:HD21 | 1:D:175:ARG:HE   | 1.72                     | 0.55              |
| 1:D:165:ASP:OD1  | 1:D:166:LYS:N    | 2.40                     | 0.55              |
| 1:C:101:ILE:HB   | 1:C:102:PRO:HD2  | 1.89                     | 0.55              |
| 1:D:98:ALA:O     | 1:D:129:VAL:HG21 | 2.06                     | 0.55              |
| 1:C:166:LYS:HE3  | 1:C:193:TRP:HZ3  | 1.71                     | 0.55              |
| 1:A:150:ASP:HB3  | 1:A:153:ASN:ND2  | 2.22                     | 0.55              |
| 1:C:183:GLY:O    | 1:C:185:VAL:N    | 2.39                     | 0.54              |
| 1:C:109:ALA:O    | 1:C:110:MET:C    | 2.46                     | 0.54              |
| 1:C:166:LYS:HE3  | 1:C:193:TRP:CZ3  | 2.42                     | 0.54              |
| 1:D:39:PHE:HB2   | 1:D:40:PRO:HD3   | 1.89                     | 0.54              |
| 1:D:198:VAL:HG22 | 1:D:199:ALA:N    | 2.23                     | 0.54              |
| 1:D:231:ILE:HA   | 1:D:243:CYS:HA   | 1.87                     | 0.54              |
| 1:A:44:GLU:HG3   | 1:A:45:ALA:N     | 2.21                     | 0.54              |
| 1:C:232:CYS:SG   | 1:C:234:LEU:HD21 | 2.48                     | 0.54              |
| 1:C:209:VAL:CG2  | 1:C:210:ARG:N    | 2.71                     | 0.54              |
| 1:D:47:LYS:HD3   | 1:D:50:ARG:NH2   | 2.22                     | 0.54              |
| 1:B:180:VAL:HG11 | 1:B:186:ILE:CG1  | 2.37                     | 0.54              |
| 1:D:101:ILE:CD1  | 1:D:132:LYS:HD3  | 2.38                     | 0.54              |
| 1:D:45:ALA:HB1   | 1:D:95:LEU:HD11  | 1.90                     | 0.54              |
| 1:A:225:VAL:CG1  | 1:A:225:VAL:O    | 2.56                     | 0.54              |
| 1:D:38:VAL:CG2   | 1:D:39:PHE:H     | 2.17                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:228:ARG:NH2  | 1:C:245:ARG:HH21 | 2.06                     | 0.54              |
| 1:D:105:GLY:O    | 1:D:132:LYS:HG2  | 2.08                     | 0.54              |
| 1:A:23:LEU:HD13  | 1:A:192:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:101:ILE:HD11 | 1:D:132:LYS:HD3  | 1.89                     | 0.53              |
| 1:C:165:ASP:O    | 1:C:166:LYS:HE2  | 2.08                     | 0.53              |
| 1:D:229:ILE:HB   | 1:D:243:CYS:HB3  | 1.89                     | 0.53              |
| 1:D:160:ILE:O    | 1:D:186:ILE:HA   | 2.07                     | 0.53              |
| 1:C:203:ALA:HB3  | 1:C:205:LEU:HD22 | 1.90                     | 0.53              |
| 1:D:230:GLU:OE1  | 1:D:244:ARG:NH1  | 2.42                     | 0.53              |
| 1:D:24:LEU:HD12  | 1:D:30:TYR:HB2   | 1.89                     | 0.53              |
| 1:A:239:GLY:C    | 1:A:240:ILE:HD13 | 2.29                     | 0.53              |
| 1:D:182:VAL:H    | 1:D:245:ARG:NH1  | 1.99                     | 0.53              |
| 1:D:34:LEU:HB3   | 1:D:39:PHE:CE1   | 2.42                     | 0.53              |
| 1:D:165:ASP:C    | 1:D:166:LYS:HD2  | 2.28                     | 0.53              |
| 1:A:229:ILE:O    | 1:C:41:ARG:NH2   | 2.41                     | 0.53              |
| 1:C:85:GLU:O     | 1:C:110:MET:HB3  | 2.09                     | 0.53              |
| 1:A:89:TYR:O     | 1:A:91:GLY:N     | 2.36                     | 0.53              |
| 1:C:97:THR:O     | 1:C:101:ILE:HG12 | 2.08                     | 0.53              |
| 1:C:181:LYS:CG   | 1:C:182:VAL:H    | 2.17                     | 0.53              |
| 1:C:87:GLY:HA2   | 3:C:303:SAH:C2   | 2.37                     | 0.53              |
| 1:B:165:ASP:O    | 1:B:166:LYS:CB   | 2.48                     | 0.52              |
| 1:C:109:ALA:HB3  | 1:C:133:ILE:HG23 | 1.91                     | 0.52              |
| 1:B:46:MET:SD    | 1:B:95:LEU:HD13  | 2.49                     | 0.52              |
| 1:C:112:ILE:HG12 | 1:C:113:ASN:H    | 1.73                     | 0.52              |
| 1:D:105:GLY:O    | 1:D:106:LYS:HD2  | 2.10                     | 0.52              |
| 1:D:192:LEU:O    | 1:D:193:TRP:C    | 2.47                     | 0.52              |
| 1:D:224:ALA:HA   | 1:D:231:ILE:HD13 | 1.90                     | 0.52              |
| 1:B:37:SER:C     | 1:B:69:GLN:HE22  | 2.12                     | 0.52              |
| 1:C:121:LEU:N    | 1:C:122:PRO:CD   | 2.73                     | 0.52              |
| 1:D:48:GLU:OE1   | 1:D:123:VAL:HG13 | 2.09                     | 0.52              |
| 1:D:75:LEU:HD21  | 1:D:97:THR:HG23  | 1.91                     | 0.52              |
| 1:B:111:ASP:OD1  | 1:B:112:ILE:N    | 2.43                     | 0.52              |
| 1:D:144:LEU:O    | 1:D:148:ILE:HG12 | 2.10                     | 0.52              |
| 1:B:30:TYR:HE1   | 1:B:34:LEU:HD11  | 1.71                     | 0.52              |
| 1:D:144:LEU:HD12 | 1:D:147:MET:HE1  | 1.92                     | 0.52              |
| 1:D:50:ARG:NH1   | 1:D:65:ALA:HB2   | 2.24                     | 0.52              |
| 1:C:109:ALA:CB   | 1:C:133:ILE:HG23 | 2.40                     | 0.52              |
| 1:A:157:TYR:O    | 1:A:181:LYS:HD2  | 2.10                     | 0.52              |
| 1:C:110:MET:O    | 1:C:111:ASP:HB3  | 2.08                     | 0.52              |
| 1:D:188:TYR:O    | 1:D:191:THR:HG23 | 2.10                     | 0.52              |
| 1:C:49:LEU:HD22  | 1:C:95:LEU:HD12  | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:89:TYR:O     | 1:C:90:THR:HB    | 2.09                     | 0.51              |
| 1:B:202:ASP:OD1  | 1:B:204:PRO:HB2  | 2.09                     | 0.51              |
| 1:D:217:LEU:O    | 1:D:221:LYS:HB2  | 2.10                     | 0.51              |
| 1:A:230:GLU:O    | 1:A:231:ILE:HG12 | 2.08                     | 0.51              |
| 1:D:53:THR:HG22  | 1:D:53:THR:O     | 2.09                     | 0.51              |
| 1:D:184:GLY:O    | 1:D:185:VAL:CB   | 2.58                     | 0.51              |
| 1:D:129:VAL:CG2  | 1:D:132:LYS:HD2  | 2.37                     | 0.51              |
