



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:17 PM GMT

PDB ID : 1O96  
Title : STRUCTURE OF ELECTRON TRANSFERRING FLAVOPROTEIN FOR METHYLOPHILUS METHYLOTROPHUS.  
Authors : Leys, D.; Basran, J.; Talfournier, F.; Sutcliffe, M.J.; Scrutton, N.S.  
Deposited on : 2002-12-11  
Resolution : 3.10 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

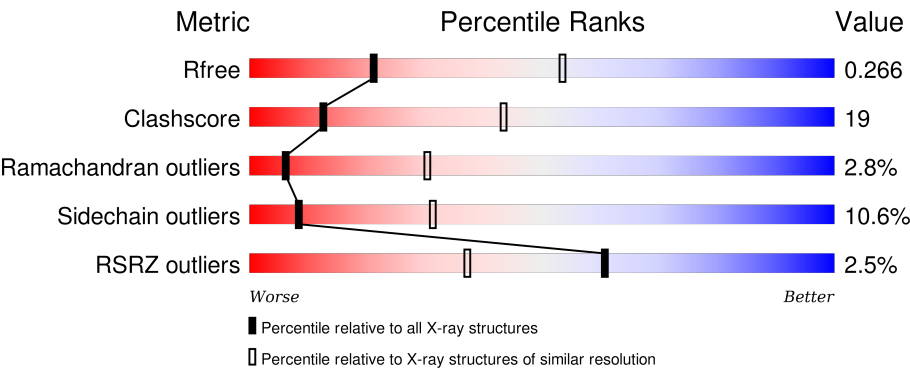
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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 <sub>free</sub>     | 91344                       | 1114 (3.14-3.06)                                      |
| Clashscore            | 102246                      | 1222 (3.14-3.06)                                      |
| Ramachandran outliers | 100387                      | 1174 (3.14-3.06)                                      |
| Sidechain outliers    | 100360                      | 1174 (3.14-3.06)                                      |
| RSRZ outliers         | 91569                       | 1119 (3.14-3.06)                                      |

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     | 264    | <div><div></div><div><div>56%</div><div>30%</div><div>11%</div><div>..</div></div></div>  |
| 1   | C     | 264    | <div><div></div><div><div>55%</div><div>36%</div><div>6%</div><div>..</div></div></div>   |
| 1   | E     | 264    | <div><div></div><div><div>53%</div><div>31%</div><div>12%</div><div>..</div></div></div>  |
| 1   | Q     | 264    | <div><div>6%</div><div><div>56%</div><div>30%</div><div>5%</div><div>7%</div></div></div> |
| 2   | B     | 320    | <div><div>%</div><div><div>61%</div><div>27%</div><div>8%</div><div>..</div></div></div>  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | D     | 320    | <div><div><div>%</div><div><div></div><div>47%</div><div>38%</div><div>13%</div><div><div></div><div></div></div></div></div></div> |
| 2   | F     | 320    | <div><div><div>%</div><div><div></div><div>58%</div><div>30%</div><div>8%</div><div><div></div><div></div></div></div></div></div>  |
| 2   | Z     | 320    | <div><div><div>10%</div><div><div></div><div>70%</div><div>24%</div><div><div></div><div></div></div></div></div></div>             |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17093 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 ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 261      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1963  | 1227 | 336 | 389 | 11 |         |         |       |
| 1   | C     | 260      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1942  | 1217 | 334 | 380 | 11 |         |         |       |
| 1   | E     | 260      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1939  | 1216 | 331 | 381 | 11 |         |         |       |
| 1   | Q     | 246      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1831  | 1147 | 311 | 363 | 10 |         |         |       |

- Molecule 2 is a protein called ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT.

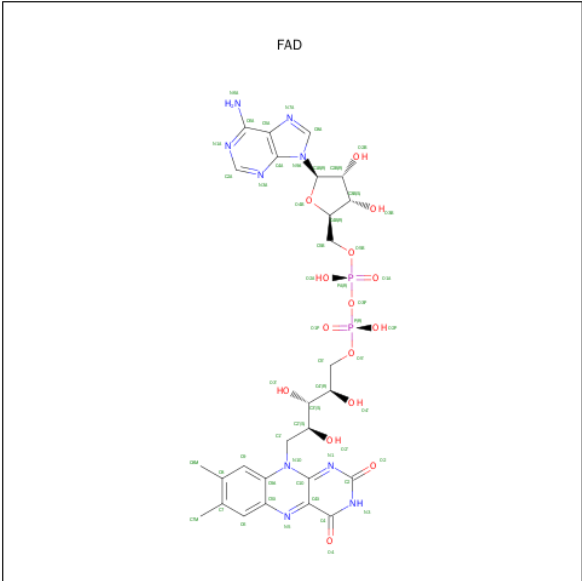
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 314      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2287  | 1444 | 384 | 452 | 7 |         |         |       |
| 2   | D     | 314      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2281  | 1440 | 383 | 451 | 7 |         |         |       |
| 2   | F     | 314      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2281  | 1440 | 383 | 451 | 7 |         |         |       |
| 2   | Z     | 312      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2265  | 1430 | 381 | 447 | 7 |         |         |       |

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |
| 3   | Q     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

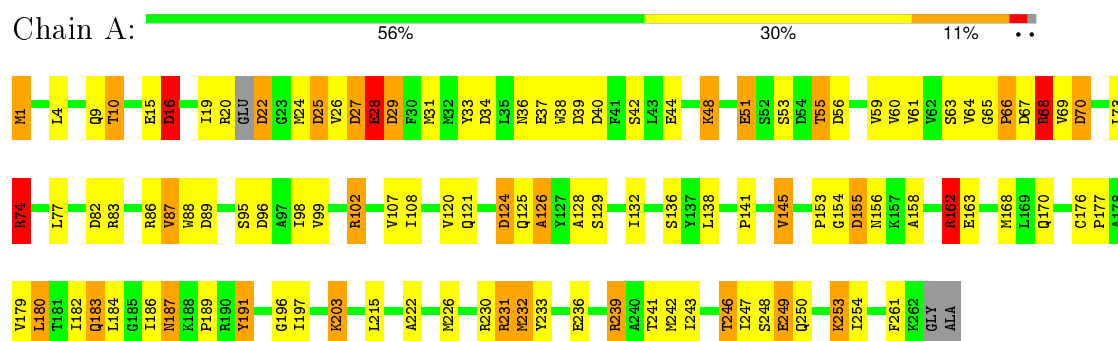


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 4   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 4   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 4   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 4   | Z     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

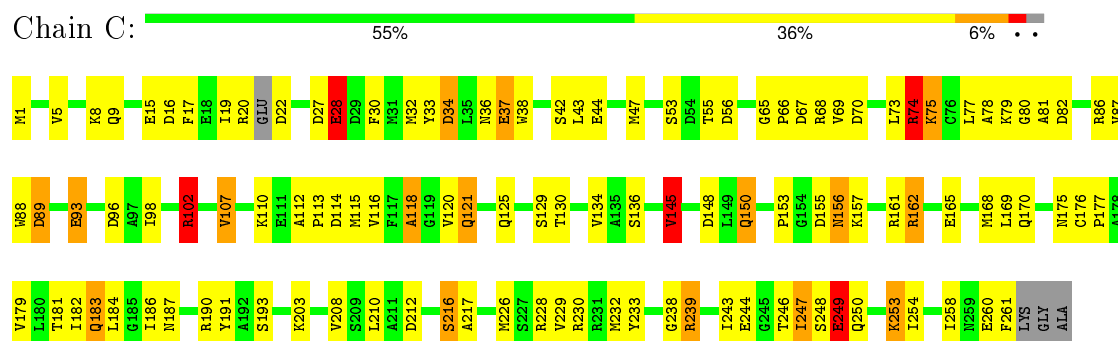
### 3 Residue-property plots

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.

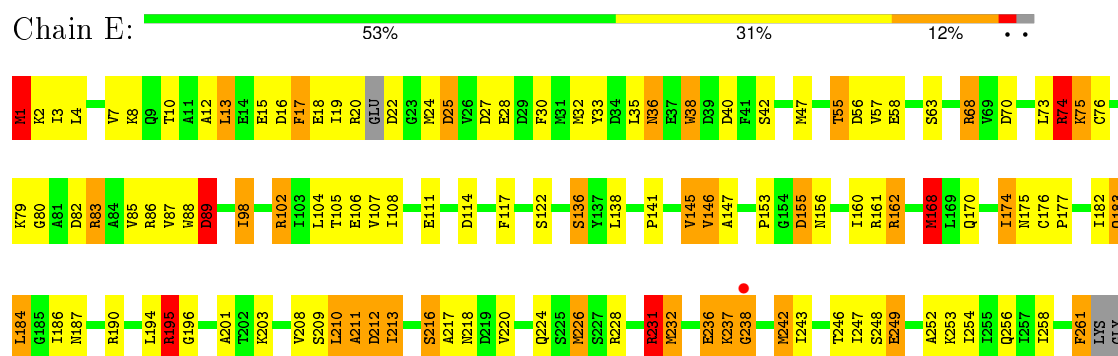
#### • Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT



#### • Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

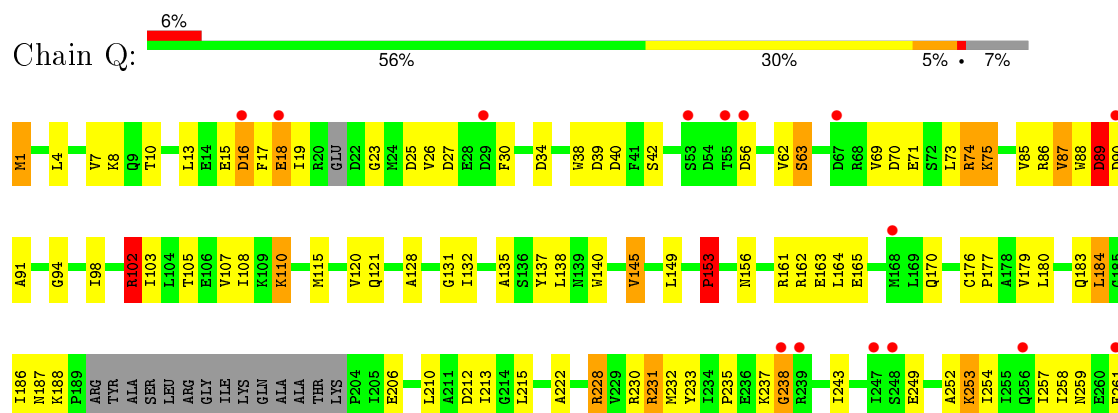


#### • Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

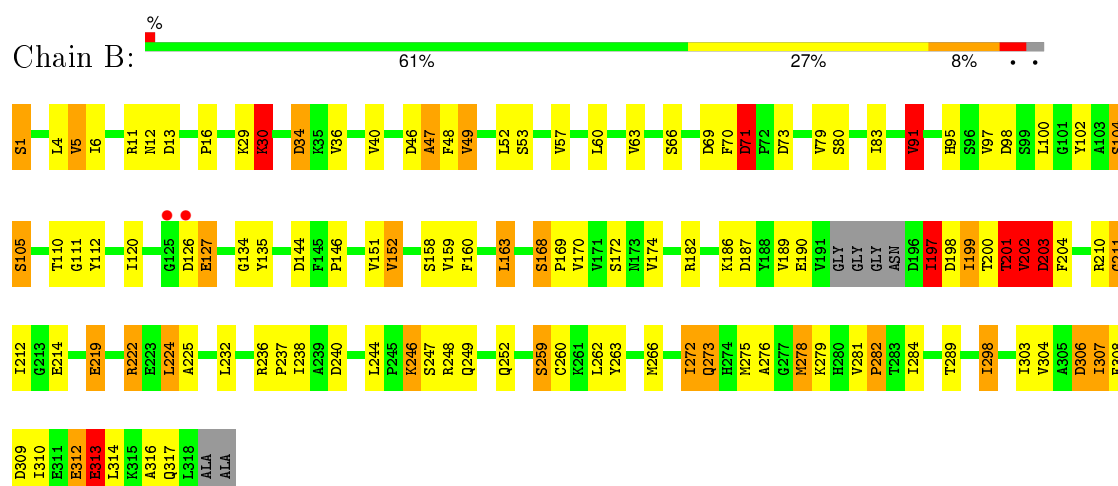


ALA

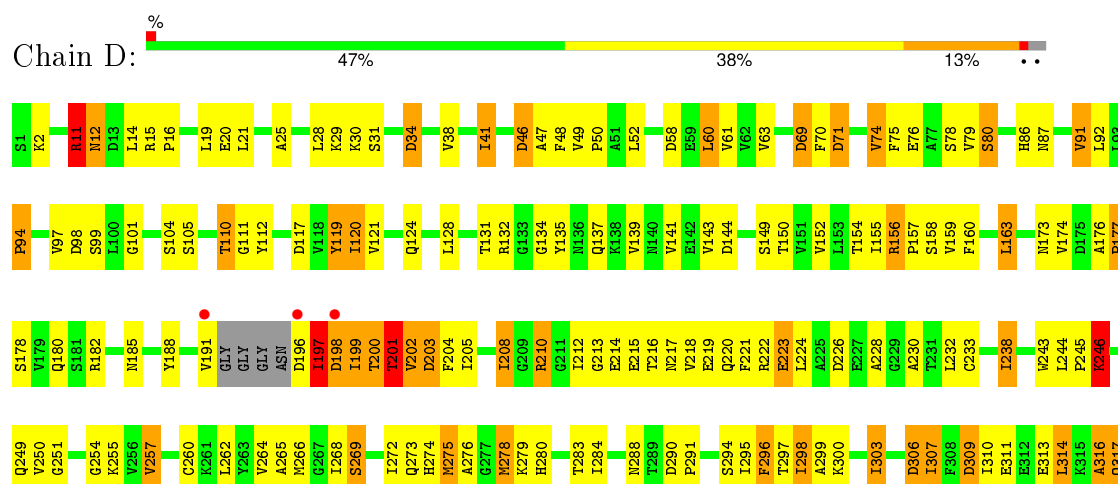
- Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

LYS  
GLY  
ALA

- Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT



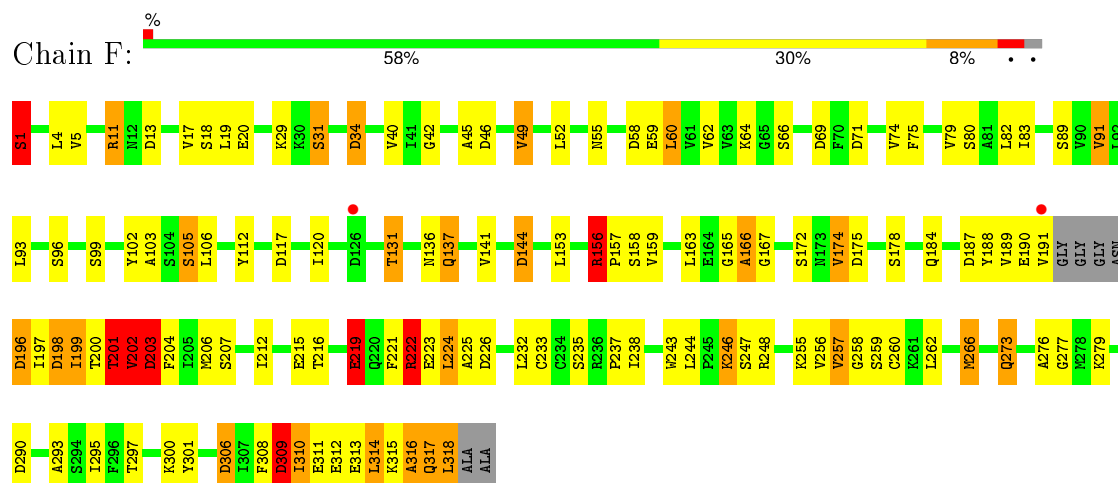
- Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT



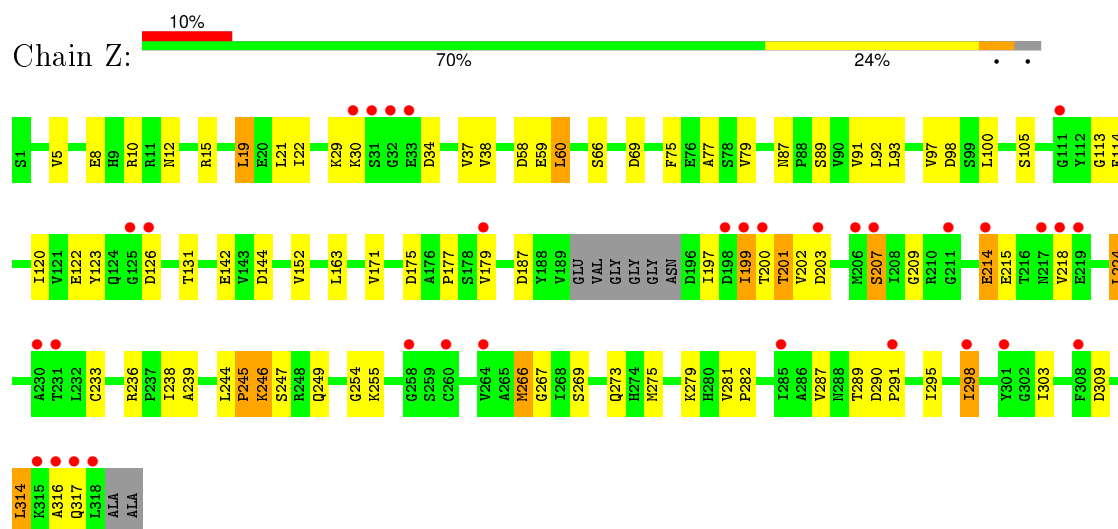




• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT



• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 117.52Å 126.88Å 221.39Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 19.92 – 3.10<br>19.93 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (19.92-3.10)<br>97.8 (19.93-3.10)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.09  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.11 (at 3.09Å)   | Xtriage          |
| Refinement program  | REFMAC 5.1.08   | Depositor        |
| R, $R_{free}$   | 0.212 , 0.278<br>0.207 , 0.266                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2989 reflections (5.32%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 61.9  | Xtriage          |
| Anisotropy  | 0.422   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 56.5   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Outliers  | 0 of 59189 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 17093   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 56.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.69         | 17/1986 (0.9%)   | 1.59        | 26/2688 (1.0%)   |
| 1   | C     | 1.72         | 20/1965 (1.0%)   | 1.53        | 24/2660 (0.9%)   |
| 1   | E     | 1.55         | 19/1962 (1.0%)   | 1.51        | 31/2657 (1.2%)   |
| 1   | Q     | 1.28         | 10/1851 (0.5%)   | 1.25        | 10/2507 (0.4%)   |
| 2   | B     | 1.49         | 20/2324 (0.9%)   | 1.48        | 28/3167 (0.9%)   |
| 2   | D     | 1.53         | 21/2318 (0.9%)   | 1.54        | 34/3159 (1.1%)   |
| 2   | F     | 1.57         | 24/2318 (1.0%)   | 1.53        | 31/3159 (1.0%)   |
| 2   | Z     | 1.06         | 6/2302 (0.3%)    | 1.17        | 11/3137 (0.4%)   |
| All | All   | 1.50         | 137/17026 (0.8%) | 1.46        | 195/23134 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | Q     | 0                   | 1                   |
| 2   | B     | 0                   | 3                   |
| 2   | D     | 0                   | 2                   |
| 2   | F     | 0                   | 2                   |
| All | All   | 0                   | 10                  |

