



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 PM GMT

PDB ID : 4I46  
Title : Crystal structure of 31kD Heat Shock Protein, VcHsp31 from *Vibrio cholerae*  
Authors : Sen, U.; Das, S.  
Deposited on : 2012-11-27  
Resolution : 2.50 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

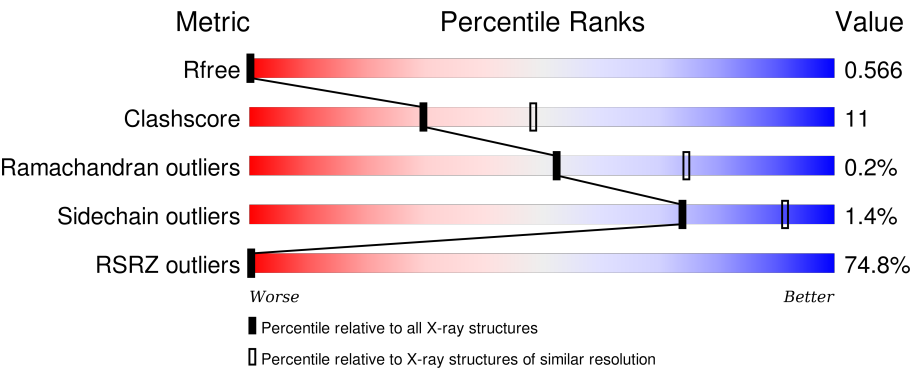
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                       | 3553 (2.50-2.50)                                      |
| Clashscore            | 102246                      | 4242 (2.50-2.50)                                      |
| Ramachandran outliers | 100387                      | 4156 (2.50-2.50)                                      |
| Sidechain outliers    | 100360                      | 4158 (2.50-2.50)                                      |
| RSRZ outliers         | 91569                       | 3562 (2.50-2.50)                                      |

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     | 286    | <div><div>72%</div><div><div></div><div></div><div></div><div></div></div><div>72%26%.</div></div>  |
| 1   | B     | 286    | <div><div>69%</div><div><div></div><div></div><div></div><div></div></div><div>81%17%.</div></div>  |
| 1   | C     | 286    | <div><div>73%</div><div><div></div><div></div><div></div><div></div></div><div>77%20%..</div></div> |
| 1   | D     | 286    | <div><div>72%</div><div><div></div><div></div><div></div><div></div></div><div>76%22%.</div></div>  |
| 1   | E     | 286    | <div><div>79%</div><div><div></div><div></div><div></div><div></div></div><div>71%27%.</div></div>  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | F     | 286    | <div> <div>76%</div> <div>73%</div> <div>25%</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | MPD  | A     | 301  | -         | -        | -       | X                |
| 2   | MPD  | B     | 5001 | -         | -        | -       | X                |
| 2   | MPD  | B     | 5002 | -         | -        | -       | X                |
| 2   | MPD  | D     | 301  | -         | -        | -       | X                |
| 2   | MPD  | F     | 301  | -         | -        | X       | X                |

## 2 Entry composition [i](#)

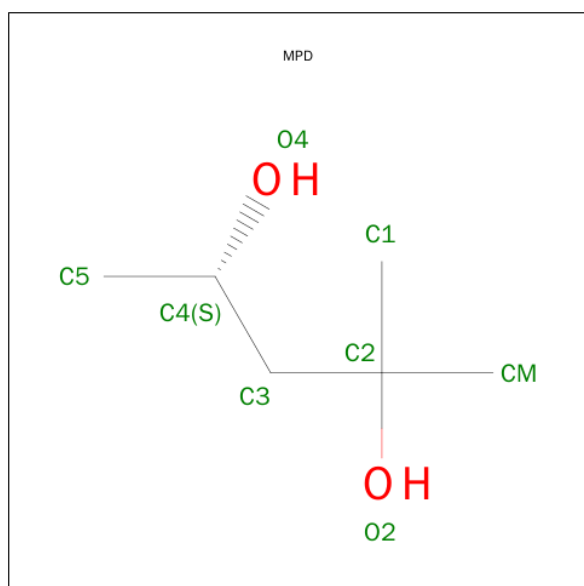
There are 3 unique types of molecules in this entry. The entry contains 13718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Intracellular protease/amidase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2163  | 1390 | 352 | 411 | 10 |         |         |       |
| 1   | B     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2163  | 1390 | 352 | 411 | 10 |         |         |       |
| 1   | C     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2163  | 1390 | 352 | 411 | 10 |         |         |       |
| 1   | D     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2163  | 1390 | 352 | 411 | 10 |         |         |       |
| 1   | E     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2163  | 1390 | 352 | 411 | 10 |         |         |       |
| 1   | F     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2163  | 1390 | 352 | 411 | 10 |         |         |       |

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).

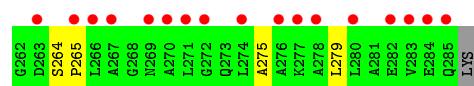


| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2   | A     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 2   | B     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 2   | B     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 2   | D     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 2   | E     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 2   | F     | 1        | Total C O<br>8 6 2 | 0       | 0       |

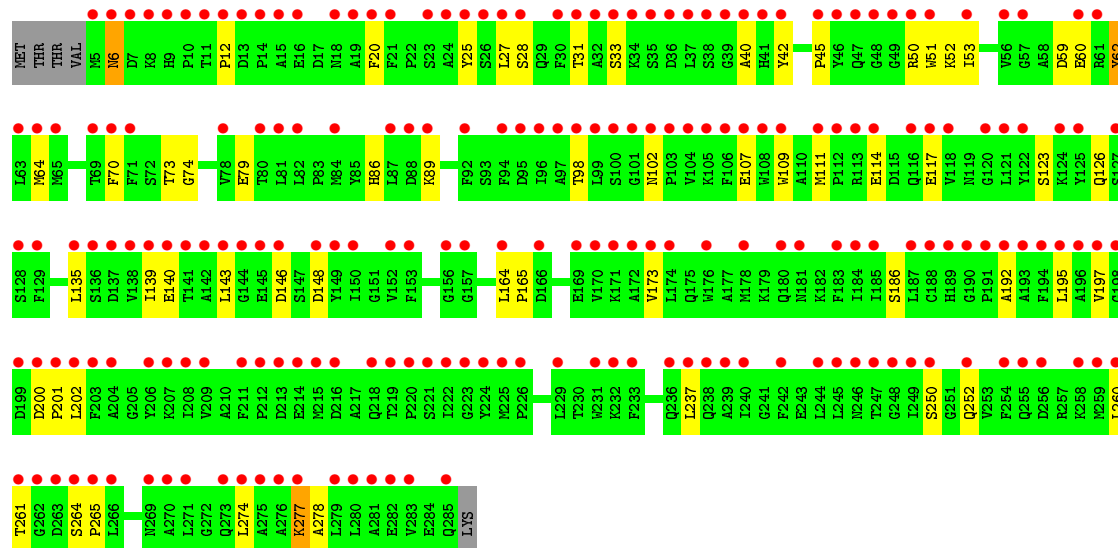
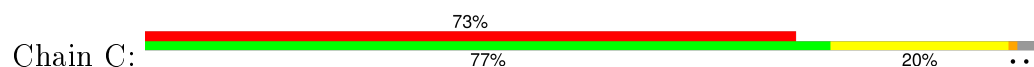
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | A     | 131      | Total O<br>131 131 | 0       | 0       |
| 3   | B     | 131      | Total O<br>131 131 | 0       | 0       |
| 3   | C     | 113      | Total O<br>113 113 | 0       | 0       |
| 3   | D     | 123      | Total O<br>123 123 | 0       | 0       |
| 3   | E     | 91       | Total O<br>91 91   | 0       | 0       |
| 3   | F     | 103      | Total O<br>103 103 | 0       | 0       |

