



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:46 PM GMT

PDB ID : 4AEZ  
Title : Crystal Structure of Mitotic Checkpoint Complex  
Authors : Kulkarni, K.A.; Chao, W.C.H.; Zhang, Z.; Barford, D.  
Deposited on : 2012-01-13  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

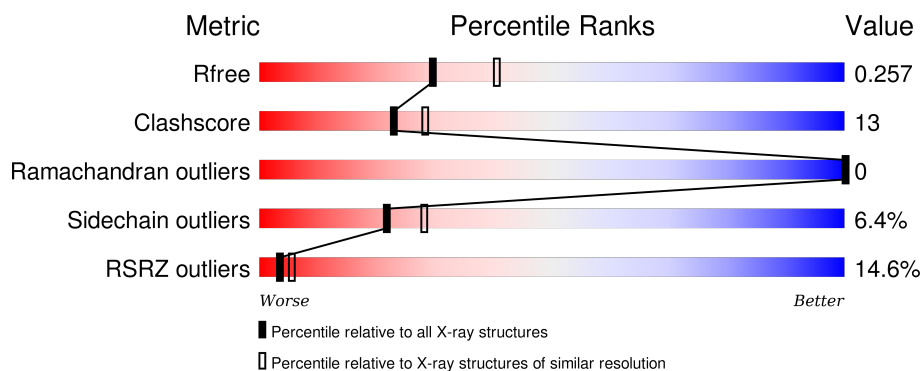
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 3852 (2.30-2.30)                                      |
| Clashscore            | 102246                      | 4452 (2.30-2.30)                                      |
| Ramachandran outliers | 100387                      | 4410 (2.30-2.30)                                      |
| Sidechain outliers    | 100360                      | 4409 (2.30-2.30)                                      |
| RSRZ outliers         | 91569                       | 3857 (2.30-2.30)                                      |

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     | 401    | <div> <div>71%</div> <div>9%</div> <div>19%</div> </div>                 |
| 1   | D     | 401    | <div> <div>3%</div> <div>61%</div> <div>16%</div> <div>22%</div> </div>  |
| 1   | G     | 401    | <div> <div>15%</div> <div>54%</div> <div>23%</div> <div>21%</div> </div> |
| 2   | B     | 203    | <div> <div>71%</div> <div>16%</div> <div>11%</div> </div>                |
| 2   | E     | 203    | <div> <div>33%</div> <div>53%</div> <div>30%</div> <div>14%</div> </div> |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | H     | 203    | <div><div></div><div>27%</div><div>60%</div><div>28%</div><div>9%</div></div>               |
| 3   | C     | 223    | <div><div></div><div>2%</div><div>77%</div><div>19%</div><div></div></div>                  |
| 3   | F     | 223    | <div><div></div><div>8%</div><div>66%</div><div>19%</div><div>12%</div></div>               |
| 3   | I     | 223    | <div><div></div><div>38%</div><div>44%</div><div>34%</div><div>9%</div><div>13%</div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16896 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 WD REPEAT-CONTAINING PROTEIN SLP1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 326      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2499  | 1565 | 445 | 483 | 6 |         |         |       |
| 1   | D     | 314      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2406  | 1507 | 426 | 467 | 6 |         |         |       |
| 1   | G     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2400  | 1502 | 425 | 467 | 6 |         |         |       |

- Molecule 2 is a protein called MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1469  | 941 | 243 | 278 | 7 |         |         |       |
| 2   | E     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1369  | 880 | 224 | 260 | 5 |         |         |       |
| 2   | H     | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1477  | 951 | 246 | 274 | 6 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 12      | ALA      | LEU    | ENGINEERED MUTATION | UNP O14417 |
| B     | 133     | ALA      | ARG    | ENGINEERED MUTATION | UNP O14417 |
| E     | 12      | ALA      | LEU    | ENGINEERED MUTATION | UNP O14417 |
| E     | 133     | ALA      | ARG    | ENGINEERED MUTATION | UNP O14417 |
| H     | 12      | ALA      | LEU    | ENGINEERED MUTATION | UNP O14417 |
| H     | 133     | ALA      | ARG    | ENGINEERED MUTATION | UNP O14417 |

- Molecule 3 is a protein called MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1799  | 1142 | 313 | 339 | 5 |         |         |       |

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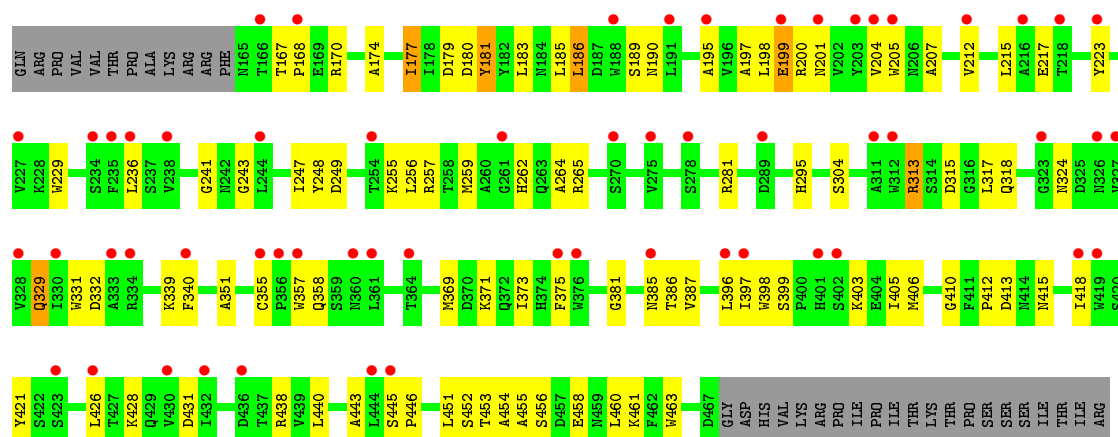
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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | F     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1013 | 265 | 302 | 5 |         |         |       |
| 3   | I     | 193      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1574  | 997  | 273 | 300 | 4 |         |         |       |

- Molecule 4 is water.

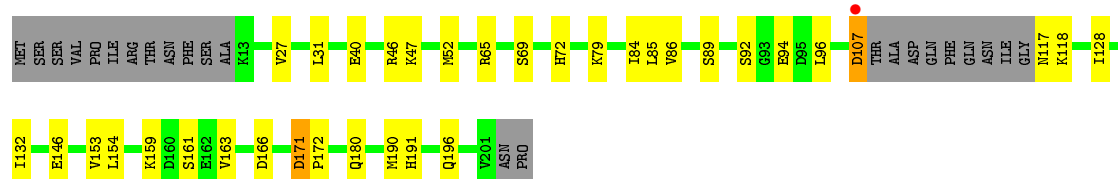
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 114      | Total | O   | 0       | 0       |
|     |       |          | 114   | 114 |         |         |
| 4   | B     | 33       | Total | O   | 0       | 0       |
|     |       |          | 33    | 33  |         |         |
| 4   | C     | 33       | Total | O   | 0       | 0       |
|     |       |          | 33    | 33  |         |         |
| 4   | D     | 61       | Total | O   | 0       | 0       |
|     |       |          | 61    | 61  |         |         |
| 4   | E     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 4   | F     | 48       | Total | O   | 0       | 0       |
|     |       |          | 48    | 48  |         |         |
| 4   | G     | 21       | Total | O   | 0       | 0       |
|     |       |          | 21    | 21  |         |         |
| 4   | H     | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 4   | I     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |





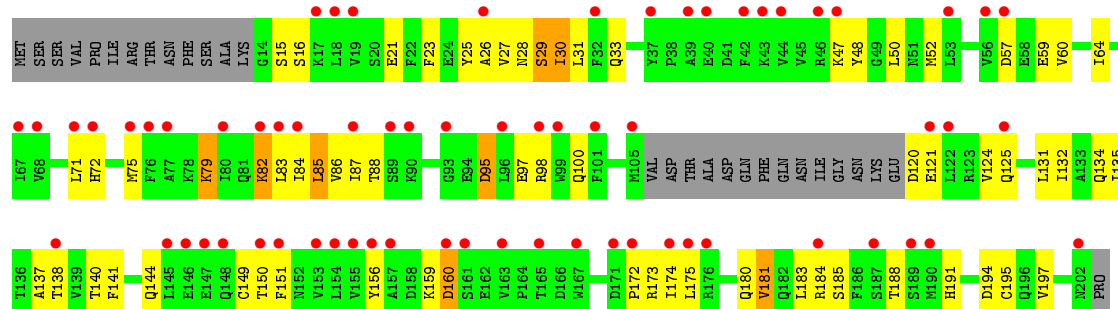
• Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2

Chain B: 71% 16% 11%



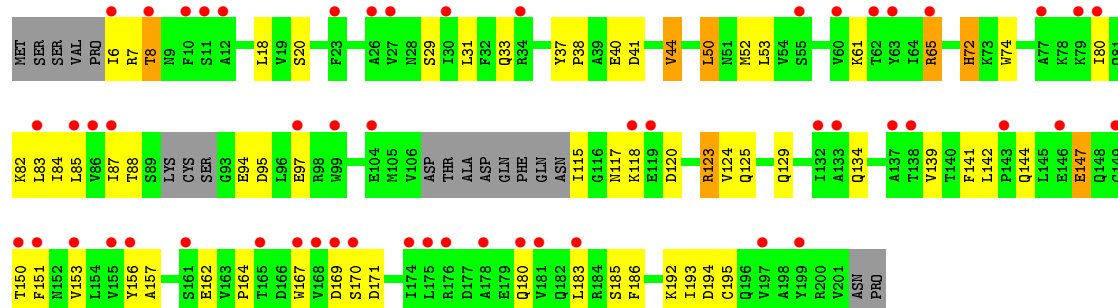
• Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2