| 1:C:133:ILE:CD1  | 1:C:133:ILE:N    | 2.73                     | 0.51              |
| 1:A:53:THR:OG1   | 1:A:90:THR:CG2   | 2.56                     | 0.51              |
| 1:A:234:LEU:HD21 | 1:C:70:PHE:CD1   | 2.46                     | 0.51              |
| 1:D:154:HIS:O    | 1:D:181:LYS:HE2  | 2.11                     | 0.51              |
| 1:D:75:LEU:CD2   | 1:D:97:THR:HA    | 2.41                     | 0.51              |
| 1:B:81:LYS:HG2   | 1:B:102:PRO:HG3  | 1.93                     | 0.51              |
| 1:A:201:PRO:O    | 1:A:202:ASP:HB3  | 2.11                     | 0.51              |
| 1:A:170:LEU:HD22 | 1:A:219:LEU:HD23 | 1.92                     | 0.51              |
| 1:D:88:VAL:HG21  | 1:D:109:ALA:HB1  | 1.92                     | 0.51              |
| 1:C:29:LEU:O     | 1:C:33:ILE:HG13  | 2.10                     | 0.51              |
| 1:B:47:LYS:O     | 1:B:51:GLU:HG3   | 2.11                     | 0.51              |
| 1:A:206:ARG:HB2  | 1:A:209:VAL:HG12 | 1.93                     | 0.51              |
| 1:B:200:PRO:N    | 1:B:201:PRO:CD   | 2.74                     | 0.51              |
| 1:B:43:HIS:HD2   | 1:B:44:GLU:N     | 2.09                     | 0.51              |
| 1:C:74:LEU:HD23  | 1:C:74:LEU:O     | 2.11                     | 0.51              |
| 1:C:60:ILE:HG21  | 1:C:89:TYR:CE2   | 2.46                     | 0.51              |
| 1:D:112:ILE:HA   | 1:D:138:GLY:HA2  | 1.93                     | 0.51              |
| 1:C:49:LEU:CD2   | 1:C:95:LEU:HD12  | 2.40                     | 0.50              |
| 1:D:182:VAL:N    | 1:D:245:ARG:HH11 | 2.00                     | 0.50              |
| 1:A:182:VAL:O    | 1:A:183:GLY:C    | 2.49                     | 0.50              |
| 1:C:168:ASN:HA   | 1:C:171:ASN:HD22 | 1.77                     | 0.50              |
| 1:D:154:HIS:O    | 1:D:181:LYS:HG3  | 2.10                     | 0.50              |
| 1:D:205:LEU:HD11 | 1:D:213:ARG:NH2  | 2.25                     | 0.50              |
| 1:D:108:LEU:HD13 | 1:D:134:ASP:HB3  | 1.92                     | 0.50              |
| 1:B:62:THR:OG1   | 1:B:63:THR:N     | 2.43                     | 0.50              |
| 1:D:146:GLU:CG   | 1:D:147:MET:HG3  | 2.39                     | 0.50              |
| 1:A:98:ALA:HB1   | 1:A:129:VAL:HG22 | 1.94                     | 0.50              |
| 1:D:160:ILE:HD12 | 1:D:180:VAL:HG13 | 1.94                     | 0.50              |
| 1:A:233:MET:HE3  | 1:C:37:SER:CB    | 2.41                     | 0.50              |
| 1:B:113:ASN:OD1  | 1:B:115:GLU:HB2  | 2.12                     | 0.50              |
| 1:D:83:THR:O     | 1:D:108:LEU:HD23 | 2.12                     | 0.50              |
| 1:C:133:ILE:HG22 | 1:C:134:ASP:N    | 2.27                     | 0.50              |
| 1:A:150:ASP:HB3  | 1:A:153:ASN:HD22 | 1.76                     | 0.50              |
| 1:C:88:VAL:HG12  | 1:C:89:TYR:N     | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:144:LEU:HA   | 1:D:147:MET:HE3  | 1.94                     | 0.49              |
| 1:C:205:LEU:HD21 | 1:C:210:ARG:NH2  | 2.27                     | 0.49              |
| 1:B:43:HIS:CD2   | 1:B:45:ALA:H     | 2.30                     | 0.49              |
| 1:B:62:THR:HG21  | 1:B:89:TYR:HE2   | 1.78                     | 0.49              |
| 1:D:89:TYR:O     | 1:D:90:THR:HB    | 2.12                     | 0.49              |
| 1:D:157:TYR:O    | 1:D:180:VAL:HA   | 2.11                     | 0.49              |
| 1:C:197:VAL:HG23 | 1:C:197:VAL:O    | 2.12                     | 0.49              |
| 1:B:48:GLU:O     | 1:B:52:VAL:HG23  | 2.12                     | 0.49              |
| 1:C:181:LYS:HG3  | 1:C:182:VAL:N    | 2.22                     | 0.49              |
| 1:C:177:ILE:HD11 | 1:C:245:ARG:HG3  | 1.93                     | 0.49              |
| 1:C:70:PHE:CZ    | 1:C:234:LEU:HD12 | 2.46                     | 0.49              |
| 1:A:32:TYR:CE1   | 1:A:36:THR:HG21  | 2.47                     | 0.49              |
| 1:D:184:GLY:HA3  | 1:D:245:ARG:H    | 1.77                     | 0.49              |
| 1:B:89:TYR:O     | 1:B:90:THR:HB    | 2.12                     | 0.49              |
| 1:D:95:LEU:HD23  | 1:D:99:LEU:HG    | 1.94                     | 0.49              |
| 1:D:146:GLU:CG   | 1:D:147:MET:N    | 2.76                     | 0.48              |
| 1:C:198:VAL:CG1  | 1:C:199:ALA:N    | 2.76                     | 0.48              |
| 1:B:38:VAL:HG22  | 1:B:69:GLN:NE2   | 2.27                     | 0.48              |
| 1:D:219:LEU:HD13 | 1:D:219:LEU:C    | 2.33                     | 0.48              |
| 1:B:165:ASP:HB2  | 1:B:167:ASP:OD1  | 2.12                     | 0.48              |
| 1:B:43:HIS:HD2   | 1:B:45:ALA:H     | 1.61                     | 0.48              |
| 1:D:106:LYS:HA   | 1:D:132:LYS:HB3  | 1.94                     | 0.48              |
| 1:C:74:LEU:O     | 1:C:78:ILE:HG12  | 2.12                     | 0.48              |
| 1:A:193:TRP:NE1  | 1:A:209:VAL:HG23 | 2.28                     | 0.48              |
| 1:D:136:ARG:HH11 | 1:D:136:ARG:HG2  | 1.78                     | 0.48              |
| 1:C:66:ASP:OD1   | 1:C:66:ASP:N     | 2.46                     | 0.48              |
| 1:D:180:VAL:HG11 | 1:D:186:ILE:HG13 | 1.96                     | 0.48              |
| 1:C:133:ILE:HG22 | 1:C:135:PHE:H    | 1.79                     | 0.48              |
| 1:B:180:VAL:HG11 | 1:B:186:ILE:HG13 | 1.95                     | 0.48              |
| 1:D:219:LEU:HD21 | 1:D:223:LEU:HD22 | 1.96                     | 0.48              |
| 1:B:83:THR:OG1   | 1:B:107:ILE:HG12 | 2.13                     | 0.48              |
| 1:C:89:TYR:C     | 1:C:89:TYR:CD1   | 2.87                     | 0.48              |
| 1:C:198:VAL:CG1  | 1:C:199:ALA:H    | 2.23                     | 0.48              |
| 1:D:188:TYR:CD1  | 1:D:223:LEU:HD21 | 2.49                     | 0.48              |
| 1:A:166:LYS:HB3  | 1:A:212:TYR:CD1  | 2.48                     | 0.48              |
| 1:A:60:ILE:O     | 1:A:60:ILE:HG12  | 2.13                     | 0.48              |