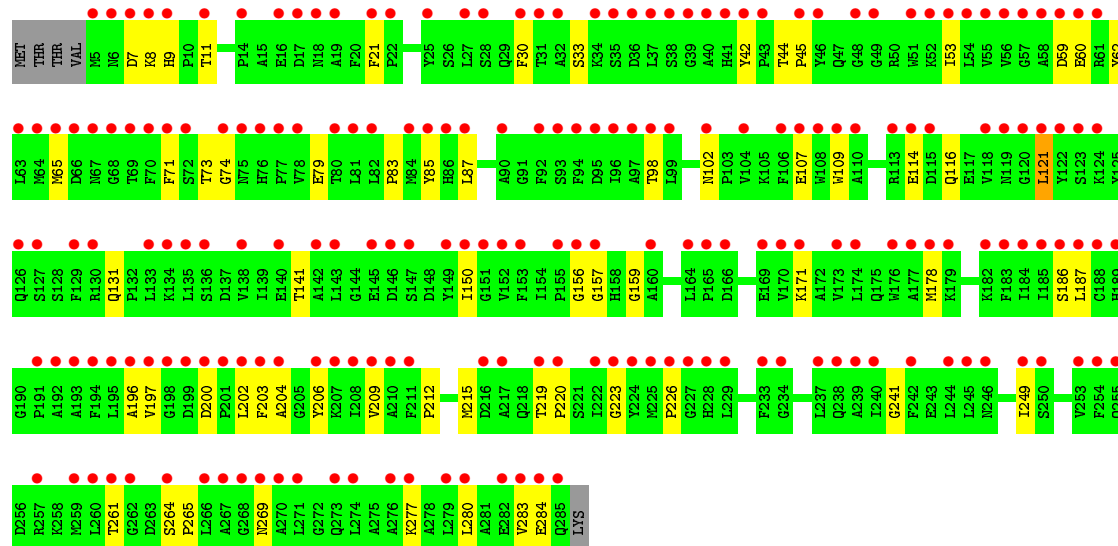
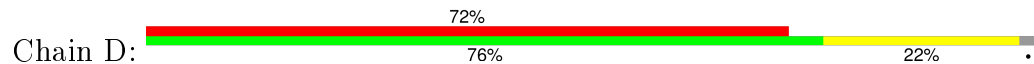




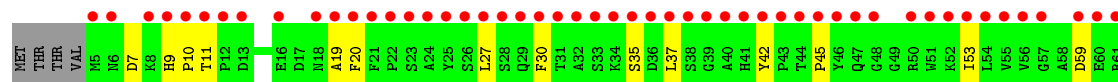
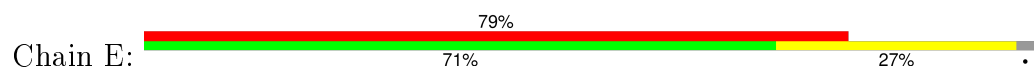
• Molecule 1: Intracellular protease/amidase

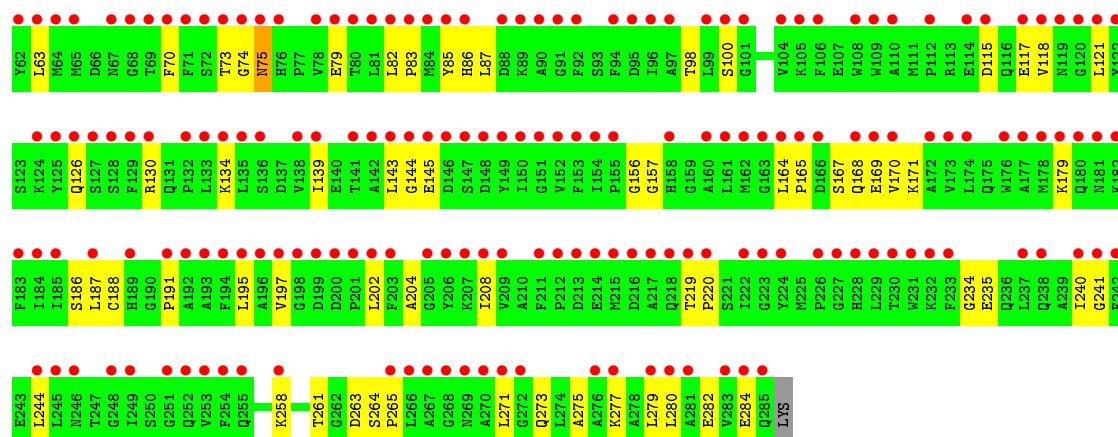


• Molecule 1: Intracellular protease/amidase

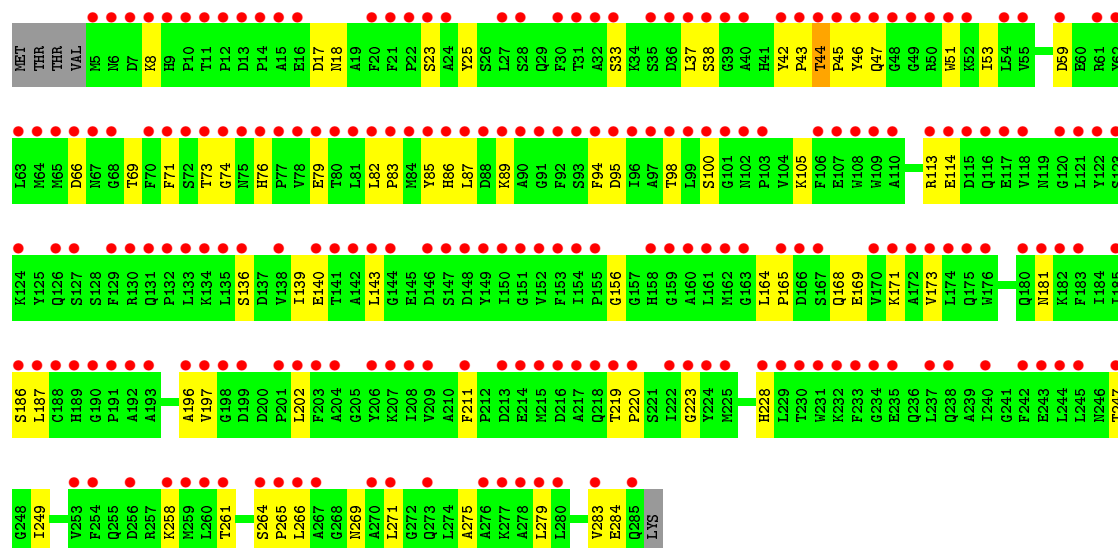
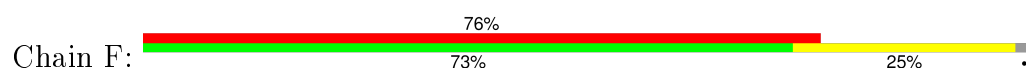


• Molecule 1: Intracellular protease/amidase





● Molecule 1: Intracellular protease/amidase





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 73.29 Å   80.03 Å   133.04 Å<br>90.00°   95.36°   90.00°    | Depositor        |
| Resolution (Å)  | 29.65 – 2.50<br>66.23 – 1.58                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.6 (29.65-2.50)<br>15.1 (66.23-1.58)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.09 (at 1.58 Å)  | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.199   ,   0.259<br>0.554   ,   0.566                      | Depositor<br>DCC |
| $R_{free}$ test set   | 1220 reflections (5.17%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 2.9   | Xtriage          |
| Anisotropy  | 2.292   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 14.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 1 of 31535 reflections (0.003%)                             | Xtriage          |
| $F_o, F_c$ correlation  | 0.24  | EDS              |
| Total number of atoms   | 13718   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 36.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: MPD