Chain E: 33% 53% 30% 14%

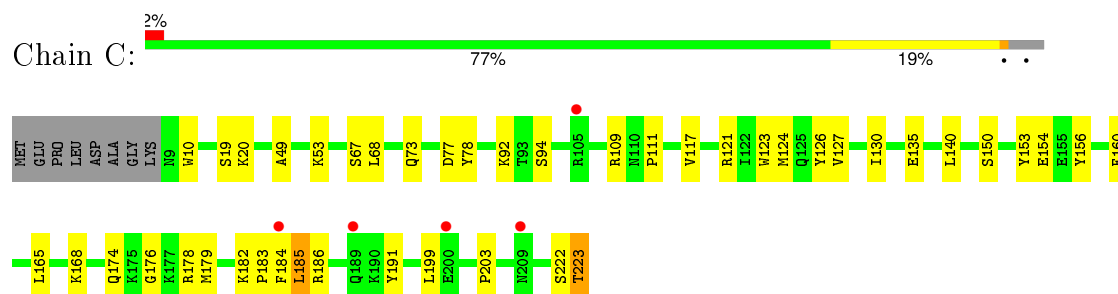


• Molecule 2: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2

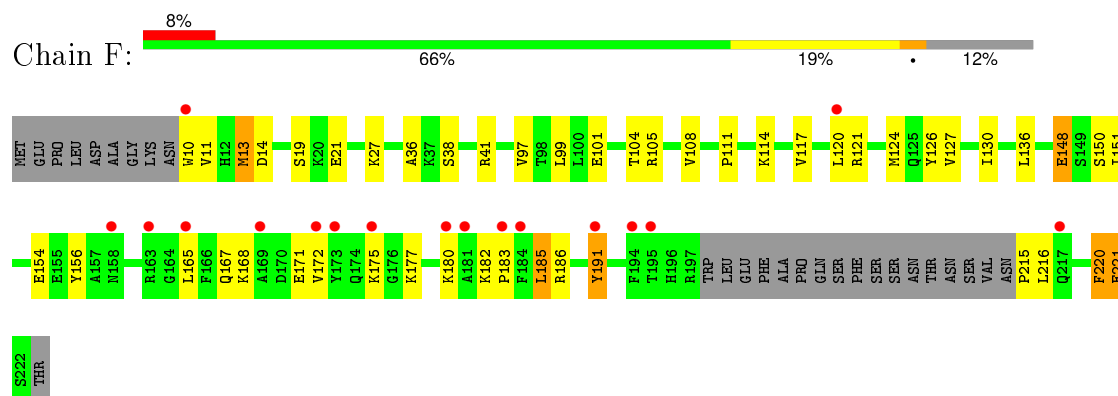
Chain H: 27% 60% 28% 9%



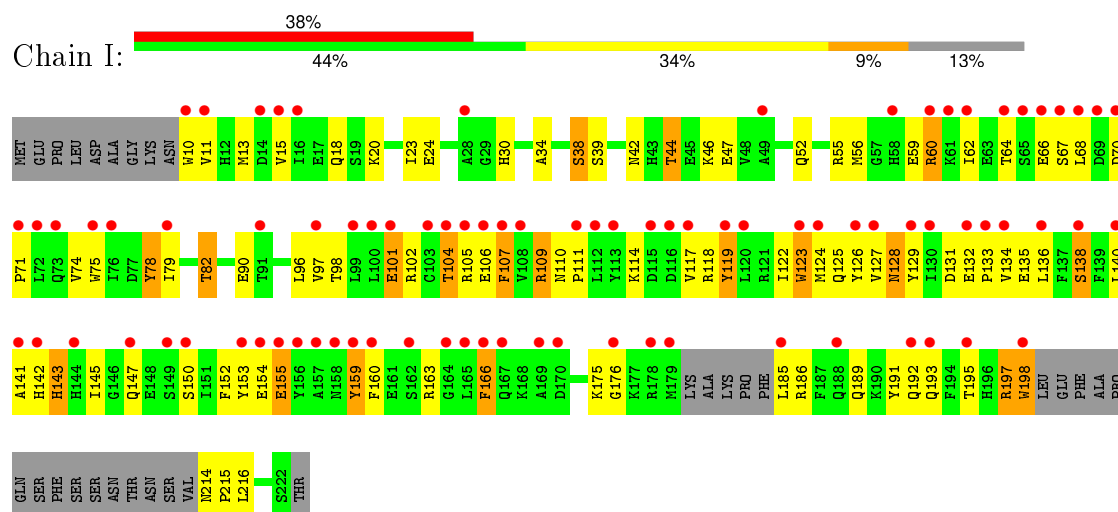
- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 1 21 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 70.81Å 286.90Å 72.01Å<br>90.00° 119.04° 90.00°   | Depositor        |
| Resolution (Å)  | 62.96 – 2.30<br>62.96 – 2.30   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (62.96-2.30)<br>99.8 (62.96-2.30)   | Depositor<br>EDS |
| $R_{merge}$   | 0.06   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.84 (at 2.29Å)  | Xtriage          |
| Refinement program  | PHENIX (PHENIX.REFINE)   | Depositor        |
| R, $R_{free}$   | 0.221 , 0.267<br>0.209 , 0.257   | Depositor<br>DCC |
| $R_{free}$ test set   | 1968 reflections (1.78%)   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.8   | Xtriage          |
| Anisotropy  | 0.217  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 54.6  | EDS              |
| Estimated twinning fraction   | 0.002 for -h-l,k,h<br>0.002 for l,k,-h-l<br>0.024 for h,-k,-h-l<br>0.022 for -h-l,-k,l<br>0.024 for l,-k,h | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$  | Xtriage          |
| Outliers  | 0 of 110586 reflections  | Xtriage          |
| $F_o, F_c$ correlation  | 0.94   | EDS              |
| Total number of atoms   | 16896  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.36         | 0/2559  | 0.54        | 0/3492  |
| 1   | D     | 0.34         | 0/2465  | 0.56        | 0/3366  |
| 1   | G     | 0.28         | 0/2458  | 0.49        | 0/3361  |
| 2   | B     | 0.36         | 0/1494  | 0.50        | 0/2016  |
| 2   | E     | 0.27         | 0/1394  | 0.43        | 0/1895  |
| 2   | H     | 0.29         | 0/1502  | 0.46        | 0/2032  |
| 3   | C     | 0.35         | 0/1847  | 0.46        | 0/2495  |
| 3   | F     | 0.34         | 0/1625  | 0.48        | 0/2198  |
| 3   | I     | 0.27         | 0/1614  | 0.44        | 0/2187  |
| All | All   | 0.32         | 0/16958 | 0.50        | 0/23042 |

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 |
|-----|-------|---------------------|---------------------|
| 3   | I     | 0                   | 1                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | I     | 107 | PHE  | Peptide |