| 1:A:75:LEU:CD1   | 1:A:97:THR:HG23  | 2.44                     | 0.48              |
| 1:D:141:LEU:HD23 | 1:D:141:LEU:O    | 2.14                     | 0.47              |
| 1:A:44:GLU:CG    | 1:A:45:ALA:N     | 2.77                     | 0.47              |
| 1:D:234:LEU:O    | 1:D:236:VAL:N    | 2.39                     | 0.47              |
| 1:D:158:ASP:O    | 1:D:185:VAL:HG11 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:144:LEU:HA   | 1:D:147:MET:CE   | 2.44                     | 0.47              |
| 1:A:113:ASN:O    | 1:A:114:LYS:CB   | 2.62                     | 0.47              |
| 1:C:217:LEU:O    | 1:C:221:LYS:HG2  | 2.14                     | 0.47              |
| 1:D:141:LEU:HD21 | 1:D:175:ARG:NE   | 2.28                     | 0.47              |
| 1:B:43:HIS:CD2   | 1:B:44:GLU:N     | 2.83                     | 0.47              |
| 1:A:75:LEU:HD21  | 1:A:159:PHE:CD2  | 2.50                     | 0.47              |
| 1:D:118:GLU:HA   | 1:D:121:LEU:HB2  | 1.96                     | 0.47              |
| 1:C:30:TYR:CE2   | 1:C:34:LEU:HD11  | 2.49                     | 0.47              |
| 1:A:145:ASP:CG   | 1:A:175:ARG:HH21 | 2.18                     | 0.47              |
| 1:C:230:GLU:HG3  | 1:C:246:ILE:HG21 | 1.95                     | 0.47              |
| 1:A:233:MET:HE2  | 1:C:37:SER:HB2   | 1.97                     | 0.47              |
| 1:C:119:LEU:HD23 | 1:C:119:LEU:O    | 2.14                     | 0.47              |
| 1:B:150:ASP:O    | 1:B:152:LYS:N    | 2.48                     | 0.47              |
| 1:D:185:VAL:CG1  | 1:D:186:ILE:N    | 2.61                     | 0.47              |
| 1:D:160:ILE:HG21 | 1:D:176:LEU:HD21 | 1.97                     | 0.47              |
| 1:C:163:ASP:CG   | 3:C:303:SAH:HG2  | 2.35                     | 0.47              |
| 1:C:103:GLU:HA   | 1:C:132:LYS:CE   | 2.45                     | 0.47              |
| 1:C:162:VAL:HG12 | 1:C:169:TYR:CE1  | 2.49                     | 0.47              |
| 1:D:189:ASP:HA   | 1:D:240:ILE:HG12 | 1.97                     | 0.47              |
| 1:B:226:ASP:HB3  | 1:B:229:ILE:HG12 | 1.97                     | 0.47              |
| 1:C:63:THR:O     | 1:C:63:THR:HG23  | 2.15                     | 0.47              |
| 1:D:21:LYS:HG2   | 1:D:22:SER:N     | 2.17                     | 0.47              |
| 1:D:163:ASP:OD1  | 1:D:189:ASP:HB3  | 2.15                     | 0.47              |
| 1:D:166:LYS:HE3  | 1:D:193:TRP:CZ3  | 2.50                     | 0.47              |
| 1:D:181:LYS:HD2  | 1:D:245:ARG:NH1  | 2.24                     | 0.47              |
| 1:D:176:LEU:HA   | 1:D:179:LEU:HD23 | 1.95                     | 0.46              |
| 1:C:133:ILE:HG22 | 1:C:135:PHE:N    | 2.29                     | 0.46              |
| 1:A:34:LEU:HB3   | 1:A:39:PHE:CE2   | 2.50                     | 0.46              |
| 1:C:230:GLU:HG3  | 1:C:246:ILE:CG2  | 2.45                     | 0.46              |
| 1:D:34:LEU:HA    | 1:D:38:VAL:CG2   | 2.44                     | 0.46              |
| 1:D:165:ASP:O    | 1:D:169:TYR:CE1  | 2.69                     | 0.46              |
| 1:A:200:PRO:HG2  | 1:A:203:ALA:CB   | 2.45                     | 0.46              |
| 1:D:171:ASN:O    | 1:D:172:TYR:C    | 2.54                     | 0.46              |
| 1:C:89:TYR:O     | 1:C:91:GLY:N     | 2.43                     | 0.46              |
| 1:B:89:TYR:C     | 1:B:91:GLY:H     | 2.18                     | 0.46              |
| 1:D:63:THR:HG23  | 1:D:92:TYR:CD1   | 2.51                     | 0.46              |
| 1:C:61:MET:CE    | 1:C:61:MET:H     | 2.29                     | 0.46              |
| 1:D:200:PRO:O    | 1:D:203:ALA:N    | 2.48                     | 0.46              |
| 1:D:141:LEU:HD21 | 1:D:175:ARG:CZ   | 2.46                     | 0.46              |
| 1:D:190:ASN:C    | 1:D:192:LEU:H    | 2.19                     | 0.46              |
| 1:D:111:ASP:OD2  | 3:D:304:SAH:H4'  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:240:ILE:HD13 | 1:A:240:ILE:N    | 2.31                     | 0.46              |
| 1:A:234:LEU:HD21 | 1:C:70:PHE:HD1   | 1.81                     | 0.46              |
| 1:B:171:ASN:O    | 1:B:175:ARG:NH1  | 2.49                     | 0.46              |
| 1:C:196:SER:OG   | 1:C:197:VAL:N    | 2.47                     | 0.46              |
| 1:D:206:ARG:HB2  | 1:D:209:VAL:HG12 | 1.98                     | 0.46              |
| 1:D:121:LEU:N    | 1:D:122:PRO:CD   | 2.79                     | 0.46              |
| 1:B:67:GLU:CG    | 1:B:240:ILE:HD11 | 2.38                     | 0.46              |
| 1:D:239:GLY:O    | 1:D:240:ILE:HG13 | 2.16                     | 0.46              |
| 1:D:47:LYS:CD    | 1:D:50:ARG:HH21  | 2.24                     | 0.46              |
| 1:A:29:LEU:HD21  | 1:C:192:LEU:HD22 | 1.97                     | 0.46              |
| 1:D:227:PRO:O    | 1:D:246:ILE:HD11 | 2.16                     | 0.46              |
| 1:A:200:PRO:HA   | 1:A:201:PRO:HD3  | 1.76                     | 0.46              |
| 1:D:165:ASP:O    | 1:D:166:LYS:HD2  | 2.16                     | 0.46              |
| 1:D:28:ALA:HA    | 1:D:31:GLN:CB    | 2.45                     | 0.46              |
| 1:B:150:ASP:C    | 1:B:152:LYS:H    | 2.19                     | 0.46              |
| 1:D:84:MET:HB2   | 1:D:157:TYR:CE2  | 2.51                     | 0.45              |
| 1:B:112:ILE:HD11 | 1:B:139:PRO:HG3  | 1.97                     | 0.45              |
| 1:A:163:ASP:CG   | 4:A:306:FRE:H131 | 2.36                     | 0.45              |
| 1:C:61:MET:SD    | 3:C:303:SAH:H5'1 | 2.56                     | 0.45              |
| 1:D:95:LEU:C     | 1:D:95:LEU:HD23  | 2.37                     | 0.45              |
| 1:C:230:GLU:O    | 1:C:231:ILE:HG12 | 2.16                     | 0.45              |
| 1:A:181:LYS:HE3  | 1:A:183:GLY:HA3  | 1.99                     | 0.45              |
| 1:A:227:PRO:O    | 1:A:246:ILE:HD11 | 2.15                     | 0.45              |