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     | 0.38         | 0/2225      | 0.65        | 0/3023         |
| 1   | B     | 0.39         | 0/2225      | 0.65        | 0/3023         |
| 1   | C     | 0.39         | 0/2225      | 0.64        | 0/3023         |
| 1   | D     | 0.38         | 0/2225      | 0.65        | 0/3023         |
| 1   | E     | 0.37         | 0/2225      | 0.64        | 1/3023 (0.0%)  |
| 1   | F     | 0.38         | 0/2225      | 0.59        | 0/3023         |
| All | All   | 0.38         | 0/13350     | 0.64        | 1/18138 (0.0%) |

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   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | E     | 157 | GLY  | N-CA-C | -5.20 | 100.09                 | 113.10              |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 62  | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 62  | TYR  | Sidechain |

## 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     | 2163  | 0        | 2072     | 50      | 0            |
| 1   | B     | 2163  | 0        | 2072     | 36      | 0            |
| 1   | C     | 2163  | 0        | 2072     | 41      | 0            |
| 1   | D     | 2163  | 0        | 2072     | 48      | 0            |
| 1   | E     | 2163  | 0        | 2072     | 61      | 0            |
| 1   | F     | 2163  | 0        | 2072     | 60      | 0            |
| 2   | A     | 8     | 0        | 14       | 3       | 0            |
| 2   | B     | 16    | 0        | 28       | 3       | 0            |
| 2   | D     | 8     | 0        | 14       | 4       | 0            |
| 2   | E     | 8     | 0        | 14       | 4       | 0            |
| 2   | F     | 8     | 0        | 14       | 6       | 0            |
| 3   | A     | 131   | 0        | 0        | 5       | 0            |
| 3   | B     | 131   | 0        | 0        | 2       | 0            |
| 3   | C     | 113   | 0        | 0        | 1       | 0            |
| 3   | D     | 123   | 0        | 0        | 4       | 0            |
| 3   | E     | 91    | 0        | 0        | 5       | 0            |
| 3   | F     | 103   | 0        | 0        | 6       | 0            |
| All | All   | 13718 | 0        | 12516    | 287     | 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 11.