All (137) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 28  | GLU  | CD-OE2 | 30.98 | 1.59        | 1.25     |
| 1   | C     | 249 | GLU  | CD-OE1 | 22.16 | 1.50        | 1.25     |
| 1   | A     | 74  | ARG  | CZ-NH2 | 15.41 | 1.53        | 1.33     |
| 1   | A     | 28  | GLU  | CD-OE2 | 13.61 | 1.40        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | F     | 222 | ARG  | NE-CZ  | 13.57 | 1.50        | 1.33     |
| 1   | E     | 195 | ARG  | NE-CZ  | 13.06 | 1.50        | 1.33     |
| 1   | Q     | 74  | ARG  | NE-CZ  | 12.98 | 1.50        | 1.33     |
| 1   | C     | 93  | GLU  | CD-OE1 | 12.89 | 1.39        | 1.25     |
| 2   | D     | 219 | GLU  | CD-OE2 | 12.20 | 1.39        | 1.25     |
| 1   | A     | 28  | GLU  | CG-CD  | 11.90 | 1.69        | 1.51     |
| 2   | F     | 222 | ARG  | CZ-NH1 | 11.43 | 1.48        | 1.33     |
| 2   | D     | 222 | ARG  | NE-CZ  | 11.35 | 1.47        | 1.33     |
| 1   | C     | 93  | GLU  | CD-OE2 | 11.34 | 1.38        | 1.25     |
| 1   | C     | 244 | GLU  | CD-OE1 | 11.15 | 1.38        | 1.25     |
| 1   | E     | 195 | ARG  | CZ-NH1 | 10.51 | 1.46        | 1.33     |
| 1   | E     | 74  | ARG  | NE-CZ  | 10.22 | 1.46        | 1.33     |
| 1   | Q     | 71  | GLU  | CD-OE2 | 9.84  | 1.36        | 1.25     |
| 2   | F     | 219 | GLU  | CD-OE2 | 9.54  | 1.36        | 1.25     |
| 1   | A     | 74  | ARG  | CG-CD  | 9.53  | 1.75        | 1.51     |
| 2   | Z     | 179 | VAL  | CB-CG2 | 9.51  | 1.72        | 1.52     |
| 2   | D     | 222 | ARG  | CZ-NH1 | 9.42  | 1.45        | 1.33     |
| 1   | Q     | 74  | ARG  | CZ-NH1 | 9.22  | 1.45        | 1.33     |
| 1   | C     | 28  | GLU  | CD-OE1 | 9.16  | 1.35        | 1.25     |
| 2   | D     | 196 | ASP  | C-O    | 9.14  | 1.40        | 1.23     |
| 1   | A     | 74  | ARG  | CZ-NH1 | 9.02  | 1.44        | 1.33     |
| 2   | Z     | 122 | GLU  | CD-OE1 | 8.88  | 1.35        | 1.25     |
| 2   | D     | 197 | ILE  | CA-CB  | 8.35  | 1.74        | 1.54     |
| 1   | C     | 249 | GLU  | CD-OE2 | 8.16  | 1.34        | 1.25     |
| 2   | B     | 30  | LYS  | CE-NZ  | 7.93  | 1.68        | 1.49     |
| 2   | F     | 226 | ASP  | CB-CG  | 7.92  | 1.68        | 1.51     |
| 2   | F     | 103 | ALA  | CA-CB  | -7.92 | 1.35        | 1.52     |
| 2   | B     | 197 | ILE  | CA-CB  | 7.89  | 1.73        | 1.54     |
| 2   | F     | 222 | ARG  | CZ-NH2 | 7.87  | 1.43        | 1.33     |
| 1   | Q     | 74  | ARG  | CZ-NH2 | 7.83  | 1.43        | 1.33     |
| 1   | E     | 232 | MET  | SD-CE  | 7.76  | 2.21        | 1.77     |
| 2   | F     | 219 | GLU  | CG-CD  | 7.75  | 1.63        | 1.51     |
| 2   | B     | 40  | VAL  | CB-CG1 | -7.73 | 1.36        | 1.52     |
| 1   | A     | 179 | VAL  | CB-CG1 | -7.71 | 1.36        | 1.52     |
| 2   | D     | 11  | ARG  | CG-CD  | 7.52  | 1.70        | 1.51     |
| 2   | D     | 309 | ASP  | CG-OD1 | 7.31  | 1.42        | 1.25     |
| 1   | Q     | 71  | GLU  | CD-OE1 | 7.24  | 1.33        | 1.25     |
| 1   | C     | 244 | GLU  | CD-OE2 | 7.18  | 1.33        | 1.25     |
| 2   | B     | 266 | MET  | CG-SD  | -7.17 | 1.62        | 1.81     |
| 2   | F     | 40  | VAL  | CB-CG2 | -7.13 | 1.37        | 1.52     |
| 1   | E     | 74  | ARG  | CZ-NH2 | 7.12  | 1.42        | 1.33     |
| 2   | Z     | 122 | GLU  | CD-OE2 | 7.08  | 1.33        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 145 | VAL  | CB-CG1  | -7.04 | 1.38        | 1.52     |
| 1   | Q     | 75  | LYS  | CD-CE   | 7.03  | 1.68        | 1.51     |
| 1   | E     | 242 | MET  | SD-CE   | 7.00  | 2.17        | 1.77     |
| 2   | B     | 170 | VAL  | CB-CG1  | 6.96  | 1.67        | 1.52     |
| 2   | B     | 222 | ARG  | NE-CZ   | 6.95  | 1.42        | 1.33     |
| 2   | D     | 196 | ASP  | CA-C    | 6.88  | 1.70        | 1.52     |
| 1   | E     | 12  | ALA  | CA-CB   | -6.86 | 1.38        | 1.52     |
| 1   | A     | 28  | GLU  | CD-OE1  | 6.81  | 1.33        | 1.25     |
| 2   | F     | 59  | GLU  | CD-OE1  | 6.76  | 1.33        | 1.25     |
| 2   | D     | 191 | VAL  | CA-CB   | 6.65  | 1.68        | 1.54     |
| 1   | E     | 122 | SER  | CB-OG   | -6.59 | 1.33        | 1.42     |
| 2   | B     | 198 | ASP  | CB-CG   | -6.50 | 1.38        | 1.51     |
| 2   | D     | 197 | ILE  | N-CA    | 6.47  | 1.59        | 1.46     |
| 2   | D     | 197 | ILE  | C-O     | 6.39  | 1.35        | 1.23     |
| 2   | F     | 266 | MET  | SD-CE   | 6.39  | 2.13        | 1.77     |
| 2   | D     | 196 | ASP  | N-CA    | 6.39  | 1.59        | 1.46     |
| 1   | C     | 93  | GLU  | CG-CD   | 6.37  | 1.61        | 1.51     |
| 1   | E     | 74  | ARG  | CG-CD   | 6.37  | 1.67        | 1.51     |
| 1   | E     | 226 | MET  | SD-CE   | 6.37  | 2.13        | 1.77     |
| 2   | B     | 97  | VAL  | CB-CG2  | -6.36 | 1.39        | 1.52     |
| 1   | Q     | 163 | GLU  | CD-OE1  | 6.35  | 1.32        | 1.25     |
| 1   | Q     | 140 | TRP  | CB-CG   | 6.32  | 1.61        | 1.50     |
| 2   | B     | 152 | VAL  | CB-CG2  | -6.27 | 1.39        | 1.52     |
| 1   | E     | 168 | MET  | SD-CE   | 6.24  | 2.12        | 1.77     |
| 2   | F     | 20  | GLU  | CD-OE1  | 6.23  | 1.32        | 1.25     |
| 2   | F     | 201 | THR  | CA-C    | 6.22  | 1.69        | 1.52     |
| 1   | A     | 87  | VAL  | CB-CG1  | -6.21 | 1.39        | 1.52     |
| 1   | C     | 107 | VAL  | CB-CG2  | -6.18 | 1.39        | 1.52     |
| 2   | B     | 5   | VAL  | CA-CB   | -6.11 | 1.42        | 1.54     |
| 2   | F     | 102 | TYR  | CE2-CZ  | 6.08  | 1.46        | 1.38     |
| 2   | D     | 222 | ARG  | CZ-NH2  | 6.07  | 1.41        | 1.33     |
| 2   | F     | 202 | VAL  | N-CA    | 6.07  | 1.58        | 1.46     |
| 1   | A     | 232 | MET  | SD-CE   | 6.00  | 2.11        | 1.77     |
| 1   | C     | 162 | ARG  | CB-CG   | -5.94 | 1.36        | 1.52     |
| 2   | F     | 257 | VAL  | CB-CG1  | -5.82 | 1.40        | 1.52     |
| 1   | A     | 163 | GLU  | CD-OE1  | 5.78  | 1.32        | 1.25     |
| 1   | A     | 48  | LYS  | CB-CG   | 5.76  | 1.68        | 1.52     |
| 2   | D     | 276 | ALA  | CA-CB   | -5.76 | 1.40        | 1.52     |
| 1   | Q     | 1   | MET  | CG-SD   | 5.73  | 1.96        | 1.81     |
| 2   | B     | 304 | VAL  | CA-CB   | -5.72 | 1.42        | 1.54     |
| 2   | F     | 204 | PHE  | CD2-CE2 | 5.71  | 1.50        | 1.39     |
| 2   | F     | 80  | SER  | CB-OG   | -5.71 | 1.34        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 195 | ARG  | CD-NE   | 5.63  | 1.56        | 1.46     |
| 2   | B     | 219 | GLU  | CG-CD   | 5.59  | 1.60        | 1.51     |
| 2   | B     | 104 | SER  | CB-OG   | -5.59 | 1.34        | 1.42     |
| 2   | F     | 293 | ALA  | CA-CB   | 5.58  | 1.64        | 1.52     |
| 2   | Z     | 187 | ASP  | CB-CG   | 5.57  | 1.63        | 1.51     |
| 1   | E     | 75  | LYS  | CD-CE   | 5.55  | 1.65        | 1.51     |
| 2   | D     | 219 | GLU  | CD-OE1  | 5.55  | 1.31        | 1.25     |
| 1   | C     | 191 | TYR  | CD2-CE2 | 5.52  | 1.47        | 1.39     |
| 1   | A     | 61  | VAL  | CB-CG2  | -5.51 | 1.41        | 1.52     |
| 1   | C     | 110 | LYS  | CD-CE   | 5.49  | 1.65        | 1.51     |
| 2   | D     | 185 | ASN  | CB-CG   | -5.48 | 1.38        | 1.51     |
| 1   | C     | 102 | ARG  | NE-CZ   | 5.48  | 1.40        | 1.33     |
| 2   | B     | 97  | VAL  | CB-CG1  | -5.47 | 1.41        | 1.52     |
| 2   | B     | 222 | ARG  | CD-NE   | 5.46  | 1.55        | 1.46     |
| 1   | E     | 74  | ARG  | CZ-NH1  | 5.45  | 1.40        | 1.33     |
| 1   | A     | 191 | TYR  | CB-CG   | -5.43 | 1.43        | 1.51     |
| 2   | B     | 91  | VAL  | CB-CG1  | -5.43 | 1.41        | 1.52     |
| 2   | B     | 225 | ALA  | CA-CB   | -5.42 | 1.41        | 1.52     |
| 2   | B     | 151 | VAL  | CB-CG2  | -5.41 | 1.41        | 1.52     |
| 1   | C     | 37  | GLU  | CD-OE1  | 5.39  | 1.31        | 1.25     |
| 1   | C     | 5   | VAL  | CB-CG1  | -5.38 | 1.41        | 1.52     |
| 1   | Q     | 75  | LYS  | CE-NZ   | 5.38  | 1.62        | 1.49     |
| 1   | E     | 38  | TRP  | CB-CG   | -5.37 | 1.40        | 1.50     |
| 1   | A     | 16  | ASP  | CB-CG   | 5.34  | 1.62        | 1.51     |
| 2   | F     | 266 | MET  | CG-SD   | -5.34 | 1.67        | 1.81     |
| 2   | Z     | 266 | MET  | SD-CE   | 5.34  | 2.07        | 1.77     |
| 2   | F     | 191 | VAL  | CB-CG1  | 5.32  | 1.64        | 1.52     |
| 2   | F     | 238 | ILE  | CA-CB   | -5.28 | 1.42        | 1.54     |
| 1   | E     | 85  | VAL  | CB-CG2  | -5.28 | 1.41        | 1.52     |
| 1   | C     | 37  | GLU  | CD-OE2  | 5.27  | 1.31        | 1.25     |
| 2   | D     | 74  | VAL  | CB-CG1  | -5.27 | 1.41        | 1.52     |
| 2   | D     | 250 | VAL  | CA-CB   | -5.25 | 1.43        | 1.54     |
| 2   | F     | 137 | GLN  | C-O     | 5.24  | 1.33        | 1.23     |
| 1   | A     | 59  | VAL  | CB-CG2  | -5.23 | 1.41        | 1.52     |
| 1   | C     | 118 | ALA  | CA-CB   | -5.22 | 1.41        | 1.52     |
| 1   | E     | 195 | ARG  | CG-CD   | 5.20  | 1.65        | 1.51     |
| 2   | B     | 144 | ASP  | CB-CG   | 5.18  | 1.62        | 1.51     |
| 2   | B     | 127 | GLU  | CD-OE2  | 5.11  | 1.31        | 1.25     |
| 2   | F     | 219 | GLU  | CB-CG   | 5.11  | 1.61        | 1.52     |
| 2   | Z     | 122 | GLU  | CG-CD   | 5.11  | 1.59        | 1.51     |
| 1   | E     | 36  | ASN  | CB-CG   | 5.09  | 1.62        | 1.51     |
| 2   | D     | 275 | MET  | SD-CE   | -5.08 | 1.49        | 1.77     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 233 | TYR  | CD1-CE1 | 5.07  | 1.47        | 1.39     |
| 1   | A     | 64  | VAL  | CA-CB   | -5.07 | 1.44        | 1.54     |
| 2   | D     | 296 | PHE  | CB-CG   | -5.07 | 1.42        | 1.51     |
| 1   | C     | 134 | VAL  | CB-CG2  | -5.06 | 1.42        | 1.52     |
| 2   | F     | 223 | GLU  | CD-OE2  | 5.06  | 1.31        | 1.25     |
| 1   | E     | 146 | VAL  | CB-CG1  | 5.04  | 1.63        | 1.52     |
| 2   | D     | 159 | VAL  | CB-CG1  | -5.04 | 1.42        | 1.52     |