| 1:C:45:ALA:O     | 1:C:48:GLU:N     | 2.50                     | 0.45              |
| 1:B:34:LEU:CD2   | 1:B:65:ALA:HB3   | 2.46                     | 0.45              |
| 1:C:159:PHE:CZ   | 1:C:161:PHE:HB2  | 2.51                     | 0.45              |
| 1:A:59:ASN:O     | 1:A:62:THR:HG22  | 2.17                     | 0.45              |
| 1:B:201:PRO:O    | 1:B:203:ALA:N    | 2.50                     | 0.45              |
| 1:D:232:CYS:HB3  | 1:D:242:ILE:CG1  | 2.46                     | 0.45              |
| 1:B:89:TYR:O     | 1:B:91:GLY:N     | 2.48                     | 0.45              |
| 1:C:112:ILE:CG1  | 1:C:113:ASN:N    | 2.79                     | 0.45              |
| 1:C:246:ILE:HG13 | 1:C:247:LYS:HG3  | 1.98                     | 0.45              |
| 1:A:121:LEU:N    | 1:A:122:PRO:CD   | 2.80                     | 0.45              |
| 1:C:112:ILE:CG1  | 1:C:113:ASN:H    | 2.28                     | 0.45              |
| 1:D:107:ILE:C    | 1:D:108:LEU:HD22 | 2.36                     | 0.45              |
| 1:D:89:TYR:O     | 1:D:91:GLY:N     | 2.45                     | 0.45              |
| 1:D:145:ASP:HA   | 1:D:148:ILE:HG12 | 1.99                     | 0.45              |
| 1:D:106:LYS:HG3  | 1:D:132:LYS:HA   | 1.98                     | 0.45              |
| 1:D:219:LEU:HD13 | 1:D:220:ASN:N    | 2.32                     | 0.45              |
| 1:D:88:VAL:O     | 1:D:89:TYR:HB3   | 2.16                     | 0.45              |
| 1:A:244:ARG:HD3  | 1:C:73:MET:CE    | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:225:VAL:O    | 1:B:225:VAL:HG12 | 2.17                     | 0.45              |
| 1:C:158:ASP:O    | 1:C:184:GLY:O    | 2.35                     | 0.45              |
| 1:B:53:THR:HG21  | 1:B:62:THR:CG2   | 2.47                     | 0.45              |
| 1:A:166:LYS:C    | 1:A:168:ASN:H    | 2.20                     | 0.45              |
| 1:D:145:ASP:HA   | 1:D:148:ILE:CG1  | 2.47                     | 0.45              |
| 1:D:230:GLU:O    | 1:D:231:ILE:HG12 | 2.17                     | 0.45              |
| 1:D:231:ILE:HG22 | 1:D:243:CYS:SG   | 2.57                     | 0.45              |
| 1:D:184:GLY:CA   | 1:D:245:ARG:H    | 2.29                     | 0.44              |
| 1:D:34:LEU:HD22  | 1:D:39:PHE:HE1   | 1.80                     | 0.44              |
| 1:D:107:ILE:N    | 1:D:132:LYS:O    | 2.49                     | 0.44              |
| 1:B:24:LEU:HD12  | 1:B:30:TYR:HB2   | 1.99                     | 0.44              |
| 1:D:60:ILE:HG13  | 1:D:60:ILE:O     | 2.17                     | 0.44              |
| 1:A:111:ASP:OD2  | 3:A:301:SAH:H4'  | 2.17                     | 0.44              |
| 1:D:145:ASP:OD1  | 1:D:175:ARG:HD2  | 2.17                     | 0.44              |
| 1:D:194:ASN:HB3  | 1:D:195:GLY:H    | 1.61                     | 0.44              |
| 1:B:81:LYS:HG2   | 1:B:102:PRO:CG   | 2.48                     | 0.44              |
| 1:B:95:LEU:HD22  | 1:B:99:LEU:HG    | 1.99                     | 0.44              |
| 1:A:200:PRO:HG2  | 1:A:203:ALA:HB3  | 1.99                     | 0.44              |
| 1:D:185:VAL:HG22 | 1:D:186:ILE:N    | 2.32                     | 0.44              |
| 1:C:107:ILE:O    | 1:C:109:ALA:N    | 2.50                     | 0.44              |
| 1:C:205:LEU:HD12 | 1:C:209:VAL:HG23 | 1.99                     | 0.44              |
| 1:D:170:LEU:HD23 | 1:D:170:LEU:O    | 2.17                     | 0.44              |
| 1:B:230:GLU:HG3  | 1:B:244:ARG:NH1  | 2.32                     | 0.44              |
| 1:B:56:HIS:NE2   | 1:B:116:ASN:ND2  | 2.65                     | 0.44              |
| 1:A:48:GLU:O     | 1:A:51:GLU:HB2   | 2.17                     | 0.44              |
| 1:C:184:GLY:O    | 1:C:185:VAL:HB   | 2.18                     | 0.44              |
| 1:D:95:LEU:HD21  | 1:D:99:LEU:HD11  | 1.99                     | 0.44              |
| 1:D:165:ASP:HB3  | 3:D:304:SAH:HN61 | 1.83                     | 0.44              |
| 1:D:209:VAL:HG13 | 1:D:210:ARG:N    | 2.33                     | 0.44              |
| 1:D:52:VAL:C     | 1:D:54:ALA:H     | 2.21                     | 0.44              |
| 1:B:53:THR:HG1   | 1:B:90:THR:HG21  | 1.77                     | 0.44              |
| 1:D:21:LYS:CG    | 1:D:22:SER:N     | 2.75                     | 0.44              |
| 1:A:231:ILE:CD1  | 1:C:41:ARG:HD3   | 2.44                     | 0.44              |
| 1:D:114:LYS:HG3  | 1:D:135:PHE:CE2  | 2.51                     | 0.44              |
| 1:C:73:MET:CE    | 1:C:73:MET:HA    | 2.46                     | 0.44              |
| 1:C:162:VAL:HG12 | 1:C:169:TYR:HE1  | 1.82                     | 0.44              |
| 1:D:240:ILE:O    | 1:D:240:ILE:HG22 | 2.17                     | 0.44              |
| 1:C:153:ASN:HD22 | 1:C:153:ASN:HA   | 1.52                     | 0.44              |
| 1:B:126:LYS:C    | 1:B:128:GLY:H    | 2.21                     | 0.43              |
| 1:B:182:VAL:HA   | 1:B:245:ARG:HD3  | 2.00                     | 0.43              |
| 1:D:180:VAL:HG11 | 1:D:186:ILE:CG1  | 2.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:LEU:O    | 1:A:180:VAL:CG2  | 2.67                     | 0.43              |
| 1:D:145:ASP:O    | 1:D:149:LYS:HE3  | 2.19                     | 0.43              |
| 1:B:172:TYR:HB3  | 1:B:176:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:61:MET:HG3   | 1:B:62:THR:N     | 2.34                     | 0.43              |
| 1:B:199:ALA:C    | 1:B:201:PRO:HD2  | 2.38                     | 0.43              |
| 1:D:136:ARG:O    | 1:D:137:GLU:HG2  | 2.19                     | 0.43              |
| 1:A:244:ARG:HD3  | 1:C:73:MET:HE1   | 1.99                     | 0.43              |
| 1:B:228:ARG:HH21 | 1:B:245:ARG:HH21 | 1.66                     | 0.43              |
| 1:B:140:ALA:O    | 1:B:144:LEU:HB2  | 2.19                     | 0.43              |
| 1:C:113:ASN:ND2  | 1:C:139:PRO:HD3  | 2.33                     | 0.43              |
| 1:C:37:SER:O     | 1:C:69:GLN:NE2   | 2.51                     | 0.43              |