All (287) 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:D:33:SER:HB2   | 1:D:114:GLU:HG3 | 1.42                     | 1.00              |
| 1:E:126:GLN:HE21 | 1:E:130:ARG:NH1 | 1.66                     | 0.93              |
| 1:E:126:GLN:HE21 | 1:E:130:ARG:CZ  | 1.85                     | 0.88              |
| 2:B:5002:MPD:HM3 | 3:B:5198:HOH:O  | 1.74                     | 0.86              |
| 1:A:58:ALA:H     | 1:A:75:ASN:HD21 | 1.31                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:249:ILE:CD1  | 2:F:301:MPD:H31  | 2.13                     | 0.78              |
| 1:C:40:ALA:O     | 1:C:89:LYS:HD3   | 1.85                     | 0.76              |
| 1:C:140:GLU:HB3  | 1:F:143:LEU:HB2  | 1.68                     | 0.76              |
| 1:D:85:TYR:HA    | 1:D:121:LEU:HD13 | 1.68                     | 0.74              |
| 1:A:58:ALA:H     | 1:A:75:ASN:ND2   | 1.89                     | 0.70              |
| 1:D:186:SER:O    | 1:D:261:THR:HA   | 1.91                     | 0.70              |
| 1:E:10:PRO:HB3   | 3:E:406:HOH:O    | 1.93                     | 0.68              |
| 1:E:208:ILE:HB   | 1:E:261:THR:HG21 | 1.75                     | 0.68              |
| 1:C:200:ASP:OD2  | 1:C:202:LEU:HB2  | 1.94                     | 0.68              |
| 1:D:204:ALA:HA   | 1:D:241:GLY:HA3  | 1.74                     | 0.68              |
| 1:D:42:TYR:O     | 1:D:45:PRO:HD3   | 1.95                     | 0.67              |
| 1:B:186:SER:O    | 1:B:261:THR:HA   | 1.96                     | 0.66              |
| 1:A:229:LEU:HA   | 3:A:484:HOH:O    | 1.94                     | 0.66              |
| 1:C:264:SER:HB2  | 1:C:265:PRO:CD   | 2.26                     | 0.66              |
| 1:E:126:GLN:NE2  | 1:E:130:ARG:NH1  | 2.42                     | 0.65              |
| 1:D:53:ILE:HD13  | 1:D:87:LEU:HD13  | 1.78                     | 0.65              |
| 1:D:280:LEU:O    | 1:D:284:GLU:HG3  | 1.97                     | 0.65              |
| 1:A:186:SER:O    | 1:A:261:THR:HA   | 1.96                     | 0.65              |
| 1:E:188:CYS:O    | 1:E:191:PRO:HD2  | 1.95                     | 0.65              |
| 1:D:202:LEU:H    | 1:D:202:LEU:HD23 | 1.62                     | 0.65              |
| 1:B:141:THR:HG22 | 3:B:5132:HOH:O   | 1.96                     | 0.64              |
| 1:E:42:TYR:O     | 1:E:45:PRO:HD3   | 1.96                     | 0.64              |
| 1:E:134:LYS:HE3  | 3:F:489:HOH:O    | 1.96                     | 0.64              |
| 1:D:197:VAL:HG11 | 1:D:202:LEU:HD21 | 1.80                     | 0.64              |
| 1:E:53:ILE:HD13  | 1:E:87:LEU:HD13  | 1.79                     | 0.64              |
| 1:F:169:GLU:O    | 1:F:173:VAL:HG23 | 1.99                     | 0.63              |
| 1:B:42:TYR:O     | 1:B:45:PRO:HD3   | 1.99                     | 0.63              |
| 1:A:179:LYS:HD3  | 3:A:480:HOH:O    | 1.98                     | 0.62              |
| 1:E:264:SER:HB2  | 1:E:265:PRO:CD   | 2.28                     | 0.62              |
| 1:E:37:LEU:HD21  | 1:E:85:TYR:CE2   | 2.34                     | 0.62              |
| 1:E:53:ILE:CD1   | 1:E:87:LEU:HD13  | 2.30                     | 0.62              |
| 1:C:277:LYS:HE2  | 3:C:345:HOH:O    | 1.98                     | 0.62              |
| 1:C:186:SER:O    | 1:C:261:THR:HA   | 2.00                     | 0.61              |
| 1:D:116:GLN:HG2  | 3:D:519:HOH:O    | 2.00                     | 0.61              |
| 1:D:264:SER:HB2  | 1:D:265:PRO:CD   | 2.31                     | 0.61              |
| 1:E:280:LEU:O    | 1:E:284:GLU:HG2  | 2.00                     | 0.61              |
| 1:B:232:LYS:O    | 1:B:236:GLN:HG2  | 2.01                     | 0.61              |
| 1:C:192:ALA:O    | 1:C:195:LEU:HB2  | 2.02                     | 0.60              |
| 1:C:139:ILE:HD11 | 1:C:173:VAL:CG2  | 2.33                     | 0.59              |
| 1:F:265:PRO:HD2  | 2:F:301:MPD:H12  | 1.84                     | 0.59              |
| 1:C:264:SER:HB2  | 1:C:265:PRO:HD2  | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:249:ILE:HD11 | 2:F:301:MPD:H31  | 1.85                     | 0.58              |
| 1:A:211:PHE:HE1  | 2:A:301:MPD:C1   | 2.16                     | 0.58              |
| 1:E:126:GLN:NE2  | 1:E:130:ARG:CZ   | 2.64                     | 0.58              |
| 1:E:277:LYS:HE3  | 3:E:484:HOH:O    | 2.02                     | 0.58              |
| 1:F:76:HIS:HE1   | 3:F:499:HOH:O    | 1.86                     | 0.57              |
| 1:B:275:ALA:O    | 1:B:279:LEU:HD13 | 2.03                     | 0.57              |
| 1:B:18:ASN:ND2   | 1:B:69:THR:HA    | 2.19                     | 0.57              |
| 1:E:164:LEU:HB2  | 1:E:165:PRO:HD3  | 1.88                     | 0.56              |
| 1:C:139:ILE:HD11 | 1:C:173:VAL:HG23 | 1.88                     | 0.56              |
| 1:A:136:SER:O    | 1:A:140:GLU:HG3  | 2.06                     | 0.56              |
| 1:D:249:ILE:CD1  | 2:D:301:MPD:HM1  | 2.35                     | 0.56              |
| 1:C:33:SER:HB2   | 1:C:114:GLU:HG3  | 1.86                     | 0.56              |
| 1:D:59:ASP:HB3   | 1:D:98:THR:HB    | 1.86                     | 0.56              |
| 1:E:264:SER:HB2  | 1:E:265:PRO:HD2  | 1.88                     | 0.56              |
| 1:E:85:TYR:HD1   | 1:E:121:LEU:HD22 | 1.71                     | 0.56              |
| 1:F:37:LEU:HD21  | 1:F:85:TYR:CE2   | 2.41                     | 0.56              |
| 1:F:187:LEU:HB3  | 1:F:271:LEU:HD22 | 1.88                     | 0.55              |
| 1:F:53:ILE:CD1   | 1:F:87:LEU:HD13  | 2.37                     | 0.55              |
| 1:C:164:LEU:HB2  | 1:C:165:PRO:HD3  | 1.88                     | 0.55              |
| 1:F:171:LYS:HB2  | 1:F:196:ALA:O    | 2.06                     | 0.55              |
| 1:F:164:LEU:HB2  | 1:F:165:PRO:HD3  | 1.87                     | 0.55              |
| 1:C:27:LEU:O     | 1:C:31:THR:HB    | 2.05                     | 0.55              |
| 1:A:130:ARG:HH22 | 1:B:18:ASN:HD22  | 1.54                     | 0.54              |
| 1:F:42:TYR:O     | 1:F:45:PRO:HD3   | 2.07                     | 0.54              |
| 1:F:220:PRO:HG2  | 1:F:228:HIS:CD2  | 2.43                     | 0.54              |
| 1:A:211:PHE:HE1  | 2:A:301:MPD:H13  | 1.73                     | 0.54              |
| 1:B:76:HIS:CD2   | 1:B:79:GLU:HG3   | 2.43                     | 0.54              |
| 1:B:145:GLU:HG3  | 1:F:284:GLU:C    | 2.27                     | 0.54              |
| 1:D:264:SER:HB2  | 1:D:265:PRO:HD2  | 1.90                     | 0.54              |
| 1:A:59:ASP:HB3   | 1:A:98:THR:HB    | 1.89                     | 0.54              |
| 1:F:249:ILE:HD12 | 2:F:301:MPD:H31  | 1.89                     | 0.53              |
| 1:F:136:SER:O    | 1:F:140:GLU:HG3  | 2.08                     | 0.53              |
| 1:C:200:ASP:C    | 1:C:202:LEU:H    | 2.10                     | 0.53              |
| 1:D:171:LYS:HG3  | 1:D:197:VAL:HA   | 1.90                     | 0.53              |
| 1:B:96:ILE:HD12  | 1:B:128:SER:CB   | 2.38                     | 0.53              |
| 1:A:279:LEU:O    | 1:A:283:VAL:HG22 | 2.09                     | 0.53              |
| 1:E:63:LEU:O     | 1:E:70:PHE:HA    | 2.08                     | 0.53              |
| 1:F:18:ASN:ND2   | 1:F:69:THR:HA    | 2.25                     | 0.52              |
| 1:A:87:LEU:HB2   | 1:A:94:PHE:HZ    | 1.74                     | 0.52              |
| 1:B:140:GLU:HB3  | 3:F:416:HOH:O    | 2.09                     | 0.52              |
| 1:E:186:SER:O    | 1:E:261:THR:HA   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:HIS:HE1  | 1:A:216:ASP:OD2  | 1.93                     | 0.52              |
| 1:D:171:LYS:HB2  | 1:D:196:ALA:O    | 2.10                     | 0.52              |
| 1:E:37:LEU:HD11  | 1:E:85:TYR:CD2   | 2.44                     | 0.52              |
| 1:D:215:MET:O    | 1:D:219:THR:HG23 | 2.10                     | 0.52              |
| 1:E:258:LYS:NZ   | 1:E:282:GLU:OE2  | 2.41                     | 0.51              |
| 1:C:135:LEU:O    | 1:C:139:ILE:HG12 | 2.10                     | 0.51              |
| 3:A:464:HOH:O    | 1:B:17:ASP:HB2   | 2.10                     | 0.51              |
| 1:F:82:LEU:HD23  | 1:F:269:ASN:N    | 2.25                     | 0.51              |
| 1:A:211:PHE:CE1  | 2:A:301:MPD:H13  | 2.45                     | 0.51              |
| 1:D:249:ILE:HD11 | 2:D:301:MPD:HM1  | 1.92                     | 0.51              |
| 1:A:253:VAL:HG12 | 1:A:262:GLY:HA2  | 1.93                     | 0.51              |