All (195) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 74  | ARG  | NE-CZ-NH2  | -12.17 | 114.22      | 120.30   |
| 2   | D     | 198 | ASP  | CB-CG-OD2  | 11.85  | 128.97      | 118.30   |
| 1   | C     | 56  | ASP  | CB-CG-OD2  | 11.16  | 128.35      | 118.30   |
| 1   | Q     | 16  | ASP  | CB-CG-OD2  | 10.98  | 128.18      | 118.30   |
| 1   | A     | 68  | ARG  | NE-CZ-NH1  | 10.87  | 125.73      | 120.30   |
| 2   | F     | 202 | VAL  | CB-CA-C    | -10.59 | 91.29       | 111.40   |
| 1   | E     | 27  | ASP  | CB-CG-OD2  | 10.56  | 127.80      | 118.30   |
| 1   | E     | 195 | ARG  | NE-CZ-NH1  | 10.54  | 125.57      | 120.30   |
| 2   | D     | 202 | VAL  | CB-CA-C    | -9.83  | 92.72       | 111.40   |
| 1   | A     | 25  | ASP  | CB-CG-OD2  | 9.65   | 126.98      | 118.30   |
| 1   | A     | 89  | ASP  | CB-CG-OD2  | 9.59   | 126.93      | 118.30   |
| 2   | F     | 58  | ASP  | CB-CG-OD2  | 9.56   | 126.91      | 118.30   |
| 2   | F     | 226 | ASP  | CB-CG-OD1  | 9.51   | 126.86      | 118.30   |
| 1   | E     | 162 | ARG  | NE-CZ-NH1  | -9.45  | 115.58      | 120.30   |
| 2   | D     | 163 | LEU  | CA-CB-CG   | 9.27   | 136.62      | 115.30   |
| 2   | B     | 187 | ASP  | CB-CG-OD1  | -9.12  | 110.09      | 118.30   |
| 2   | F     | 69  | ASP  | CB-CG-OD1  | 9.10   | 126.49      | 118.30   |
| 1   | C     | 102 | ARG  | NE-CZ-NH1  | 9.05   | 124.83      | 120.30   |
| 1   | A     | 67  | ASP  | CB-CG-OD2  | 9.04   | 126.44      | 118.30   |
| 2   | D     | 58  | ASP  | CB-CG-OD2  | 9.01   | 126.41      | 118.30   |
| 2   | D     | 15  | ARG  | NE-CZ-NH1  | -8.96  | 115.82      | 120.30   |
| 1   | A     | 39  | ASP  | CB-CG-OD2  | 8.87   | 126.28      | 118.30   |
| 1   | C     | 82  | ASP  | CB-CG-OD2  | 8.86   | 126.28      | 118.30   |
| 1   | E     | 195 | ARG  | NH1-CZ-NH2 | -8.79  | 109.73      | 119.40   |
| 2   | Z     | 144 | ASP  | CB-CG-OD2  | 8.76   | 126.19      | 118.30   |
| 2   | B     | 202 | VAL  | CB-CA-C    | -8.64  | 94.98       | 111.40   |
| 1   | C     | 28  | GLU  | OE1-CD-OE2 | 8.53   | 133.53      | 123.30   |
| 2   | D     | 98  | ASP  | CB-CG-OD2  | 8.35   | 125.81      | 118.30   |
| 1   | Q     | 27  | ASP  | CB-CG-OD2  | 8.30   | 125.77      | 118.30   |
| 1   | C     | 27  | ASP  | CB-CG-OD2  | 8.27   | 125.75      | 118.30   |
| 2   | Z     | 98  | ASP  | CB-CG-OD2  | 8.23   | 125.71      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Q     | 102 | ARG  | NE-CZ-NH1  | 8.12  | 124.36      | 120.30   |
| 2   | Z     | 58  | ASP  | CB-CG-OD2  | 8.09  | 125.58      | 118.30   |
| 2   | B     | 187 | ASP  | CB-CG-OD2  | 7.78  | 125.30      | 118.30   |
| 2   | Z     | 34  | ASP  | CB-CG-OD2  | 7.74  | 125.26      | 118.30   |
| 2   | F     | 156 | ARG  | NE-CZ-NH1  | 7.52  | 124.06      | 120.30   |
| 1   | E     | 68  | ARG  | NE-CZ-NH2  | -7.47 | 116.56      | 120.30   |
| 2   | B     | 126 | ASP  | CB-CG-OD2  | 7.28  | 124.86      | 118.30   |
| 1   | C     | 68  | ARG  | NE-CZ-NH1  | 7.25  | 123.92      | 120.30   |
| 2   | D     | 180 | GLN  | N-CA-C     | -7.22 | 91.51       | 111.00   |
| 1   | Q     | 16  | ASP  | CB-CG-OD1  | -7.19 | 111.83      | 118.30   |
| 2   | B     | 69  | ASP  | CB-CG-OD2  | 7.17  | 124.75      | 118.30   |
| 1   | E     | 83  | ARG  | NE-CZ-NH1  | -7.17 | 116.72      | 120.30   |
| 2   | B     | 201 | THR  | CA-CB-CG2  | -7.14 | 102.40      | 112.40   |
| 1   | A     | 48  | LYS  | CA-CB-CG   | 7.08  | 128.98      | 113.40   |
| 2   | Z     | 126 | ASP  | CB-CG-OD2  | 7.05  | 124.65      | 118.30   |
| 2   | D     | 182 | ARG  | NE-CZ-NH1  | 7.04  | 123.82      | 120.30   |
| 1   | E     | 24  | MET  | CB-CA-C    | 6.99  | 124.39      | 110.40   |
| 2   | D     | 306 | ASP  | CB-CA-C    | 6.97  | 124.34      | 110.40   |
| 1   | A     | 241 | THR  | OG1-CB-CG2 | -6.97 | 93.97       | 110.00   |
| 2   | F     | 13  | ASP  | CB-CG-OD2  | 6.97  | 124.57      | 118.30   |
| 1   | C     | 68  | ARG  | NE-CZ-NH2  | -6.95 | 116.83      | 120.30   |
| 2   | B     | 98  | ASP  | CB-CG-OD2  | 6.93  | 124.53      | 118.30   |
| 1   | E     | 89  | ASP  | CB-CG-OD1  | -6.91 | 112.08      | 118.30   |
| 1   | A     | 29  | ASP  | CB-CG-OD2  | 6.89  | 124.50      | 118.30   |
| 1   | E     | 70  | ASP  | CB-CG-OD2  | 6.88  | 124.49      | 118.30   |
| 1   | E     | 89  | ASP  | CB-CG-OD2  | 6.88  | 124.49      | 118.30   |
| 1   | C     | 244 | GLU  | OE1-CD-OE2 | 6.87  | 131.54      | 123.30   |
| 2   | F     | 1   | SER  | N-CA-C     | -6.87 | 92.45       | 111.00   |
| 2   | D     | 198 | ASP  | N-CA-CB    | -6.86 | 98.25       | 110.60   |
| 1   | C     | 249 | GLU  | CB-CA-C    | -6.78 | 96.83       | 110.40   |
| 2   | F     | 156 | ARG  | NE-CZ-NH2  | -6.78 | 116.91      | 120.30   |
| 2   | F     | 34  | ASP  | CB-CG-OD2  | 6.77  | 124.39      | 118.30   |
| 1   | A     | 162 | ARG  | NE-CZ-NH1  | -6.75 | 116.93      | 120.30   |
| 1   | Q     | 212 | ASP  | CB-CG-OD2  | 6.74  | 124.37      | 118.30   |
| 1   | C     | 70  | ASP  | CB-CG-OD1  | 6.67  | 124.30      | 118.30   |
| 2   | B     | 34  | ASP  | CB-CG-OD2  | 6.66  | 124.29      | 118.30   |
| 1   | A     | 40  | ASP  | CB-CG-OD2  | 6.64  | 124.27      | 118.30   |
| 2   | F     | 309 | ASP  | CB-CG-OD2  | 6.61  | 124.25      | 118.30   |
| 1   | C     | 74  | ARG  | CG-CD-NE   | -6.57 | 98.00       | 111.80   |
| 1   | E     | 162 | ARG  | NE-CZ-NH2  | 6.57  | 123.58      | 120.30   |
| 2   | F     | 11  | ARG  | NE-CZ-NH1  | -6.55 | 117.02      | 120.30   |
| 2   | F     | 201 | THR  | N-CA-CB    | -6.55 | 97.86       | 110.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 74  | ARG  | NE-CZ-NH2  | 6.51  | 123.55      | 120.30   |
| 1   | C     | 89  | ASP  | CB-CG-OD2  | 6.50  | 124.14      | 118.30   |
| 1   | C     | 212 | ASP  | CB-CG-OD2  | 6.45  | 124.11      | 118.30   |
| 2   | D     | 180 | GLN  | CB-CA-C    | 6.45  | 123.30      | 110.40   |
| 1   | A     | 74  | ARG  | NH1-CZ-NH2 | 6.45  | 126.50      | 119.40   |
| 1   | A     | 27  | ASP  | CB-CG-OD2  | 6.42  | 124.08      | 118.30   |
| 2   | D     | 46  | ASP  | CB-CA-C    | -6.42 | 97.57       | 110.40   |
| 2   | B     | 163 | LEU  | CB-CG-CD2  | -6.39 | 100.14      | 111.00   |
| 2   | F     | 187 | ASP  | CB-CG-OD2  | 6.38  | 124.04      | 118.30   |
| 2   | Z     | 175 | ASP  | CB-CG-OD2  | 6.36  | 124.03      | 118.30   |
| 1   | E     | 102 | ARG  | NE-CZ-NH1  | 6.36  | 123.48      | 120.30   |
| 2   | F     | 306 | ASP  | CB-CG-OD1  | 6.36  | 124.02      | 118.30   |
| 1   | E     | 190 | ARG  | NE-CZ-NH1  | 6.34  | 123.47      | 120.30   |
| 2   | D     | 198 | ASP  | CB-CG-OD1  | -6.34 | 112.60      | 118.30   |
| 1   | E     | 231 | ARG  | NE-CZ-NH1  | 6.30  | 123.45      | 120.30   |
| 1   | A     | 242 | MET  | CG-SD-CE   | 6.28  | 110.25      | 100.20   |
| 1   | C     | 155 | ASP  | CB-CG-OD2  | 6.28  | 123.95      | 118.30   |
| 2   | Z     | 309 | ASP  | CB-CG-OD2  | 6.19  | 123.87      | 118.30   |
| 1   | C     | 168 | MET  | CB-CG-SD   | -6.16 | 93.91       | 112.40   |
| 2   | D     | 15  | ARG  | NE-CZ-NH2  | 6.16  | 123.38      | 120.30   |
| 2   | D     | 69  | ASP  | CB-CG-OD1  | 6.16  | 123.84      | 118.30   |
| 2   | Z     | 69  | ASP  | CB-CG-OD1  | 6.15  | 123.83      | 118.30   |
| 2   | D     | 201 | THR  | C-N-CA     | 6.13  | 137.01      | 121.70   |
| 2   | B     | 309 | ASP  | CB-CG-OD1  | 6.11  | 123.80      | 118.30   |
| 2   | F     | 153 | LEU  | CB-CG-CD1  | -6.10 | 100.63      | 111.00   |
| 1   | C     | 148 | ASP  | CB-CG-OD2  | 6.09  | 123.78      | 118.30   |
| 1   | A     | 180 | LEU  | CB-CG-CD2  | -6.05 | 100.71      | 111.00   |
| 2   | B     | 198 | ASP  | CB-CG-OD2  | 6.05  | 123.75      | 118.30   |
| 1   | A     | 231 | ARG  | NE-CZ-NH2  | -6.05 | 117.28      | 120.30   |
| 2   | F     | 198 | ASP  | CB-CA-C    | -6.04 | 98.31       | 110.40   |
| 2   | F     | 144 | ASP  | CB-CG-OD2  | 6.00  | 123.70      | 118.30   |
| 1   | A     | 124 | ASP  | CB-CG-OD2  | 6.00  | 123.70      | 118.30   |
| 1   | E     | 190 | ARG  | NE-CZ-NH2  | -5.96 | 117.32      | 120.30   |
| 2   | F     | 318 | LEU  | CA-CB-CG   | 5.96  | 129.00      | 115.30   |
| 1   | E     | 13  | LEU  | CB-CG-CD2  | -5.95 | 100.88      | 111.00   |
| 2   | D     | 213 | GLY  | N-CA-C     | 5.94  | 127.95      | 113.10   |
| 2   | D     | 34  | ASP  | CB-CG-OD2  | 5.94  | 123.64      | 118.30   |
| 2   | D     | 16  | PRO  | N-CD-CG    | -5.91 | 94.33       | 103.20   |
| 2   | D     | 254 | GLY  | N-CA-C     | -5.90 | 98.36       | 113.10   |
| 2   | D     | 210 | ARG  | NE-CZ-NH2  | 5.85  | 123.23      | 120.30   |
| 2   | D     | 303 | ILE  | N-CA-C     | -5.85 | 95.21       | 111.00   |
| 1   | C     | 168 | MET  | CB-CA-C    | -5.84 | 98.71       | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 244 | GLU  | CG-CD-OE1  | -5.83 | 106.63      | 118.30   |
| 2   | B     | 146 | PRO  | N-CD-CG    | -5.81 | 94.48       | 103.20   |
| 1   | C     | 34  | ASP  | CB-CG-OD1  | 5.80  | 123.52      | 118.30   |
| 2   | F     | 198 | ASP  | CB-CG-OD1  | -5.80 | 113.08      | 118.30   |
| 2   | D     | 94  | PRO  | N-CD-CG    | -5.79 | 94.51       | 103.20   |
| 2   | B     | 13  | ASP  | CB-CG-OD2  | 5.77  | 123.49      | 118.30   |
| 2   | D     | 12  | ASN  | CB-CA-C    | -5.76 | 98.88       | 110.40   |
| 1   | A     | 67  | ASP  | CB-CG-OD1  | -5.76 | 113.12      | 118.30   |
| 2   | Z     | 100 | LEU  | CA-CB-CG   | 5.76  | 128.54      | 115.30   |
| 1   | E     | 238 | GLY  | N-CA-C     | -5.75 | 98.74       | 113.10   |
| 2   | B     | 182 | ARG  | NE-CZ-NH1  | -5.72 | 117.44      | 120.30   |
| 1   | E     | 86  | ARG  | NE-CZ-NH1  | -5.70 | 117.45      | 120.30   |
| 2   | D     | 14  | LEU  | CB-CG-CD1  | 5.70  | 120.68      | 111.00   |
| 2   | Z     | 98  | ASP  | CB-CG-OD1  | -5.69 | 113.18      | 118.30   |
| 2   | F     | 201 | THR  | C-N-CA     | 5.67  | 135.89      | 121.70   |
| 1   | Q     | 184 | LEU  | CA-CB-CG   | 5.59  | 128.16      | 115.30   |
| 2   | F     | 198 | ASP  | CB-CG-OD2  | 5.59  | 123.33      | 118.30   |
| 1   | Q     | 40  | ASP  | CB-CG-OD2  | 5.58  | 123.32      | 118.30   |
| 2   | D     | 314 | LEU  | CA-CB-CG   | 5.55  | 128.08      | 115.30   |
| 1   | C     | 74  | ARG  | NE-CZ-NH2  | -5.53 | 117.53      | 120.30   |
| 2   | F     | 131 | THR  | OG1-CB-CG2 | -5.51 | 97.33       | 110.00   |
| 1   | A     | 31  | MET  | CG-SD-CE   | -5.50 | 91.40       | 100.20   |
| 2   | B     | 278 | MET  | CG-SD-CE   | -5.49 | 91.41       | 100.20   |
| 2   | B     | 71  | ASP  | CB-CG-OD2  | 5.49  | 123.24      | 118.30   |
| 1   | A     | 138 | LEU  | CB-CG-CD1  | -5.48 | 101.68      | 111.00   |
| 1   | A     | 83  | ARG  | NE-CZ-NH1  | 5.47  | 123.04      | 120.30   |
| 2   | B     | 313 | GLU  | N-CA-CB    | -5.47 | 100.75      | 110.60   |
| 2   | F     | 1   | SER  | C-N-CA     | -5.46 | 108.04      | 121.70   |
| 2   | D     | 198 | ASP  | C-N-CA     | -5.45 | 108.08      | 121.70   |
| 2   | F     | 196 | ASP  | C-N-CA     | 5.45  | 135.32      | 121.70   |
| 2   | D     | 128 | LEU  | CB-CG-CD2  | -5.44 | 101.76      | 111.00   |
| 2   | D     | 110 | THR  | C-N-CA     | -5.43 | 110.89      | 122.30   |
| 1   | E     | 108 | ILE  | CG1-CB-CG2 | -5.41 | 99.50       | 111.40   |
| 1   | Q     | 228 | ARG  | NE-CZ-NH1  | -5.41 | 117.59      | 120.30   |
| 2   | D     | 41  | ILE  | CG1-CB-CG2 | -5.40 | 99.52       | 111.40   |
| 2   | B     | 73  | ASP  | CB-CG-OD2  | 5.39  | 123.15      | 118.30   |
| 1   | A     | 70  | ASP  | CB-CG-OD1  | 5.38  | 123.14      | 118.30   |
| 2   | B     | 272 | ILE  | CG1-CB-CG2 | -5.37 | 99.59       | 111.40   |
| 1   | C     | 161 | ARG  | NE-CZ-NH2  | -5.35 | 117.62      | 120.30   |
| 2   | D     | 71  | ASP  | CB-CG-OD2  | 5.35  | 123.11      | 118.30   |
| 2   | D     | 219 | GLU  | CA-CB-CG   | 5.33  | 125.12      | 113.40   |
| 1   | A     | 82  | ASP  | CB-CG-OD2  | 5.32  | 123.09      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 32  | MET  | CG-SD-CE   | 5.32  | 108.71      | 100.20   |
| 2   | F     | 222 | ARG  | NE-CZ-NH2  | 5.30  | 122.95      | 120.30   |
| 2   | F     | 203 | ASP  | N-CA-C     | 5.29  | 125.28      | 111.00   |
| 2   | F     | 246 | LYS  | CD-CE-NZ   | 5.29  | 123.87      | 111.70   |
| 2   | B     | 120 | ILE  | CG1-CB-CG2 | -5.28 | 99.79       | 111.40   |
| 1   | E     | 102 | ARG  | CG-CD-NE   | 5.27  | 122.86      | 111.80   |
| 2   | B     | 201 | THR  | C-N-CA     | 5.25  | 134.82      | 121.70   |
| 2   | B     | 222 | ARG  | NE-CZ-NH2  | 5.23  | 122.91      | 120.30   |
| 2   | B     | 306 | ASP  | CB-CG-OD1  | -5.23 | 113.60      | 118.30   |
| 1   | A     | 180 | LEU  | CA-CB-CG   | 5.20  | 127.26      | 115.30   |
| 1   | C     | 162 | ARG  | CB-CA-C    | 5.20  | 120.80      | 110.40   |
| 2   | F     | 318 | LEU  | CB-CG-CD1  | -5.20 | 102.16      | 111.00   |
| 2   | B     | 110 | THR  | C-N-CA     | -5.19 | 111.39      | 122.30   |
| 1   | E     | 184 | LEU  | CB-CG-CD1  | -5.18 | 102.19      | 111.00   |
| 1   | A     | 68  | ARG  | NE-CZ-NH2  | -5.17 | 117.72      | 120.30   |
| 2   | B     | 240 | ASP  | CB-CG-OD2  | 5.17  | 122.95      | 118.30   |
| 2   | B     | 203 | ASP  | CB-CG-OD2  | 5.17  | 122.95      | 118.30   |
| 1   | E     | 161 | ARG  | NE-CZ-NH1  | -5.15 | 117.73      | 120.30   |
| 2   | B     | 105 | SER  | N-CA-CB    | 5.14  | 118.21      | 110.50   |
| 1   | Q     | 25  | ASP  | CB-CG-OD2  | 5.14  | 122.92      | 118.30   |
| 1   | E     | 98  | ILE  | CG1-CB-CG2 | -5.13 | 100.12      | 111.40   |
| 1   | A     | 40  | ASP  | CB-CG-OD1  | -5.12 | 113.70      | 118.30   |
| 1   | E     | 17  | PHE  | N-CA-CB    | -5.10 | 101.41      | 110.60   |
| 2   | D     | 156 | ARG  | NE-CZ-NH2  | -5.10 | 117.75      | 120.30   |
| 2   | Z     | 21  | LEU  | CA-CB-CG   | 5.10  | 127.03      | 115.30   |
| 1   | Q     | 87  | VAL  | CB-CA-C    | -5.09 | 101.74      | 111.40   |
| 1   | E     | 184 | LEU  | CB-CG-CD2  | 5.06  | 119.60      | 111.00   |
| 1   | E     | 195 | ARG  | NE-CZ-NH2  | 5.06  | 122.83      | 120.30   |
| 2   | B     | 214 | GLU  | OE1-CD-OE2 | -5.05 | 117.24      | 123.30   |
| 2   | F     | 167 | GLY  | N-CA-C     | -5.05 | 100.48      | 113.10   |
| 1   | C     | 175 | ASN  | CB-CA-C    | -5.04 | 100.32      | 110.40   |
| 1   | E     | 155 | ASP  | CB-CA-C    | -5.03 | 100.35      | 110.40   |
| 2   | F     | 290 | ASP  | CB-CG-OD2  | 5.02  | 122.82      | 118.30   |
| 1   | E     | 40  | ASP  | CB-CG-OD2  | 5.01  | 122.81      | 118.30   |
| 2   | F     | 5   | VAL  | CB-CA-C    | -5.01 | 101.88      | 111.40   |
| 1   | C     | 169 | LEU  | CB-CG-CD2  | -5.01 | 102.49      | 111.00   |
| 2   | D     | 61  | VAL  | CB-CA-C    | -5.00 | 101.89      | 111.40   |
| 1   | E     | 1   | MET  | CB-CG-SD   | 5.00  | 127.41      | 112.40   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 22  | ASP  | Peptide |
| 2   | B     | 201 | THR  | Peptide |
| 2   | B     | 312 | GLU  | Peptide |
| 2   | B     | 313 | GLU  | Peptide |
| 2   | D     | 197 | ILE  | Peptide |
| 2   | D     | 200 | THR  | Peptide |
| 1   | E     | 210 | LEU  | Peptide |
| 2   | F     | 196 | ASP  | Peptide |
| 2   | F     | 201 | THR  | Peptide |
| 1   | Q     | 231 | ARG  | Peptide |

## 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     | 1963  | 0        | 1916     | 87      | 1            |
| 1   | C     | 1942  | 0        | 1901     | 99      | 0            |
| 1   | E     | 1939  | 0        | 1891     | 107     | 0            |
| 1   | Q     | 1831  | 0        | 1768     | 68      | 0            |
| 2   | B     | 2287  | 0        | 2250     | 81      | 0            |
| 2   | D     | 2281  | 0        | 2237     | 125     | 0            |
| 2   | F     | 2281  | 0        | 2237     | 85      | 1            |
| 2   | Z     | 2265  | 0        | 2222     | 52      | 0            |
| 3   | A     | 23    | 0        | 12       | 0       | 0            |
| 3   | C     | 23    | 0        | 12       | 3       | 0            |
| 3   | E     | 23    | 0        | 12       | 2       | 0            |
| 3   | Q     | 23    | 0        | 12       | 2       | 0            |
| 4   | B     | 53    | 0        | 31       | 1       | 0            |
| 4   | D     | 53    | 0        | 31       | 8       | 0            |
| 4   | F     | 53    | 0        | 31       | 0       | 0            |
| 4   | Z     | 53    | 0        | 31       | 4       | 0            |
| All | All   | 17093 | 0        | 16594    | 655     | 1            |

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 19.