| 1:B:159:PHE:CE2  | 1:B:161:PHE:HB2  | 2.53                     | 0.43              |
| 1:A:165:ASP:HB2  | 1:A:168:ASN:HB2  | 2.01                     | 0.43              |
| 1:D:67:GLU:OE2   | 1:D:240:ILE:HG13 | 2.19                     | 0.43              |
| 1:D:107:ILE:HG22 | 1:D:108:LEU:N    | 2.34                     | 0.43              |
| 1:B:203:ALA:O    | 1:B:205:LEU:N    | 2.52                     | 0.43              |
| 1:D:170:LEU:HD12 | 1:D:218:GLU:CG   | 2.46                     | 0.43              |
| 1:C:182:VAL:CG1  | 1:C:183:GLY:N    | 2.74                     | 0.43              |
| 1:D:246:ILE:CG1  | 1:D:247:LYS:N    | 2.82                     | 0.43              |
| 1:A:246:ILE:O    | 1:A:247:LYS:HB3  | 2.19                     | 0.43              |
| 1:C:160:ILE:HD12 | 1:C:180:VAL:HG13 | 2.01                     | 0.43              |
| 1:D:22:SER:OG    | 1:D:23:LEU:N     | 2.52                     | 0.42              |
| 1:C:130:ASP:C    | 1:C:132:LYS:H    | 2.22                     | 0.42              |
| 1:B:37:SER:C     | 1:B:69:GLN:NE2   | 2.72                     | 0.42              |
| 1:A:200:PRO:O    | 1:A:202:ASP:N    | 2.47                     | 0.42              |
| 1:A:118:GLU:O    | 1:A:122:PRO:HD3  | 2.19                     | 0.42              |
| 1:C:175:ARG:H    | 1:C:175:ARG:HG2  | 1.52                     | 0.42              |
| 1:B:50:ARG:HG2   | 1:B:63:THR:CG2   | 2.49                     | 0.42              |
| 1:D:26:SER:C     | 1:D:28:ALA:N     | 2.71                     | 0.42              |
| 1:B:163:ASP:CG   | 3:B:302:SAH:HG1  | 2.39                     | 0.42              |
| 1:D:63:THR:CG2   | 1:D:93:SER:HB3   | 2.49                     | 0.42              |
| 1:C:46:MET:CE    | 1:C:95:LEU:HD13  | 2.48                     | 0.42              |
| 1:C:44:GLU:CD    | 1:C:44:GLU:H     | 2.21                     | 0.42              |
| 1:A:244:ARG:CB   | 1:C:73:MET:HE1   | 2.48                     | 0.42              |
| 1:A:165:ASP:CB   | 1:A:168:ASN:HB2  | 2.50                     | 0.42              |
| 1:A:170:LEU:CD2  | 1:A:219:LEU:HA   | 2.49                     | 0.42              |
| 1:D:181:LYS:HA   | 1:D:245:ARG:HG3  | 2.02                     | 0.42              |
| 1:D:180:VAL:HG23 | 1:D:181:LYS:H    | 1.83                     | 0.42              |
| 1:D:225:VAL:O    | 1:D:227:PRO:HD3  | 2.20                     | 0.42              |
| 1:D:41:ARG:N     | 1:D:41:ARG:NE    | 2.67                     | 0.42              |
| 1:C:42:GLU:OE2   | 1:C:50:ARG:NH2   | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:88:VAL:O     | 3:D:304:SAH:HA   | 2.19                     | 0.42              |
| 1:D:180:VAL:O    | 1:D:181:LYS:O    | 2.37                     | 0.42              |
| 1:D:181:LYS:CA   | 1:D:245:ARG:NH1  | 2.81                     | 0.42              |
| 1:C:113:ASN:HD21 | 1:C:139:PRO:HD3  | 1.85                     | 0.42              |
| 1:A:180:VAL:HG22 | 1:A:186:ILE:HD11 | 1.94                     | 0.42              |
| 1:D:141:LEU:CD1  | 1:D:175:ARG:HH21 | 2.32                     | 0.42              |
| 1:D:95:LEU:HD21  | 1:D:99:LEU:CD1   | 2.49                     | 0.42              |
| 1:C:177:ILE:HD12 | 1:C:228:ARG:CZ   | 2.49                     | 0.42              |
| 1:B:135:PHE:CD1  | 1:B:136:ARG:N    | 2.87                     | 0.42              |
| 1:C:134:ASP:OD1  | 1:C:134:ASP:O    | 2.38                     | 0.42              |
| 1:A:181:LYS:HG2  | 1:A:183:GLY:H    | 1.84                     | 0.42              |
| 1:D:203:ALA:O    | 1:D:205:LEU:CD2  | 2.67                     | 0.42              |
| 1:B:175:ARG:HG2  | 1:B:175:ARG:HH11 | 1.83                     | 0.42              |
| 1:D:97:THR:O     | 1:D:101:ILE:HG23 | 2.20                     | 0.41              |
| 1:D:225:VAL:O    | 1:D:225:VAL:HG12 | 2.20                     | 0.41              |
| 1:D:208:TYR:N    | 1:D:208:TYR:CD1  | 2.87                     | 0.41              |
| 1:D:226:ASP:C    | 1:D:228:ARG:H    | 2.22                     | 0.41              |
| 1:D:41:ARG:CA    | 1:D:41:ARG:NE    | 2.83                     | 0.41              |
| 1:C:33:ILE:O     | 1:C:37:SER:HB3   | 2.21                     | 0.41              |
| 1:D:59:ASN:C     | 1:D:61:MET:H     | 2.24                     | 0.41              |
| 1:C:140:ALA:O    | 1:C:141:LEU:C    | 2.58                     | 0.41              |
| 1:C:46:MET:HE2   | 1:C:95:LEU:HD13  | 2.02                     | 0.41              |
| 1:D:108:LEU:N    | 1:D:108:LEU:HD22 | 2.35                     | 0.41              |
| 1:A:40:PRO:O     | 1:A:41:ARG:CB    | 2.68                     | 0.41              |
| 1:C:137:GLU:HG2  | 1:C:138:GLY:N    | 2.35                     | 0.41              |
| 1:D:163:ASP:OD2  | 3:D:304:SAH:HB1  | 2.21                     | 0.41              |
| 1:A:193:TRP:CD1  | 1:A:209:VAL:HG23 | 2.56                     | 0.41              |
| 1:D:155:GLY:C    | 1:D:157:TYR:N    | 2.73                     | 0.41              |
| 1:A:185:VAL:H    | 1:A:244:ARG:HA   | 1.86                     | 0.41              |
| 1:A:75:LEU:HD11  | 1:A:97:THR:HG23  | 2.03                     | 0.41              |
| 1:B:224:ALA:HA   | 1:B:231:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:148:ILE:HA   | 1:A:148:ILE:HD13 | 1.93                     | 0.41              |
| 1:B:192:LEU:HA   | 1:B:192:LEU:HD23 | 1.77                     | 0.41              |
| 1:D:159:PHE:CD1  | 1:D:185:VAL:CG2  | 2.99                     | 0.41              |
| 1:D:84:MET:HG2   | 1:D:85:GLU:N     | 2.36                     | 0.41              |
| 1:D:158:ASP:O    | 1:D:185:VAL:CG1  | 2.69                     | 0.40              |
| 1:C:206:ARG:HD2  | 1:C:206:ARG:N    | 2.36                     | 0.40              |
| 1:A:224:ALA:HA   | 1:A:231:ILE:HD13 | 2.03                     | 0.40              |
| 1:C:190:ASN:C    | 1:C:192:LEU:H    | 2.25                     | 0.40              |