| 1:F:82:LEU:HB3   | 1:F:83:PRO:HD3   | 1.93                     | 0.51              |
| 1:F:46:TYR:O     | 1:F:47:GLN:HG3   | 2.11                     | 0.51              |
| 1:A:8:LYS:O      | 1:A:223:GLY:HA3  | 2.11                     | 0.51              |
| 1:E:115:ASP:OD1  | 1:E:117:GLU:HB2  | 2.11                     | 0.51              |
| 1:E:168:GLN:HB3  | 3:E:482:HOH:O    | 2.11                     | 0.51              |
| 1:E:195:LEU:HD23 | 1:E:240:ILE:HD13 | 1.92                     | 0.51              |
| 1:F:186:SER:O    | 1:F:261:THR:HA   | 2.12                     | 0.50              |
| 1:F:47:GLN:NE2   | 3:F:490:HOH:O    | 2.45                     | 0.50              |
| 1:B:207:LYS:HE3  | 1:B:243:GLU:OE1  | 2.11                     | 0.50              |
| 1:C:73:THR:OG1   | 1:C:74:GLY:N     | 2.45                     | 0.50              |
| 1:A:42:TYR:OH    | 1:A:86:HIS:HD2   | 1.94                     | 0.50              |
| 1:C:277:LYS:HG3  | 1:C:278:ALA:N    | 2.26                     | 0.49              |
| 1:E:79:GLU:OE1   | 1:E:156:GLY:HA3  | 2.13                     | 0.49              |
| 1:B:107:GLU:HB3  | 1:B:109:TRP:CE2  | 2.47                     | 0.49              |
| 1:F:219:THR:N    | 1:F:220:PRO:CD   | 2.75                     | 0.49              |
| 1:F:187:LEU:N    | 1:F:187:LEU:HD23 | 2.28                     | 0.49              |
| 1:E:30:PHE:CG    | 2:E:301:MPD:H11  | 2.48                     | 0.49              |
| 1:F:264:SER:HB2  | 1:F:265:PRO:CD   | 2.42                     | 0.49              |
| 1:F:171:LYS:HG3  | 1:F:197:VAL:HA   | 1.94                     | 0.49              |
| 1:C:42:TYR:OH    | 1:C:86:HIS:HD2   | 1.96                     | 0.49              |
| 1:A:65:MET:HG3   | 1:A:226:PRO:HG2  | 1.95                     | 0.49              |
| 1:B:96:ILE:HD12  | 1:B:128:SER:HB3  | 1.93                     | 0.48              |
| 1:B:199:ASP:OD1  | 1:B:200:ASP:N    | 2.46                     | 0.48              |
| 1:A:171:LYS:O    | 1:A:175:GLN:HG3  | 2.12                     | 0.48              |
| 1:B:51:TRP:CE3   | 1:B:51:TRP:HA    | 2.48                     | 0.48              |
| 1:D:7:ASP:OD2    | 1:D:9:HIS:HB2    | 2.14                     | 0.48              |
| 1:F:264:SER:HB2  | 1:F:265:PRO:HD2  | 1.95                     | 0.48              |
| 1:F:275:ALA:O    | 1:F:279:LEU:HD13 | 2.13                     | 0.48              |
| 1:A:79:GLU:OE2   | 1:A:265:PRO:HG3  | 2.13                     | 0.48              |
| 1:F:73:THR:OG1   | 1:F:74:GLY:N     | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:95:ASP:HA    | 3:F:425:HOH:O    | 2.12                     | 0.48              |
| 1:F:197:VAL:HG11 | 1:F:202:LEU:HD21 | 1.96                     | 0.48              |
| 1:C:60:GLU:OE1   | 1:D:102:ASN:HB3  | 2.13                     | 0.48              |
| 1:E:167:SER:OG   | 1:E:170:VAL:HG23 | 2.13                     | 0.47              |
| 1:F:266:LEU:HD21 | 2:F:301:MPD:H51  | 1.96                     | 0.47              |
| 1:E:167:SER:CB   | 1:E:170:VAL:HG23 | 2.45                     | 0.47              |
| 1:C:59:ASP:HB3   | 1:C:98:THR:HB    | 1.96                     | 0.47              |
| 1:E:11:THR:O     | 1:E:20:PHE:HA    | 2.14                     | 0.47              |
| 1:E:167:SER:HB3  | 1:E:170:VAL:CG2  | 2.45                     | 0.47              |
| 1:A:96:ILE:HD13  | 1:A:129:PHE:CE1  | 2.49                     | 0.47              |
| 1:D:79:GLU:O     | 1:D:83:PRO:HG2   | 2.14                     | 0.47              |
| 1:D:187:LEU:N    | 1:D:187:LEU:HD23 | 2.29                     | 0.47              |
| 1:A:275:ALA:O    | 1:A:279:LEU:HD13 | 2.15                     | 0.47              |
| 1:E:235:GLU:HB3  | 3:E:440:HOH:O    | 2.15                     | 0.47              |
| 1:D:107:GLU:HB3  | 1:D:109:TRP:CE2  | 2.49                     | 0.47              |
| 1:D:8:LYS:O      | 1:D:223:GLY:HA3  | 2.14                     | 0.47              |
| 1:E:85:TYR:CD1   | 1:E:121:LEU:HD22 | 2.50                     | 0.46              |
| 1:C:42:TYR:O     | 1:C:45:PRO:HD3   | 2.15                     | 0.46              |
| 1:D:85:TYR:HA    | 1:D:121:LEU:CD1  | 2.41                     | 0.46              |
| 1:B:264:SER:HB2  | 1:B:265:PRO:CD   | 2.46                     | 0.46              |
| 1:F:82:LEU:CB    | 1:F:83:PRO:HD3   | 2.45                     | 0.46              |
| 1:E:30:PHE:HB3   | 2:E:301:MPD:H31  | 1.98                     | 0.46              |
| 1:F:71:PHE:CD1   | 1:F:73:THR:HB    | 2.51                     | 0.46              |
| 1:A:61:ARG:HH12  | 1:B:16:GLU:HG2   | 1.80                     | 0.46              |
| 1:A:264:SER:HB2  | 1:A:265:PRO:CD   | 2.46                     | 0.46              |
| 1:B:194:PHE:O    | 1:B:197:VAL:HG22 | 2.16                     | 0.46              |
| 1:C:140:GLU:HA   | 1:F:140:GLU:HA   | 1.97                     | 0.46              |
| 1:D:212:PRO:HG2  | 1:D:215:MET:HG3  | 1.98                     | 0.46              |
| 1:D:150:ILE:HG12 | 1:D:150:ILE:O    | 2.16                     | 0.46              |
| 1:D:30:PHE:CD1   | 2:D:301:MPD:H11  | 2.51                     | 0.46              |
| 1:F:8:LYS:HE2    | 1:F:25:TYR:CD2   | 2.50                     | 0.46              |
| 1:E:204:ALA:HA   | 1:E:241:GLY:HA3  | 1.98                     | 0.46              |
| 1:C:195:LEU:HD13 | 1:C:237:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:42:TYR:O     | 1:A:45:PRO:HD3   | 2.16                     | 0.46              |
| 1:F:44:THR:HG23  | 3:F:421:HOH:O    | 2.16                     | 0.46              |
| 1:A:73:THR:OG1   | 1:A:74:GLY:N     | 2.49                     | 0.46              |
| 1:D:197:VAL:CG1  | 1:D:202:LEU:HD21 | 2.46                     | 0.45              |
| 1:A:191:PRO:O    | 1:A:237:LEU:HD21 | 2.16                     | 0.45              |
| 1:F:105:LYS:HD3  | 1:F:105:LYS:HA   | 1.69                     | 0.45              |
| 1:C:51:TRP:HA    | 1:C:148:ASP:O    | 2.16                     | 0.45              |
| 1:A:76:HIS:CE1   | 1:A:78:VAL:HB    | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:30:PHE:O     | 2:E:301:MPD:H52  | 2.16                     | 0.45              |
| 1:E:143:LEU:HB3  | 1:E:144:GLY:H    | 1.51                     | 0.45              |
| 1:F:139:ILE:HG22 | 1:F:173:VAL:HG22 | 1.98                     | 0.45              |
| 1:F:89:LYS:HA    | 1:F:89:LYS:HD3   | 1.79                     | 0.45              |
| 1:F:53:ILE:HD13  | 1:F:87:LEU:HD13  | 1.98                     | 0.45              |
| 1:A:96:ILE:HD13  | 1:A:129:PHE:CD1  | 2.52                     | 0.45              |
| 1:E:86:HIS:NE2   | 1:E:273:GLN:HG2  | 2.32                     | 0.45              |
| 1:E:79:GLU:OE2   | 1:E:265:PRO:HG3  | 2.17                     | 0.45              |
| 1:A:79:GLU:OE1   | 1:A:156:GLY:HA3  | 2.17                     | 0.45              |
| 1:D:141:THR:HB   | 3:D:505:HOH:O    | 2.16                     | 0.45              |
| 1:C:260:LEU:HD22 | 1:C:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:F:211:PHE:CE1  | 2:F:301:MPD:H11  | 2.52                     | 0.45              |
| 1:A:43:PRO:HG2   | 3:A:494:HOH:O    | 2.15                     | 0.45              |
| 1:E:30:PHE:CD1   | 2:E:301:MPD:H11  | 2.51                     | 0.45              |
| 1:F:37:LEU:HD12  | 1:F:38:SER:N     | 2.32                     | 0.45              |
| 1:F:87:LEU:HB2   | 1:F:94:PHE:HZ    | 1.82                     | 0.45              |
| 1:B:171:LYS:O    | 1:B:175:GLN:HG3  | 2.16                     | 0.45              |
| 1:A:102:ASN:HB3  | 1:A:103:PRO:HD2  | 1.99                     | 0.45              |
| 1:B:187:LEU:N    | 1:B:187:LEU:HD23 | 2.32                     | 0.44              |
| 1:E:100:SER:HB2  | 1:F:100:SER:HB3  | 1.99                     | 0.44              |
| 1:A:104:VAL:HG23 | 1:A:132:PRO:HG3  | 1.98                     | 0.44              |
| 1:A:269:ASN:O    | 1:A:273:GLN:HG3  | 2.18                     | 0.44              |
| 1:A:227:GLY:HA2  | 3:A:513:HOH:O    | 2.16                     | 0.44              |
| 1:F:23:SER:HB3   | 1:F:223:GLY:HA3  | 1.98                     | 0.44              |
| 1:A:74:GLY:HA2   | 1:A:159:GLY:HA3  | 2.00                     | 0.44              |
| 1:E:59:ASP:HB3   | 1:E:98:THR:HB    | 1.98                     | 0.44              |
| 1:E:27:LEU:HD12  | 3:E:424:HOH:O    | 2.18                     | 0.44              |
| 1:A:236:GLN:O    | 1:A:239:ALA:HB3  | 2.17                     | 0.44              |