All (655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:74:ARG:CG    | 1:A:74:ARG:CD    | 1.75                     | 1.56              |
| 2:B:30:LYS:NZ    | 2:B:30:LYS:CE    | 1.68                     | 1.54              |
| 1:Q:115:MET:CE   | 1:Q:115:MET:SD   | 2.03                     | 1.46              |
| 1:Q:232:MET:SD   | 1:Q:232:MET:CE   | 2.05                     | 1.44              |
| 2:Z:266:MET:CE   | 2:Z:266:MET:SD   | 2.07                     | 1.42              |
| 1:A:232:MET:CE   | 1:A:232:MET:SD   | 2.11                     | 1.39              |
| 2:F:266:MET:SD   | 2:F:266:MET:CE   | 2.13                     | 1.36              |
| 1:E:226:MET:CE   | 1:E:226:MET:SD   | 2.13                     | 1.36              |
| 1:E:168:MET:SD   | 1:E:168:MET:CE   | 2.12                     | 1.36              |
| 1:E:242:MET:CE   | 1:E:242:MET:SD   | 2.17                     | 1.32              |
| 1:E:232:MET:SD   | 1:E:232:MET:CE   | 2.21                     | 1.29              |
| 1:A:239:ARG:O    | 1:A:239:ARG:CG   | 1.80                     | 1.27              |
| 1:C:53:SER:OG    | 1:C:55:THR:HG22  | 1.45                     | 1.16              |
| 1:C:243:ILE:HD13 | 1:C:253:LYS:HG3  | 1.23                     | 1.16              |
| 1:A:74:ARG:NH2   | 1:A:203:LYS:O    | 1.77                     | 1.15              |
| 1:Q:235:PRO:HG2  | 1:Q:237:LYS:HG3  | 1.21                     | 1.14              |
| 1:A:239:ARG:O    | 1:A:239:ARG:HG2  | 1.32                     | 1.08              |
| 1:E:1:MET:HG3    | 1:E:153:PRO:HB3  | 1.27                     | 1.08              |
| 2:D:202:VAL:HG12 | 2:D:203:ASP:H    | 0.93                     | 1.06              |
| 2:F:202:VAL:HG12 | 2:F:203:ASP:N    | 1.67                     | 1.05              |
| 1:E:236:GLU:O    | 1:E:237:LYS:HB2  | 1.52                     | 1.03              |
| 1:C:47:MET:HE2   | 1:C:80:GLY:HA3   | 1.39                     | 1.03              |
| 1:A:246:THR:H    | 1:A:249:GLU:HG3  | 1.19                     | 1.03              |
| 1:E:246:THR:H    | 1:E:249:GLU:HG3  | 1.24                     | 1.02              |
| 2:D:202:VAL:CG1  | 2:D:203:ASP:H    | 1.74                     | 1.01              |
| 2:F:202:VAL:CG1  | 2:F:203:ASP:N    | 2.24                     | 1.01              |
| 2:D:202:VAL:HG12 | 2:D:203:ASP:N    | 1.72                     | 1.00              |
| 1:A:1:MET:HG3    | 1:A:153:PRO:HB3  | 1.43                     | 1.00              |
| 2:B:313:GLU:O    | 2:B:317:GLN:HG3  | 1.61                     | 0.99              |
| 2:B:202:VAL:HG12 | 2:B:203:ASP:N    | 1.72                     | 0.98              |
| 2:D:310:ILE:HG22 | 2:D:314:LEU:HD22 | 1.45                     | 0.96              |
| 2:F:1:SER:N      | 2:F:34:ASP:OD1   | 2.00                     | 0.94              |
| 1:Q:235:PRO:HG2  | 1:Q:237:LYS:CG   | 1.97                     | 0.94              |
| 2:F:202:VAL:CG1  | 2:F:203:ASP:H    | 1.79                     | 0.94              |
| 2:D:205:ILE:HG13 | 2:D:260:CYS:SG   | 2.07                     | 0.93              |
| 1:Q:102:ARG:HH11 | 1:Q:102:ARG:HG2  | 1.34                     | 0.93              |
| 1:C:246:THR:H    | 1:C:249:GLU:HG3  | 1.34                     | 0.92              |
| 2:Z:202:VAL:HG12 | 2:Z:203:ASP:N    | 1.85                     | 0.92              |
| 1:Q:183:GLN:HE21 | 1:Q:184:LEU:H    | 0.93                     | 0.91              |
| 2:F:31:SER:HA    | 1:Q:91:ALA:HA    | 1.53                     | 0.91              |
| 1:Q:102:ARG:HG2  | 1:Q:102:ARG:NH1  | 1.83                     | 0.91              |
| 2:Z:202:VAL:HG12 | 2:Z:203:ASP:H    | 1.37                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Z:202:VAL:CG1  | 2:Z:203:ASP:H    | 1.84                     | 0.90              |
| 2:B:197:ILE:CD1  | 2:B:248:ARG:HE   | 1.84                     | 0.89              |
| 1:E:168:MET:HB2  | 1:E:168:MET:CE   | 2.03                     | 0.89              |
| 2:F:219:GLU:OE2  | 2:F:222:ARG:HD2  | 1.73                     | 0.89              |
| 1:C:246:THR:O    | 1:C:247:ILE:C    | 2.10                     | 0.89              |
| 1:A:246:THR:N    | 1:A:249:GLU:HG3  | 1.87                     | 0.88              |
| 1:C:47:MET:CE    | 1:C:80:GLY:HA3   | 2.05                     | 0.86              |
| 2:F:1:SER:N      | 2:F:34:ASP:CG    | 2.28                     | 0.86              |
| 1:Q:183:GLN:NE2  | 1:Q:184:LEU:H    | 1.72                     | 0.85              |
| 1:C:230:ARG:NH2  | 2:D:124:GLN:HE22 | 1.75                     | 0.84              |
| 1:A:239:ARG:O    | 1:A:239:ARG:HG3  | 1.75                     | 0.84              |
| 1:Q:183:GLN:HE21 | 1:Q:184:LEU:N    | 1.75                     | 0.83              |
| 1:E:226:MET:HE3  | 2:F:112:TYR:O    | 1.77                     | 0.83              |
| 1:C:243:ILE:CD1  | 1:C:253:LYS:HG3  | 2.05                     | 0.83              |
| 2:B:202:VAL:HG12 | 2:B:203:ASP:H    | 1.41                     | 0.83              |
| 2:Z:246:LYS:HE2  | 2:Z:249:GLN:HE22 | 1.44                     | 0.82              |
| 1:C:74:ARG:NH2   | 1:C:203:LYS:O    | 2.13                     | 0.82              |
| 2:B:202:VAL:CG1  | 2:B:203:ASP:N    | 2.42                     | 0.81              |
| 1:C:66:PRO:O     | 1:C:86:ARG:HD2   | 1.80                     | 0.81              |
| 1:A:28:GLU:OE2   | 1:A:33:TYR:OH    | 1.99                     | 0.81              |
| 2:F:219:GLU:OE2  | 2:F:222:ARG:CD   | 2.28                     | 0.81              |
| 2:B:197:ILE:HD13 | 2:B:248:ARG:HE   | 1.46                     | 0.81              |
| 1:Q:102:ARG:HH11 | 1:Q:102:ARG:CG   | 1.92                     | 0.80              |
| 2:F:120:ILE:HB   | 2:F:131:THR:HB   | 1.63                     | 0.80              |
| 1:C:15:GLU:O     | 1:C:16:ASP:HB2   | 1.79                     | 0.80              |
| 1:A:20:ARG:CB    | 1:A:22:ASP:HA    | 2.10                     | 0.80              |
| 1:C:162:ARG:HE   | 1:C:170:GLN:NE2  | 1.79                     | 0.80              |
| 1:A:102:ARG:HG3  | 1:A:102:ARG:HH11 | 1.48                     | 0.80              |
| 1:A:246:THR:H    | 1:A:249:GLU:CG   | 1.93                     | 0.79              |
| 2:D:243:TRP:O    | 2:D:244:LEU:HG   | 1.81                     | 0.79              |
| 2:Z:202:VAL:CG1  | 2:Z:203:ASP:N    | 2.44                     | 0.78              |
| 2:F:219:GLU:CD   | 2:F:222:ARG:HD2  | 2.03                     | 0.77              |
| 1:C:129:SER:HB3  | 2:D:104:SER:HB3  | 1.66                     | 0.77              |
| 1:Q:1:MET:HG3    | 1:Q:153:PRO:HB3  | 1.67                     | 0.77              |
| 2:D:223:GLU:O    | 2:D:226:ASP:HB2  | 1.84                     | 0.76              |
| 1:Q:108:ILE:HG21 | 1:Q:138:LEU:HD11 | 1.66                     | 0.76              |
| 1:A:247:ILE:HG22 | 2:B:313:GLU:HG2  | 1.66                     | 0.76              |
| 1:A:254:ILE:HD11 | 2:B:303:ILE:HD13 | 1.66                     | 0.76              |
| 2:F:310:ILE:O    | 2:F:314:LEU:HB2  | 1.85                     | 0.76              |
| 2:D:200:THR:HA   | 2:D:202:VAL:HG23 | 1.68                     | 0.75              |
| 2:D:264:VAL:HG12 | 2:D:266:MET:HE2  | 1.67                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:202:VAL:HG13 | 2:F:203:ASP:H    | 1.52                     | 0.75              |
| 2:B:202:VAL:CG1  | 2:B:203:ASP:H    | 1.97                     | 0.75              |
| 1:E:42:SER:HB2   | 1:E:182:ILE:HG13 | 1.67                     | 0.75              |
| 1:E:15:GLU:O     | 1:E:16:ASP:HB2   | 1.86                     | 0.74              |
| 1:Q:243:ILE:HD13 | 1:Q:253:LYS:HG3  | 1.70                     | 0.74              |
| 2:F:313:GLU:O    | 2:F:316:ALA:N    | 2.21                     | 0.73              |
| 1:E:232:MET:HG3  | 2:F:141:VAL:HG22 | 1.70                     | 0.73              |
| 2:D:204:PHE:CE1  | 2:D:230:ALA:HB2  | 2.22                     | 0.73              |
| 2:F:31:SER:HB3   | 1:Q:90:ASP:O     | 1.88                     | 0.73              |
| 2:D:310:ILE:O    | 2:D:314:LEU:HB2  | 1.88                     | 0.73              |
| 1:E:246:THR:N    | 1:E:249:GLU:HG3  | 2.02                     | 0.73              |
| 1:C:53:SER:HG    | 1:C:55:THR:HG22  | 1.52                     | 0.72              |
| 1:E:105:THR:HG23 | 1:E:138:LEU:HG   | 1.71                     | 0.72              |
| 2:B:313:GLU:HA   | 2:B:316:ALA:HB3  | 1.70                     | 0.72              |
| 1:A:136:SER:HB2  | 2:B:105:SER:OG   | 1.88                     | 0.72              |
| 1:E:1:MET:CG     | 1:E:153:PRO:HB3  | 2.16                     | 0.72              |
| 2:F:206:MET:SD   | 2:F:224:LEU:HD13 | 2.30                     | 0.72              |
| 1:E:246:THR:H    | 1:E:249:GLU:CG   | 2.00                     | 0.71              |
| 2:D:208:ILE:HG12 | 2:D:232:LEU:HD11 | 1.73                     | 0.71              |
| 1:C:53:SER:OG    | 1:C:55:THR:CG2   | 2.35                     | 0.70              |
| 2:D:278:MET:CE   | 2:D:284:ILE:HD13 | 2.22                     | 0.69              |
| 1:A:20:ARG:HB2   | 1:A:22:ASP:HA    | 1.74                     | 0.69              |
| 1:A:236:GLU:OE2  | 2:F:184:GLN:NE2  | 2.26                     | 0.69              |
| 1:Q:105:THR:HG21 | 1:Q:137:TYR:HB3  | 1.75                     | 0.69              |
| 2:D:21:LEU:HD11  | 2:D:94:PRO:HG3   | 1.74                     | 0.69              |
| 2:D:204:PHE:CD2  | 2:D:262:LEU:HD23 | 2.27                     | 0.68              |
| 2:B:95:HIS:CE1   | 2:B:100:LEU:HD21 | 2.27                     | 0.68              |
| 1:E:20:ARG:O     | 1:E:22:ASP:CB    | 2.41                     | 0.68              |
| 1:A:19:ILE:O     | 1:A:20:ARG:C     | 2.32                     | 0.68              |
| 1:E:55:THR:OG1   | 1:E:56:ASP:N     | 2.28                     | 0.67              |
| 2:Z:22:ILE:HD11  | 2:Z:38:VAL:HG21  | 1.74                     | 0.67              |
| 1:A:25:ASP:OD1   | 1:A:26:VAL:N     | 2.24                     | 0.67              |
| 1:E:211:ALA:O    | 1:E:213:ILE:N    | 2.28                     | 0.66              |
| 1:E:10:THR:HG23  | 1:E:36:ASN:HB2   | 1.77                     | 0.66              |
| 1:E:58:GLU:OE2   | 1:E:83:ARG:NH1   | 2.27                     | 0.66              |
| 1:A:183:GLN:HE21 | 1:A:184:LEU:H    | 1.43                     | 0.66              |
| 2:B:246:LYS:NZ   | 2:B:249:GLN:HE22 | 1.94                     | 0.65              |
| 1:A:74:ARG:CG    | 1:A:74:ARG:NE    | 2.57                     | 0.65              |
| 1:C:162:ARG:HE   | 1:C:170:GLN:HE21 | 1.44                     | 0.65              |
| 2:D:25:ALA:HB2   | 2:D:92:LEU:HD12  | 1.78                     | 0.65              |
| 2:F:313:GLU:O    | 2:F:314:LEU:C    | 2.35                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:162:ARG:HH21 | 1:Q:170:GLN:HE22 | 1.45                     | 0.65              |
| 1:Q:121:GLN:HB3  | 1:Q:128:ALA:HB2  | 1.78                     | 0.65              |
| 2:F:157:PRO:O    | 2:F:158:SER:HB2  | 1.97                     | 0.65              |
| 2:F:117:ASP:OD1  | 2:F:156:ARG:HD3  | 1.97                     | 0.65              |
| 1:E:147:ALA:O    | 1:E:186:ILE:HG13 | 1.96                     | 0.65              |
| 2:B:46:ASP:O     | 2:B:48:PHE:N     | 2.29                     | 0.64              |
| 2:D:173:ASN:O    | 2:D:174:VAL:HG12 | 1.97                     | 0.64              |
| 2:Z:8:GLU:O      | 2:Z:15:ARG:HB2   | 1.96                     | 0.64              |
| 1:Q:132:ILE:HG22 | 2:Z:105:SER:HB2  | 1.80                     | 0.64              |
| 1:C:87:VAL:HG21  | 1:C:107:VAL:HG21 | 1.78                     | 0.64              |
| 2:D:310:ILE:CG2  | 2:D:314:LEU:HD22 | 2.25                     | 0.64              |
| 1:C:246:THR:OG1  | 1:C:249:GLU:HG2  | 1.98                     | 0.64              |
| 1:A:38:TRP:HE1   | 1:A:183:GLN:NE2  | 1.95                     | 0.64              |
| 1:A:176:CYS:HA   | 1:A:177:PRO:C    | 2.19                     | 0.63              |
| 2:B:199:ILE:C    | 2:B:201:THR:H    | 2.00                     | 0.63              |
| 2:D:257:VAL:O    | 2:D:257:VAL:HG23 | 1.99                     | 0.63              |
| 1:E:63:SER:HA    | 3:E:1262:AMP:H2  | 1.64                     | 0.63              |
| 1:Q:252:ALA:HA   | 2:Z:317:GLN:HE22 | 1.63                     | 0.63              |
| 2:F:309:ASP:HA   | 2:F:312:GLU:HG2  | 1.81                     | 0.62              |
| 2:B:189:VAL:HG12 | 2:B:190:GLU:N    | 2.14                     | 0.62              |
| 2:D:63:VAL:HG22  | 2:D:174:VAL:HG22 | 1.80                     | 0.62              |
| 1:Q:132:ILE:CG2  | 2:Z:105:SER:HB2  | 2.30                     | 0.62              |
| 2:Z:30:LYS:HE3   | 2:Z:123:TYR:CD2  | 2.35                     | 0.62              |
| 1:C:114:ASP:O    | 1:C:115:MET:HG2  | 2.00                     | 0.61              |
| 1:C:230:ARG:HH22 | 2:D:124:GLN:HE22 | 1.47                     | 0.61              |
| 1:E:236:GLU:O    | 1:E:237:LYS:CB   | 2.39                     | 0.61              |
| 1:C:47:MET:HE2   | 1:C:80:GLY:CA    | 2.21                     | 0.61              |
| 2:B:199:ILE:O    | 2:B:201:THR:N    | 2.33                     | 0.61              |
| 1:C:9:GLN:HG2    | 1:C:33:TYR:HB3   | 1.81                     | 0.61              |
| 2:D:313:GLU:O    | 2:D:317:GLN:HG3  | 2.00                     | 0.61              |
| 2:B:197:ILE:HD11 | 2:B:247:SER:CB   | 2.31                     | 0.61              |
| 2:D:11:ARG:HG3   | 2:D:188:TYR:CE1  | 2.35                     | 0.61              |
| 2:Z:246:LYS:HE2  | 2:Z:249:GLN:NE2  | 2.14                     | 0.61              |
| 2:D:275:MET:HG2  | 2:D:298:ILE:HD11 | 1.81                     | 0.61              |
| 1:A:27:ASP:O     | 1:A:29:ASP:N     | 2.34                     | 0.60              |
| 2:B:238:ILE:HG21 | 2:B:244:LEU:HD12 | 1.83                     | 0.60              |
| 2:F:198:ASP:OD1  | 2:F:198:ASP:N    | 2.33                     | 0.60              |
| 2:D:246:LYS:NZ   | 2:D:249:GLN:HE22 | 2.00                     | 0.60              |
| 1:E:1:MET:HG3    | 1:E:153:PRO:CB   | 2.18                     | 0.60              |
| 2:D:217:ASN:O    | 2:D:220:GLN:HG2  | 2.01                     | 0.60              |
| 2:D:288:ASN:ND2  | 4:D:1319:FAD:H1B | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:87:VAL:HG21  | 1:Q:107:VAL:HG21 | 1.84                     | 0.60              |
| 1:A:74:ARG:CB    | 1:A:74:ARG:CD    | 2.76                     | 0.60              |
| 2:Z:209:GLY:HA3  | 2:Z:267:GLY:O    | 2.01                     | 0.60              |
| 2:D:99:SER:C     | 2:D:101:GLY:H    | 2.05                     | 0.60              |
| 1:A:20:ARG:HB3   | 1:A:22:ASP:HA    | 1.84                     | 0.59              |
| 2:B:46:ASP:O     | 2:B:47:ALA:C     | 2.40                     | 0.59              |
| 2:Z:114:PHE:HA   | 2:Z:152:VAL:O    | 2.03                     | 0.59              |
| 1:C:249:GLU:O    | 1:C:253:LYS:N    | 2.29                     | 0.59              |
| 1:C:65:GLY:O     | 1:C:88:TRP:HB2   | 2.02                     | 0.59              |
| 2:F:199:ILE:C    | 2:F:201:THR:H    | 2.05                     | 0.59              |
| 1:C:1:MET:HG3    | 1:C:153:PRO:HB3  | 1.84                     | 0.59              |
| 2:Z:207:SER:HA   | 2:Z:233:CYS:O    | 2.02                     | 0.59              |
| 2:F:79:VAL:HA    | 2:F:82:LEU:HD12  | 1.84                     | 0.59              |
| 2:F:136:ASN:O    | 2:F:137:GLN:HB2  | 2.03                     | 0.59              |
| 2:B:306:ASP:OD1  | 2:B:308:PHE:N    | 2.35                     | 0.58              |
| 1:E:1:MET:HE2    | 1:E:2:LYS:N      | 2.17                     | 0.58              |
| 2:F:316:ALA:O    | 2:F:317:GLN:C    | 2.42                     | 0.58              |
| 1:Q:254:ILE:HD11 | 2:Z:303:ILE:HD13 | 1.86                     | 0.58              |
| 1:C:98:ILE:O     | 1:C:98:ILE:CG2   | 2.52                     | 0.58              |
| 2:D:76:GLU:O     | 2:D:80:SER:HB3   | 2.04                     | 0.58              |
| 2:D:110:THR:HG21 | 2:D:112:TYR:CE2  | 2.38                     | 0.58              |
| 2:F:266:MET:CG   | 2:F:266:MET:CE   | 2.81                     | 0.58              |
| 2:B:91:VAL:HG13  | 2:B:152:VAL:HG22 | 1.84                     | 0.58              |
| 1:E:1:MET:HE1    | 1:E:3:ILE:HG13   | 1.85                     | 0.58              |
| 2:F:189:VAL:HG12 | 2:F:190:GLU:N    | 2.18                     | 0.58              |
| 2:D:117:ASP:N    | 2:D:154:THR:O    | 2.35                     | 0.58              |
| 1:A:158:ALA:HB2  | 1:A:176:CYS:SG   | 2.43                     | 0.58              |
| 2:Z:120:ILE:HB   | 2:Z:131:THR:HB   | 1.86                     | 0.58              |
| 1:E:1:MET:CE     | 1:E:3:ILE:HG13   | 2.34                     | 0.57              |
| 1:A:186:ILE:O    | 1:A:187:ASN:HB3  | 2.02                     | 0.57              |
| 1:C:47:MET:CE    | 1:C:80:GLY:CA    | 2.78                     | 0.57              |
| 2:F:219:GLU:OE2  | 2:F:222:ARG:HD3  | 2.04                     | 0.57              |
| 2:B:197:ILE:HD12 | 2:B:248:ARG:HE   | 1.67                     | 0.57              |
| 1:E:25:ASP:HA    | 1:E:232:MET:SD   | 2.44                     | 0.57              |
| 2:D:204:PHE:CD1  | 2:D:230:ALA:HB2  | 2.39                     | 0.57              |
| 2:F:199:ILE:HG13 | 2:F:201:THR:OG1  | 2.04                     | 0.57              |
| 1:A:243:ILE:HD13 | 1:A:253:LYS:HG3  | 1.86                     | 0.57              |
| 2:F:316:ALA:O    | 2:F:318:LEU:N    | 2.38                     | 0.57              |
| 2:Z:37:VAL:HG22  | 2:Z:59:GLU:HB2   | 1.85                     | 0.57              |
| 1:Q:259:ASN:C    | 1:Q:261:PHE:N    | 2.58                     | 0.57              |
| 1:E:145:VAL:HG12 | 1:E:145:VAL:O    | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:269:SER:H    | 4:D:1319:FAD:H4B | 1.70                     | 0.56              |
| 1:Q:88:TRP:CG    | 1:Q:89:ASP:N     | 2.73                     | 0.56              |
| 1:Q:230:ARG:HD3  | 2:Z:142:GLU:HG2  | 1.87                     | 0.56              |
| 2:B:134:GLY:O    | 2:B:135:TYR:C    | 2.43                     | 0.56              |
| 2:Z:254:GLY:C    | 2:Z:255:LYS:HE2  | 2.25                     | 0.56              |
| 2:D:46:ASP:O     | 2:D:49:VAL:HG13  | 2.04                     | 0.56              |
| 2:D:63:VAL:HG11  | 2:D:78:SER:HB3   | 1.87                     | 0.56              |
| 2:D:91:VAL:HG13  | 2:D:152:VAL:HG22 | 1.87                     | 0.56              |
| 2:B:312:GLU:O    | 2:B:316:ALA:N    | 2.39                     | 0.56              |
| 2:D:157:PRO:O    | 2:D:158:SER:HB2  | 2.04                     | 0.56              |
| 1:C:98:ILE:O     | 1:C:98:ILE:HG22  | 2.05                     | 0.56              |
| 2:D:99:SER:C     | 2:D:101:GLY:N    | 2.57                     | 0.56              |
| 2:F:232:LEU:O    | 2:F:248:ARG:HD2  | 2.05                     | 0.56              |
| 1:A:247:ILE:HD13 | 1:A:247:ILE:N    | 2.19                     | 0.56              |
| 1:C:89:ASP:OD2   | 1:C:210:LEU:HG   | 2.05                     | 0.56              |
| 1:A:102:ARG:HG3  | 1:A:102:ARG:NH1  | 2.21                     | 0.55              |
| 2:D:264:VAL:HG12 | 2:D:266:MET:CE   | 2.36                     | 0.55              |
| 2:D:99:SER:O     | 2:D:101:GLY:N    | 2.39                     | 0.55              |
| 1:A:63:SER:HB2   | 1:A:73:LEU:HD21  | 1.88                     | 0.55              |
| 1:E:176:CYS:HA   | 1:E:177:PRO:C    | 2.27                     | 0.55              |
| 1:E:17:PHE:HA    | 1:E:30:PHE:CD2   | 2.41                     | 0.55              |
| 2:D:265:ALA:HB1  | 2:D:268:ILE:HD12 | 1.89                     | 0.55              |
| 1:A:87:VAL:HG21  | 1:A:107:VAL:HG21 | 1.89                     | 0.55              |
| 1:C:232:MET:HG2  | 2:D:141:VAL:HG22 | 1.89                     | 0.55              |
| 2:D:246:LYS:HZ2  | 2:D:249:GLN:HE22 | 1.54                     | 0.55              |
| 1:Q:186:ILE:HG23 | 1:Q:187:ASN:ND2  | 2.21                     | 0.55              |
| 1:E:168:MET:HE3  | 1:E:168:MET:HB2  | 1.86                     | 0.55              |
| 1:C:246:THR:O    | 1:C:247:ILE:O    | 2.23                     | 0.55              |
| 1:E:211:ALA:O    | 1:E:212:ASP:C    | 2.43                     | 0.55              |
| 2:B:263:TYR:CE2  | 2:B:278:MET:HE2  | 2.42                     | 0.55              |
| 1:Q:259:ASN:C    | 1:Q:261:PHE:H    | 2.11                     | 0.55              |
| 2:B:224:LEU:HD11 | 2:B:314:LEU:HD23 | 1.89                     | 0.54              |
| 1:C:247:ILE:HG22 | 2:D:313:GLU:HG2  | 1.88                     | 0.54              |
| 2:Z:239:ALA:HB3  | 2:Z:249:GLN:HE21 | 1.71                     | 0.54              |
| 1:E:10:THR:CG2   | 1:E:36:ASN:HB2   | 2.37                     | 0.54              |
| 2:F:309:ASP:O    | 2:F:312:GLU:N    | 2.37                     | 0.54              |
| 2:F:219:GLU:OE1  | 2:F:222:ARG:HD2  | 2.07                     | 0.54              |
| 1:C:75:LYS:O     | 1:C:79:LYS:HG3   | 2.08                     | 0.54              |
| 1:C:246:THR:OG1  | 1:C:249:GLU:CG   | 2.55                     | 0.54              |
| 2:D:266:MET:HG2  | 2:D:307:ILE:HG22 | 1.89                     | 0.54              |
| 2:F:313:GLU:O    | 2:F:315:LYS:N    | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:183:GLN:HG3  | 1:A:184:LEU:N    | 2.23                     | 0.54              |
| 2:Z:60:LEU:HB3   | 2:Z:171:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:246:THR:HB   | 1:A:248:SER:H    | 1.73                     | 0.54              |
| 2:Z:275:MET:HG2  | 2:Z:298:ILE:HD11 | 1.90                     | 0.54              |
| 1:A:226:MET:CE   | 2:B:112:TYR:O    | 2.56                     | 0.54              |
| 2:B:246:LYS:HZ1  | 2:B:249:GLN:HE22 | 1.53                     | 0.53              |
| 1:E:63:SER:HA    | 3:E:1262:AMP:C2  | 2.43                     | 0.53              |
| 1:A:168:MET:CE   | 2:B:190:GLU:OE1  | 2.56                     | 0.53              |
| 2:B:273:GLN:H    | 2:B:273:GLN:NE2  | 2.06                     | 0.53              |
| 1:C:38:TRP:HE1   | 1:C:183:GLN:NE2  | 2.07                     | 0.53              |
| 2:D:200:THR:C    | 2:D:202:VAL:H    | 2.11                     | 0.53              |
| 2:F:256:VAL:HG13 | 2:F:277:GLY:HA2  | 1.89                     | 0.53              |
| 1:A:26:VAL:HG12  | 1:A:27:ASP:N     | 2.23                     | 0.53              |
| 2:F:207:SER:HA   | 2:F:233:CYS:O    | 2.09                     | 0.53              |
| 1:Q:94:GLY:HA3   | 1:Q:222:ALA:HB2  | 1.91                     | 0.53              |
| 2:F:300:LYS:HG2  | 2:F:301:TYR:CE1  | 2.43                     | 0.53              |
| 1:E:162:ARG:HE   | 1:E:170:GLN:NE2  | 2.06                     | 0.53              |
| 1:E:209:SER:OG   | 1:E:211:ALA:HB3  | 2.09                     | 0.53              |
| 1:E:237:LYS:O    | 1:E:238:GLY:C    | 2.47                     | 0.53              |
| 1:A:10:THR:HG22  | 1:A:124:ASP:OD1  | 2.09                     | 0.53              |
| 2:B:275:MET:HG2  | 2:B:298:ILE:HD13 | 1.89                     | 0.53              |
| 2:B:79:VAL:O     | 2:B:83:ILE:HG13  | 2.10                     | 0.52              |
| 2:Z:266:MET:HG2  | 2:Z:287:VAL:HB   | 1.90                     | 0.52              |
| 2:F:309:ASP:N    | 2:F:309:ASP:OD1  | 2.41                     | 0.52              |
| 1:E:254:ILE:O    | 1:E:258:ILE:HG13 | 2.10                     | 0.52              |
| 1:C:230:ARG:NH2  | 2:D:124:GLN:NE2  | 2.53                     | 0.52              |
| 1:Q:210:LEU:HB3  | 1:Q:215:LEU:HB2  | 1.91                     | 0.52              |
| 1:C:28:GLU:OE2   | 1:C:33:TYR:OH    | 2.28                     | 0.52              |
| 1:E:226:MET:CE   | 2:F:112:TYR:O    | 2.56                     | 0.52              |
| 2:D:119:TYR:CE2  | 2:D:132:ARG:HA   | 2.44                     | 0.52              |
| 2:Z:77:ALA:HB1   | 2:Z:177:PRO:HG2  | 1.92                     | 0.52              |
| 2:B:36:VAL:HG12  | 2:B:36:VAL:O     | 2.09                     | 0.52              |
| 1:E:252:ALA:HA   | 2:F:317:GLN:HE22 | 1.74                     | 0.52              |
| 1:E:183:GLN:HE21 | 1:E:184:LEU:H    | 1.57                     | 0.52              |
| 2:D:251:GLY:HA3  | 4:D:1319:FAD:C4  | 2.40                     | 0.52              |
| 1:A:44:GLU:HG2   | 1:A:189:PRO:HA   | 1.92                     | 0.51              |
| 2:D:290:ASP:O    | 2:D:296:PHE:HE1  | 1.92                     | 0.51              |
| 1:Q:161:ARG:HA   | 1:Q:170:GLN:O    | 2.10                     | 0.51              |
| 1:C:77:LEU:HA    | 1:C:81:ALA:HB3   | 1.91                     | 0.51              |
| 2:F:4:LEU:HB3    | 2:F:91:VAL:HB    | 1.92                     | 0.51              |
| 1:Q:17:PHE:HA    | 1:Q:30:PHE:CD1   | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:208:ILE:HG13 | 2:D:233:CYS:O    | 2.10                     | 0.51              |
| 1:E:15:GLU:O     | 1:E:16:ASP:CB    | 2.54                     | 0.51              |
| 2:D:25:ALA:HB2   | 2:D:92:LEU:CD1   | 2.40                     | 0.51              |
| 1:A:187:ASN:OD1  | 1:A:187:ASN:C    | 2.49                     | 0.51              |
| 1:Q:19:ILE:HD13  | 1:Q:26:VAL:HG22  | 1.92                     | 0.51              |
| 2:Z:75:PHE:O     | 2:Z:79:VAL:HG23  | 2.10                     | 0.51              |
| 1:E:247:ILE:N    | 1:E:247:ILE:HD13 | 2.25                     | 0.51              |
| 1:C:38:TRP:NE1   | 1:C:184:LEU:HG   | 2.25                     | 0.51              |
| 2:D:290:ASP:OD1  | 2:D:290:ASP:C    | 2.49                     | 0.51              |
| 1:C:247:ILE:HD12 | 2:D:309:ASP:HB3  | 1.93                     | 0.51              |
| 2:F:235:SER:OG   | 2:F:237:PRO:HD2  | 2.10                     | 0.51              |
| 1:C:186:ILE:HG23 | 1:C:187:ASN:N    | 2.25                     | 0.51              |
| 1:C:183:GLN:HA   | 1:C:183:GLN:HE21 | 1.77                     | 0.50              |
| 1:A:33:TYR:CE1   | 1:A:68:ARG:HD2   | 2.46                     | 0.50              |
| 1:Q:63:SER:HB2   | 1:Q:73:LEU:HD21  | 1.93                     | 0.50              |
| 2:F:17:VAL:O     | 2:F:18:SER:C     | 2.49                     | 0.50              |
| 2:F:314:LEU:O    | 2:F:318:LEU:HG   | 2.10                     | 0.50              |
| 1:E:183:GLN:HG3  | 1:E:184:LEU:N    | 2.25                     | 0.50              |
| 1:E:38:TRP:HE1   | 1:E:183:GLN:NE2  | 2.09                     | 0.50              |
| 1:E:162:ARG:HE   | 1:E:170:GLN:HE21 | 1.59                     | 0.50              |
| 1:C:233:TYR:O    | 2:D:139:VAL:HB   | 2.11                     | 0.50              |
| 1:A:24:MET:O     | 1:A:25:ASP:HB2   | 2.10                     | 0.50              |
| 1:A:102:ARG:HH11 | 1:A:102:ARG:CG   | 2.22                     | 0.50              |
| 2:B:199:ILE:C    | 2:B:201:THR:N    | 2.64                     | 0.50              |
| 1:E:243:ILE:HD11 | 2:F:301:TYR:HB3  | 1.93                     | 0.50              |
| 2:Z:289:THR:H    | 4:Z:1319:FAD:C2A | 2.23                     | 0.50              |
| 1:E:186:ILE:HG23 | 1:E:187:ASN:ND2  | 2.27                     | 0.50              |
| 2:D:20:GLU:HG2   | 2:D:160:PHE:O    | 2.11                     | 0.50              |
| 2:Z:273:GLN:NE2  | 2:Z:273:GLN:H    | 2.10                     | 0.50              |
| 2:D:202:VAL:CG1  | 2:D:203:ASP:N    | 2.45                     | 0.50              |
| 1:E:216:SER:O    | 1:E:218:ASN:N    | 2.44                     | 0.50              |
| 2:D:176:ALA:C    | 2:D:177:PRO:O    | 2.46                     | 0.50              |
| 2:D:120:ILE:HG13 | 2:D:131:THR:HB   | 1.94                     | 0.50              |
| 1:C:19:ILE:O     | 1:C:20:ARG:C     | 2.50                     | 0.50              |
| 1:E:258:ILE:O    | 1:E:261:PHE:HB3  | 2.12                     | 0.49              |
| 2:Z:236:ARG:HB2  | 4:Z:1319:FAD:C2  | 2.42                     | 0.49              |
| 2:F:273:GLN:H    | 2:F:273:GLN:NE2  | 2.10                     | 0.49              |
| 1:Q:131:GLY:O    | 1:Q:179:VAL:HG11 | 2.12                     | 0.49              |
| 1:E:74:ARG:NH2   | 1:E:201:ALA:O    | 2.37                     | 0.49              |
| 1:C:165:GLU:OE2  | 2:D:97:VAL:HG23  | 2.13                     | 0.49              |