| 1:C:49:LEU:HD11  | 1:C:90:THR:CG2   | 2.51                     | 0.40              |
| 1:A:240:ILE:HB   | 1:A:242:ILE:CD1  | 2.52                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:112:ILE:HD12 | 1:B:138:GLY:C   | 2.41                     | 0.40              |
| 1:D:73:MET:HA    | 1:D:73:MET:CE   | 2.52                     | 0.40              |
| 1:A:171:ASN:O    | 1:A:175:ARG:HD3 | 2.20                     | 0.40              |
| 1:B:225:VAL:O    | 1:B:225:VAL:CG1 | 2.69                     | 0.40              |
| 1:B:125:LYS:HA   | 1:B:130:ASP:OD1 | 2.22                     | 0.40              |
| 1:A:56:HIS:HA    | 1:A:57:PRO:HD3  | 1.89                     | 0.40              |
| 1:D:180:VAL:CG2  | 1:D:181:LYS:N   | 2.84                     | 0.40              |
| 1:C:112:ILE:HG13 | 3:C:303:SAH:C2  | 2.52                     | 0.40              |
| 1:A:40:PRO:O     | 1:A:41:ARG:HB2  | 2.22                     | 0.40              |
| 1:A:94:LEU:HD23  | 1:A:94:LEU:HA   | 1.81                     | 0.40              |
| 1:D:191:THR:HB   | 1:D:220:ASN:OD1 | 2.22                     | 0.40              |
| 1:A:104:ASP:N    | 1:A:104:ASP:OD1 | 2.54                     | 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     | 225/247 (91%) | 196 (87%) | 18 (8%)   | 11 (5%)  | 3           | 5 |
| 1   | B     | 225/247 (91%) | 197 (88%) | 18 (8%)   | 10 (4%)  | 3           | 6 |
| 1   | C     | 225/247 (91%) | 170 (76%) | 30 (13%)  | 25 (11%) | 0           | 0 |
| 1   | D     | 225/247 (91%) | 155 (69%) | 41 (18%)  | 29 (13%) | 0           | 0 |
| All | All   | 900/988 (91%) | 718 (80%) | 107 (12%) | 75 (8%)  | 1           | 1 |

All (75) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | HIS  |
| 1   | A     | 89  | TYR  |
| 1   | A     | 165 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 202 | ASP  |
| 1   | A     | 231 | ILE  |
| 1   | B     | 62  | THR  |
| 1   | B     | 63  | THR  |
| 1   | B     | 89  | TYR  |
| 1   | B     | 202 | ASP  |
| 1   | C     | 60  | ILE  |
| 1   | C     | 104 | ASP  |
| 1   | C     | 110 | MET  |
| 1   | C     | 166 | LYS  |
| 1   | C     | 182 | VAL  |
| 1   | C     | 201 | PRO  |
| 1   | C     | 231 | ILE  |
| 1   | D     | 102 | PRO  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 181 | LYS  |
| 1   | D     | 185 | VAL  |
| 1   | D     | 186 | ILE  |
| 1   | D     | 207 | LYS  |
| 1   | D     | 231 | ILE  |
| 1   | A     | 44  | GLU  |
| 1   | A     | 166 | LYS  |
| 1   | B     | 151 | GLU  |
| 1   | B     | 166 | LYS  |
| 1   | B     | 231 | ILE  |
| 1   | C     | 105 | GLY  |
| 1   | C     | 165 | ASP  |
| 1   | C     | 184 | GLY  |
| 1   | C     | 194 | ASN  |
| 1   | C     | 196 | SER  |
| 1   | C     | 197 | VAL  |
| 1   | D     | 37  | SER  |
| 1   | D     | 182 | VAL  |
| 1   | D     | 193 | TRP  |
| 1   | A     | 114 | LYS  |
| 1   | B     | 204 | PRO  |
| 1   | C     | 59  | ASN  |
| 1   | C     | 139 | PRO  |
| 1   | C     | 200 | PRO  |
| 1   | C     | 202 | ASP  |
| 1   | D     | 156 | SER  |
| 1   | D     | 204 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 165 | ASP  |
| 1   | C     | 111 | ASP  |
| 1   | C     | 164 | ALA  |
| 1   | C     | 181 | LYS  |
| 1   | D     | 41  | ARG  |
| 1   | D     | 79  | ASN  |
| 1   | D     | 89  | TYR  |
| 1   | D     | 164 | ALA  |
| 1   | D     | 165 | ASP  |
| 1   | D     | 240 | ILE  |
| 1   | A     | 185 | VAL  |
| 1   | C     | 88  | VAL  |
| 1   | C     | 185 | VAL  |
| 1   | C     | 191 | THR  |
| 1   | D     | 42  | GLU  |
| 1   | D     | 124 | ILE  |
| 1   | D     | 191 | THR  |
| 1   | D     | 232 | CYS  |
| 1   | D     | 129 | VAL  |
| 1   | D     | 199 | ALA  |
| 1   | B     | 57  | PRO  |
| 1   | A     | 204 | PRO  |
| 1   | C     | 112 | ILE  |
| 1   | C     | 128 | GLY  |
| 1   | D     | 138 | GLY  |
| 1   | D     | 201 | PRO  |
| 1   | A     | 201 | PRO  |
| 1   | D     | 200 | PRO  |
| 1   | D     | 235 | PRO  |
| 1   | D     | 57  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 196/214 (92%) | 177 (90%) | 19 (10%) | 10          | 23 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | B     | 196/214 (92%) | 177 (90%) | 19 (10%) | 10          | 23 |
| 1   | C     | 196/214 (92%) | 174 (89%) | 22 (11%) | 7           | 17 |
| 1   | D     | 192/214 (90%) | 181 (94%) | 11 (6%)  | 25          | 53 |
| All | All   | 780/856 (91%) | 709 (91%) | 71 (9%)  | 12          | 26 |

All (71) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | LEU  |
| 1   | A     | 69  | GLN  |
| 1   | A     | 79  | ASN  |
| 1   | A     | 90  | THR  |
| 1   | A     | 94  | LEU  |
| 1   | A     | 95  | LEU  |
| 1   | A     | 115 | GLU  |
| 1   | A     | 136 | ARG  |
| 1   | A     | 144 | LEU  |
| 1   | A     | 170 | LEU  |
| 1   | A     | 175 | ARG  |
| 1   | A     | 176 | LEU  |
| 1   | A     | 180 | VAL  |
| 1   | A     | 181 | LYS  |
| 1   | A     | 205 | LEU  |
| 1   | A     | 210 | ARG  |
| 1   | A     | 223 | LEU  |
| 1   | A     | 240 | ILE  |
| 1   | A     | 247 | LYS  |
| 1   | B     | 25  | GLN  |
| 1   | B     | 57  | PRO  |
| 1   | B     | 58  | TRP  |
| 1   | B     | 59  | ASN  |
| 1   | B     | 74  | LEU  |
| 1   | B     | 94  | LEU  |
| 1   | B     | 95  | LEU  |
| 1   | B     | 103 | GLU  |
| 1   | B     | 144 | LEU  |
| 1   | B     | 165 | ASP  |
| 1   | B     | 170 | LEU  |
| 1   | B     | 176 | LEU  |
| 1   | B     | 177 | ILE  |
| 1   | B     | 180 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 185 | VAL  |
| 1   | B     | 198 | VAL  |
| 1   | B     | 206 | ARG  |
| 1   | B     | 219 | LEU  |
| 1   | B     | 223 | LEU  |
| 1   | C     | 27  | ASP  |
| 1   | C     | 36  | THR  |
| 1   | C     | 44  | GLU  |
| 1   | C     | 61  | MET  |
| 1   | C     | 66  | ASP  |
| 1   | C     | 73  | MET  |
| 1   | C     | 79  | ASN  |
| 1   | C     | 83  | THR  |
| 1   | C     | 89  | TYR  |
| 1   | C     | 95  | LEU  |
| 1   | C     | 103 | GLU  |
| 1   | C     | 108 | LEU  |
| 1   | C     | 139 | PRO  |
| 1   | C     | 145 | ASP  |
| 1   | C     | 152 | LYS  |
| 1   | C     | 153 | ASN  |
| 1   | C     | 170 | LEU  |