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2499  | 0        | 2393     | 33      | 0            |
| 1   | D     | 2406  | 0        | 2290     | 46      | 0            |
| 1   | G     | 2400  | 0        | 2269     | 76      | 0            |
| 2   | B     | 1469  | 0        | 1476     | 23      | 0            |
| 2   | E     | 1369  | 0        | 1312     | 83      | 0            |
| 2   | H     | 1477  | 0        | 1462     | 48      | 0            |
| 3   | C     | 1799  | 0        | 1718     | 27      | 0            |
| 3   | F     | 1585  | 0        | 1472     | 41      | 0            |
| 3   | I     | 1574  | 0        | 1434     | 88      | 0            |
| 4   | A     | 114   | 0        | 0        | 3       | 0            |
| 4   | B     | 33    | 0        | 0        | 0       | 0            |
| 4   | C     | 33    | 0        | 0        | 0       | 0            |
| 4   | D     | 61    | 0        | 0        | 3       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 48    | 0        | 0        | 0       | 0            |
| 4   | G     | 21    | 0        | 0        | 0       | 0            |
| 4   | H     | 6     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 16896 | 0        | 15826    | 436     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (436) 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:466:TYR:O    | 1:A:467:ASP:HB3  | 1.49                     | 1.08              |
| 3:C:222:SER:O    | 3:C:223:THR:HB   | 1.54                     | 1.05              |
| 1:G:177:ILE:HD11 | 1:G:458:GLU:HA   | 1.42                     | 0.99              |
| 1:D:164:PHE:HE1  | 1:D:432:ILE:HD11 | 1.25                     | 0.97              |
| 3:I:122:ILE:HG22 | 3:I:126:TYR:CE1  | 2.01                     | 0.95              |
| 3:I:123:TRP:HA   | 3:I:126:TYR:CD2  | 2.07                     | 0.89              |
| 1:D:268:CYS:SG   | 1:D:308:CYS:O    | 2.31                     | 0.88              |
| 3:I:118:ARG:O    | 3:I:122:ILE:HG13 | 1.75                     | 0.86              |
| 3:I:109:ARG:HD3  | 3:I:110:ASN:H    | 1.41                     | 0.85              |
| 3:I:133:PRO:O    | 3:I:136:LEU:HG   | 1.77                     | 0.85              |
| 1:A:133:LYS:HE2  | 2:B:166:ASP:HA   | 1.59                     | 0.84              |
| 1:D:164:PHE:CE1  | 1:D:432:ILE:HD11 | 2.10                     | 0.84              |
| 3:I:198:TRP:HD1  | 3:I:198:TRP:H    | 1.26                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:50:LEU:HD11  | 2:H:129:GLN:HB3  | 1.61                     | 0.81              |
| 2:E:87:ILE:CG2   | 2:E:97:GLU:HB3   | 2.11                     | 0.80              |
| 3:I:127:VAL:HB   | 3:I:136:LEU:HD22 | 1.63                     | 0.80              |
| 3:F:38:SER:O     | 3:F:41:ARG:HG2   | 1.81                     | 0.79              |
| 3:F:220:PHE:HD1  | 3:F:221:GLU:N    | 1.80                     | 0.78              |
| 2:E:172:PRO:HB2  | 2:E:174:ILE:HG13 | 1.64                     | 0.77              |
| 2:E:50:LEU:HD12  | 2:E:52:MET:HE1   | 1.67                     | 0.77              |
| 2:H:120:ASP:O    | 2:H:124:VAL:HG23 | 1.88                     | 0.73              |
| 1:D:313:ARG:HG3  | 1:D:354:TRP:CD2  | 2.23                     | 0.73              |
| 3:I:122:ILE:HG22 | 3:I:126:TYR:HE1  | 1.52                     | 0.72              |
| 2:E:134:GLN:O    | 2:E:138:THR:HG23 | 1.88                     | 0.72              |
| 2:E:87:ILE:HD12  | 2:E:150:THR:O    | 1.90                     | 0.72              |
| 3:F:220:PHE:HD1  | 3:F:221:GLU:H    | 1.38                     | 0.71              |
| 3:F:120:LEU:HD12 | 3:F:121:ARG:N    | 2.05                     | 0.71              |
| 2:H:164:PRO:HB2  | 2:H:167:TRP:HD1  | 1.56                     | 0.71              |
| 3:F:117:VAL:HA   | 3:F:120:LEU:HG   | 1.73                     | 0.70              |
| 2:E:25:TYR:CE1   | 2:E:47:LYS:HD2   | 2.26                     | 0.70              |
| 1:D:368:THR:HG22 | 1:D:369:MET:HE2  | 1.73                     | 0.70              |
| 3:I:198:TRP:N    | 3:I:198:TRP:CD1  | 2.58                     | 0.70              |
| 1:G:167:THR:HG23 | 1:G:168:PRO:HD2  | 1.73                     | 0.70              |
| 1:A:313:ARG:HG3  | 1:A:354:TRP:CD2  | 2.26                     | 0.70              |
| 3:I:56:MET:O     | 3:I:60:ARG:HD2   | 1.92                     | 0.69              |
| 1:A:467:ASP:OD1  | 1:A:467:ASP:C    | 2.30                     | 0.69              |
| 2:E:25:TYR:CZ    | 2:E:47:LYS:HD2   | 2.27                     | 0.69              |
| 2:H:8:THR:HG23   | 2:H:117:ASN:HD21 | 1.57                     | 0.69              |
| 1:G:180:ASP:HB3  | 1:G:183:LEU:HG   | 1.73                     | 0.68              |
| 2:E:23:PHE:CE2   | 2:E:75:MET:HE3   | 2.28                     | 0.68              |
| 1:G:177:ILE:HD11 | 1:G:458:GLU:CA   | 2.22                     | 0.68              |
| 3:I:15:VAL:HG12  | 3:I:39:SER:HB2   | 1.76                     | 0.68              |
| 2:E:138:THR:HA   | 2:E:141:PHE:CE2  | 2.27                     | 0.67              |
| 2:H:125:GLN:O    | 2:H:129:GLN:HG2  | 1.94                     | 0.67              |
| 1:D:413:ASP:HB3  | 1:D:415:ASN:OD1  | 1.95                     | 0.67              |
| 1:D:369:MET:SD   | 2:E:140:THR:HG22 | 2.36                     | 0.66              |
| 2:E:23:PHE:CD2   | 2:E:71:LEU:HD11  | 2.30                     | 0.66              |
| 1:A:126:ASN:HD22 | 2:B:159:LYS:HG2  | 1.60                     | 0.66              |
| 2:H:180:GLN:HB3  | 3:I:10:TRP:CZ3   | 2.31                     | 0.65              |
| 1:G:177:ILE:HG23 | 1:G:198:LEU:CD2  | 2.27                     | 0.65              |
| 2:E:121:GLU:O    | 2:E:125:GLN:HG2  | 1.97                     | 0.65              |
| 1:D:415:ASN:ND2  | 1:D:431:ASP:OD1  | 2.29                     | 0.65              |
| 3:C:174:GLN:O    | 3:C:178:ARG:HG3  | 1.96                     | 0.64              |
| 1:A:126:ASN:O    | 2:B:159:LYS:HG2  | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:181:VAL:HG13 | 2:E:197:VAL:HG13 | 1.78                     | 0.64              |
| 1:A:126:ASN:ND2  | 1:A:126:ASN:O    | 2.30                     | 0.64              |
| 3:C:199:LEU:O    | 3:C:203:PRO:HG3  | 1.98                     | 0.64              |
| 2:E:88:THR:HG21  | 2:E:173:ARG:NH2  | 2.13                     | 0.64              |
| 3:I:44:THR:HG22  | 3:I:47:GLU:HG3   | 1.80                     | 0.63              |
| 3:I:97:VAL:HG13  | 3:I:98:THR:N     | 2.13                     | 0.63              |
| 2:E:87:ILE:HG22  | 2:E:97:GLU:HB3   | 1.80                     | 0.62              |
| 2:B:180:GLN:HB2  | 3:C:10:TRP:CZ3   | 2.34                     | 0.62              |
| 2:E:120:ASP:O    | 2:E:124:VAL:HG23 | 2.00                     | 0.62              |
| 3:C:182:LYS:HB3  | 3:C:183:PRO:HA   | 1.82                     | 0.62              |
| 1:D:180:ASP:HB3  | 1:D:183:LEU:HG   | 1.80                     | 0.61              |
| 3:I:78:TYR:O     | 3:I:82:THR:HG22  | 2.01                     | 0.61              |
| 3:F:220:PHE:CD1  | 3:F:221:GLU:N    | 2.67                     | 0.61              |
| 1:G:428:LYS:HD3  | 1:G:431:ASP:HB2  | 1.81                     | 0.61              |
| 1:G:177:ILE:CD1  | 1:G:458:GLU:HA   | 2.24                     | 0.61              |
| 2:E:23:PHE:HE2   | 2:E:75:MET:HE3   | 1.65                     | 0.61              |
| 2:E:82:LYS:HD3   | 2:E:100:GLN:OE1  | 2.01                     | 0.61              |
| 1:G:179:ASP:HB2  | 1:G:456:SER:CB   | 2.31                     | 0.60              |
| 2:E:47:LYS:HD3   | 2:E:48:TYR:CE2   | 2.37                     | 0.60              |
| 1:D:249:ASP:OD1  | 1:D:251:GLU:HG2  | 2.01                     | 0.60              |
| 1:G:421:TYR:HD2  | 1:G:426:LEU:HD11 | 1.66                     | 0.60              |
| 3:I:97:VAL:HG13  | 3:I:98:THR:H     | 1.66                     | 0.60              |
| 3:I:66:GLU:OE1   | 3:I:66:GLU:N     | 2.34                     | 0.60              |
| 3:C:185:LEU:HD12 | 3:C:186:ARG:H    | 1.66                     | 0.60              |
| 1:G:249:ASP:HB2  | 1:G:256:LEU:HD11 | 1.83                     | 0.60              |
| 2:E:26:ALA:O     | 2:E:30:ILE:HG23  | 2.02                     | 0.60              |
| 1:G:179:ASP:HB2  | 1:G:456:SER:HB3  | 1.83                     | 0.59              |
| 1:D:410:GLY:HA2  | 1:D:438:ARG:HB3  | 1.84                     | 0.59              |
| 2:E:82:LYS:HB2   | 2:E:82:LYS:HZ3   | 1.66                     | 0.59              |
| 1:G:189:SER:HB3  | 1:G:229:TRP:CD2  | 2.37                     | 0.59              |
| 1:A:190:ASN:HA   | 1:A:446:PRO:HB3  | 1.84                     | 0.59              |
| 3:I:109:ARG:HD3  | 3:I:110:ASN:N    | 2.15                     | 0.59              |
| 2:B:117:ASN:HB2  | 1:D:436:ASP:OD1  | 2.01                     | 0.59              |
| 1:A:406:MET:HG2  | 1:A:418:ILE:HG12 | 1.84                     | 0.59              |
| 1:A:184:ASN:O    | 1:A:226:SER:HA   | 2.02                     | 0.59              |
| 2:H:147:GLU:CD   | 2:H:147:GLU:H    | 2.05                     | 0.59              |
| 2:B:118:LYS:NZ   | 1:D:433:PRO:O    | 2.29                     | 0.58              |
| 3:F:127:VAL:HG23 | 3:F:136:LEU:HD13 | 1.86                     | 0.58              |
| 2:E:79:LYS:HE3   | 2:E:79:LYS:HA    | 1.86                     | 0.57              |
| 1:G:128:ARG:N    | 2:H:157:ALA:O    | 2.37                     | 0.57              |
| 1:G:357:TRP:HZ3  | 1:G:399:SER:O    | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:133:PRO:HA   | 3:I:136:LEU:HD23 | 1.86                     | 0.57              |
| 3:F:148:GLU:HG3  | 3:F:180:LYS:HB2  | 1.87                     | 0.57              |
| 2:E:47:LYS:NZ    | 2:E:48:TYR:OH    | 2.29                     | 0.57              |
| 2:E:52:MET:HE3   | 2:E:132:ILE:HD13 | 1.87                     | 0.57              |
| 1:D:268:CYS:SG   | 1:D:308:CYS:C    | 2.83                     | 0.56              |
| 1:D:179:ASP:HB2  | 1:D:456:SER:HB3  | 1.86                     | 0.56              |
| 3:I:90:GLU:HB2   | 3:I:129:TYR:HE2  | 1.70                     | 0.56              |