| 1:C:8:LYS:HG3    | 3:C:1262:AMP:N7  | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:146:VAL:HG22 | 1:E:160:ILE:HD13 | 1.94                     | 0.49              |
| 2:D:38:VAL:HG11  | 2:D:52:LEU:HD22  | 1.95                     | 0.49              |
| 2:F:71:ASP:OD1   | 2:F:74:VAL:HG23  | 2.12                     | 0.49              |
| 1:A:65:GLY:HA3   | 1:A:69:VAL:HG21  | 1.94                     | 0.49              |
| 1:E:246:THR:O    | 1:E:247:ILE:C    | 2.51                     | 0.49              |
| 2:D:134:GLY:O    | 2:D:135:TYR:C    | 2.50                     | 0.49              |
| 2:B:49:VAL:O     | 2:B:53:SER:OG    | 2.13                     | 0.49              |
| 2:F:165:GLY:O    | 2:F:166:ALA:O    | 2.30                     | 0.49              |
| 1:E:36:ASN:HD21  | 1:E:38:TRP:HB2   | 1.77                     | 0.49              |
| 1:C:20:ARG:HB3   | 1:C:22:ASP:HA    | 1.95                     | 0.49              |
| 1:A:129:SER:HB3  | 2:B:104:SER:HB3  | 1.95                     | 0.49              |
| 1:Q:149:LEU:HD13 | 1:Q:180:LEU:CD1  | 2.43                     | 0.49              |
| 2:D:238:ILE:HG21 | 2:D:244:LEU:HD12 | 1.95                     | 0.49              |
| 2:D:269:SER:HB3  | 4:D:1319:FAD:O1P | 2.12                     | 0.49              |
| 2:D:46:ASP:O     | 2:D:47:ALA:C     | 2.52                     | 0.49              |
| 2:D:264:VAL:HG12 | 2:D:264:VAL:O    | 2.13                     | 0.48              |
| 1:A:230:ARG:O    | 1:A:231:ARG:HB3  | 2.12                     | 0.48              |
| 2:B:310:ILE:O    | 2:B:314:LEU:HB2  | 2.12                     | 0.48              |
| 1:Q:63:SER:HA    | 3:Q:1262:AMP:H2  | 1.78                     | 0.48              |
| 2:B:57:VAL:HG12  | 2:B:169:PRO:HB3  | 1.95                     | 0.48              |
| 1:A:26:VAL:CG1   | 1:A:27:ASP:N     | 2.76                     | 0.48              |
| 1:A:183:GLN:NE2  | 1:A:184:LEU:H    | 2.09                     | 0.48              |
| 2:F:199:ILE:C    | 2:F:201:THR:N    | 2.67                     | 0.48              |
| 1:Q:252:ALA:CA   | 2:Z:317:GLN:HE22 | 2.27                     | 0.48              |
| 1:C:183:GLN:HE21 | 1:C:184:LEU:H    | 1.62                     | 0.48              |
| 1:C:254:ILE:O    | 1:C:258:ILE:HG13 | 2.12                     | 0.48              |
| 2:Z:202:VAL:HG13 | 2:Z:203:ASP:H    | 1.72                     | 0.48              |
| 1:Q:8:LYS:HB2    | 3:Q:1262:AMP:C5  | 2.48                     | 0.48              |
| 1:A:231:ARG:HG3  | 1:A:231:ARG:O    | 2.11                     | 0.48              |
| 1:Q:120:VAL:HG22 | 1:Q:145:VAL:HA   | 1.96                     | 0.48              |
| 2:F:46:ASP:O     | 2:F:49:VAL:HG13  | 2.13                     | 0.48              |
| 1:E:2:LYS:NZ     | 1:E:111:GLU:OE1  | 2.47                     | 0.48              |
| 1:C:130:THR:OG1  | 3:C:1262:AMP:O2P | 2.25                     | 0.48              |
| 2:Z:5:VAL:HG22   | 2:Z:92:LEU:HB2   | 1.94                     | 0.48              |
| 2:F:199:ILE:HG12 | 2:F:201:THR:HB   | 1.95                     | 0.48              |
| 2:D:215:GLU:O    | 2:D:218:VAL:HG23 | 2.14                     | 0.48              |
| 1:E:237:LYS:HA   | 2:F:297:THR:HG22 | 1.96                     | 0.48              |
| 2:F:189:VAL:CG1  | 2:F:190:GLU:N    | 2.77                     | 0.47              |
| 1:A:226:MET:HE2  | 2:B:112:TYR:O    | 2.14                     | 0.47              |
| 1:C:102:ARG:HH11 | 1:C:102:ARG:HG2  | 1.78                     | 0.47              |
| 1:E:237:LYS:C    | 1:E:238:GLY:O    | 2.51                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:110:LYS:HD2  | 1:Q:213:ILE:HG22 | 1.95                     | 0.47              |
| 1:E:4:LEU:C      | 1:E:4:LEU:HD23   | 2.34                     | 0.47              |
| 2:F:219:GLU:OE1  | 2:F:222:ARG:NH1  | 2.46                     | 0.47              |
| 2:B:201:THR:HG22 | 2:B:259:SER:OG   | 2.14                     | 0.47              |
| 2:D:228:ALA:HA   | 2:D:318:LEU:CD1  | 2.45                     | 0.47              |
| 1:Q:15:GLU:O     | 1:Q:16:ASP:HB2   | 2.14                     | 0.47              |
| 2:D:205:ILE:HG13 | 2:D:260:CYS:HG   | 1.77                     | 0.47              |
| 1:E:183:GLN:NE2  | 1:E:184:LEU:H    | 2.12                     | 0.47              |
| 1:C:102:ARG:HH11 | 1:C:102:ARG:CG   | 2.28                     | 0.47              |
| 1:C:226:MET:HE1  | 2:D:111:GLY:HA2  | 1.95                     | 0.47              |
| 1:C:129:SER:HB3  | 2:D:104:SER:CB   | 2.41                     | 0.47              |
| 1:E:106:GLU:HB3  | 1:E:213:ILE:HB   | 1.96                     | 0.47              |
| 2:B:273:GLN:H    | 2:B:273:GLN:HE21 | 1.62                     | 0.47              |
| 2:B:168:SER:O    | 2:B:169:PRO:C    | 2.52                     | 0.47              |
| 1:C:176:CYS:HA   | 1:C:177:PRO:C    | 2.35                     | 0.47              |
| 1:A:66:PRO:O     | 1:A:86:ARG:HD2   | 2.13                     | 0.47              |
| 1:A:15:GLU:O     | 1:A:16:ASP:HB2   | 2.14                     | 0.47              |
| 1:A:162:ARG:HH21 | 1:A:170:GLN:HE22 | 1.62                     | 0.47              |
| 2:B:52:LEU:HD23  | 2:B:52:LEU:HA    | 1.81                     | 0.47              |
| 1:E:141:PRO:HG2  | 1:E:177:PRO:O    | 2.15                     | 0.47              |
| 1:A:77:LEU:HD23  | 1:A:77:LEU:HA    | 1.56                     | 0.47              |
| 1:E:98:ILE:N     | 1:E:98:ILE:HD12  | 2.28                     | 0.47              |
| 2:D:228:ALA:HA   | 2:D:318:LEU:HD12 | 1.97                     | 0.47              |
| 1:E:1:MET:HA     | 1:E:114:ASP:OD1  | 2.14                     | 0.47              |
| 1:C:239:ARG:HG2  | 2:D:297:THR:HA   | 1.96                     | 0.47              |
| 2:D:86:HIS:O     | 2:D:87:ASN:C     | 2.52                     | 0.47              |
| 2:B:63:VAL:HG13  | 2:B:174:VAL:HG23 | 1.96                     | 0.47              |
| 2:D:199:ILE:HG13 | 2:D:201:THR:HB   | 1.97                     | 0.47              |
| 2:B:238:ILE:CG2  | 2:B:244:LEU:HD12 | 2.45                     | 0.47              |
| 1:C:156:ASN:ND2  | 1:C:157:LYS:HG3  | 2.29                     | 0.47              |
| 1:C:36:ASN:O     | 1:C:37:GLU:C     | 2.52                     | 0.47              |
| 2:F:215:GLU:HB2  | 2:F:243:TRP:CD2  | 2.50                     | 0.47              |
| 2:D:11:ARG:CG    | 2:D:188:TYR:CE1  | 2.98                     | 0.46              |
| 1:C:102:ARG:NH1  | 1:C:102:ARG:HG2  | 2.29                     | 0.46              |
| 2:F:215:GLU:HB2  | 2:F:243:TRP:CE2  | 2.50                     | 0.46              |
| 1:C:112:ALA:N    | 1:C:113:PRO:CD   | 2.78                     | 0.46              |
| 1:A:102:ARG:CG   | 1:A:102:ARG:NH1  | 2.77                     | 0.46              |
| 2:D:283:THR:HG23 | 2:D:300:LYS:HD3  | 1.96                     | 0.46              |
| 1:E:210:LEU:O    | 1:E:213:ILE:HG13 | 2.16                     | 0.46              |
| 2:Z:269:SER:HB3  | 4:Z:1319:FAD:O5B | 2.16                     | 0.46              |
| 2:Z:19:LEU:HA    | 2:Z:19:LEU:HD22  | 1.54                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:163:LEU:HD22 | 2:B:163:LEU:H    | 1.80                     | 0.46              |
| 1:A:247:ILE:N    | 1:A:247:ILE:CD1  | 2.75                     | 0.46              |
| 2:D:278:MET:HE2  | 2:D:278:MET:C    | 2.35                     | 0.46              |
| 1:E:170:GLN:HB2  | 2:F:188:TYR:CD2  | 2.50                     | 0.46              |
| 1:Q:63:SER:HB3   | 1:Q:69:VAL:HG11  | 1.98                     | 0.46              |
| 1:C:67:ASP:C     | 1:C:69:VAL:H     | 2.17                     | 0.46              |
| 1:E:216:SER:C    | 1:E:218:ASN:N    | 2.67                     | 0.46              |
| 1:Q:165:GLU:OE2  | 2:Z:97:VAL:HG23  | 2.15                     | 0.46              |
| 1:E:168:MET:HE2  | 1:E:168:MET:HB2  | 1.95                     | 0.46              |
| 1:C:186:ILE:CG2  | 1:C:187:ASN:N    | 2.78                     | 0.46              |
| 1:Q:164:LEU:HD13 | 2:Z:10:ARG:NE    | 2.31                     | 0.46              |
| 2:D:137:GLN:NE2  | 2:D:156:ARG:HH12 | 2.13                     | 0.46              |
| 2:B:272:ILE:HD13 | 2:B:272:ILE:HA   | 1.73                     | 0.46              |
| 2:B:1:SER:HB2    | 2:B:34:ASP:OD1   | 2.16                     | 0.46              |
| 1:Q:38:TRP:HE1   | 1:Q:183:GLN:HE22 | 1.64                     | 0.46              |
| 2:B:46:ASP:C     | 2:B:48:PHE:N     | 2.69                     | 0.46              |
| 2:D:273:GLN:NE2  | 4:D:1319:FAD:O2' | 2.49                     | 0.46              |
| 2:D:284:ILE:HB   | 2:D:299:ALA:HA   | 1.98                     | 0.46              |
| 1:A:65:GLY:O     | 1:A:88:TRP:HB2   | 2.16                     | 0.45              |
| 2:F:212:ILE:HG22 | 2:F:221:PHE:CE1  | 2.51                     | 0.45              |
| 1:E:168:MET:CB   | 1:E:168:MET:CE   | 2.85                     | 0.45              |
| 2:F:1:SER:H3     | 2:F:34:ASP:CG    | 2.15                     | 0.45              |
| 1:Q:4:LEU:HD22   | 1:Q:108:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:182:ILE:N    | 1:A:182:ILE:HD13 | 2.31                     | 0.45              |
| 1:A:36:ASN:O     | 1:A:37:GLU:C     | 2.53                     | 0.45              |
| 1:E:98:ILE:CD1   | 1:E:98:ILE:N     | 2.79                     | 0.45              |
| 1:Q:164:LEU:HD13 | 2:Z:10:ARG:CZ    | 2.46                     | 0.45              |
| 1:C:162:ARG:HH21 | 1:C:170:GLN:HE22 | 1.62                     | 0.45              |
| 2:D:197:ILE:CB   | 2:D:198:ASP:CG   | 2.85                     | 0.45              |
| 1:A:36:ASN:HD21  | 1:A:38:TRP:HB2   | 1.79                     | 0.45              |
| 1:Q:254:ILE:O    | 1:Q:258:ILE:HG13 | 2.17                     | 0.45              |
| 1:E:216:SER:O    | 1:E:217:ALA:C    | 2.54                     | 0.45              |
| 2:D:176:ALA:O    | 2:D:177:PRO:O    | 2.34                     | 0.45              |
| 1:A:196:GLY:O    | 1:A:197:ILE:C    | 2.54                     | 0.45              |
| 1:C:145:VAL:HG12 | 1:C:145:VAL:O    | 2.15                     | 0.45              |
| 2:D:204:PHE:CZ   | 2:D:230:ALA:HB2  | 2.51                     | 0.45              |
| 1:Q:132:ILE:O    | 1:Q:135:ALA:HB3  | 2.17                     | 0.45              |
| 1:C:183:GLN:NE2  | 1:C:184:LEU:H    | 2.14                     | 0.45              |
| 1:C:44:GLU:HB3   | 1:C:187:ASN:ND2  | 2.31                     | 0.45              |
| 2:B:260:CYS:O    | 2:B:281:VAL:HG13 | 2.17                     | 0.45              |
| 2:D:264:VAL:CG1  | 2:D:266:MET:CE   | 2.95                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:73:LEU:O     | 1:E:76:CYS:HB2   | 2.16                     | 0.45              |
| 2:D:92:LEU:HD22  | 2:D:155:ILE:HD11 | 1.99                     | 0.45              |
| 2:D:251:GLY:HA3  | 4:D:1319:FAD:O4  | 2.16                     | 0.45              |
| 2:B:197:ILE:HD13 | 2:B:248:ARG:NE   | 2.23                     | 0.45              |
| 2:B:189:VAL:CG1  | 2:B:190:GLU:N    | 2.76                     | 0.45              |
| 2:D:251:GLY:HA3  | 4:D:1319:FAD:N3  | 2.32                     | 0.45              |
| 2:F:306:ASP:OD1  | 2:F:308:PHE:CD1  | 2.70                     | 0.45              |
| 1:C:79:LYS:O     | 1:C:190:ARG:HD2  | 2.17                     | 0.45              |
| 2:D:69:ASP:O     | 2:D:70:PHE:C     | 2.51                     | 0.45              |
| 1:C:150:GLN:HE21 | 1:C:150:GLN:HB3  | 1.43                     | 0.45              |
| 2:F:174:VAL:HG23 | 2:F:175:ASP:N    | 2.32                     | 0.45              |
| 1:C:216:SER:O    | 1:C:217:ALA:C    | 2.54                     | 0.45              |
| 1:A:20:ARG:HB3   | 1:A:22:ASP:CA    | 2.47                     | 0.45              |
| 2:D:41:ILE:HG12  | 2:D:63:VAL:HB    | 1.99                     | 0.45              |
| 1:A:53:SER:OG    | 1:A:55:THR:HG23  | 2.17                     | 0.45              |
| 2:D:273:GLN:HG2  | 4:D:1319:FAD:C9A | 2.47                     | 0.44              |
| 2:D:218:VAL:O    | 2:D:221:PHE:N    | 2.50                     | 0.44              |
| 2:B:281:VAL:HG13 | 2:B:282:PRO:HD2  | 1.98                     | 0.44              |
| 1:Q:102:ARG:NH1  | 1:Q:102:ARG:CG   | 2.54                     | 0.44              |
| 1:Q:253:LYS:HD2  | 1:Q:257:ILE:HD11 | 1.97                     | 0.44              |
| 2:D:273:GLN:O    | 2:D:274:HIS:C    | 2.53                     | 0.44              |
| 1:C:183:GLN:HE21 | 1:C:183:GLN:CA   | 2.29                     | 0.44              |
| 2:B:284:ILE:HG21 | 2:B:284:ILE:HD13 | 1.64                     | 0.44              |
| 2:D:112:TYR:CD1  | 2:D:150:THR:HB   | 2.53                     | 0.44              |
| 1:A:124:ASP:OD1  | 1:A:124:ASP:N    | 2.50                     | 0.44              |
| 2:F:260:CYS:SG   | 2:F:262:LEU:O    | 2.76                     | 0.44              |
| 1:C:136:SER:HB2  | 2:D:105:SER:OG   | 2.17                     | 0.44              |
| 2:D:208:ILE:HD11 | 2:D:244:LEU:HD11 | 1.98                     | 0.44              |
| 1:Q:231:ARG:CZ   | 1:Q:233:TYR:CE2  | 3.01                     | 0.44              |
| 2:F:60:LEU:HD23  | 2:F:60:LEU:HA    | 1.62                     | 0.44              |
| 2:Z:8:GLU:HG2    | 2:Z:15:ARG:HD3   | 2.00                     | 0.44              |
| 1:E:216:SER:C    | 1:E:218:ASN:H    | 2.21                     | 0.44              |
| 2:B:159:VAL:HG12 | 2:B:160:PHE:CD1  | 2.53                     | 0.44              |
| 1:C:96:ASP:OD1   | 1:C:96:ASP:C     | 2.54                     | 0.44              |
| 1:E:242:MET:CE   | 1:E:242:MET:CG   | 2.94                     | 0.44              |
| 1:C:230:ARG:HH22 | 2:D:124:GLN:NE2  | 2.14                     | 0.44              |
| 2:B:263:TYR:CD2  | 2:B:278:MET:HE2  | 2.53                     | 0.44              |
| 1:C:156:ASN:HD22 | 1:C:157:LYS:HG3  | 1.82                     | 0.44              |
| 2:D:238:ILE:HA   | 2:D:238:ILE:HD12 | 1.93                     | 0.44              |
| 1:Q:39:ASP:HA    | 1:Q:42:SER:HB3   | 1.98                     | 0.44              |
| 1:E:75:LYS:O     | 1:E:79:LYS:HG3   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:20:ARG:O     | 1:A:22:ASP:CB     | 2.65                     | 0.44              |
| 2:B:314:LEU:HA   | 2:B:314:LEU:HD12  | 1.82                     | 0.44              |
| 2:D:119:TYR:CD2  | 2:D:119:TYR:N     | 2.85                     | 0.44              |
| 1:C:121:GLN:C    | 3:C:1262:AMP:H5'2 | 2.38                     | 0.43              |
| 1:C:228:ARG:NH2  | 2:D:144:ASP:OD2   | 2.50                     | 0.43              |
| 1:E:174:ILE:HG12 | 1:E:175:ASN:N     | 2.31                     | 0.43              |
| 2:D:316:ALA:O    | 2:D:318:LEU:N     | 2.50                     | 0.43              |
| 1:C:102:ARG:HD3  | 1:C:102:ARG:O     | 2.17                     | 0.43              |
| 1:Q:23:GLY:O     | 1:Q:231:ARG:HA    | 2.18                     | 0.43              |
| 2:Z:295:ILE:HG13 | 2:Z:295:ILE:O     | 2.17                     | 0.43              |
| 1:E:246:THR:C    | 1:E:248:SER:N     | 2.71                     | 0.43              |
| 1:E:136:SER:HB2  | 2:F:105:SER:OG    | 2.19                     | 0.43              |
| 1:E:88:TRP:CG    | 1:E:89:ASP:N      | 2.87                     | 0.43              |
| 1:C:120:VAL:HG23 | 1:C:182:ILE:O     | 2.18                     | 0.43              |
| 1:E:252:ALA:O    | 1:E:256:GLN:HG3   | 2.19                     | 0.43              |
| 1:A:168:MET:HE3  | 2:B:190:GLU:OE1   | 2.18                     | 0.43              |
| 2:Z:113:GLY:O    | 2:Z:114:PHE:HB2   | 2.17                     | 0.43              |
| 2:B:4:LEU:HB3    | 2:B:91:VAL:HB     | 1.98                     | 0.43              |
| 2:D:49:VAL:HB    | 2:D:60:LEU:HD13   | 2.00                     | 0.43              |
| 2:D:290:ASP:HA   | 2:D:291:PRO:HD3   | 1.77                     | 0.43              |
| 1:C:243:ILE:HG22 | 1:C:250:GLN:HG2   | 2.00                     | 0.43              |
| 1:Q:18:GLU:HG3   | 1:Q:30:PHE:CE1    | 2.52                     | 0.43              |
| 1:Q:13:LEU:HD22  | 1:Q:26:VAL:HG11   | 2.01                     | 0.43              |
| 1:E:47:MET:CE    | 1:E:80:GLY:HA3    | 2.48                     | 0.43              |
| 1:E:87:VAL:HG21  | 1:E:107:VAL:HG21  | 2.00                     | 0.43              |
| 1:C:249:GLU:H    | 1:C:249:GLU:HG2   | 1.44                     | 0.43              |
| 1:A:243:ILE:HG21 | 1:A:253:LYS:HG3   | 1.99                     | 0.43              |
| 1:E:117:PHE:CD1  | 1:E:117:PHE:N     | 2.85                     | 0.43              |
| 1:E:33:TYR:CD1   | 1:E:68:ARG:HD2    | 2.53                     | 0.43              |
| 1:C:258:ILE:O    | 1:C:261:PHE:HB3   | 2.19                     | 0.43              |
| 2:D:2:LYS:NZ     | 2:D:86:HIS:ND1    | 2.65                     | 0.43              |
| 2:B:163:LEU:HD22 | 2:B:163:LEU:N     | 2.34                     | 0.43              |
| 2:F:306:ASP:OD1  | 2:F:308:PHE:N     | 2.46                     | 0.43              |
| 2:B:222:ARG:HA   | 2:B:232:LEU:HD22  | 2.00                     | 0.43              |
| 1:Q:38:TRP:HE1   | 1:Q:183:GLN:NE2   | 2.17                     | 0.43              |
| 2:D:264:VAL:HG11 | 2:D:266:MET:HE1   | 2.01                     | 0.43              |
| 1:E:73:LEU:HD23  | 1:E:73:LEU:HA     | 1.56                     | 0.43              |
| 1:A:120:VAL:HG22 | 1:A:145:VAL:HA    | 2.01                     | 0.43              |
| 1:A:226:MET:HE3  | 2:B:112:TYR:O     | 2.18                     | 0.43              |
| 2:Z:214:GLU:N    | 2:Z:214:GLU:OE2   | 2.52                     | 0.43              |
| 1:E:35:LEU:HD12  | 1:E:35:LEU:HA     | 1.77                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:272:ILE:HG23 | 2:D:272:ILE:HD12 | 1.77                     | 0.42              |
| 2:B:127:GLU:HA   | 2:B:127:GLU:OE2  | 2.19                     | 0.42              |
| 1:C:87:VAL:HG22  | 1:C:208:VAL:HB   | 2.01                     | 0.42              |
| 1:C:182:ILE:HG23 | 1:C:182:ILE:HD12 | 1.76                     | 0.42              |
| 1:E:253:LYS:O    | 1:E:254:ILE:C    | 2.56                     | 0.42              |
| 2:B:11:ARG:O     | 2:B:12:ASN:HB2   | 2.19                     | 0.42              |
| 2:B:6:ILE:HD12   | 2:B:79:VAL:HG22  | 2.01                     | 0.42              |
| 1:C:20:ARG:CB    | 1:C:22:ASP:HA    | 2.50                     | 0.42              |
| 1:Q:7:VAL:HG12   | 1:Q:39:ASP:HB3   | 2.00                     | 0.42              |
| 2:Z:199:ILE:C    | 2:Z:201:THR:H    | 2.23                     | 0.42              |
| 1:E:104:LEU:HA   | 1:E:104:LEU:HD23 | 1.55                     | 0.42              |
| 2:D:46:ASP:C     | 2:D:48:PHE:N     | 2.69                     | 0.42              |
| 1:E:261:PHE:CD1  | 1:E:261:PHE:C    | 2.93                     | 0.42              |
| 1:A:162:ARG:HD2  | 1:A:162:ARG:HH11 | 1.59                     | 0.42              |
| 1:Q:103:ILE:HD13 | 1:Q:103:ILE:HG21 | 1.79                     | 0.42              |
| 2:B:186:LYS:HA   | 2:B:186:LYS:HD2  | 1.72                     | 0.42              |
| 1:E:8:LYS:HD3    | 1:E:10:THR:HG22  | 2.01                     | 0.42              |
| 2:D:71:ASP:OD1   | 2:D:74:VAL:HG23  | 2.20                     | 0.42              |
| 2:B:204:PHE:CE2  | 2:B:262:LEU:HD23 | 2.54                     | 0.42              |
| 2:F:42:GLY:O     | 2:F:64:LYS:HA    | 2.20                     | 0.42              |
| 2:B:236:ARG:HB2  | 4:B:1319:FAD:C2  | 2.50                     | 0.42              |
| 1:A:25:ASP:HA    | 1:A:232:MET:SD   | 2.59                     | 0.42              |
| 2:D:266:MET:HB3  | 2:D:307:ILE:HG21 | 2.00                     | 0.42              |
| 2:D:298:ILE:H    | 2:D:298:ILE:HG13 | 1.65                     | 0.42              |
| 2:F:273:GLN:H    | 2:F:273:GLN:HE21 | 1.66                     | 0.42              |
| 2:D:28:LEU:HD13  | 2:D:121:VAL:HG13 | 2.01                     | 0.42              |
| 2:B:210:ARG:O    | 2:B:212:ILE:N    | 2.53                     | 0.42              |
| 1:E:38:TRP:NE1   | 1:E:184:LEU:HG   | 2.35                     | 0.42              |
| 1:E:58:GLU:HA    | 1:E:82:ASP:OD2   | 2.20                     | 0.42              |
| 1:A:182:ILE:HG22 | 1:A:183:GLN:N    | 2.34                     | 0.42              |
| 1:A:215:LEU:HA   | 1:A:215:LEU:HD23 | 1.85                     | 0.42              |
| 1:C:116:VAL:O    | 1:C:179:VAL:HA   | 2.20                     | 0.42              |
| 1:E:13:LEU:HA    | 1:E:13:LEU:HD23  | 1.81                     | 0.42              |
| 2:Z:238:ILE:HG21 | 2:Z:244:LEU:HD12 | 2.02                     | 0.42              |
| 1:E:17:PHE:HA    | 1:E:30:PHE:CG    | 2.55                     | 0.42              |
| 2:D:244:LEU:HA   | 2:D:245:PRO:HD2  | 1.79                     | 0.41              |
| 2:F:75:PHE:O     | 2:F:79:VAL:HG23  | 2.20                     | 0.41              |
| 2:D:75:PHE:O     | 2:D:79:VAL:HG23  | 2.20                     | 0.41              |
| 1:C:118:ALA:O    | 1:C:181:THR:HA   | 2.20                     | 0.41              |
| 1:C:73:LEU:HA    | 1:C:73:LEU:HD23  | 1.85                     | 0.41              |
| 1:C:53:SER:C     | 1:C:55:THR:H     | 2.23                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:GLN:OE1    | 1:A:68:ARG:HG3   | 2.20                     | 0.41              |
| 2:B:252:GLN:HB3  | 2:B:273:GLN:HB3  | 2.01                     | 0.41              |
| 2:F:45:ALA:HB3   | 2:F:62:VAL:CG1   | 2.50                     | 0.41              |
| 2:F:106:LEU:HD12 | 2:F:106:LEU:HA   | 1.91                     | 0.41              |
| 2:F:224:LEU:HD23 | 2:F:224:LEU:HA   | 1.83                     | 0.41              |
| 1:A:70:ASP:OD1   | 1:A:86:ARG:NE    | 2.52                     | 0.41              |
| 1:E:220:VAL:O    | 1:E:224:GLN:HG2  | 2.20                     | 0.41              |
| 2:F:156:ARG:HG2  | 2:F:159:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:168:MET:HE2  | 2:B:190:GLU:OE1  | 2.20                     | 0.41              |
| 2:F:199:ILE:CG1  | 2:F:201:THR:HB   | 2.49                     | 0.41              |
| 1:E:87:VAL:HG22  | 1:E:208:VAL:HB   | 2.01                     | 0.41              |
| 1:A:125:GLN:O    | 1:A:126:ALA:C    | 2.58                     | 0.41              |
| 1:E:19:ILE:H     | 1:E:19:ILE:HG12  | 1.62                     | 0.41              |
| 1:A:154:GLY:O    | 1:A:155:ASP:O    | 2.39                     | 0.41              |
| 2:Z:245:PRO:C    | 2:Z:247:SER:N    | 2.74                     | 0.41              |
| 1:E:231:ARG:HG3  | 1:E:232:MET:N    | 2.36                     | 0.41              |
| 1:E:246:THR:OG1  | 1:E:249:GLU:HG2  | 2.20                     | 0.41              |
| 1:E:249:GLU:O    | 1:E:252:ALA:N    | 2.54                     | 0.41              |
| 1:C:16:ASP:C     | 1:C:17:PHE:O     | 2.58                     | 0.41              |
| 1:C:9:GLN:CG     | 1:C:33:TYR:HB3   | 2.49                     | 0.41              |
| 1:A:226:MET:HE3  | 2:B:111:GLY:C    | 2.41                     | 0.41              |
| 1:E:228:ARG:NH2  | 2:F:144:ASP:OD2  | 2.42                     | 0.41              |
| 1:E:194:LEU:HA   | 1:E:194:LEU:HD23 | 1.76                     | 0.41              |
| 2:F:224:LEU:O    | 2:F:225:ALA:C    | 2.58                     | 0.41              |
| 2:D:278:MET:O    | 2:D:280:HIS:N    | 2.54                     | 0.41              |
| 2:D:278:MET:HE1  | 2:D:284:ILE:HD13 | 2.01                     | 0.41              |
| 1:C:75:LYS:O     | 1:C:78:ALA:HB3   | 2.21                     | 0.41              |
| 2:Z:215:GLU:O    | 2:Z:218:VAL:HG23 | 2.21                     | 0.41              |
| 1:Q:254:ILE:HD11 | 2:Z:303:ILE:CD1  | 2.50                     | 0.41              |
| 2:D:49:VAL:N     | 2:D:50:PRO:HD2   | 2.35                     | 0.41              |
| 2:F:257:VAL:HG22 | 2:F:277:GLY:O    | 2.20                     | 0.41              |
| 2:B:5:VAL:HG12   | 2:B:6:ILE:N      | 2.32                     | 0.41              |
| 2:D:197:ILE:CB   | 2:D:198:ASP:CB   | 2.99                     | 0.41              |
| 2:Z:199:ILE:O    | 2:Z:201:THR:N    | 2.54                     | 0.41              |
| 1:C:42:SER:O     | 1:C:43:LEU:C     | 2.59                     | 0.41              |
| 2:F:244:LEU:HD23 | 2:F:244:LEU:HA   | 1.89                     | 0.41              |
| 2:B:307:ILE:H    | 2:B:307:ILE:HG12 | 1.61                     | 0.41              |
| 1:E:7:VAL:O      | 1:E:7:VAL:HG23   | 2.20                     | 0.41              |
| 1:Q:176:CYS:HA   | 1:Q:177:PRO:C    | 2.41                     | 0.41              |
| 1:A:27:ASP:C     | 1:A:29:ASP:H     | 2.24                     | 0.41              |
| 1:A:249:GLU:O    | 1:A:250:GLN:C    | 2.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:310:ILE:HD12 | 2:F:310:ILE:HG23 | 1.74                     | 0.41              |
| 2:D:310:ILE:HG22 | 2:D:314:LEU:CD2  | 2.34                     | 0.41              |
| 2:B:102:TYR:O    | 2:B:105:SER:N    | 2.51                     | 0.41              |
| 1:C:87:VAL:CG2   | 1:C:107:VAL:HG21 | 2.49                     | 0.41              |
| 2:B:275:MET:HG2  | 2:B:298:ILE:CD1  | 2.51                     | 0.41              |
| 1:Q:18:GLU:HG3   | 1:Q:30:PHE:HE1   | 1.86                     | 0.41              |
| 2:D:197:ILE:CB   | 2:D:198:ASP:HB2  | 2.50                     | 0.41              |
| 2:B:70:PHE:CG    | 2:B:71:ASP:N     | 2.89                     | 0.41              |
| 1:Q:237:LYS:O    | 1:Q:238:GLY:C    | 2.59                     | 0.41              |
| 1:Q:89:ASP:CB    | 1:Q:210:LEU:HD12 | 2.51                     | 0.41              |
| 1:C:17:PHE:HA    | 1:C:30:PHE:CD1   | 2.56                     | 0.40              |
| 1:E:83:ARG:HH11  | 1:E:83:ARG:HD3   | 1.55                     | 0.40              |
| 1:Q:162:ARG:HH21 | 1:Q:170:GLN:NE2  | 2.15                     | 0.40              |
| 2:F:79:VAL:O     | 2:F:83:ILE:HG13  | 2.21                     | 0.40              |
| 1:E:243:ILE:HG21 | 1:E:253:LYS:HG3  | 2.03                     | 0.40              |
| 1:C:67:ASP:C     | 1:C:69:VAL:N     | 2.73                     | 0.40              |
| 1:A:121:GLN:HB3  | 1:A:128:ALA:HB2  | 2.03                     | 0.40              |
| 1:E:57:VAL:HG12  | 1:E:58:GLU:N     | 2.36                     | 0.40              |
| 2:Z:289:THR:HG23 | 4:Z:1319:FAD:N1A | 2.36                     | 0.40              |
| 2:D:120:ILE:HD13 | 2:D:120:ILE:HG21 | 1.62                     | 0.40              |
| 2:B:272:ILE:HG23 | 2:B:272:ILE:HD12 | 1.84                     | 0.40              |
| 2:F:308:PHE:O    | 2:F:311:GLU:HB3  | 2.20                     | 0.40              |
| 2:B:210:ARG:O    | 2:B:211:GLY:C    | 2.59                     | 0.40              |
| 1:C:229:VAL:HA   | 2:D:143:VAL:HG12 | 2.03                     | 0.40              |
| 2:Z:281:VAL:HA   | 2:Z:282:PRO:HD3  | 1.86                     | 0.40              |
| 1:A:96:ASP:C     | 1:A:96:ASP:OD1   | 2.59                     | 0.40              |
| 2:F:52:LEU:HD23  | 2:F:52:LEU:HA    | 1.87                     | 0.40              |
| 2:D:316:ALA:O    | 2:D:317:GLN:C    | 2.60                     | 0.40              |
| 1:Q:62:VAL:HG22  | 1:Q:85:VAL:HB    | 2.03                     | 0.40              |
| 2:F:96:SER:H     | 2:F:99:SER:HB2   | 1.87                     | 0.40              |
| 1:C:246:THR:N    | 1:C:249:GLU:HG3  | 2.17                     | 0.40              |
| 2:D:278:MET:HE3  | 2:D:278:MET:HB2  | 1.92                     | 0.40              |
| 1:Q:70:ASP:OD1   | 1:Q:86:ARG:NE    | 2.54                     | 0.40              |
| 2:Z:290:ASP:HA   | 2:Z:291:PRO:HD2  | 1.79                     | 0.40              |
| 1:C:246:THR:O    | 1:C:248:SER:N    | 2.54                     | 0.40              |
| 1:C:77:LEU:HD23  | 1:C:81:ALA:HB3   | 2.03                     | 0.40              |
| 1:A:4:LEU:HD22   | 1:A:108:ILE:HG12 | 2.03                     | 0.40              |
| 2:Z:224:LEU:HD21 | 2:Z:314:LEU:HB3  | 2.03                     | 0.40              |
| 1:A:95:SER:HB3   | 1:A:99:VAL:HB    | 2.04                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:191:TYR:OH | 2:F:216:THR:CG2[4_456] | 2.19                     | 0.01              |