| 1   | C     | 175 | ARG  |
| 1   | C     | 176 | LEU  |
| 1   | C     | 177 | ILE  |
| 1   | C     | 180 | VAL  |
| 1   | C     | 223 | LEU  |
| 1   | D     | 27  | ASP  |
| 1   | D     | 41  | ARG  |
| 1   | D     | 42  | GLU  |
| 1   | D     | 136 | ARG  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 167 | ASP  |
| 1   | D     | 174 | LYS  |
| 1   | D     | 177 | ILE  |
| 1   | D     | 208 | TYR  |
| 1   | D     | 221 | LYS  |
| 1   | D     | 245 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | GLN  |
| 1   | A     | 153 | ASN  |
| 1   | A     | 194 | ASN  |
| 1   | B     | 43  | HIS  |
| 1   | B     | 69  | GLN  |
| 1   | B     | 116 | ASN  |
| 1   | C     | 31  | GLN  |
| 1   | C     | 43  | HIS  |
| 1   | C     | 69  | GLN  |
| 1   | C     | 79  | ASN  |
| 1   | C     | 113 | ASN  |
| 1   | C     | 168 | ASN  |
| 1   | C     | 171 | ASN  |
| 1   | C     | 220 | ASN  |
| 1   | D     | 31  | GLN  |
| 1   | D     | 69  | GLN  |
| 1   | D     | 116 | ASN  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 190 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SAH  | A     | 301 | -    | 20,28,28     | 1.64 | 3 (15%)     | 19,40,40    | 3.54 | 10 (52%)    |
| 4   | FRE  | A     | 306 | -    | 53,65,65     | 1.50 | 11 (20%)    | 71,96,96    | 1.98 | 12 (16%)    |
| 3   | SAH  | B     | 302 | -    | 20,28,28     | 1.60 | 3 (15%)     | 19,40,40    | 3.03 | 11 (57%)    |
| 3   | SAH  | C     | 303 | -    | 20,28,28     | 1.80 | 3 (15%)     | 19,40,40    | 3.11 | 8 (42%)     |
| 3   | SAH  | D     | 304 | 2    | 20,28,28     | 1.73 | 3 (15%)     | 19,40,40    | 3.10 | 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     | 301 | -    | -         | 0/7/31/31  | 0/3/3/3 |
| 4   | FRE  | A     | 306 | -    | 1/1/12/16 | 0/53/74/74 | 0/4/4/4 |
| 3   | SAH  | B     | 302 | -    | -         | 0/7/31/31  | 0/3/3/3 |
| 3   | SAH  | C     | 303 | -    | -         | 0/7/31/31  | 0/3/3/3 |
| 3   | SAH  | D     | 304 | 2    | -         | 0/7/31/31  | 0/3/3/3 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 303 | SAH  | C8-N7   | -3.64 | 1.27        | 1.34     |
| 3   | D     | 304 | SAH  | C8-N7   | -3.52 | 1.27        | 1.34     |
| 3   | A     | 301 | SAH  | C8-N7   | -3.42 | 1.28        | 1.34     |
| 3   | B     | 302 | SAH  | C8-N7   | -3.37 | 1.28        | 1.34     |
| 3   | A     | 301 | SAH  | C5-C4   | -2.58 | 1.34        | 1.40     |
| 3   | B     | 302 | SAH  | O2'-C2' | -2.29 | 1.37        | 1.43     |
| 4   | A     | 306 | FRE  | P2A-O6A | -2.26 | 1.48        | 1.59     |
| 4   | A     | 306 | FRE  | O4B-C1B | -2.25 | 1.38        | 1.41     |
| 3   | D     | 304 | SAH  | O2'-C2' | -2.23 | 1.37        | 1.43     |
| 3   | C     | 303 | SAH  | O2'-C2' | -2.12 | 1.37        | 1.43     |
| 4   | A     | 306 | FRE  | C5-C6   | 2.02  | 1.42        | 1.38     |
| 4   | A     | 306 | FRE  | C3-C2   | 2.03  | 1.41        | 1.38     |
| 4   | A     | 306 | FRE  | C6-C1   | 2.39  | 1.43        | 1.40     |
| 4   | A     | 306 | FRE  | C5-C4   | 2.54  | 1.44        | 1.39     |
| 4   | A     | 306 | FRE  | C2-C1   | 2.75  | 1.43        | 1.39     |
| 4   | A     | 306 | FRE  | P3B-O9A | 2.82  | 1.60        | 1.51     |
| 4   | A     | 306 | FRE  | OAP-CAP | 3.02  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | A     | 306 | FRE  | C3P-N4P | 3.69 | 1.54        | 1.46     |
| 4   | A     | 306 | FRE  | C7P-N8P | 3.95 | 1.55        | 1.46     |
| 3   | A     | 301 | SAH  | O4'-C1' | 4.59 | 1.47        | 1.41     |
| 3   | B     | 302 | SAH  | O4'-C1' | 4.81 | 1.47        | 1.41     |
| 3   | D     | 304 | SAH  | O4'-C1' | 5.44 | 1.48        | 1.41     |
| 3   | C     | 303 | SAH  | O4'-C1' | 5.95 | 1.48        | 1.41     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 301 | SAH  | C4'-O4'-C1' | -9.06 | 99.77       | 109.72   |
| 3   | A     | 301 | SAH  | N3-C2-N1    | -8.41 | 122.46      | 128.89   |
| 3   | D     | 304 | SAH  | N3-C2-N1    | -7.98 | 122.79      | 128.89   |
| 3   | B     | 302 | SAH  | N3-C2-N1    | -7.71 | 122.99      | 128.89   |
| 3   | C     | 303 | SAH  | C4'-O4'-C1' | -7.53 | 101.44      | 109.72   |
| 3   | C     | 303 | SAH  | N3-C2-N1    | -7.41 | 123.22      | 128.89   |
| 3   | D     | 304 | SAH  | C4'-O4'-C1' | -6.92 | 102.11      | 109.72   |
| 4   | A     | 306 | FRE  | O5P-C5P-C6P | -6.39 | 110.95      | 121.98   |
| 3   | B     | 302 | SAH  | C4'-O4'-C1' | -5.83 | 103.31      | 109.72   |
| 4   | A     | 306 | FRE  | C3P-N4P-C5P | -5.08 | 112.81      | 122.79   |
| 4   | A     | 306 | FRE  | C7P-N8P-C9P | -4.70 | 113.23      | 122.53   |
| 4   | A     | 306 | FRE  | C5-C6-C1    | -3.43 | 117.11      | 120.56   |
| 3   | B     | 302 | SAH  | O4'-C1'-N9  | -3.01 | 101.80      | 108.10   |
| 3   | D     | 304 | SAH  | O4'-C1'-N9  | -2.78 | 102.29      | 108.10   |
| 3   | C     | 303 | SAH  | O4'-C1'-N9  | -2.48 | 102.92      | 108.10   |
| 4   | A     | 306 | FRE  | O3B-P3B-O9A | -2.42 | 101.05      | 107.11   |
| 3   | A     | 301 | SAH  | O4'-C4'-C3' | -2.10 | 100.91      | 105.15   |
| 3   | B     | 302 | SAH  | O4'-C4'-C3' | -2.08 | 100.95      | 105.15   |
| 3   | A     | 301 | SAH  | N6-C6-N1    | 2.11  | 123.72      | 119.20   |
| 3   | D     | 304 | SAH  | O4'-C4'-C5' | 2.12  | 114.61      | 108.85   |
| 3   | A     | 301 | SAH  | O4'-C4'-C5' | 2.14  | 114.67      | 108.85   |
| 3   | B     | 302 | SAH  | C4'-C5'-SD  | 2.23  | 120.40      | 113.53   |
| 4   | A     | 306 | FRE  | C3-C2-C1    | 2.31  | 121.85      | 120.42   |
| 3   | A     | 301 | SAH  | C5'-C4'-C3' | 2.34  | 121.04      | 114.98   |
| 3   | C     | 303 | SAH  | O4'-C4'-C5' | 2.37  | 115.30      | 108.85   |
| 3   | B     | 302 | SAH  | N6-C6-N1    | 2.52  | 124.60      | 119.20   |
| 4   | A     | 306 | FRE  | O3A-P2A-O6A | 2.60  | 109.83      | 102.94   |
| 3   | C     | 303 | SAH  | N6-C6-N1    | 2.62  | 124.83      | 119.20   |
| 3   | B     | 302 | SAH  | C2'-C1'-N9  | 2.65  | 118.34      | 114.29   |
| 3   | D     | 304 | SAH  | N6-C6-N1    | 2.71  | 125.01      | 119.20   |