| 2:E:85:LEU:HG    | 2:E:151:PHE:CZ   | 2.41                     | 0.56              |
| 2:E:23:PHE:HD2   | 2:E:71:LEU:HD11  | 1.70                     | 0.56              |
| 3:F:182:LYS:HA   | 3:F:183:PRO:C    | 2.25                     | 0.56              |
| 2:H:8:THR:CG2    | 2:H:117:ASN:HD21 | 2.19                     | 0.56              |
| 3:F:124:MET:O    | 3:F:127:VAL:HG12 | 2.05                     | 0.56              |
| 3:I:123:TRP:O    | 3:I:127:VAL:HG12 | 2.05                     | 0.56              |
| 1:G:397:ILE:HG23 | 1:G:406:MET:HB2  | 1.86                     | 0.56              |
| 2:B:196:GLN:HB3  | 3:C:10:TRP:CZ3   | 2.41                     | 0.55              |
| 3:I:150:SER:O    | 3:I:154:GLU:HG3  | 2.06                     | 0.55              |
| 3:F:105:ARG:O    | 3:F:108:VAL:HG22 | 2.06                     | 0.55              |
| 3:I:124:MET:SD   | 3:I:155:GLU:HG2  | 2.47                     | 0.55              |
| 2:E:181:VAL:HG13 | 2:E:197:VAL:CG1  | 2.35                     | 0.55              |
| 3:I:141:ALA:HA   | 3:I:147:GLN:NE2  | 2.21                     | 0.55              |
| 2:E:15:SER:OG    | 2:E:188:THR:HG21 | 2.06                     | 0.55              |
| 3:F:150:SER:O    | 3:F:154:GLU:HG3  | 2.06                     | 0.55              |
| 3:I:79:ILE:HA    | 3:I:82:THR:CG2   | 2.37                     | 0.55              |
| 2:E:52:MET:CE    | 2:E:132:ILE:HD13 | 2.37                     | 0.55              |
| 1:G:445:SER:HB2  | 1:G:446:PRO:HD2  | 1.88                     | 0.55              |
| 2:E:98:ARG:HH12  | 2:E:100:GLN:HE21 | 1.56                     | 0.54              |
| 2:E:27:VAL:HG22  | 2:E:85:LEU:HD21  | 1.90                     | 0.54              |
| 2:E:184:ARG:HG3  | 2:E:185:SER:N    | 2.22                     | 0.54              |
| 3:I:185:LEU:O    | 3:I:189:GLN:HG3  | 2.08                     | 0.54              |
| 1:G:324:ASN:OD1  | 3:I:20:LYS:HE2   | 2.07                     | 0.54              |
| 1:G:243:GLY:O    | 1:G:262:HIS:HB2  | 2.06                     | 0.54              |
| 3:I:24:GLU:O     | 3:I:30:HIS:NE2   | 2.32                     | 0.54              |
| 3:I:123:TRP:HA   | 3:I:126:TYR:CE2  | 2.43                     | 0.54              |
| 3:I:153:TYR:CZ   | 3:I:176:GLY:HA2  | 2.42                     | 0.54              |
| 2:B:47:LYS:HB3   | 2:B:52:MET:HG3   | 1.90                     | 0.54              |
| 1:G:177:ILE:HG23 | 1:G:198:LEU:HD23 | 1.88                     | 0.54              |
| 1:G:243:GLY:HA2  | 1:G:264:ALA:O    | 2.08                     | 0.54              |
| 3:I:191:TYR:O    | 3:I:195:THR:HG23 | 2.08                     | 0.54              |
| 3:I:52:GLN:O     | 3:I:56:MET:HG2   | 2.08                     | 0.54              |
| 1:G:412:PRO:HG2  | 1:G:413:ASP:OD1  | 2.07                     | 0.53              |
| 2:H:141:PHE:HB3  | 3:I:23:ILE:HG21  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:123:TRP:O    | 3:I:127:VAL:CG1  | 2.56                     | 0.53              |
| 3:F:172:VAL:HA   | 3:F:175:LYS:CE   | 2.38                     | 0.53              |
| 1:G:281:ARG:HH21 | 3:I:18:GLN:HB3   | 1.72                     | 0.53              |
| 2:E:131:LEU:HD23 | 2:E:131:LEU:C    | 2.29                     | 0.53              |
| 3:I:133:PRO:HA   | 3:I:136:LEU:CD2  | 2.39                     | 0.53              |
| 3:I:109:ARG:C    | 3:I:111:PRO:HD3  | 2.30                     | 0.53              |
| 3:I:166:PHE:HB3  | 3:I:197:ARG:HD3  | 1.91                     | 0.52              |
| 3:F:185:LEU:HD12 | 3:F:186:ARG:N    | 2.24                     | 0.52              |
| 1:G:177:ILE:HG13 | 1:G:456:SER:HA   | 1.91                     | 0.52              |
| 2:E:172:PRO:HB2  | 2:E:174:ILE:CG1  | 2.36                     | 0.52              |
| 2:E:84:ILE:HD12  | 2:E:84:ILE:N     | 2.24                     | 0.52              |
| 1:G:454:ALA:HB2  | 1:G:460:LEU:HD13 | 1.89                     | 0.52              |
| 3:I:128:ASN:ND2  | 3:I:128:ASN:H    | 2.07                     | 0.52              |
| 1:D:288:HIS:HA   | 1:D:295:HIS:O    | 2.10                     | 0.52              |
| 3:C:124:MET:O    | 3:C:127:VAL:HG12 | 2.09                     | 0.52              |
| 2:E:48:TYR:HD2   | 2:E:52:MET:HE3   | 1.73                     | 0.52              |
| 1:A:185:LEU:HD22 | 1:A:441:TYR:CZ   | 2.45                     | 0.52              |
| 2:H:50:LEU:HD11  | 2:H:129:GLN:CB   | 2.35                     | 0.52              |
| 2:E:160:ASP:OD1  | 2:E:160:ASP:N    | 2.43                     | 0.52              |
| 2:B:107:ASP:OD1  | 2:B:107:ASP:N    | 2.42                     | 0.52              |
| 2:H:85:LEU:N     | 2:H:85:LEU:HD12  | 2.25                     | 0.52              |
| 1:D:340:PHE:HE2  | 1:D:378:ALA:O    | 1.93                     | 0.51              |
| 1:G:355:CYS:SG   | 1:G:358:GLN:HB2  | 2.50                     | 0.51              |
| 1:G:369:MET:HA   | 1:G:369:MET:HE2  | 1.92                     | 0.51              |
| 2:E:21:GLU:HG2   | 2:E:47:LYS:NZ    | 2.24                     | 0.51              |
| 1:D:292:ILE:HG22 | 1:D:294:ASN:H    | 1.74                     | 0.51              |
| 2:H:31:LEU:HD21  | 2:H:151:PHE:CZ   | 2.44                     | 0.51              |
| 3:F:177:LYS:CD   | 3:F:191:TYR:HE2  | 2.24                     | 0.51              |
| 2:H:164:PRO:HB2  | 2:H:167:TRP:CD1  | 2.42                     | 0.51              |
| 2:E:57:ASP:HB3   | 2:E:60:VAL:CG1   | 2.40                     | 0.51              |
| 1:A:313:ARG:HD3  | 1:A:318:GLN:HB2  | 1.93                     | 0.51              |
| 3:F:126:TYR:CZ   | 3:F:130:ILE:HD11 | 2.46                     | 0.51              |
| 3:I:134:VAL:O    | 3:I:138:SER:OG   | 2.26                     | 0.51              |
| 1:G:259:MET:HB3  | 1:G:295:HIS:CD2  | 2.46                     | 0.51              |
| 3:I:71:PRO:HB2   | 3:I:107:PHE:HZ   | 1.76                     | 0.50              |
| 2:E:159:LYS:HD3  | 2:E:159:LYS:H    | 1.76                     | 0.50              |
| 3:I:122:ILE:O    | 3:I:125:GLN:HB2  | 2.11                     | 0.50              |
| 2:E:23:PHE:HE2   | 2:E:75:MET:CE    | 2.24                     | 0.50              |
| 2:B:163:VAL:HG23 | 2:B:163:VAL:O    | 2.11                     | 0.50              |
| 2:H:74:TRP:HB3   | 2:H:80:ILE:HB    | 1.93                     | 0.50              |
| 1:G:223:TYR:CE1  | 1:G:241:GLY:HA3  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:30:ILE:HG13  | 2:E:31:LEU:N     | 2.27                     | 0.50              |
| 1:D:292:ILE:HG22 | 1:D:293:ALA:N    | 2.27                     | 0.50              |
| 2:H:180:GLN:HB3  | 3:I:10:TRP:CE3   | 2.46                     | 0.50              |
| 2:H:38:PRO:O     | 2:H:41:ASP:HB2   | 2.11                     | 0.50              |
| 3:I:123:TRP:CD1  | 3:I:126:TYR:HD2  | 2.30                     | 0.50              |
| 3:F:168:LYS:O    | 3:F:171:GLU:HB2  | 2.11                     | 0.50              |
| 1:D:345:HIS:HB2  | 4:D:2040:HOH:O   | 2.11                     | 0.50              |
| 3:F:11:VAL:HG13  | 3:F:36:ALA:HB2   | 1.94                     | 0.50              |
| 3:I:127:VAL:HB   | 3:I:136:LEU:CD2  | 2.39                     | 0.49              |
| 3:C:183:PRO:HB2  | 3:C:185:LEU:CD1  | 2.42                     | 0.49              |
| 1:G:247:ILE:O    | 1:G:256:LEU:N    | 2.44                     | 0.49              |
| 2:B:89:SER:HB2   | 2:B:96:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:201:ASN:HA   | 1:A:216:ALA:O    | 2.12                     | 0.49              |
| 3:I:106:GLU:HG3  | 3:I:107:PHE:CD1  | 2.46                     | 0.49              |
| 3:C:182:LYS:HA   | 3:C:183:PRO:C    | 2.32                     | 0.49              |
| 2:E:86:VAL:HG22  | 2:E:98:ARG:HG3   | 1.93                     | 0.49              |
| 1:A:467:ASP:OD1  | 1:A:467:ASP:O    | 2.30                     | 0.49              |
| 3:I:140:LEU:HD12 | 3:I:152:PHE:CE1  | 2.47                     | 0.49              |
| 1:G:415:ASN:ND2  | 1:G:431:ASP:OD1  | 2.45                     | 0.49              |
| 3:F:171:GLU:O    | 3:F:175:LYS:HG3  | 2.13                     | 0.49              |
| 1:G:315:ASP:OD2  | 1:G:317:LEU:HD12 | 2.13                     | 0.49              |
| 1:A:169:GLU:OE2  | 1:A:464:ARG:HD2  | 2.12                     | 0.49              |
| 1:A:131:ALA:HB2  | 2:B:154:LEU:HD22 | 1.93                     | 0.49              |
| 1:D:300:LEU:HD21 | 1:D:336:SER:HA   | 1.95                     | 0.49              |
| 2:E:82:LYS:HE2   | 2:E:156:TYR:CD2  | 2.48                     | 0.49              |
| 2:E:184:ARG:HG3  | 2:E:185:SER:H    | 1.78                     | 0.49              |
| 1:G:313:ARG:HE   | 1:G:318:GLN:HB2  | 1.77                     | 0.49              |
| 1:G:313:ARG:HH21 | 1:G:318:GLN:HG3  | 1.78                     | 0.49              |
| 1:G:229:TRP:CD2  | 1:G:236:LEU:HD13 | 2.48                     | 0.48              |
| 3:I:159:TYR:CE1  | 3:I:163:ARG:CZ   | 2.96                     | 0.48              |
| 1:A:370:ASP:O    | 1:A:371:LYS:HB2  | 2.13                     | 0.48              |
| 2:H:185:SER:HB3  | 2:H:194:ASP:HB3  | 1.94                     | 0.48              |
| 3:C:73:GLN:NE2   | 3:C:77:ASP:OD1   | 2.45                     | 0.48              |
| 2:E:88:THR:HG21  | 2:E:173:ARG:HH21 | 1.77                     | 0.48              |
| 2:H:44:VAL:HA    | 2:H:52:MET:O     | 2.12                     | 0.48              |
| 3:I:44:THR:HG22  | 3:I:47:GLU:H     | 1.78                     | 0.48              |
| 2:E:23:PHE:HD2   | 2:E:71:LEU:HD21  | 1.78                     | 0.48              |
| 2:E:159:LYS:CD   | 2:E:159:LYS:H    | 2.27                     | 0.48              |
| 3:F:165:LEU:N    | 3:F:165:LEU:HD12 | 2.28                     | 0.48              |
| 1:D:389:ALA:HB1  | 1:D:409:HIS:CE1  | 2.49                     | 0.48              |
| 3:F:97:VAL:O     | 3:F:101:GLU:HG3  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:87:ILE:HB    | 2:H:97:GLU:HB3   | 1.96                     | 0.48              |
| 2:E:50:LEU:CD1   | 2:E:52:MET:HE1   | 2.40                     | 0.47              |