## 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     | 257/264 (97%)   | 228 (89%)  | 22 (9%)  | 7 (3%)   | 6           | 31 |
| 1   | C     | 256/264 (97%)   | 221 (86%)  | 29 (11%) | 6 (2%)   | 8           | 35 |
| 1   | E     | 256/264 (97%)   | 227 (89%)  | 20 (8%)  | 9 (4%)   | 4           | 24 |
| 1   | Q     | 240/264 (91%)   | 221 (92%)  | 15 (6%)  | 4 (2%)   | 11          | 43 |
| 2   | B     | 310/320 (97%)   | 269 (87%)  | 33 (11%) | 8 (3%)   | 7           | 32 |
| 2   | D     | 310/320 (97%)   | 272 (88%)  | 26 (8%)  | 12 (4%)  | 4           | 22 |
| 2   | F     | 310/320 (97%)   | 272 (88%)  | 25 (8%)  | 13 (4%)  | 3           | 19 |
| 2   | Z     | 308/320 (96%)   | 279 (91%)  | 24 (8%)  | 5 (2%)   | 12          | 44 |
| All | All   | 2247/2336 (96%) | 1989 (88%) | 194 (9%) | 64 (3%)  | 6           | 30 |

All (64) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 155 | ASP  |
| 2   | B     | 211 | GLY  |
| 1   | C     | 247 | ILE  |
| 2   | D     | 197 | ILE  |
| 2   | D     | 201 | THR  |
| 2   | D     | 269 | SER  |
| 2   | D     | 316 | ALA  |
| 1   | E     | 155 | ASP  |
| 1   | E     | 211 | ALA  |
| 1   | E     | 237 | LYS  |
| 2   | F     | 166 | ALA  |
| 2   | F     | 197 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 202 | VAL  |
| 2   | F     | 314 | LEU  |
| 1   | Q     | 145 | VAL  |
| 2   | B     | 47  | ALA  |
| 2   | B     | 202 | VAL  |
| 1   | C     | 28  | GLU  |
| 2   | D     | 257 | VAL  |
| 2   | D     | 279 | LYS  |
| 1   | E     | 145 | VAL  |
| 1   | E     | 212 | ASP  |
| 2   | F     | 222 | ARG  |
| 2   | F     | 247 | SER  |
| 2   | F     | 276 | ALA  |
| 2   | F     | 310 | ILE  |
| 2   | F     | 316 | ALA  |
| 2   | F     | 317 | GLN  |
| 1   | Q     | 238 | GLY  |
| 1   | A     | 28  | GLU  |
| 2   | B     | 200 | THR  |
| 2   | B     | 276 | ALA  |
| 1   | C     | 93  | GLU  |
| 1   | C     | 145 | VAL  |
| 2   | D     | 12  | ASN  |
| 2   | D     | 34  | ASP  |
| 2   | D     | 177 | PRO  |
| 1   | E     | 195 | ARG  |
| 1   | E     | 236 | GLU  |
| 2   | F     | 258 | GLY  |
| 2   | Z     | 12  | ASN  |
| 2   | Z     | 316 | ALA  |
| 1   | A     | 126 | ALA  |
| 1   | A     | 187 | ASN  |
| 2   | B     | 197 | ILE  |
| 1   | E     | 196 | GLY  |
| 2   | F     | 55  | ASN  |
| 2   | F     | 200 | THR  |
| 1   | Q     | 89  | ASP  |
| 2   | Z     | 200 | THR  |
| 1   | A     | 222 | ALA  |
| 1   | C     | 260 | GLU  |
| 2   | D     | 246 | LYS  |
| 1   | E     | 25  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 51  | GLU  |
| 1   | A     | 66  | PRO  |
| 2   | D     | 210 | ARG  |
| 2   | D     | 317 | GLN  |
| 1   | Q     | 153 | PRO  |
| 2   | B     | 298 | ILE  |
| 2   | Z     | 87  | ASN  |
| 1   | C     | 238 | GLY  |
| 2   | Z     | 197 | ILE  |
| 2   | B     | 282 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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     | 200/216 (93%)   | 173 (86%)  | 27 (14%)  | 5           | 20 |
| 1   | C     | 196/216 (91%)   | 181 (92%)  | 15 (8%)   | 16          | 50 |
| 1   | E     | 195/216 (90%)   | 176 (90%)  | 19 (10%)  | 10          | 36 |
| 1   | Q     | 184/216 (85%)   | 166 (90%)  | 18 (10%)  | 10          | 36 |
| 2   | B     | 245/258 (95%)   | 220 (90%)  | 25 (10%)  | 9           | 33 |
| 2   | D     | 243/258 (94%)   | 209 (86%)  | 34 (14%)  | 4           | 18 |
| 2   | F     | 243/258 (94%)   | 213 (88%)  | 30 (12%)  | 6           | 23 |
| 2   | Z     | 241/258 (93%)   | 223 (92%)  | 18 (8%)   | 17          | 51 |
| All | All   | 1747/1896 (92%) | 1561 (89%) | 186 (11%) | 8           | 31 |