| 3   | B     | 302 | SAH  | C5'-C4'-C3' | 2.71  | 122.00      | 114.98   |
| 3   | A     | 301 | SAH  | C4-C5-N7    | 2.82  | 112.07      | 109.48   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4   | A     | 306 | FRE  | C4-C5-C6    | 2.83 | 123.92      | 120.17   |
| 3   | B     | 302 | SAH  | O2'-C2'-C3' | 3.00 | 121.58      | 111.83   |
| 3   | D     | 304 | SAH  | O2'-C2'-C3' | 3.12 | 121.97      | 111.83   |
| 3   | A     | 301 | SAH  | O2'-C2'-C3' | 3.26 | 122.42      | 111.83   |
| 3   | C     | 303 | SAH  | O2'-C2'-C3' | 3.37 | 122.79      | 111.83   |
| 3   | B     | 302 | SAH  | C4-C5-N7    | 3.53 | 112.72      | 109.48   |
| 3   | B     | 302 | SAH  | C2-N1-C6    | 3.58 | 125.16      | 118.77   |
| 3   | D     | 304 | SAH  | C4-C5-N7    | 3.59 | 112.78      | 109.48   |
| 3   | D     | 304 | SAH  | C2-N1-C6    | 3.60 | 125.20      | 118.77   |
| 3   | C     | 303 | SAH  | C2-N1-C6    | 3.61 | 125.22      | 118.77   |
| 4   | A     | 306 | FRE  | O13-C6-C1   | 3.65 | 118.15      | 114.47   |
| 3   | A     | 301 | SAH  | C2-N1-C6    | 3.66 | 125.31      | 118.77   |
| 3   | C     | 303 | SAH  | C4-C5-N7    | 3.76 | 112.94      | 109.48   |
| 4   | A     | 306 | FRE  | C13-O13-C6  | 4.77 | 124.77      | 117.54   |
| 3   | A     | 301 | SAH  | C2'-C1'-N9  | 4.82 | 121.65      | 114.29   |
| 4   | A     | 306 | FRE  | C2P-S1P-C9  | 5.40 | 106.47      | 99.59    |
| 4   | A     | 306 | FRE  | C6P-C5P-N4P | 5.89 | 126.70      | 116.46   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 4   | A     | 306 | FRE  | CAP  |

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 301 | SAH  | 3       | 0            |
| 4   | A     | 306 | FRE  | 6       | 0            |
| 3   | B     | 302 | SAH  | 2       | 0            |
| 3   | C     | 303 | SAH  | 6       | 0            |
| 3   | D     | 304 | SAH  | 4       | 0            |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 227/247 (91%) | -0.10  | 4 (1%) 71 72  | 37, 54, 83, 98        | 0     |
| 1   | B     | 227/247 (91%) | 0.02   | 10 (4%) 38 37 | 41, 56, 87, 103       | 0     |
| 1   | C     | 227/247 (91%) | 0.43   | 19 (8%) 14 11 | 53, 84, 117, 130      | 0     |
| 1   | D     | 227/247 (91%) | 0.99   | 39 (17%) 2 1  | 89, 122, 140, 147     | 0     |
| All | All   | 908/988 (91%) | 0.33   | 72 (7%) 15 13 | 37, 72, 134, 147      | 0     |

All (72) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 41  | ARG  | 6.3  |
| 1   | B     | 203 | ALA  | 5.6  |
| 1   | C     | 201 | PRO  | 5.2  |
| 1   | D     | 201 | PRO  | 5.2  |
| 1   | D     | 161 | PHE  | 4.9  |
| 1   | D     | 162 | VAL  | 4.5  |
| 1   | D     | 246 | ILE  | 4.4  |
| 1   | D     | 104 | ASP  | 4.3  |
| 1   | D     | 175 | ARG  | 4.3  |
| 1   | C     | 84  | MET  | 4.1  |
| 1   | B     | 62  | THR  | 4.0  |
| 1   | D     | 102 | PRO  | 3.9  |
| 1   | C     | 162 | VAL  | 3.9  |
| 1   | C     | 202 | ASP  | 3.8  |
| 1   | D     | 247 | LYS  | 3.8  |
| 1   | B     | 201 | PRO  | 3.7  |
| 1   | C     | 111 | ASP  | 3.6  |
| 1   | B     | 202 | ASP  | 3.6  |
| 1   | C     | 161 | PHE  | 3.5  |
| 1   | B     | 187 | GLY  | 3.5  |
| 1   | C     | 247 | LYS  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 200 | PRO  | 3.3  |
| 1   | D     | 85  | GLU  | 3.3  |
| 1   | C     | 85  | GLU  | 3.2  |
| 1   | D     | 86  | ILE  | 3.1  |
| 1   | D     | 187 | GLY  | 3.0  |
| 1   | D     | 48  | GLU  | 3.0  |
| 1   | D     | 152 | LYS  | 3.0  |
| 1   | C     | 86  | ILE  | 3.0  |
| 1   | D     | 80  | ALA  | 2.9  |
| 1   | D     | 93  | SER  | 2.9  |
| 1   | D     | 160 | ILE  | 2.9  |
| 1   | C     | 93  | SER  | 2.9  |
| 1   | C     | 203 | ALA  | 2.8  |
| 1   | D     | 27  | ASP  | 2.8  |
| 1   | D     | 188 | TYR  | 2.7  |
| 1   | C     | 83  | THR  | 2.6  |
| 1   | D     | 84  | MET  | 2.6  |
| 1   | D     | 163 | ASP  | 2.6  |
| 1   | C     | 204 | PRO  | 2.6  |
| 1   | D     | 181 | LYS  | 2.5  |
| 1   | D     | 103 | GLU  | 2.5  |
| 1   | D     | 151 | GLU  | 2.5  |
| 1   | C     | 188 | TYR  | 2.5  |
| 1   | D     | 105 | GLY  | 2.5  |
| 1   | B     | 161 | PHE  | 2.4  |
| 1   | B     | 204 | PRO  | 2.4  |
| 1   | B     | 152 | LYS  | 2.4  |
| 1   | C     | 110 | MET  | 2.4  |
| 1   | D     | 125 | LYS  | 2.4  |
| 1   | D     | 79  | ASN  | 2.4  |
| 1   | D     | 87  | GLY  | 2.4  |
| 1   | C     | 61  | MET  | 2.4  |
| 1   | D     | 166 | LYS  | 2.3  |
| 1   | D     | 241 | THR  | 2.3  |
| 1   | A     | 161 | PHE  | 2.3  |
| 1   | C     | 60  | ILE  | 2.3  |
| 1   | B     | 195 | GLY  | 2.3  |
| 1   | D     | 95  | LEU  | 2.3  |
| 1   | D     | 132 | LYS  | 2.2  |
| 1   | D     | 81  | LYS  | 2.2  |
| 1   | A     | 86  | ILE  | 2.2  |
| 1   | B     | 115 | GLU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 187 | GLY  | 2.2  |
| 1   | D     | 129 | VAL  | 2.2  |
| 1   | A     | 240 | ILE  | 2.1  |
| 1   | D     | 115 | GLU  | 2.1  |
| 1   | A     | 85  | GLU  | 2.1  |
| 1   | D     | 112 | ILE  | 2.1  |
| 1   | D     | 42  | GLU  | 2.1  |
| 1   | D     | 191 | THR  | 2.0  |
| 1   | D     | 108 | LEU  | 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 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | FRE  | A     | 306 | 62/62 | 0.26 | 0.78 | 12.76 | 158,178,190,190            | 1     |
| 3   | SAH  | C     | 303 | 26/26 | 0.30 | 0.69 | 4.44  | 167,180,181,181            | 0     |
| 3   | SAH  | B     | 302 | 26/26 | 0.46 | 0.49 | 3.92  | 116,133,134,135            | 0     |
| 2   | CA   | A     | 305 | 1/1   | 0.92 | 0.26 | 1.24  | 59,59,59,59                | 0     |
| 3   | SAH  | A     | 301 | 26/26 | 0.91 | 0.24 | 0.44  | 41,54,65,69                | 0     |
| 3   | SAH  | D     | 304 | 26/26 | 0.74 | 0.29 | 0.37  | 139,142,144,145            | 0     |
| 2   | CA   | D     | 308 | 1/1   | 0.97 | 0.24 | -0.23 | 88,88,88,88                | 0     |
| 2   | CA   | C     | 307 | 1/1   | 0.86 | 0.16 | -     | 90,90,90,90                | 0     |
| 2   | CA   | B     | 306 | 1/1   | 0.93 | 0.17 | -     | 63,63,63,63                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.