| 2:E:16:SER:HB3   | 2:E:75:MET:HB3   | 1.96                     | 0.47              |
| 2:H:18:LEU:C     | 2:H:18:LEU:HD23  | 2.34                     | 0.47              |
| 1:G:329:GLN:HG2  | 1:G:331:TRP:CZ2  | 2.49                     | 0.47              |
| 2:E:87:ILE:HD11  | 2:E:149:CYS:CB   | 2.44                     | 0.47              |
| 1:G:248:TYR:CE2  | 1:G:255:LYS:HB2  | 2.49                     | 0.47              |
| 3:I:44:THR:HG23  | 3:I:46:LYS:H     | 1.79                     | 0.47              |
| 3:C:222:SER:O    | 3:C:223:THR:CB   | 2.40                     | 0.47              |
| 1:D:438:ARG:NH2  | 3:F:21:GLU:O     | 2.47                     | 0.47              |
| 3:F:172:VAL:HG12 | 3:F:175:LYS:HE3  | 1.97                     | 0.47              |
| 2:E:83:LEU:C     | 2:E:84:ILE:HD12  | 2.34                     | 0.47              |
| 3:I:119:TYR:CE2  | 3:I:123:TRP:HZ3  | 2.31                     | 0.47              |
| 1:G:177:ILE:CD1  | 1:G:455:ALA:O    | 2.63                     | 0.47              |
| 3:I:119:TYR:CE2  | 3:I:123:TRP:CZ3  | 3.02                     | 0.47              |
| 3:I:68:LEU:HD11  | 3:I:71:PRO:HA    | 1.96                     | 0.47              |
| 1:G:375:PHE:HB2  | 1:G:385:ASN:HB2  | 1.97                     | 0.47              |
| 2:H:20:SER:OG    | 2:H:72:HIS:HA    | 2.15                     | 0.47              |
| 2:B:190:MET:HG2  | 2:B:191:HIS:CE1  | 2.50                     | 0.47              |
| 1:A:196:VAL:HG11 | 3:I:216:LEU:HD11 | 1.97                     | 0.47              |
| 2:H:183:LEU:HB2  | 2:H:195:CYS:O    | 2.14                     | 0.47              |
| 1:G:215:LEU:HD23 | 1:G:236:LEU:HD23 | 1.95                     | 0.47              |
| 2:B:171:ASP:HB2  | 2:B:172:PRO:HD2  | 1.97                     | 0.46              |
| 2:B:27:VAL:O     | 2:B:31:LEU:HG    | 2.15                     | 0.46              |
| 3:C:126:TYR:CZ   | 3:C:130:ILE:HD11 | 2.50                     | 0.46              |
| 3:I:166:PHE:CB   | 3:I:197:ARG:HD3  | 2.45                     | 0.46              |
| 1:G:177:ILE:CG2  | 1:G:198:LEU:HD23 | 2.46                     | 0.46              |
| 3:I:111:PRO:O    | 3:I:114:LYS:HG2  | 2.15                     | 0.46              |
| 2:B:85:LEU:HD23  | 2:B:85:LEU:C     | 2.36                     | 0.46              |
| 3:F:168:LYS:HA   | 3:F:171:GLU:CD   | 2.36                     | 0.46              |
| 3:C:160:PHE:HD1  | 3:C:165:LEU:HD12 | 1.81                     | 0.46              |
| 3:I:104:THR:OG1  | 3:I:126:TYR:CD2  | 2.63                     | 0.46              |
| 2:E:29:SER:O     | 2:E:33:GLN:HG3   | 2.15                     | 0.46              |
| 1:A:466:TYR:O    | 1:A:467:ASP:CB   | 2.35                     | 0.46              |
| 3:C:49:ALA:O     | 3:C:53:LYS:HD3   | 2.15                     | 0.46              |
| 1:G:205:TRP:CZ3  | 1:G:207:ALA:HA   | 2.51                     | 0.46              |
| 1:D:361:LEU:HD13 | 1:D:398:TRP:CH2  | 2.50                     | 0.46              |
| 3:F:104:THR:O    | 3:F:108:VAL:HG13 | 2.16                     | 0.46              |
| 2:B:146:GLU:HG3  | 3:C:186:ARG:HH12 | 1.81                     | 0.45              |
| 1:G:410:GLY:HA2  | 1:G:438:ARG:HG2  | 1.98                     | 0.45              |
| 1:A:263:GLN:NE2  | 4:A:2042:HOH:O   | 2.49                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:68:LEU:HD13  | 3:I:70:ASP:C     | 2.37                     | 0.45              |
| 2:H:83:LEU:C     | 2:H:84:ILE:HD13  | 2.36                     | 0.45              |
| 1:G:127:THR:HG23 | 2:H:156:TYR:HB3  | 1.98                     | 0.45              |
| 2:E:30:ILE:HD11  | 2:E:151:PHE:CE1  | 2.52                     | 0.45              |
| 3:F:185:LEU:HD12 | 3:F:186:ARG:H    | 1.81                     | 0.45              |
| 3:I:106:GLU:HG3  | 3:I:107:PHE:CE1  | 2.52                     | 0.45              |
| 2:H:87:ILE:HD12  | 2:H:97:GLU:HB3   | 1.98                     | 0.45              |
| 1:D:243:GLY:O    | 1:D:262:HIS:HB2  | 2.17                     | 0.45              |
| 1:D:420:SER:OG   | 1:D:427:THR:HB   | 2.16                     | 0.45              |
| 3:I:101:GLU:OE1  | 3:I:102:ARG:HG3  | 2.16                     | 0.45              |
| 1:G:174:ALA:CB   | 1:G:177:ILE:HD13 | 2.47                     | 0.45              |
| 1:D:369:MET:HA   | 1:D:369:MET:CE   | 2.46                     | 0.45              |
| 3:I:97:VAL:CG1   | 3:I:98:THR:N     | 2.80                     | 0.45              |
| 1:A:180:ASP:HB3  | 1:A:183:LEU:HG   | 1.98                     | 0.45              |
| 3:C:109:ARG:O    | 3:C:111:PRO:HD3  | 2.17                     | 0.45              |
| 3:C:183:PRO:HB2  | 3:C:185:LEU:HD11 | 1.99                     | 0.45              |
| 2:H:38:PRO:HB2   | 2:H:40:GLU:HG2   | 1.99                     | 0.45              |
| 3:I:56:MET:HA    | 3:I:59:GLU:CG    | 2.47                     | 0.45              |
| 1:G:357:TRP:CZ3  | 1:G:399:SER:O    | 2.68                     | 0.45              |
| 1:D:411:PHE:HA   | 1:D:412:PRO:HA   | 1.62                     | 0.45              |
| 3:F:120:LEU:HD13 | 3:F:151:ILE:HG21 | 1.98                     | 0.44              |
| 3:F:148:GLU:OE2  | 3:F:180:LYS:CG   | 2.65                     | 0.44              |
| 2:H:170:SER:OG   | 2:H:171:ASP:N    | 2.50                     | 0.44              |
| 2:H:192:LYS:C    | 2:H:193:ILE:HD12 | 2.37                     | 0.44              |
| 1:G:340:PHE:CE1  | 1:G:381:GLY:HA3  | 2.52                     | 0.44              |
| 1:G:351:ALA:HB1  | 1:G:396:LEU:HG   | 1.99                     | 0.44              |
| 3:I:123:TRP:CD1  | 3:I:126:TYR:CD2  | 3.05                     | 0.44              |
| 2:E:134:GLN:O    | 2:E:137:ALA:HB3  | 2.17                     | 0.44              |
| 1:G:256:LEU:O    | 1:G:257:ARG:HB3  | 2.18                     | 0.44              |
| 2:B:84:ILE:HB    | 2:B:154:LEU:HB2  | 1.99                     | 0.44              |
| 1:D:184:ASN:O    | 1:D:226:SER:HA   | 2.17                     | 0.44              |
| 1:G:201:ASN:OD1  | 1:G:217:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:184:ASN:C    | 1:A:185:LEU:HD13 | 2.38                     | 0.44              |
| 2:H:156:TYR:CD1  | 2:H:156:TYR:N    | 2.86                     | 0.44              |
| 1:D:305:SER:HB2  | 4:D:2037:HOH:O   | 2.17                     | 0.44              |
| 2:H:120:ASP:O    | 2:H:123:ARG:HG3  | 2.18                     | 0.44              |
| 3:I:62:ILE:HD11  | 3:I:75:TRP:CZ2   | 2.53                     | 0.44              |
| 1:D:348:ALA:HB3  | 3:F:21:GLU:HG3   | 1.99                     | 0.44              |
| 1:G:195:ALA:HB2  | 1:G:229:TRP:CZ2  | 2.52                     | 0.44              |
| 1:D:181:TYR:CZ   | 1:D:350:LYS:HB2  | 2.52                     | 0.44              |
| 3:F:167:GLN:O    | 3:F:171:GLU:HG3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:29:SER:O     | 2:H:33:GLN:HG3   | 2.17                     | 0.44              |
| 3:F:117:VAL:HG23 | 3:F:120:LEU:HD11 | 2.00                     | 0.44              |
| 1:G:421:TYR:CD2  | 1:G:426:LEU:HD11 | 2.49                     | 0.44              |
| 2:H:82:LYS:HD2   | 2:H:156:TYR:CD2  | 2.52                     | 0.44              |
| 1:G:398:TRP:CD2  | 1:G:405:ILE:HD12 | 2.52                     | 0.44              |
| 3:I:34:ALA:O     | 3:I:38:SER:OG    | 2.34                     | 0.44              |
| 2:E:86:VAL:HG13  | 2:E:95:ASP:HB3   | 2.00                     | 0.44              |
| 2:E:159:LYS:N    | 2:E:159:LYS:HD3  | 2.32                     | 0.44              |
| 3:C:168:LYS:HB3  | 3:C:168:LYS:HE3  | 1.74                     | 0.44              |
| 1:D:464:ARG:NH2  | 4:D:2060:HOH:O   | 2.49                     | 0.44              |
| 1:D:287:HIS:O    | 1:D:296:GLN:HA   | 2.18                     | 0.44              |
| 1:G:387:VAL:CG1  | 1:G:426:LEU:HB2  | 2.47                     | 0.43              |
| 1:G:126:ASN:HD22 | 1:G:126:ASN:N    | 2.16                     | 0.43              |
| 3:F:172:VAL:HA   | 3:F:175:LYS:HE3  | 2.00                     | 0.43              |
| 2:E:180:GLN:HB3  | 3:F:10:TRP:CZ3   | 2.53                     | 0.43              |
| 2:E:87:ILE:HD11  | 2:E:149:CYS:HB2  | 2.01                     | 0.43              |
| 2:E:180:GLN:HB3  | 3:F:10:TRP:CH2   | 2.53                     | 0.43              |
| 1:D:228:LYS:HG3  | 1:D:269:LEU:O    | 2.18                     | 0.43              |
| 3:C:153:TYR:OH   | 3:C:179:MET:HG3  | 2.18                     | 0.43              |
| 1:A:185:LEU:HG   | 1:A:197:ALA:HB3  | 2.01                     | 0.43              |
| 1:A:131:ALA:HB2  | 2:B:154:LEU:CD2  | 2.48                     | 0.43              |
| 3:I:104:THR:HG22 | 3:I:105:ARG:N    | 2.33                     | 0.43              |
| 1:G:451:LEU:O    | 1:G:463:TRP:HD1  | 2.01                     | 0.43              |
| 1:A:296:GLN:NE2  | 4:A:2039:HOH:O   | 2.42                     | 0.43              |
| 1:D:415:ASN:HB2  | 1:D:432:ILE:O    | 2.19                     | 0.43              |
| 3:I:55:ARG:O     | 3:I:59:GLU:HG2   | 2.18                     | 0.43              |
| 2:E:84:ILE:HG12  | 2:E:98:ARG:NH2   | 2.33                     | 0.43              |
| 1:D:189:SER:HB3  | 1:D:229:TRP:CD2  | 2.54                     | 0.43              |
| 2:E:137:ALA:HB3  | 3:F:13:MET:CE    | 2.49                     | 0.43              |
| 1:D:340:PHE:CE2  | 1:D:378:ALA:O    | 2.71                     | 0.43              |
| 3:F:111:PRO:HA   | 3:F:114:LYS:HD3  | 2.01                     | 0.43              |
| 3:I:64:THR:HG22  | 3:I:67:SER:HB2   | 2.01                     | 0.43              |
| 1:G:177:ILE:H    | 1:G:177:ILE:HG12 | 1.66                     | 0.43              |
| 1:G:190:ASN:HA   | 1:G:446:PRO:HB3  | 2.01                     | 0.43              |
| 1:G:186:LEU:HD11 | 1:G:460:LEU:HD11 | 2.01                     | 0.43              |
| 3:C:176:GLY:HA2  | 3:C:179:MET:HB2  | 2.00                     | 0.43              |
| 1:A:195:ALA:HB2  | 1:A:229:TRP:CZ2  | 2.54                     | 0.43              |