All (186) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 10  | THR  |
| 1   | A     | 16  | ASP  |
| 1   | A     | 34  | ASP  |
| 1   | A     | 42  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | LYS  |
| 1   | A     | 51  | GLU  |
| 1   | A     | 55  | THR  |
| 1   | A     | 56  | ASP  |
| 1   | A     | 60  | VAL  |
| 1   | A     | 68  | ARG  |
| 1   | A     | 74  | ARG  |
| 1   | A     | 98  | ILE  |
| 1   | A     | 102 | ARG  |
| 1   | A     | 132 | ILE  |
| 1   | A     | 141 | PRO  |
| 1   | A     | 145 | VAL  |
| 1   | A     | 156 | ASN  |
| 1   | A     | 162 | ARG  |
| 1   | A     | 180 | LEU  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 203 | LYS  |
| 1   | A     | 239 | ARG  |
| 1   | A     | 246 | THR  |
| 1   | A     | 249 | GLU  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 261 | PHE  |
| 2   | B     | 1   | SER  |
| 2   | B     | 16  | PRO  |
| 2   | B     | 29  | LYS  |
| 2   | B     | 30  | LYS  |
| 2   | B     | 49  | VAL  |
| 2   | B     | 60  | LEU  |
| 2   | B     | 66  | SER  |
| 2   | B     | 71  | ASP  |
| 2   | B     | 80  | SER  |
| 2   | B     | 91  | VAL  |
| 2   | B     | 158 | SER  |
| 2   | B     | 168 | SER  |
| 2   | B     | 172 | SER  |
| 2   | B     | 199 | ILE  |
| 2   | B     | 201 | THR  |
| 2   | B     | 203 | ASP  |
| 2   | B     | 219 | GLU  |
| 2   | B     | 224 | LEU  |
| 2   | B     | 237 | PRO  |
| 2   | B     | 246 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 259 | SER  |
| 2   | B     | 273 | GLN  |
| 2   | B     | 279 | LYS  |
| 2   | B     | 289 | THR  |
| 2   | B     | 307 | ILE  |
| 1   | C     | 32  | MET  |
| 1   | C     | 34  | ASP  |
| 1   | C     | 74  | ARG  |
| 1   | C     | 75  | LYS  |
| 1   | C     | 102 | ARG  |
| 1   | C     | 121 | GLN  |
| 1   | C     | 125 | GLN  |
| 1   | C     | 150 | GLN  |
| 1   | C     | 156 | ASN  |
| 1   | C     | 183 | GLN  |
| 1   | C     | 193 | SER  |
| 1   | C     | 216 | SER  |
| 1   | C     | 239 | ARG  |
| 1   | C     | 249 | GLU  |
| 1   | C     | 253 | LYS  |
| 2   | D     | 11  | ARG  |
| 2   | D     | 19  | LEU  |
| 2   | D     | 29  | LYS  |
| 2   | D     | 30  | LYS  |
| 2   | D     | 31  | SER  |
| 2   | D     | 60  | LEU  |
| 2   | D     | 80  | SER  |
| 2   | D     | 91  | VAL  |
| 2   | D     | 119 | TYR  |
| 2   | D     | 120 | ILE  |
| 2   | D     | 149 | SER  |
| 2   | D     | 163 | LEU  |
| 2   | D     | 178 | SER  |
| 2   | D     | 199 | ILE  |
| 2   | D     | 201 | THR  |
| 2   | D     | 203 | ASP  |
| 2   | D     | 208 | ILE  |
| 2   | D     | 212 | ILE  |
| 2   | D     | 214 | GLU  |
| 2   | D     | 216 | THR  |
| 2   | D     | 223 | GLU  |
| 2   | D     | 224 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 238 | ILE  |
| 2   | D     | 246 | LYS  |
| 2   | D     | 255 | LYS  |
| 2   | D     | 278 | MET  |
| 2   | D     | 294 | SER  |
| 2   | D     | 295 | ILE  |
| 2   | D     | 298 | ILE  |
| 2   | D     | 303 | ILE  |
| 2   | D     | 306 | ASP  |
| 2   | D     | 307 | ILE  |
| 2   | D     | 311 | GLU  |
| 2   | D     | 318 | LEU  |
| 1   | E     | 1   | MET  |
| 1   | E     | 18  | GLU  |
| 1   | E     | 28  | GLU  |
| 1   | E     | 55  | THR  |
| 1   | E     | 74  | ARG  |
| 1   | E     | 89  | ASP  |
| 1   | E     | 102 | ARG  |
| 1   | E     | 136 | SER  |
| 1   | E     | 156 | ASN  |
| 1   | E     | 168 | MET  |
| 1   | E     | 174 | ILE  |
| 1   | E     | 183 | GLN  |
| 1   | E     | 195 | ARG  |
| 1   | E     | 203 | LYS  |
| 1   | E     | 213 | ILE  |
| 1   | E     | 216 | SER  |
| 1   | E     | 231 | ARG  |
| 1   | E     | 249 | GLU  |
| 1   | E     | 261 | PHE  |
| 2   | F     | 1   | SER  |
| 2   | F     | 11  | ARG  |
| 2   | F     | 19  | LEU  |
| 2   | F     | 29  | LYS  |
| 2   | F     | 31  | SER  |
| 2   | F     | 49  | VAL  |
| 2   | F     | 60  | LEU  |
| 2   | F     | 66  | SER  |
| 2   | F     | 89  | SER  |
| 2   | F     | 91  | VAL  |
| 2   | F     | 93  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 105 | SER  |
| 2   | F     | 156 | ARG  |
| 2   | F     | 163 | LEU  |
| 2   | F     | 172 | SER  |
| 2   | F     | 174 | VAL  |
| 2   | F     | 178 | SER  |
| 2   | F     | 199 | ILE  |
| 2   | F     | 201 | THR  |
| 2   | F     | 203 | ASP  |
| 2   | F     | 219 | GLU  |
| 2   | F     | 222 | ARG  |
| 2   | F     | 224 | LEU  |
| 2   | F     | 246 | LYS  |
| 2   | F     | 255 | LYS  |
| 2   | F     | 259 | SER  |
| 2   | F     | 273 | GLN  |
| 2   | F     | 279 | LYS  |
| 2   | F     | 295 | ILE  |
| 2   | F     | 309 | ASP  |
| 1   | Q     | 10  | THR  |
| 1   | Q     | 18  | GLU  |
| 1   | Q     | 34  | ASP  |
| 1   | Q     | 56  | ASP  |
| 1   | Q     | 63  | SER  |
| 1   | Q     | 74  | ARG  |
| 1   | Q     | 75  | LYS  |
| 1   | Q     | 89  | ASP  |
| 1   | Q     | 98  | ILE  |
| 1   | Q     | 102 | ARG  |
| 1   | Q     | 110 | LYS  |
| 1   | Q     | 153 | PRO  |
| 1   | Q     | 156 | ASN  |
| 1   | Q     | 188 | LYS  |
| 1   | Q     | 206 | GLU  |
| 1   | Q     | 228 | ARG  |
| 1   | Q     | 249 | GLU  |
| 1   | Q     | 253 | LYS  |
| 2   | Z     | 19  | LEU  |
| 2   | Z     | 29  | LYS  |
| 2   | Z     | 60  | LEU  |
| 2   | Z     | 66  | SER  |
| 2   | Z     | 89  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Z     | 91  | VAL  |
| 2   | Z     | 93  | LEU  |
| 2   | Z     | 163 | LEU  |
| 2   | Z     | 199 | ILE  |
| 2   | Z     | 201 | THR  |
| 2   | Z     | 207 | SER  |
| 2   | Z     | 214 | GLU  |
| 2   | Z     | 224 | LEU  |
| 2   | Z     | 245 | PRO  |
| 2   | Z     | 246 | LYS  |
| 2   | Z     | 279 | LYS  |
| 2   | Z     | 298 | ILE  |
| 2   | Z     | 314 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 170 | GLN  |
| 1   | A     | 175 | ASN  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 199 | GLN  |
| 1   | A     | 250 | GLN  |
| 2   | B     | 124 | GLN  |
| 2   | B     | 173 | ASN  |
| 2   | B     | 249 | GLN  |
| 2   | B     | 273 | GLN  |
| 2   | B     | 317 | GLN  |
| 1   | C     | 121 | GLN  |
| 1   | C     | 150 | GLN  |
| 1   | C     | 156 | ASN  |
| 1   | C     | 170 | GLN  |
| 1   | C     | 175 | ASN  |
| 1   | C     | 183 | GLN  |
| 1   | C     | 199 | GLN  |
| 1   | C     | 250 | GLN  |
| 2   | D     | 124 | GLN  |
| 2   | D     | 137 | GLN  |
| 2   | D     | 249 | GLN  |
| 2   | D     | 273 | GLN  |
| 2   | D     | 317 | GLN  |
| 1   | E     | 121 | GLN  |
| 1   | E     | 170 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 175 | ASN  |
| 1   | E     | 183 | GLN  |
| 1   | E     | 199 | GLN  |
| 1   | E     | 250 | GLN  |
| 1   | E     | 256 | GLN  |
| 2   | F     | 124 | GLN  |
| 2   | F     | 173 | ASN  |
| 2   | F     | 249 | GLN  |
| 2   | F     | 273 | GLN  |
| 2   | F     | 317 | GLN  |
| 1   | Q     | 121 | GLN  |
| 1   | Q     | 150 | GLN  |
| 1   | Q     | 156 | ASN  |
| 1   | Q     | 170 | GLN  |
| 1   | Q     | 175 | ASN  |
| 1   | Q     | 183 | GLN  |
| 1   | Q     | 250 | GLN  |
| 1   | Q     | 256 | GLN  |
| 2   | Z     | 44  | GLN  |
| 2   | Z     | 173 | ASN  |
| 2   | Z     | 249 | GLN  |
| 2   | Z     | 273 | GLN  |
| 2   | Z     | 317 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | AMP  | A     | 1263 | -    | 20,25,25     | 1.81 | 4 (20%)     | 22,38,38    | 2.64 | 9 (40%)     |
| 4   | FAD  | B     | 1319 | -    | 48,58,58     | 1.87 | 12 (25%)    | 54,89,89    | 2.22 | 9 (16%)     |
| 3   | AMP  | C     | 1262 | -    | 20,25,25     | 1.48 | 4 (20%)     | 22,38,38    | 3.58 | 7 (31%)     |
| 4   | FAD  | D     | 1319 | -    | 48,58,58     | 2.43 | 17 (35%)    | 54,89,89    | 2.15 | 10 (18%)    |
| 3   | AMP  | E     | 1262 | -    | 20,25,25     | 1.76 | 4 (20%)     | 22,38,38    | 3.74 | 7 (31%)     |
| 4   | FAD  | F     | 1319 | -    | 48,58,58     | 1.87 | 12 (25%)    | 54,89,89    | 1.73 | 12 (22%)    |
| 3   | AMP  | Q     | 1262 | -    | 20,25,25     | 1.50 | 4 (20%)     | 22,38,38    | 4.45 | 6 (27%)     |
| 4   | FAD  | Z     | 1319 | -    | 48,58,58     | 1.59 | 8 (16%)     | 54,89,89    | 2.47 | 12 (22%)    |

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   | AMP  | A     | 1263 | -    | -       | 0/6/26/26  | 0/3/3/3 |
| 4   | FAD  | B     | 1319 | -    | -       | 0/30/50/50 | 0/6/6/6 |
| 3   | AMP  | C     | 1262 | -    | -       | 0/6/26/26  | 0/3/3/3 |
| 4   | FAD  | D     | 1319 | -    | -       | 0/30/50/50 | 0/6/6/6 |
| 3   | AMP  | E     | 1262 | -    | -       | 0/6/26/26  | 0/3/3/3 |
| 4   | FAD  | F     | 1319 | -    | -       | 0/30/50/50 | 0/6/6/6 |
| 3   | AMP  | Q     | 1262 | -    | -       | 0/6/26/26  | 0/3/3/3 |
| 4   | FAD  | Z     | 1319 | -    | -       | 0/30/50/50 | 0/6/6/6 |