| 1:D:178:MET:HG3  | 1:D:202:LEU:HD12 | 2.00                     | 0.44              |
| 1:B:44:THR:O     | 1:B:44:THR:HG23  | 2.18                     | 0.44              |
| 1:E:197:VAL:HG11 | 1:E:202:LEU:HD21 | 2.00                     | 0.44              |
| 1:B:234:GLY:O    | 1:B:238:GLN:HG3  | 2.18                     | 0.44              |
| 1:B:265:PRO:HB2  | 2:B:5001:MPD:H53 | 2.00                     | 0.44              |
| 1:E:275:ALA:O    | 1:E:279:LEU:HD13 | 2.18                     | 0.44              |
| 1:B:203:PHE:CG   | 1:B:242:PHE:CZ   | 3.06                     | 0.44              |
| 1:E:73:THR:HG23  | 1:E:74:GLY:N     | 2.33                     | 0.44              |
| 1:D:277:LYS:HB2  | 3:D:473:HOH:O    | 2.17                     | 0.44              |
| 1:C:62:TYR:HB3   | 1:C:70:PHE:CD1   | 2.53                     | 0.44              |
| 1:A:123:SER:O    | 1:A:126:GLN:HG2  | 2.18                     | 0.43              |
| 1:B:96:ILE:HD12  | 1:B:128:SER:HB2  | 2.00                     | 0.43              |
| 1:E:171:LYS:HG3  | 1:E:197:VAL:HA   | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:65:MET:HG3   | 1:D:226:PRO:HG2  | 2.00                     | 0.43              |
| 1:A:115:ASP:HB3  | 1:A:118:VAL:HB   | 1.99                     | 0.43              |
| 1:F:53:ILE:HB    | 1:F:94:PHE:CD1   | 2.54                     | 0.43              |
| 1:B:16:GLU:HB2   | 1:B:62:TYR:CE1   | 2.54                     | 0.43              |
| 1:C:64:MET:CE    | 1:D:131:GLN:HE21 | 2.32                     | 0.43              |
| 1:D:73:THR:HG23  | 1:D:74:GLY:N     | 2.34                     | 0.43              |
| 1:D:73:THR:OG1   | 1:D:74:GLY:N     | 2.52                     | 0.43              |
| 1:C:107:GLU:HB3  | 1:C:109:TRP:CE2  | 2.54                     | 0.43              |
| 1:C:79:GLU:OE2   | 1:C:265:PRO:HG3  | 2.19                     | 0.43              |
| 1:D:79:GLU:OE1   | 1:D:156:GLY:HA3  | 2.18                     | 0.43              |
| 1:A:108:TRP:CZ3  | 1:A:111:MET:CE   | 3.01                     | 0.43              |
| 1:A:231:TRP:CZ3  | 1:A:233:PHE:HA   | 2.54                     | 0.43              |
| 1:D:249:ILE:HG13 | 1:D:249:ILE:O    | 2.19                     | 0.43              |
| 1:B:79:GLU:OE2   | 1:B:265:PRO:HG3  | 2.18                     | 0.43              |
| 1:E:219:THR:N    | 1:E:220:PRO:CD   | 2.82                     | 0.42              |
| 1:D:11:THR:HB    | 1:D:21:PHE:HB2   | 2.01                     | 0.42              |
| 1:D:280:LEU:HA   | 1:D:283:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:42:TYR:HA    | 1:A:43:PRO:HD2   | 1.85                     | 0.42              |
| 1:C:6:ASN:HD22   | 1:C:6:ASN:HA     | 1.56                     | 0.42              |
| 1:B:6:ASN:HB3    | 1:B:9:HIS:NE2    | 2.34                     | 0.42              |
| 1:A:256:ASP:O    | 1:A:257:ARG:HB2  | 2.18                     | 0.42              |
| 1:D:203:PHE:O    | 1:D:206:TYR:HB2  | 2.19                     | 0.42              |
| 1:E:167:SER:HB3  | 1:E:170:VAL:HG23 | 2.02                     | 0.42              |
| 1:C:50:ARG:HG3   | 1:C:148:ASP:OD1  | 2.19                     | 0.42              |
| 1:E:35:SER:HB3   | 1:E:118:VAL:HG21 | 2.00                     | 0.42              |
| 1:D:71:PHE:CD1   | 1:D:73:THR:HB    | 2.54                     | 0.42              |
| 1:D:157:GLY:C    | 1:D:159:GLY:H    | 2.23                     | 0.42              |
| 1:A:200:ASP:C    | 1:A:202:LEU:H    | 2.21                     | 0.42              |
| 1:A:82:LEU:HD23  | 1:A:269:ASN:HB2  | 2.02                     | 0.42              |
| 1:E:139:ILE:HD11 | 1:E:169:GLU:O    | 2.20                     | 0.42              |
| 1:E:7:ASP:OD2    | 1:E:9:HIS:HB2    | 2.19                     | 0.42              |
| 1:C:197:VAL:HG11 | 1:C:202:LEU:HD23 | 2.02                     | 0.42              |
| 1:D:265:PRO:HG2  | 2:D:301:MPD:O4   | 2.19                     | 0.42              |
| 1:F:79:GLU:OE1   | 1:F:156:GLY:HA3  | 2.20                     | 0.42              |
| 1:A:52:LYS:HB3   | 1:A:93:SER:HB2   | 2.02                     | 0.42              |
| 1:F:42:TYR:OH    | 1:F:86:HIS:HD2   | 2.01                     | 0.42              |
| 1:F:51:TRP:CE3   | 1:F:51:TRP:HA    | 2.55                     | 0.42              |
| 1:E:75:ASN:HA    | 1:E:75:ASN:HD22  | 1.74                     | 0.42              |
| 1:C:52:LYS:C     | 1:C:53:ILE:HD12  | 2.40                     | 0.42              |
| 1:C:25:TYR:O     | 1:C:28:SER:HB3   | 2.20                     | 0.41              |
| 1:A:260:LEU:CD1  | 1:A:260:LEU:N    | 2.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:37:LEU:HD12  | 1:F:38:SER:H     | 1.85                     | 0.41              |
| 1:E:73:THR:OG1   | 1:E:74:GLY:N     | 2.50                     | 0.41              |
| 1:E:263:ASP:OD1  | 1:E:264:SER:N    | 2.53                     | 0.41              |
| 1:E:19:ALA:HA    | 1:E:70:PHE:O     | 2.21                     | 0.41              |
| 1:B:22:PRO:HG2   | 1:B:109:TRP:CZ3  | 2.54                     | 0.41              |
| 1:B:179:LYS:HG3  | 1:B:180:GLN:NE2  | 2.35                     | 0.41              |
| 1:E:187:LEU:HB3  | 1:E:271:LEU:HD22 | 2.02                     | 0.41              |
| 1:D:269:ASN:HB3  | 3:D:416:HOH:O    | 2.21                     | 0.41              |
| 1:C:140:GLU:HA   | 1:F:139:ILE:O    | 2.21                     | 0.41              |
| 1:C:123:SER:O    | 1:C:126:GLN:HG2  | 2.20                     | 0.41              |
| 1:F:136:SER:O    | 1:F:139:ILE:HG12 | 2.21                     | 0.41              |
| 1:E:42:TYR:OH    | 1:E:86:HIS:HD2   | 2.03                     | 0.41              |
| 1:F:59:ASP:HB3   | 1:F:98:THR:HB    | 2.02                     | 0.41              |
| 1:E:234:GLY:O    | 1:E:244:LEU:HD11 | 2.21                     | 0.41              |
| 1:C:143:LEU:HB2  | 1:F:140:GLU:HB3  | 2.03                     | 0.41              |
| 1:B:236:GLN:O    | 1:B:239:ALA:HB3  | 2.21                     | 0.41              |
| 1:F:53:ILE:HD12  | 1:F:94:PHE:CE1   | 2.56                     | 0.41              |
| 1:A:108:TRP:CZ3  | 1:A:111:MET:HE2  | 2.56                     | 0.41              |
| 1:A:150:ILE:HG12 | 1:A:150:ILE:O    | 2.21                     | 0.41              |
| 1:F:33:SER:OG    | 1:F:114:GLU:HB2  | 2.20                     | 0.41              |
| 1:B:59:ASP:HB3   | 1:B:98:THR:HB    | 2.03                     | 0.41              |
| 1:B:252:GLN:HE21 | 1:B:252:GLN:HB2  | 1.76                     | 0.41              |
| 1:C:102:ASN:HB3  | 1:D:60:GLU:OE1   | 2.21                     | 0.41              |
| 1:C:200:ASP:O    | 1:C:202:LEU:N    | 2.45                     | 0.41              |
| 1:C:12:PRO:HG3   | 1:C:20:PHE:HE1   | 1.85                     | 0.41              |
| 1:D:200:ASP:CG   | 1:D:202:LEU:HD22 | 2.41                     | 0.40              |
| 1:E:82:LEU:HB2   | 1:E:83:PRO:HD3   | 2.03                     | 0.40              |
| 1:A:207:LYS:HB3  | 1:A:245:LEU:HD11 | 2.03                     | 0.40              |
| 1:F:168:GLN:HE22 | 1:F:171:LYS:HD3  | 1.86                     | 0.40              |
| 2:B:5001:MPD:C1  | 2:B:5001:MPD:O4  | 2.69                     | 0.40              |
| 1:F:181:ASN:ND2  | 1:F:258:LYS:NZ   | 2.70                     | 0.40              |
| 1:C:40:ALA:HA    | 1:C:86:HIS:CD2   | 2.56                     | 0.40              |
| 1:F:42:TYR:HA    | 1:F:43:PRO:HD2   | 1.95                     | 0.40              |
| 1:D:219:THR:N    | 1:D:220:PRO:CD   | 2.84                     | 0.40              |
| 1:E:202:LEU:N    | 1:E:202:LEU:HD23 | 2.35                     | 0.40              |
| 1:B:73:THR:HG23  | 1:B:74:GLY:N     | 2.36                     | 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     | 279/286 (98%)   | 267 (96%)  | 12 (4%) | 0        | 100         | 100 |
| 1   | B     | 279/286 (98%)   | 262 (94%)  | 17 (6%) | 0        | 100         | 100 |
| 1   | C     | 279/286 (98%)   | 262 (94%)  | 15 (5%) | 2 (1%)   | 26          | 46  |
| 1   | D     | 279/286 (98%)   | 262 (94%)  | 17 (6%) | 0        | 100         | 100 |
| 1   | E     | 279/286 (98%)   | 264 (95%)  | 15 (5%) | 0        | 100         | 100 |
| 1   | F     | 279/286 (98%)   | 259 (93%)  | 19 (7%) | 1 (0%)   | 39          | 61  |
| All | All   | 1674/1716 (98%) | 1576 (94%) | 95 (6%) | 3 (0%)   | 52          | 75  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 250 | SER  |
| 1   | C     | 201 | PRO  |
| 1   | F     | 283 | VAL  |