| 2:H:88:THR:HG23  | 2:H:95:ASP:N     | 2.34                     | 0.43              |
| 1:G:387:VAL:HG11 | 1:G:426:LEU:HB2  | 2.00                     | 0.42              |
| 2:E:28:ASN:HD21  | 2:E:64:ILE:CD1   | 2.32                     | 0.42              |
| 2:H:7:ARG:HB2    | 2:H:115:ILE:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:114:LYS:NZ   | 3:I:143:HIS:O    | 2.48                     | 0.42              |
| 3:I:97:VAL:CG1   | 3:I:98:THR:H     | 2.32                     | 0.42              |
| 1:D:179:ASP:HB2  | 1:D:456:SER:CB   | 2.50                     | 0.42              |
| 1:G:443:ALA:O    | 1:G:451:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:340:PHE:CE1  | 1:D:211:SER:HB2  | 2.55                     | 0.42              |
| 2:H:8:THR:O      | 2:H:8:THR:OG1    | 2.35                     | 0.42              |
| 3:I:96:LEU:HD23  | 3:I:129:TYR:OH   | 2.19                     | 0.42              |
| 3:I:155:GLU:HA   | 3:I:155:GLU:OE1  | 2.18                     | 0.42              |
| 2:E:28:ASN:HD21  | 2:E:64:ILE:HD12  | 1.84                     | 0.42              |
| 2:B:79:LYS:HB3   | 2:B:161:SER:OG   | 2.19                     | 0.42              |
| 2:E:57:ASP:OD2   | 2:E:60:VAL:HG12  | 2.19                     | 0.42              |
| 1:G:339:LYS:HG2  | 1:G:340:PHE:CD2  | 2.54                     | 0.42              |
| 2:E:52:MET:HE3   | 2:E:132:ILE:CD1  | 2.49                     | 0.42              |
| 3:I:90:GLU:CB    | 3:I:129:TYR:HE2  | 2.33                     | 0.42              |
| 3:C:123:TRP:CD2  | 3:C:140:LEU:HD21 | 2.54                     | 0.42              |
| 3:C:117:VAL:O    | 3:C:121:ARG:HG3  | 2.19                     | 0.42              |
| 2:H:162:GLU:O    | 2:H:164:PRO:HD3  | 2.19                     | 0.42              |
| 2:E:188:THR:N    | 2:E:191:HIS:O    | 2.53                     | 0.42              |
| 1:G:205:TRP:CH2  | 1:G:207:ALA:HA   | 2.55                     | 0.42              |
| 1:G:452:SER:HA   | 1:G:461:LYS:O    | 2.19                     | 0.42              |
| 3:F:215:PRO:O    | 3:F:216:LEU:HB2  | 2.19                     | 0.42              |
| 2:H:139:VAL:HA   | 2:H:142:LEU:HD12 | 2.01                     | 0.42              |
| 2:B:128:ILE:O    | 2:B:132:ILE:HG12 | 2.19                     | 0.42              |
| 3:I:136:LEU:HD12 | 3:I:136:LEU:C    | 2.40                     | 0.42              |
| 1:G:453:THR:O    | 1:G:460:LEU:HD12 | 2.20                     | 0.42              |
| 2:E:135:ILE:HA   | 2:E:138:THR:HG23 | 2.02                     | 0.42              |
| 3:I:56:MET:O     | 3:I:59:GLU:HG3   | 2.19                     | 0.42              |
| 2:E:23:PHE:CD2   | 2:E:71:LEU:HD21  | 2.55                     | 0.42              |
| 1:G:398:TRP:CE2  | 1:G:405:ILE:HD12 | 2.55                     | 0.42              |
| 3:F:27:LYS:HE2   | 3:F:27:LYS:HB3   | 1.74                     | 0.42              |
| 2:E:183:LEU:HB2  | 2:E:195:CYS:O    | 2.19                     | 0.42              |
| 1:G:181:TYR:HA   | 1:G:440:LEU:HD22 | 2.02                     | 0.42              |
| 1:G:373:ILE:O    | 1:G:386:THR:HA   | 2.19                     | 0.42              |
| 2:E:71:LEU:HD23  | 2:E:71:LEU:C     | 2.41                     | 0.41              |
| 2:E:84:ILE:HG22  | 2:E:86:VAL:HG23  | 2.00                     | 0.41              |
| 3:I:197:ARG:O    | 3:I:197:ARG:HG3  | 2.18                     | 0.41              |
| 1:G:185:LEU:HD22 | 1:G:197:ALA:HB3  | 2.02                     | 0.41              |
| 3:I:106:GLU:HA   | 3:I:106:GLU:OE1  | 2.19                     | 0.41              |
| 1:D:406:MET:HG2  | 1:D:418:ILE:HG12 | 2.02                     | 0.41              |
| 1:G:199:GLU:HB3  | 1:G:200:ARG:H    | 1.48                     | 0.41              |
| 1:A:200:ARG:HD3  | 1:A:220:GLU:HA   | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:313:ARG:HG3  | 1:D:354:TRP:CG   | 2.54                     | 0.41              |
| 1:G:167:THR:HG23 | 1:G:168:PRO:CD   | 2.47                     | 0.41              |
| 2:E:30:ILE:HG12  | 2:E:85:LEU:HD23  | 2.02                     | 0.41              |
| 1:A:185:LEU:HD13 | 1:A:185:LEU:N    | 2.36                     | 0.41              |
| 2:H:84:ILE:C     | 2:H:85:LEU:HD12  | 2.40                     | 0.41              |
| 2:H:134:GLN:HB2  | 3:I:13:MET:HG2   | 2.02                     | 0.41              |
| 2:H:61:LYS:O     | 2:H:65:ARG:HD2   | 2.20                     | 0.41              |
| 3:I:122:ILE:HG22 | 3:I:126:TYR:CZ   | 2.52                     | 0.41              |
| 1:D:387:VAL:HG11 | 1:D:426:LEU:HB2  | 2.03                     | 0.41              |
| 1:D:375:PHE:CZ   | 1:D:426:LEU:HD21 | 2.55                     | 0.41              |
| 3:I:136:LEU:O    | 3:I:140:LEU:HB2  | 2.20                     | 0.41              |
| 2:E:95:ASP:HB2   | 2:E:175:LEU:HD21 | 2.02                     | 0.41              |
| 3:I:189:GLN:O    | 3:I:193:GLN:HG3  | 2.19                     | 0.41              |
| 2:H:61:LYS:O     | 2:H:65:ARG:HB2   | 2.20                     | 0.41              |
| 2:E:21:GLU:HG2   | 2:E:47:LYS:HZ1   | 1.85                     | 0.41              |
| 1:G:406:MET:HG2  | 1:G:418:ILE:HG12 | 2.03                     | 0.41              |
| 2:H:156:TYR:HD1  | 2:H:156:TYR:N    | 2.18                     | 0.41              |
| 3:C:123:TRP:CE2  | 3:C:140:LEU:HD21 | 2.56                     | 0.41              |
| 1:D:220:GLU:HG3  | 1:D:220:GLU:H    | 1.60                     | 0.41              |
| 3:I:107:PHE:HE1  | 3:I:109:ARG:NH1  | 2.19                     | 0.41              |
| 3:I:192:GLN:O    | 3:I:195:THR:OG1  | 2.36                     | 0.41              |
| 3:F:172:VAL:HA   | 3:F:175:LYS:HE2  | 2.02                     | 0.41              |
| 3:I:143:HIS:HB3  | 3:I:145:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:133:LYS:HG3  | 1:A:134:LEU:HD23 | 2.02                     | 0.41              |
| 2:E:21:GLU:CG    | 2:E:47:LYS:HZ1   | 2.33                     | 0.41              |
| 2:E:137:ALA:HB3  | 3:F:13:MET:HE3   | 2.03                     | 0.41              |
| 3:I:59:GLU:O     | 3:I:62:ILE:HG22  | 2.21                     | 0.41              |
| 2:B:180:GLN:HB2  | 3:C:10:TRP:CE3   | 2.55                     | 0.41              |
| 1:G:249:ASP:HB2  | 1:G:256:LEU:HD21 | 2.03                     | 0.41              |
| 2:H:37:TYR:HB3   | 2:H:38:PRO:HD2   | 2.02                     | 0.41              |
| 1:G:205:TRP:HD1  | 1:G:212:VAL:HG22 | 1.86                     | 0.41              |
| 1:A:290:VAL:HG12 | 1:A:290:VAL:O    | 2.20                     | 0.41              |
| 2:E:87:ILE:HD11  | 2:E:149:CYS:HB3  | 2.03                     | 0.41              |
| 2:E:47:LYS:NZ    | 2:E:48:TYR:CZ    | 2.86                     | 0.41              |
| 1:D:361:LEU:HD11 | 1:D:421:TYR:CZ   | 2.56                     | 0.41              |
| 2:E:134:GLN:NE2  | 3:F:14:ASP:OD1   | 2.51                     | 0.40              |
| 2:E:85:LEU:HG    | 2:E:151:PHE:CE1  | 2.56                     | 0.40              |
| 1:G:265:ARG:NH2  | 1:G:281:ARG:NH1  | 2.69                     | 0.40              |
| 3:C:150:SER:O    | 3:C:154:GLU:HG3  | 2.21                     | 0.40              |
| 1:A:397:ILE:HD12 | 1:A:451:LEU:HD11 | 2.04                     | 0.40              |
| 2:H:186:PHE:CD1  | 2:H:186:PHE:C    | 2.94                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:H:53:LEU:N     | 2:H:53:LEU:HD22 | 2.36                     | 0.40              |
| 3:I:214:ASN:HA   | 3:I:215:PRO:HD2 | 1.90                     | 0.40              |
| 2:B:92:SER:OG    | 2:B:94:GLU:HG2  | 2.21                     | 0.40              |
| 2:E:87:ILE:CG2   | 2:E:97:GLU:CB   | 2.93                     | 0.40              |
| 2:H:120:ASP:OD1  | 2:H:123:ARG:NE  | 2.49                     | 0.40              |
| 3:I:134:VAL:HG12 | 3:I:135:GLU:N   | 2.36                     | 0.40              |
| 1:G:332:ASP:OD1  | 1:G:339:LYS:HD2 | 2.21                     | 0.40              |
| 4:A:2068:HOH:O   | 3:C:20:LYS:NZ   | 2.53                     | 0.40              |
| 1:A:272:ASN:HB2  | 1:A:312:TRP:CG  | 2.57                     | 0.40              |
| 3:I:119:TYR:CD2  | 3:I:123:TRP:HZ3 | 2.39                     | 0.40              |
| 1:G:357:TRP:CH2  | 1:G:403:LYS:HA  | 2.56                     | 0.40              |
| 2:E:59:GLU:N     | 2:E:59:GLU:OE1  | 2.55                     | 0.40              |
| 2:H:144:GLN:O    | 2:H:144:GLN:HG3 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 322/401 (80%)   | 318 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | D     | 310/401 (77%)   | 303 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 1   | G     | 313/401 (78%)   | 306 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 2   | B     | 176/203 (87%)   | 176 (100%) | 0       | 0        | 100         | 100 |
| 2   | E     | 171/203 (84%)   | 169 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 2   | H     | 179/203 (88%)   | 178 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 3   | C     | 213/223 (96%)   | 213 (100%) | 0       | 0        | 100         | 100 |
| 3   | F     | 192/223 (86%)   | 191 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 3   | I     | 187/223 (84%)   | 185 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| All | All   | 2063/2481 (83%) | 2039 (99%) | 24 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 269/340 (79%)   | 260 (97%)  | 9 (3%)   | 45          | 61 |
| 1   | D     | 259/340 (76%)   | 248 (96%)  | 11 (4%)  | 36          | 49 |
| 1   | G     | 255/340 (75%)   | 244 (96%)  | 11 (4%)  | 35          | 47 |
| 2   | B     | 166/187 (89%)   | 157 (95%)  | 9 (5%)   | 27          | 36 |
| 2   | E     | 145/187 (78%)   | 134 (92%)  | 11 (8%)  | 16          | 20 |
| 2   | H     | 160/187 (86%)   | 147 (92%)  | 13 (8%)  | 15          | 18 |
| 3   | C     | 196/203 (97%)   | 184 (94%)  | 12 (6%)  | 23          | 30 |
| 3   | F     | 163/203 (80%)   | 154 (94%)  | 9 (6%)   | 27          | 36 |
| 3   | I     | 162/203 (80%)   | 134 (83%)  | 28 (17%) | 2           | 2  |
| All | All   | 1775/2190 (81%) | 1662 (94%) | 113 (6%) | 22          | 28 |