All (65) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | D     | 1319 | FAD  | C6-C5X  | -2.99 | 1.37        | 1.41     |
| 4   | Z     | 1319 | FAD  | C9A-C5X | -2.51 | 1.37        | 1.42     |
| 4   | F     | 1319 | FAD  | C10-N10 | -2.50 | 1.36        | 1.39     |
| 3   | C     | 1262 | AMP  | O4'-C4' | -2.27 | 1.39        | 1.45     |
| 3   | C     | 1262 | AMP  | P-O2P   | -2.15 | 1.47        | 1.54     |
| 4   | D     | 1319 | FAD  | C9A-C5X | -2.06 | 1.38        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | A     | 1263 | AMP  | O4'-C4' | -2.04 | 1.40        | 1.45     |
| 3   | E     | 1262 | AMP  | P-O2P   | -2.02 | 1.47        | 1.54     |
| 3   | Q     | 1262 | AMP  | C4-N3   | 2.00  | 1.38        | 1.35     |
| 4   | B     | 1319 | FAD  | C4-N3   | 2.07  | 1.36        | 1.33     |
| 4   | D     | 1319 | FAD  | C5B-C4B | 2.10  | 1.58        | 1.51     |
| 4   | F     | 1319 | FAD  | C4-N3   | 2.11  | 1.37        | 1.33     |
| 3   | E     | 1262 | AMP  | C2-N1   | 2.16  | 1.38        | 1.33     |
| 4   | F     | 1319 | FAD  | C9-C8   | 2.21  | 1.43        | 1.37     |
| 4   | D     | 1319 | FAD  | C3B-C4B | 2.24  | 1.59        | 1.53     |
| 4   | B     | 1319 | FAD  | O2'-C2' | 2.25  | 1.48        | 1.43     |
| 4   | B     | 1319 | FAD  | C2A-N1A | 2.28  | 1.38        | 1.33     |
| 3   | Q     | 1262 | AMP  | P-O1P   | 2.36  | 1.58        | 1.51     |
| 4   | F     | 1319 | FAD  | O4B-C1B | 2.40  | 1.44        | 1.41     |
| 4   | F     | 1319 | FAD  | C4A-N3A | 2.41  | 1.39        | 1.35     |
| 3   | C     | 1262 | AMP  | C2-N1   | 2.42  | 1.38        | 1.33     |
| 4   | B     | 1319 | FAD  | C9-C8   | 2.53  | 1.44        | 1.37     |
| 4   | B     | 1319 | FAD  | C8A-N7A | 2.59  | 1.39        | 1.34     |
| 4   | B     | 1319 | FAD  | C10-N1  | 2.60  | 1.39        | 1.35     |
| 4   | D     | 1319 | FAD  | P-O1P   | 2.62  | 1.60        | 1.51     |
| 3   | A     | 1263 | AMP  | C2-N1   | 2.66  | 1.38        | 1.33     |
| 4   | D     | 1319 | FAD  | C8M-C8  | 2.68  | 1.56        | 1.51     |
| 4   | F     | 1319 | FAD  | C8A-N7A | 2.69  | 1.39        | 1.34     |
| 4   | F     | 1319 | FAD  | PA-O1A  | 2.69  | 1.61        | 1.51     |
| 4   | B     | 1319 | FAD  | PA-O1A  | 2.71  | 1.61        | 1.51     |
| 3   | E     | 1262 | AMP  | P-O1P   | 2.77  | 1.60        | 1.51     |
| 4   | Z     | 1319 | FAD  | C2A-N1A | 2.94  | 1.39        | 1.33     |
| 4   | Z     | 1319 | FAD  | C8A-N7A | 2.95  | 1.40        | 1.34     |
| 4   | F     | 1319 | FAD  | C1'-N10 | 3.04  | 1.51        | 1.48     |
| 4   | Z     | 1319 | FAD  | C4-N3   | 3.04  | 1.38        | 1.33     |
| 4   | Z     | 1319 | FAD  | C4X-N5  | 3.09  | 1.38        | 1.33     |
| 4   | B     | 1319 | FAD  | C2A-N3A | 3.15  | 1.37        | 1.32     |
| 3   | Q     | 1262 | AMP  | C2-N3   | 3.21  | 1.37        | 1.32     |
| 3   | Q     | 1262 | AMP  | C2-N1   | 3.26  | 1.40        | 1.33     |
| 4   | D     | 1319 | FAD  | O4B-C1B | 3.27  | 1.45        | 1.41     |
| 4   | Z     | 1319 | FAD  | C5'-C4' | 3.35  | 1.56        | 1.51     |
| 4   | D     | 1319 | FAD  | C4-N3   | 3.38  | 1.39        | 1.33     |
| 3   | C     | 1262 | AMP  | C2-N3   | 3.39  | 1.38        | 1.32     |
| 4   | D     | 1319 | FAD  | PA-O1A  | 3.46  | 1.63        | 1.51     |
| 4   | B     | 1319 | FAD  | C5X-N5  | 3.47  | 1.40        | 1.35     |
| 4   | B     | 1319 | FAD  | C1'-N10 | 3.69  | 1.52        | 1.48     |
| 3   | A     | 1263 | AMP  | P-O1P   | 3.72  | 1.63        | 1.51     |
| 4   | D     | 1319 | FAD  | C9A-N10 | 3.72  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | Z     | 1319 | FAD  | C1'-N10 | 3.76 | 1.52        | 1.48     |
| 4   | D     | 1319 | FAD  | C8A-N7A | 4.00 | 1.42        | 1.34     |
| 4   | D     | 1319 | FAD  | C5X-N5  | 4.02 | 1.41        | 1.35     |
| 4   | F     | 1319 | FAD  | C2A-N3A | 4.06 | 1.39        | 1.32     |
| 4   | D     | 1319 | FAD  | C2A-N1A | 4.15 | 1.41        | 1.33     |
| 4   | F     | 1319 | FAD  | C5'-C4' | 4.38 | 1.58        | 1.51     |
| 4   | F     | 1319 | FAD  | C2A-N1A | 4.41 | 1.42        | 1.33     |
| 4   | D     | 1319 | FAD  | C5'-C4' | 4.46 | 1.58        | 1.51     |
| 4   | B     | 1319 | FAD  | C4X-N5  | 4.51 | 1.40        | 1.33     |
| 4   | Z     | 1319 | FAD  | C2A-N3A | 4.75 | 1.40        | 1.32     |
| 4   | F     | 1319 | FAD  | C4X-N5  | 4.76 | 1.40        | 1.33     |
| 3   | A     | 1263 | AMP  | C2-N3   | 4.79 | 1.40        | 1.32     |
| 4   | D     | 1319 | FAD  | C4X-N5  | 5.17 | 1.41        | 1.33     |
| 4   | D     | 1319 | FAD  | C2A-N3A | 5.42 | 1.41        | 1.32     |
| 3   | E     | 1262 | AMP  | C2-N3   | 5.43 | 1.41        | 1.32     |
| 4   | B     | 1319 | FAD  | C5'-C4' | 6.07 | 1.61        | 1.51     |
| 4   | D     | 1319 | FAD  | C1'-N10 | 6.60 | 1.55        | 1.48     |

All (72) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 3   | Q     | 1262 | AMP  | N3-C2-N1    | -18.77 | 114.52      | 128.89   |
| 3   | E     | 1262 | AMP  | N3-C2-N1    | -14.24 | 117.99      | 128.89   |
| 3   | C     | 1262 | AMP  | N3-C2-N1    | -13.17 | 118.81      | 128.89   |
| 4   | Z     | 1319 | FAD  | N3A-C2A-N1A | -12.89 | 119.03      | 128.89   |
| 4   | B     | 1319 | FAD  | N3A-C2A-N1A | -11.61 | 120.00      | 128.89   |
| 4   | D     | 1319 | FAD  | N3A-C2A-N1A | -11.04 | 120.44      | 128.89   |
| 3   | C     | 1262 | AMP  | O2P-P-O1P   | -7.10  | 87.74       | 110.58   |
| 3   | A     | 1263 | AMP  | O4'-C1'-N9  | -6.85  | 93.75       | 108.10   |
| 3   | A     | 1263 | AMP  | N3-C2-N1    | -5.88  | 124.39      | 128.89   |
| 3   | E     | 1262 | AMP  | O5'-P-O1P   | -5.49  | 93.16       | 107.14   |
| 4   | F     | 1319 | FAD  | C4B-O4B-C1B | -5.16  | 104.05      | 109.72   |
| 4   | D     | 1319 | FAD  | P-O3P-PA    | -4.85  | 119.11      | 132.73   |
| 3   | Q     | 1262 | AMP  | C4'-O4'-C1' | -4.45  | 104.83      | 109.72   |
| 3   | E     | 1262 | AMP  | O4'-C1'-N9  | -4.28  | 99.15       | 108.10   |
| 4   | Z     | 1319 | FAD  | P-O3P-PA    | -4.22  | 120.89      | 132.73   |
| 3   | Q     | 1262 | AMP  | O5'-P-O1P   | -4.05  | 96.83       | 107.14   |
| 4   | F     | 1319 | FAD  | N3A-C2A-N1A | -3.20  | 126.44      | 128.89   |
| 4   | D     | 1319 | FAD  | C1B-N9A-C4A | -3.18  | 122.15      | 126.94   |
| 4   | Z     | 1319 | FAD  | C4B-O4B-C1B | -3.09  | 106.33      | 109.72   |
| 4   | Z     | 1319 | FAD  | C4X-C4-N3   | -2.97  | 119.53      | 123.59   |
| 3   | Q     | 1262 | AMP  | C2'-C3'-C4' | -2.94  | 96.57       | 102.61   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | F     | 1319 | FAD  | C1B-N9A-C4A | -2.88 | 122.59      | 126.94   |
| 4   | F     | 1319 | FAD  | C9A-C5X-N5  | -2.84 | 118.15      | 122.36   |
| 3   | A     | 1263 | AMP  | C4-C5-N7    | -2.82 | 106.89      | 109.48   |
| 4   | F     | 1319 | FAD  | P-O3P-PA    | -2.77 | 124.94      | 132.73   |
| 3   | C     | 1262 | AMP  | C2'-C1'-N9  | -2.75 | 110.09      | 114.29   |
| 4   | F     | 1319 | FAD  | C4X-C10-N10 | -2.72 | 118.92      | 120.52   |
| 3   | C     | 1262 | AMP  | O5'-P-O1P   | -2.64 | 100.41      | 107.14   |
| 4   | Z     | 1319 | FAD  | C1B-N9A-C4A | -2.61 | 123.01      | 126.94   |
| 3   | E     | 1262 | AMP  | O4'-C4'-C3' | -2.54 | 100.02      | 105.15   |
| 4   | B     | 1319 | FAD  | C4X-C4-N3   | -2.52 | 120.15      | 123.59   |
| 4   | B     | 1319 | FAD  | C1B-N9A-C4A | -2.46 | 123.24      | 126.94   |
| 3   | A     | 1263 | AMP  | C2'-C3'-C4' | -2.34 | 97.80       | 102.61   |
| 4   | D     | 1319 | FAD  | C9-C8-C7    | -2.32 | 115.62      | 120.04   |
| 4   | Z     | 1319 | FAD  | C9A-C5X-N5  | -2.27 | 119.00      | 122.36   |
| 3   | A     | 1263 | AMP  | O3P-P-O5'   | -2.22 | 100.17      | 106.56   |
| 4   | B     | 1319 | FAD  | C9-C8-C7    | -2.14 | 115.95      | 120.04   |
| 4   | D     | 1319 | FAD  | O5B-C5B-C4B | -2.04 | 101.61      | 109.12   |
| 3   | A     | 1263 | AMP  | C4'-O4'-C1' | -2.01 | 107.51      | 109.72   |
| 3   | A     | 1263 | AMP  | C5'-C4'-C3' | 2.08  | 123.45      | 115.21   |
| 3   | C     | 1262 | AMP  | O3P-P-O5'   | 2.10  | 112.60      | 106.56   |
| 4   | F     | 1319 | FAD  | C6-C5X-C9A  | 2.11  | 121.75      | 118.98   |
| 4   | D     | 1319 | FAD  | C5X-C9A-N10 | 2.14  | 119.24      | 117.62   |
| 4   | B     | 1319 | FAD  | C1'-N10-C9A | 2.16  | 121.28      | 118.86   |
| 4   | Z     | 1319 | FAD  | C1'-N10-C9A | 2.18  | 121.31      | 118.86   |
| 4   | F     | 1319 | FAD  | C4-N3-C2    | 2.25  | 117.19      | 115.25   |
| 4   | D     | 1319 | FAD  | C6-C5X-N5   | 2.26  | 121.87      | 118.96   |
| 4   | D     | 1319 | FAD  | O4'-C4'-C5' | 2.30  | 115.20      | 110.19   |
| 4   | Z     | 1319 | FAD  | O2P-P-O3P   | 2.38  | 115.89      | 105.09   |
| 4   | B     | 1319 | FAD  | O4'-C4'-C5' | 2.55  | 115.75      | 110.19   |
| 4   | Z     | 1319 | FAD  | O3P-PA-O5B  | 2.58  | 109.79      | 102.94   |
| 3   | Q     | 1262 | AMP  | O3P-P-O5'   | 2.60  | 114.05      | 106.56   |
| 4   | F     | 1319 | FAD  | O4B-C4B-C3B | 2.63  | 110.44      | 105.15   |
| 4   | F     | 1319 | FAD  | C1'-N10-C9A | 2.65  | 121.84      | 118.86   |
| 4   | B     | 1319 | FAD  | O3P-PA-O5B  | 2.75  | 110.22      | 102.94   |
| 3   | E     | 1262 | AMP  | O3P-P-O1P   | 2.80  | 119.58      | 110.58   |
| 3   | E     | 1262 | AMP  | C4'-O4'-C1' | 2.83  | 112.82      | 109.72   |
| 4   | F     | 1319 | FAD  | C4X-N5-C5X  | 2.85  | 120.04      | 116.76   |
| 4   | D     | 1319 | FAD  | C4X-N5-C5X  | 2.88  | 120.08      | 116.76   |
| 4   | Z     | 1319 | FAD  | C4-C4X-N5   | 3.06  | 122.43      | 118.72   |
| 3   | C     | 1262 | AMP  | O3P-P-O2P   | 3.12  | 119.26      | 107.38   |
| 3   | E     | 1262 | AMP  | O3P-P-O5'   | 3.43  | 116.44      | 106.56   |
| 3   | A     | 1263 | AMP  | O2P-P-O5'   | 3.51  | 116.68      | 106.56   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3   | A     | 1263 | AMP  | O5'-C5'-C4' | 3.73 | 122.87      | 109.12   |
| 3   | Q     | 1262 | AMP  | O2P-P-O5'   | 3.87 | 117.69      | 106.56   |
| 4   | D     | 1319 | FAD  | O2A-PA-O3P  | 3.97 | 123.11      | 105.09   |
| 3   | C     | 1262 | AMP  | O2P-P-O5'   | 4.37 | 119.16      | 106.56   |
| 4   | B     | 1319 | FAD  | C5X-C9A-N10 | 4.48 | 121.02      | 117.62   |
| 4   | F     | 1319 | FAD  | C5X-C9A-N10 | 4.62 | 121.13      | 117.62   |
| 4   | Z     | 1319 | FAD  | C4X-N5-C5X  | 5.17 | 122.71      | 116.76   |
| 4   | B     | 1319 | FAD  | C4-N3-C2    | 5.36 | 119.88      | 115.25   |
| 4   | Z     | 1319 | FAD  | C4-N3-C2    | 5.67 | 120.14      | 115.25   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | B     | 1319 | FAD  | 1       | 0            |
| 3   | C     | 1262 | AMP  | 3       | 0            |
| 4   | D     | 1319 | FAD  | 8       | 0            |
| 3   | E     | 1262 | AMP  | 2       | 0            |
| 3   | Q     | 1262 | AMP  | 2       | 0            |
| 4   | Z     | 1319 | FAD  | 4       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



















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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  | OWAB(Å <sup>2</sup> ) | Q<0.9     |
|-----|-------|-----------------|--------|--|-----------------------|-----------|
| 1   | A     | 261/264 (98%)   | -0.74  | 0  100  100           | 20, 43, 65, 83        | 0         |
| 1   | C     | 260/264 (98%)   | -0.59  | 0  100  100           | 29, 52, 90, 112       | 0         |
| 1   | E     | 260/264 (98%)   | -0.59  | 1 (0%)  93  85      | 27, 52, 77, 88        | 0         |
| 1   | Q     | 246/264 (93%)   | 0.11   | 15 (6%)  25  10     | 41, 76, 93, 102       | 27 (10%)  |
| 2   | B     | 314/320 (98%)   | -0.64  | 2 (0%)  90  80      | 25, 47, 68, 86        | 0         |
| 2   | D     | 314/320 (98%)   | -0.57  | 3 (0%)  84  69      | 2, 50, 83, 98         | 0         |
| 2   | F     | 314/320 (98%)   | -0.65  | 2 (0%)  90  80    | 31, 49, 70, 88        | 0         |
| 2   | Z     | 312/320 (97%)   | 0.47   | 33 (10%)  8  3  | 46, 77, 95, 114       | 123 (39%) |
| All | All   | 2281/2336 (97%) | -0.40  | 56 (2%)  61  37 | 2, 54, 86, 114        | 150 (6%)  |

All (56) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | Z     | 198 | ASP  | 8.0  |
| 2   | Z     | 203 | ASP  | 5.3  |
| 2   | Z     | 315 | LYS  | 5.2  |
| 2   | Z     | 316 | ALA  | 4.9  |
| 2   | Z     | 219 | GLU  | 4.7  |
| 2   | B     | 126 | ASP  | 4.3  |
| 1   | Q     | 238 | GLY  | 4.0  |
| 1   | Q     | 239 | ARG  | 3.9  |
| 2   | Z     | 317 | GLN  | 3.9  |
| 2   | Z     | 218 | VAL  | 3.8  |
| 2   | D     | 196 | ASP  | 3.7  |
| 2   | Z     | 231 | THR  | 3.6  |
| 2   | D     | 191 | VAL  | 3.6  |
| 2   | Z     | 126 | ASP  | 3.5  |
| 2   | Z     | 111 | GLY  | 3.4  |
| 2   | Z     | 206 | MET  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 247 | ILE  | 3.4  |
| 2   | Z     | 264 | VAL  | 3.3  |
| 2   | Z     | 32  | GLY  | 3.3  |
| 2   | Z     | 30  | LYS  | 3.1  |
| 2   | D     | 198 | ASP  | 3.0  |
| 2   | Z     | 214 | GLU  | 3.0  |
| 2   | Z     | 207 | SER  | 2.9  |
| 2   | Z     | 318 | LEU  | 2.8  |
| 2   | Z     | 258 | GLY  | 2.7  |
| 2   | F     | 126 | ASP  | 2.7  |
| 1   | Q     | 16  | ASP  | 2.7  |
| 1   | Q     | 261 | PHE  | 2.7  |
| 1   | Q     | 90  | ASP  | 2.6  |
| 1   | Q     | 256 | GLN  | 2.6  |
| 2   | Z     | 199 | ILE  | 2.5  |
| 2   | Z     | 291 | PRO  | 2.5  |
| 2   | B     | 125 | GLY  | 2.5  |
| 2   | Z     | 211 | GLY  | 2.5  |
| 2   | Z     | 308 | PHE  | 2.5  |
| 2   | Z     | 301 | TYR  | 2.4  |
| 2   | Z     | 125 | GLY  | 2.4  |
| 1   | Q     | 67  | ASP  | 2.4  |
| 2   | Z     | 33  | GLU  | 2.4  |
| 2   | Z     | 260 | CYS  | 2.3  |
| 2   | Z     | 179 | VAL  | 2.3  |
| 1   | E     | 238 | GLY  | 2.3  |
| 1   | Q     | 18  | GLU  | 2.2  |
| 1   | Q     | 29  | ASP  | 2.2  |
| 1   | Q     | 53  | SER  | 2.2  |
| 2   | Z     | 31  | SER  | 2.2  |
| 1   | Q     | 56  | ASP  | 2.1  |
| 1   | Q     | 55  | THR  | 2.1  |
| 1   | Q     | 248 | SER  | 2.1  |
| 2   | Z     | 298 | ILE  | 2.1  |
| 2   | Z     | 230 | ALA  | 2.1  |
| 2   | Z     | 285 | ILE  | 2.0  |
| 1   | Q     | 168 | MET  | 2.0  |
| 2   | F     | 191 | VAL  | 2.0  |
| 2   | Z     | 217 | ASN  | 2.0  |
| 2   | Z     | 200 | THR  | 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   | FAD  | B     | 1319 | 53/53 | 0.96 | 0.14 | 0.26  | 17,24,31,33                | 0     |
| 4   | FAD  | D     | 1319 | 53/53 | 0.95 | 0.15 | 0.02  | 21,28,38,42                | 0     |
| 4   | FAD  | F     | 1319 | 53/53 | 0.97 | 0.12 | -0.27 | 17,24,29,35                | 0     |
| 3   | AMP  | A     | 1263 | 23/23 | 0.98 | 0.12 | -0.46 | 23,28,34,37                | 0     |
| 4   | FAD  | Z     | 1319 | 53/53 | 0.89 | 0.22 | -0.59 | 17,28,36,42                | 53    |
| 3   | AMP  | C     | 1262 | 23/23 | 0.99 | 0.12 | -0.61 | 30,46,52,52                | 0     |
| 3   | AMP  | E     | 1262 | 23/23 | 0.98 | 0.11 | -0.80 | 25,33,38,39                | 0     |
| 3   | AMP  | Q     | 1262 | 23/23 | 0.96 | 0.13 | -1.02 | 57,62,69,74                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.