### 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     | 226/233 (97%) | 225 (100%) | 1 (0%)   | 93          | 98 |
| 1   | B     | 226/233 (97%) | 225 (100%) | 1 (0%)   | 93          | 98 |
| 1   | C     | 226/233 (97%) | 220 (97%)  | 6 (3%)   | 52          | 79 |
| 1   | D     | 226/233 (97%) | 223 (99%)  | 3 (1%)   | 76          | 92 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | E     | 226/233 (97%)   | 223 (99%)  | 3 (1%)   | 76          | 92 |
| 1   | F     | 226/233 (97%)   | 221 (98%)  | 5 (2%)   | 60          | 84 |
| All | All   | 1356/1398 (97%) | 1337 (99%) | 19 (1%)  | 74          | 91 |

All (19) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 146 | ASP  |
| 1   | B     | 252 | GLN  |
| 1   | C     | 6   | ASN  |
| 1   | C     | 111 | MET  |
| 1   | C     | 117 | GLU  |
| 1   | C     | 146 | ASP  |
| 1   | C     | 252 | GLN  |
| 1   | C     | 277 | LYS  |
| 1   | D     | 44  | THR  |
| 1   | D     | 121 | LEU  |
| 1   | D     | 209 | VAL  |
| 1   | E     | 75  | ASN  |
| 1   | E     | 145 | GLU  |
| 1   | E     | 179 | LYS  |
| 1   | F     | 17  | ASP  |
| 1   | F     | 44  | THR  |
| 1   | F     | 66  | ASP  |
| 1   | F     | 113 | ARG  |
| 1   | F     | 247 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | ASN  |
| 1   | A     | 86  | HIS  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 189 | HIS  |
| 1   | B     | 18  | ASN  |
| 1   | B     | 29  | GLN  |
| 1   | B     | 76  | HIS  |
| 1   | B     | 86  | HIS  |
| 1   | B     | 131 | GLN  |
| 1   | B     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 236 | GLN  |
| 1   | B     | 238 | GLN  |
| 1   | B     | 252 | GLN  |
| 1   | C     | 6   | ASN  |
| 1   | C     | 86  | HIS  |
| 1   | C     | 273 | GLN  |
| 1   | D     | 76  | HIS  |
| 1   | D     | 86  | HIS  |
| 1   | D     | 102 | ASN  |
| 1   | D     | 131 | GLN  |
| 1   | D     | 168 | GLN  |
| 1   | E     | 47  | GLN  |
| 1   | E     | 86  | HIS  |
| 1   | E     | 126 | GLN  |
| 1   | E     | 218 | GLN  |
| 1   | F     | 18  | ASN  |
| 1   | F     | 76  | HIS  |
| 1   | F     | 86  | HIS  |
| 1   | F     | 168 | GLN  |
| 1   | F     | 181 | ASN  |
| 1   | F     | 189 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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 |
| 2   | MPD  | A     | 301  | -    | 6,7,7        | 0.45 | 0        | 7,10,10     | 0.52 | 0        |
| 2   | MPD  | B     | 5001 | -    | 6,7,7        | 1.18 | 1 (16%)  | 7,10,10     | 4.10 | 4 (57%)  |
| 2   | MPD  | B     | 5002 | -    | 6,7,7        | 0.44 | 0        | 7,10,10     | 0.49 | 0        |
| 2   | MPD  | D     | 301  | -    | 6,7,7        | 0.34 | 0        | 7,10,10     | 0.35 | 0        |
| 2   | MPD  | E     | 301  | -    | 6,7,7        | 0.45 | 0        | 7,10,10     | 0.31 | 0        |
| 2   | MPD  | F     | 301  | -    | 6,7,7        | 0.71 | 0        | 7,10,10     | 0.31 | 0        |