All (113) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 125 | LEU  |
| 1   | A     | 126 | ASN  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 185 | LEU  |
| 1   | A     | 186 | LEU  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 263 | GLN  |
| 1   | A     | 464 | ARG  |
| 1   | A     | 467 | ASP  |
| 2   | B     | 40  | GLU  |
| 2   | B     | 46  | ARG  |
| 2   | B     | 65  | ARG  |
| 2   | B     | 69  | SER  |
| 2   | B     | 72  | HIS  |
| 2   | B     | 86  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 107 | ASP  |
| 2   | B     | 153 | VAL  |
| 2   | B     | 171 | ASP  |
| 3   | C     | 19  | SER  |
| 3   | C     | 67  | SER  |
| 3   | C     | 68  | LEU  |
| 3   | C     | 78  | TYR  |
| 3   | C     | 92  | LYS  |
| 3   | C     | 94  | SER  |
| 3   | C     | 135 | GLU  |
| 3   | C     | 156 | TYR  |
| 3   | C     | 184 | PHE  |
| 3   | C     | 185 | LEU  |
| 3   | C     | 191 | TYR  |
| 3   | C     | 223 | THR  |
| 1   | D     | 186 | LEU  |
| 1   | D     | 220 | GLU  |
| 1   | D     | 244 | LEU  |
| 1   | D     | 281 | ARG  |
| 1   | D     | 359 | SER  |
| 1   | D     | 361 | LEU  |
| 1   | D     | 371 | LYS  |
| 1   | D     | 397 | ILE  |
| 1   | D     | 416 | LEU  |
| 1   | D     | 431 | ASP  |
| 1   | D     | 464 | ARG  |
| 2   | E     | 29  | SER  |
| 2   | E     | 30  | ILE  |
| 2   | E     | 72  | HIS  |
| 2   | E     | 79  | LYS  |
| 2   | E     | 82  | LYS  |
| 2   | E     | 85  | LEU  |
| 2   | E     | 95  | ASP  |
| 2   | E     | 144 | GLN  |
| 2   | E     | 160 | ASP  |
| 2   | E     | 181 | VAL  |
| 2   | E     | 194 | ASP  |
| 3   | F     | 13  | MET  |
| 3   | F     | 19  | SER  |
| 3   | F     | 99  | LEU  |
| 3   | F     | 148 | GLU  |
| 3   | F     | 156 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 185 | LEU  |
| 3   | F     | 191 | TYR  |
| 3   | F     | 220 | PHE  |
| 3   | F     | 221 | GLU  |
| 1   | G     | 126 | ASN  |
| 1   | G     | 170 | ARG  |
| 1   | G     | 177 | ILE  |
| 1   | G     | 181 | TYR  |
| 1   | G     | 186 | LEU  |
| 1   | G     | 199 | GLU  |
| 1   | G     | 204 | VAL  |
| 1   | G     | 304 | SER  |
| 1   | G     | 313 | ARG  |
| 1   | G     | 329 | GLN  |
| 1   | G     | 371 | LYS  |
| 2   | H     | 6   | ILE  |
| 2   | H     | 8   | THR  |
| 2   | H     | 44  | VAL  |
| 2   | H     | 50  | LEU  |
| 2   | H     | 65  | ARG  |
| 2   | H     | 72  | HIS  |
| 2   | H     | 94  | GLU  |
| 2   | H     | 118 | LYS  |
| 2   | H     | 123 | ARG  |
| 2   | H     | 147 | GLU  |
| 2   | H     | 150 | THR  |
| 2   | H     | 153 | VAL  |
| 2   | H     | 169 | ASP  |
| 3   | I     | 11  | VAL  |
| 3   | I     | 38  | SER  |
| 3   | I     | 42  | ASN  |
| 3   | I     | 44  | THR  |
| 3   | I     | 60  | ARG  |
| 3   | I     | 74  | VAL  |
| 3   | I     | 78  | TYR  |
| 3   | I     | 82  | THR  |
| 3   | I     | 101 | GLU  |
| 3   | I     | 104 | THR  |
| 3   | I     | 109 | ARG  |
| 3   | I     | 117 | VAL  |
| 3   | I     | 119 | TYR  |
| 3   | I     | 123 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 128 | ASN  |
| 3   | I     | 131 | ASP  |
| 3   | I     | 132 | GLU  |
| 3   | I     | 138 | SER  |
| 3   | I     | 142 | HIS  |
| 3   | I     | 143 | HIS  |
| 3   | I     | 155 | GLU  |
| 3   | I     | 159 | TYR  |
| 3   | I     | 160 | PHE  |
| 3   | I     | 166 | PHE  |
| 3   | I     | 175 | LYS  |
| 3   | I     | 186 | ARG  |
| 3   | I     | 197 | ARG  |
| 3   | I     | 198 | TRP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 126 | ASN  |
| 1   | A     | 429 | GLN  |
| 2   | E     | 70  | GLN  |
| 2   | H     | 70  | GLN  |
| 2   | H     | 117 | ASN  |
| 3   | I     | 128 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 326/401 (81%)   | 0.50   | 4 (1%) 81 85  | 17, 33, 64, 116       | 0     |
| 1   | D     | 314/401 (78%)   | 0.64   | 14 (4%) 37 46 | 19, 42, 84, 116       | 0     |
| 1   | G     | 317/401 (79%)   | 1.23   | 61 (19%) 2 2  | 43, 72, 103, 124      | 0     |
| 2   | B     | 180/203 (88%)   | 0.45   | 1 (0%) 90 93  | 25, 44, 69, 109       | 0     |
| 2   | E     | 175/203 (86%)   | 1.69   | 66 (37%) 0 0  | 40, 85, 127, 150      | 0     |
| 2   | H     | 185/203 (91%)   | 1.54   | 54 (29%) 1 1  | 47, 70, 117, 139      | 0     |
| 3   | C     | 215/223 (96%)   | 0.53   | 5 (2%) 64 72  | 19, 46, 81, 118       | 0     |
| 3   | F     | 196/223 (87%)   | 0.75   | 17 (8%) 13 18 | 21, 53, 115, 149      | 0     |
| 3   | I     | 193/223 (86%)   | 2.11   | 85 (44%) 0 0  | 40, 97, 133, 147      | 0     |
| All | All   | 2101/2481 (84%) | 0.99   | 307 (14%) 3 5 | 17, 56, 111, 150      | 0     |

All (307) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 151 | PHE  | 9.7  |
| 3   | I     | 117 | VAL  | 8.8  |
| 3   | I     | 141 | ALA  | 8.6  |
| 3   | I     | 158 | ASN  | 8.3  |
| 2   | E     | 153 | VAL  | 8.3  |
| 3   | I     | 134 | VAL  | 8.2  |
| 2   | H     | 87  | ILE  | 7.5  |
| 3   | I     | 103 | CYS  | 7.4  |
| 3   | I     | 133 | PRO  | 7.3  |
| 2   | E     | 155 | VAL  | 7.2  |
| 3   | F     | 165 | LEU  | 7.0  |
| 3   | I     | 69  | ASP  | 7.0  |
| 3   | I     | 115 | ASP  | 6.9  |
| 3   | I     | 107 | PHE  | 6.8  |
| 1   | D     | 134 | LEU  | 5.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 131 | ALA  | 5.9  |
| 2   | H     | 85  | LEU  | 5.9  |
| 2   | E     | 93  | GLY  | 5.8  |
| 1   | G     | 334 | ARG  | 5.7  |
| 3   | I     | 100 | LEU  | 5.7  |
| 1   | D     | 133 | LYS  | 5.6  |
| 3   | I     | 198 | TRP  | 5.6  |
| 3   | I     | 123 | TRP  | 5.6  |
| 2   | H     | 97  | GLU  | 5.4  |
| 3   | I     | 108 | VAL  | 5.4  |
| 2   | E     | 147 | GLU  | 5.4  |
| 2   | E     | 80  | ILE  | 5.1  |
| 3   | I     | 70  | ASP  | 5.1  |
| 2   | E     | 96  | LEU  | 5.1  |
| 1   | G     | 375 | PHE  | 5.1  |
| 1   | D     | 136 | ALA  | 5.0  |
| 2   | E     | 68  | VAL  | 5.0  |
| 2   | H     | 63  | TYR  | 5.0  |
| 3   | F     | 10  | TRP  | 4.9  |
| 2   | H     | 30  | ILE  | 4.9  |
| 3   | I     | 120 | LEU  | 4.9  |
| 3   | I     | 156 | TYR  | 4.8  |
| 2   | E     | 82  | LYS  | 4.8  |
| 2   | E     | 72  | HIS  | 4.7  |
| 3   | I     | 157 | ALA  | 4.6  |
| 3   | I     | 142 | HIS  | 4.6  |
| 2   | E     | 172 | PRO  | 4.5  |
| 2   | E     | 17  | LYS  | 4.5  |
| 2   | E     | 53  | LEU  | 4.5  |
| 3   | F     | 194 | PHE  | 4.5  |
| 1   | G     | 376 | TRP  | 4.5  |
| 3   | I     | 10  | TRP  | 4.4  |
| 2   | E     | 83  | LEU  | 4.4  |
| 3   | F     | 183 | PRO  | 4.4  |
| 3   | I     | 185 | LEU  | 4.3  |
| 2   | H     | 137 | ALA  | 4.3  |
| 2   | E     | 160 | ASP  | 4.3  |
| 3   | I     | 166 | PHE  | 4.3  |
| 1   | G     | 397 | ILE  | 4.2  |
| 2   | E     | 101 | PHE  | 4.2  |
| 3   | I     | 126 | TYR  | 4.2  |
| 3   | I     | 112 | LEU  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | I     | 111 | PRO  | 4.2  |
| 3   | I     | 127 | VAL  | 4.2  |
| 1   | G     | 261 | GLY  | 4.1  |
| 3   | I     | 150 | SER  | 4.1  |
| 2   | H     | 197 | VAL  | 4.0  |
| 3   | I     | 58  | HIS  | 4.0  |
| 1   | D     | 137 | PRO  | 4.0  |
| 2   | E     | 42  | PHE  | 4.0  |
| 1   | G     | 201 | ASN  | 3.9  |
| 2   | H     | 175 | LEU  | 3.9  |
| 3   | F     | 163 | ARG  | 3.9  |
| 1   | G     | 423 | SER  | 3.9  |
| 3   | I     | 140 | LEU  | 3.8  |
| 3   | I     | 76  | ILE  | 3.8  |
| 1   | D     | 130 | LEU  | 3.8  |
| 3   | F     | 195 | THR  | 3.8  |
| 1   | G     | 136 | ALA  | 3.8  |
| 3   | I     | 97  | VAL  | 3.8  |
| 3   | I     | 155 | GLU  | 3.7  |
| 2   | H     | 83  | LEU  | 3.7  |
| 2   | E     | 146 | GLU  | 3.7  |
| 2   | H     | 146 | GLU  | 3.7  |
| 3   | I     | 154 | GLU  | 3.7  |
| 1   | G     | 191 | LEU  | 3.7  |
| 2   | E     | 56  | VAL  | 3.7  |
| 1   | G     | 289 | ASP  | 3.7  |
| 1   | G     | 401 | HIS  | 3.7  |
| 2   | H     | 174 | ILE  | 3.6  |
| 3   | I     | 104 | THR  | 3.6  |
| 2   | E     | 77  | ALA  | 3.6  |
| 3   | I     | 99  | LEU  | 3.6  |
| 1   | G     | 357 | TRP  | 3.6  |
| 2   | E     | 18  | LEU  | 3.6  |
| 2   | B     | 107 | ASP  | 3.6  |
| 2   | H     | 143 | PRO  | 3.6  |
| 3   | I     | 75  | TRP  | 3.6  |
| 3   | I     | 160 | PHE  | 3.6  |
| 3   | F     | 120 | LEU  | 3.6  |
| 3   | I     | 105 | ARG  | 3.5  |
| 3   | I     | 15  | VAL  | 3.5  |
| 2   | E     | 87  | ILE  | 3.5  |
| 3   | C     | 184 | PHE  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 356 | PRO  | 3.5  |
| 2   | E     | 150 | THR  | 3.5  |
| 2   | H     | 6   | ILE  | 3.5  |
| 2   | H     | 55  | SER  | 3.4  |
| 3   | I     | 72  | LEU  | 3.4  |
| 2   | H     | 150 | THR  | 3.4  |
| 3   | I     | 178 | ARG  | 3.4  |
| 3   | I     | 147 | GLN  | 3.3  |
| 2   | H     | 86  | VAL  | 3.3  |
| 3   | I     | 68  | LEU  | 3.3  |
| 3   | I     | 16  | ILE  | 3.3  |
| 3   | I     | 106 | GLU  | 3.3  |
| 3   | I     | 153 | TYR  | 3.3  |
| 3   | I     | 162 | SER  | 3.2  |
| 3   | F     | 191 | TYR  | 3.2  |
| 1   | G     | 244 | LEU  | 3.2  |
| 1   | G     | 323 | GLY  | 3.2  |
| 3   | C     | 200 | GLU  | 3.2  |
| 3   | I     | 62  | ILE  | 3.1  |
| 2   | H     | 170 | SER  | 3.1  |
| 1   | G     | 361 | LEU  | 3.1  |
| 1   | G     | 327 | VAL  | 3.1  |
| 2   | H     | 62  | THR  | 3.1  |
| 2   | H     | 10  | PHE  | 3.1  |
| 2   | H     | 149 | CYS  | 3.1  |
| 3   | I     | 64  | THR  | 3.1  |
| 2   | H     | 99  | TRP  | 3.1  |
| 2   | H     | 80  | ILE  | 3.1  |
| 3   | I     | 170 | ASP  | 3.1  |
| 1   | G     | 235 | PHE  | 3.1  |
| 1   | G     | 216 | ALA  | 3.0  |
| 2   | H     | 181 | VAL  | 3.0  |
| 3   | I     | 165 | LEU  | 3.0  |
| 2   | H     | 168 | VAL  | 3.0  |
| 1   | G     | 311 | ALA  | 3.0  |
| 2   | E     | 175 | LEU  | 3.0  |
| 3   | I     | 28  | ALA  | 3.0  |
| 3   | I     | 164 | GLY  | 3.0  |
| 2   | E     | 76  | PHE  | 3.0  |
| 2   | E     | 43  | LYS  | 2.9  |
| 1   | G     | 205 | TRP  | 2.9  |
| 2   | H     | 77  | ALA  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 364 | THR  | 2.9  |
| 1   | G     | 168 | PRO  | 2.9  |
| 1   | G     | 203 | TYR  | 2.9  |
| 1   | G     | 436 | ASP  | 2.9  |
| 3   | I     | 91  | THR  | 2.9  |
| 1   | G     | 204 | VAL  | 2.9  |
| 3   | F     | 184 | PHE  | 2.9  |
| 3   | I     | 138 | SER  | 2.9  |
| 2   | E     | 44  | VAL  | 2.8  |
| 2   | E     | 156 | TYR  | 2.8  |
| 2   | E     | 40  | GLU  | 2.8  |
| 3   | I     | 66  | GLU  | 2.8  |
| 3   | I     | 11  | VAL  | 2.8  |
| 2   | E     | 84  | ILE  | 2.8  |
| 3   | I     | 149 | SER  | 2.8  |
| 2   | H     | 133 | ALA  | 2.8  |
| 3   | I     | 65  | SER  | 2.8  |
| 2   | E     | 184 | ARG  | 2.8  |
| 3   | C     | 209 | ASN  | 2.8  |
| 3   | I     | 61  | LYS  | 2.8  |
| 1   | G     | 328 | VAL  | 2.8  |
| 1   | G     | 312 | TRP  | 2.8  |
| 1   | G     | 330 | ILE  | 2.7  |
| 1   | D     | 466 | TYR  | 2.7  |
| 2   | E     | 99  | TRP  | 2.7  |
| 1   | D     | 268 | CYS  | 2.7  |
| 1   | G     | 360 | ASN  | 2.7  |
| 2   | E     | 19  | VAL  | 2.7  |
| 2   | H     | 155 | VAL  | 2.7  |
| 3   | I     | 176 | GLY  | 2.7  |
| 2   | E     | 39  | ALA  | 2.7  |
| 3   | C     | 189 | GLN  | 2.7  |
| 2   | H     | 79  | LYS  | 2.7  |
| 1   | G     | 234 | SER  | 2.7  |
| 1   | G     | 254 | THR  | 2.7  |
| 2   | H     | 60  | VAL  | 2.7  |
| 3   | F     | 172 | VAL  | 2.7  |
| 1   | D     | 132 | PHE  | 2.7  |
| 1   | G     | 340 | PHE  | 2.7  |
| 1   | G     | 402 | SER  | 2.7  |
| 3   | I     | 113 | TYR  | 2.7  |
| 1   | G     | 426 | LEU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 105 | MET  | 2.6  |
| 1   | G     | 270 | SER  | 2.6  |
| 3   | I     | 144 | HIS  | 2.6  |
| 2   | E     | 89  | SER  | 2.6  |
| 2   | H     | 183 | LEU  | 2.6  |
| 1   | G     | 166 | THR  | 2.6  |
| 2   | H     | 34  | ARG  | 2.6  |
| 1   | G     | 355 | CYS  | 2.6  |
| 2   | E     | 157 | ALA  | 2.6  |
| 2   | H     | 178 | ALA  | 2.6  |
| 2   | E     | 67  | ILE  | 2.6  |
| 2   | H     | 153 | VAL  | 2.5  |
| 2   | H     | 180 | GLN  | 2.5  |
| 3   | I     | 124 | MET  | 2.5  |
| 1   | G     | 238 | VAL  | 2.5  |
| 1   | D     | 341 | THR  | 2.5  |
| 1   | G     | 278 | SER  | 2.5  |
| 2   | H     | 132 | ILE  | 2.5  |
| 3   | I     | 132 | GLU  | 2.5  |
| 3   | I     | 193 | GLN  | 2.5  |
| 3   | I     | 49  | ALA  | 2.4  |
| 2   | E     | 71  | LEU  | 2.4  |
| 2   | H     | 199 | TYR  | 2.4  |
| 3   | I     | 130 | ILE  | 2.4  |
| 2   | E     | 190 | MET  | 2.4  |
| 1   | D     | 387 | VAL  | 2.4  |
| 1   | G     | 188 | TRP  | 2.4  |
| 1   | G     | 418 | ILE  | 2.4  |
| 1   | G     | 432 | ILE  | 2.4  |
| 3   | I     | 188 | GLN  | 2.4  |
| 3   | F     | 169 | ALA  | 2.4  |
| 1   | G     | 212 | VAL  | 2.4  |
| 2   | E     | 161 | SER  | 2.4  |
| 2   | E     | 171 | ASP  | 2.4  |
| 2   | H     | 169 | ASP  | 2.4  |
| 2   | E     | 26  | ALA  | 2.4  |
| 2   | E     | 165 | THR  | 2.4  |
| 2   | H     | 165 | THR  | 2.4  |
| 2   | E     | 122 | LEU  | 2.4  |
| 3   | I     | 119 | TYR  | 2.4  |
| 2   | E     | 174 | ILE  | 2.4  |
| 3   | F     | 173 | TYR  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | I     | 192 | GLN  | 2.4  |
| 3   | I     | 67  | SER  | 2.3  |
| 1   | G     | 223 | TYR  | 2.3  |
| 2   | H     | 27  | VAL  | 2.3  |
| 2   | E     | 90  | LYS  | 2.3  |
| 1   | G     | 333 | ALA  | 2.3  |
| 2   | E     | 32  | PHE  | 2.3  |
| 2   | H     | 12  | ALA  | 2.3  |
| 3   | I     | 73  | GLN  | 2.3  |
| 2   | E     | 138 | THR  | 2.3  |
| 1   | A     | 125 | LEU  | 2.3  |
| 1   | G     | 236 | LEU  | 2.3  |
| 2   | E     | 154 | LEU  | 2.3  |
| 2   | H     | 11  | SER  | 2.3  |
| 2   | H     | 119 | GLU  | 2.3  |
| 3   | I     | 14  | ASP  | 2.3  |
| 2   | H     | 23  | PHE  | 2.3  |
| 2   | H     | 176 | ARG  | 2.3  |
| 2   | E     | 167 | TRP  | 2.3  |
| 1   | G     | 326 | ASN  | 2.3  |
| 3   | F     | 175 | LYS  | 2.3  |
| 1   | G     | 430 | VAL  | 2.3  |
| 2   | H     | 8   | THR  | 2.3  |
| 3   | I     | 195 | THR  | 2.3  |
| 3   | F     | 217 | GLN  | 2.3  |
| 3   | I     | 136 | LEU  | 2.3  |
| 3   | F     | 181 | ALA  | 2.3  |
| 2   | E     | 121 | GLU  | 2.3  |
| 2   | H     | 138 | THR  | 2.2  |
| 1   | G     | 275 | VAL  | 2.2  |
| 2   | E     | 145 | LEU  | 2.2  |
| 1   | A     | 144 | ASP  | 2.2  |
| 2   | E     | 163 | VAL  | 2.2  |
| 2   | H     | 104 | GLU  | 2.2  |
| 2   | E     | 176 | ARG  | 2.2  |
| 2   | H     | 167 | TRP  | 2.2  |
| 1   | A     | 309 | GLY  | 2.2  |
| 3   | I     | 71  | PRO  | 2.2  |
| 3   | I     | 116 | ASP  | 2.2  |
| 2   | E     | 47  | LYS  | 2.2  |
| 3   | I     | 101 | GLU  | 2.2  |
| 1   | G     | 396 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 444 | LEU  | 2.2  |
| 2   | E     | 187 | SER  | 2.1  |
| 2   | H     | 161 | SER  | 2.1  |
| 1   | G     | 218 | THR  | 2.1  |
| 1   | G     | 195 | ALA  | 2.1  |
| 2   | H     | 26  | ALA  | 2.1  |
| 2   | H     | 118 | LYS  | 2.1  |
| 3   | F     | 180 | LYS  | 2.1  |
| 1   | D     | 430 | VAL  | 2.1  |
| 1   | G     | 126 | ASN  | 2.1  |
| 1   | G     | 385 | ASN  | 2.1  |
| 3   | F     | 158 | ASN  | 2.1  |
| 3   | I     | 179 | MET  | 2.1  |
| 3   | I     | 169 | ALA  | 2.1  |
| 1   | G     | 227 | VAL  | 2.1  |
| 2   | E     | 189 | SER  | 2.1  |
| 2   | H     | 156 | TYR  | 2.1  |
| 3   | I     | 129 | TYR  | 2.1  |
| 2   | E     | 148 | GLN  | 2.1  |
| 3   | I     | 60  | ARG  | 2.1  |
| 2   | E     | 125 | GLN  | 2.1  |
| 3   | I     | 167 | GLN  | 2.1  |
| 1   | A     | 126 | ASN  | 2.1  |
| 2   | E     | 37  | TYR  | 2.1  |
| 3   | I     | 159 | TYR  | 2.1  |
| 2   | E     | 46  | ARG  | 2.1  |
| 1   | D     | 291 | ARG  | 2.0  |
| 2   | H     | 65  | ARG  | 2.0  |
| 1   | G     | 419 | TRP  | 2.0  |
| 1   | G     | 445 | SER  | 2.0  |
| 1   | G     | 199 | GLU  | 2.0  |
| 3   | I     | 79  | ILE  | 2.0  |
| 2   | E     | 57  | ASP  | 2.0  |
| 1   | G     | 131 | ALA  | 2.0  |
| 2   | E     | 98  | ARG  | 2.0  |
| 3   | C     | 105 | ARG  | 2.0  |
| 2   | E     | 202 | ASN  | 2.0  |
| 1   | D     | 129 | VAL  | 2.0  |
| 2   | E     | 75  | MET  | 2.0  |
| 2   | E     | 151 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.