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   |
|-----|------|-------|------|------|---------|----------|---------|
| 2   | MPD  | A     | 301  | -    | -       | 0/5/5/5  | 0/0/0/0 |
| 2   | MPD  | B     | 5001 | -    | -       | 0/5/5/5  | 0/0/0/0 |
| 2   | MPD  | B     | 5002 | -    | -       | 0/5/5/5  | 0/0/0/0 |
| 2   | MPD  | D     | 301  | -    | -       | 0/5/5/5  | 0/0/0/0 |
| 2   | MPD  | E     | 301  | -    | -       | 0/5/5/5  | 0/0/0/0 |
| 2   | MPD  | F     | 301  | -    | -       | 0/5/5/5  | 0/0/0/0 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | B     | 5001 | MPD  | CM-C2 | -2.04 | 1.45        | 1.52     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 5001 | MPD  | O2-C2-CM | -8.09 | 78.45       | 108.09   |
| 2   | B     | 5001 | MPD  | C1-C2-C3 | -2.68 | 94.35       | 109.90   |
| 2   | B     | 5001 | MPD  | CM-C2-C1 | -2.27 | 105.30      | 110.24   |
| 2   | B     | 5001 | MPD  | CM-C2-C3 | 5.96  | 144.39      | 109.90   |

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 |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 301  | MPD  | 3       | 0            |
| 2   | B     | 5001 | MPD  | 2       | 0            |
| 2   | B     | 5002 | MPD  | 1       | 0            |
| 2   | D     | 301  | MPD  | 4       | 0            |
| 2   | E     | 301  | MPD  | 4       | 0            |
| 2   | F     | 301  | MPD  | 6       | 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     | 281/286 (98%)   | 4.98   | 206 (73%) <b>0</b> <b>0</b>  | 22, 32, 48, 66        | 0     |
| 1   | B     | 281/286 (98%)   | 5.48   | 197 (70%) <b>0</b> <b>0</b>  | 19, 31, 48, 84        | 0     |
| 1   | C     | 281/286 (98%)   | 5.73   | 208 (74%) <b>0</b> <b>0</b>  | 22, 35, 51, 85        | 0     |
| 1   | D     | 281/286 (98%)   | 5.35   | 205 (72%) <b>0</b> <b>0</b>  | 20, 33, 53, 95        | 0     |
| 1   | E     | 281/286 (98%)   | 6.08   | 227 (80%) <b>0</b> <b>0</b>  | 26, 40, 58, 84        | 0     |
| 1   | F     | 281/286 (98%)   | 5.87   | 218 (77%) <b>0</b> <b>0</b>  | 25, 37, 58, 79        | 0     |
| All | All   | 1686/1716 (98%) | 5.58   | 1261 (74%) <b>0</b> <b>0</b> | 19, 35, 55, 95        | 0     |

All (1261) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 211 | PHE  | 57.0 |
| 1   | F     | 143 | LEU  | 46.1 |
| 1   | C     | 40  | ALA  | 44.9 |
| 1   | E     | 55  | VAL  | 44.4 |
| 1   | B     | 28  | SER  | 43.7 |
| 1   | C     | 5   | MET  | 42.9 |
| 1   | C     | 191 | PRO  | 38.9 |
| 1   | C     | 104 | VAL  | 38.6 |
| 1   | E     | 244 | LEU  | 36.0 |
| 1   | B     | 38  | SER  | 34.1 |
| 1   | F     | 217 | ALA  | 32.2 |
| 1   | E     | 40  | ALA  | 31.7 |
| 1   | B     | 27  | LEU  | 30.4 |
| 1   | D     | 5   | MET  | 30.1 |
| 1   | D     | 222 | ILE  | 30.0 |
| 1   | D     | 70  | PHE  | 29.7 |
| 1   | E     | 41  | HIS  | 29.5 |
| 1   | C     | 143 | LEU  | 29.4 |
| 1   | B     | 49  | GLY  | 28.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 44  | THR  | 28.3 |
| 1   | A     | 106 | PHE  | 27.8 |
| 1   | E     | 56  | VAL  | 25.8 |
| 1   | F     | 260 | LEU  | 25.8 |
| 1   | B     | 210 | ALA  | 25.5 |
| 1   | B     | 155 | PRO  | 25.3 |
| 1   | D     | 39  | GLY  | 24.7 |
| 1   | B     | 56  | VAL  | 24.7 |
| 1   | C     | 8   | LYS  | 24.6 |
| 1   | E     | 132 | PRO  | 24.2 |
| 1   | B     | 270 | ALA  | 24.1 |
| 1   | E     | 184 | ILE  | 23.7 |
| 1   | B     | 97  | ALA  | 23.5 |
| 1   | F     | 147 | SER  | 23.3 |
| 1   | E     | 245 | LEU  | 23.1 |
| 1   | C     | 280 | LEU  | 22.7 |
| 1   | F     | 46  | TYR  | 22.7 |
| 1   | C     | 184 | ILE  | 22.5 |
| 1   | E     | 114 | GLU  | 21.9 |
| 1   | D     | 40  | ALA  | 21.8 |
| 1   | F     | 39  | GLY  | 21.1 |
| 1   | B     | 95  | ASP  | 21.0 |
| 1   | F     | 152 | VAL  | 20.9 |
| 1   | B     | 81  | LEU  | 20.7 |
| 1   | F     | 265 | PRO  | 20.6 |
| 1   | F     | 21  | PHE  | 20.6 |
| 1   | C     | 193 | ALA  | 20.5 |
| 1   | A     | 284 | GLU  | 20.4 |
| 1   | D     | 81  | LEU  | 20.2 |
| 1   | C     | 15  | ALA  | 19.7 |
| 1   | E     | 106 | PHE  | 19.5 |
| 1   | A     | 206 | TYR  | 19.3 |
| 1   | C     | 138 | VAL  | 19.2 |
| 1   | D     | 194 | PHE  | 19.2 |
| 1   | F     | 107 | GLU  | 19.2 |
| 1   | C     | 149 | TYR  | 19.1 |
| 1   | A     | 135 | LEU  | 19.0 |
| 1   | A     | 283 | VAL  | 18.8 |
| 1   | D     | 30  | PHE  | 18.8 |
| 1   | E     | 43  | PRO  | 18.7 |
| 1   | D     | 262 | GLY  | 18.6 |
| 1   | A     | 183 | PHE  | 18.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 231 | TRP  | 18.5 |
| 1   | A     | 149 | TYR  | 18.4 |
| 1   | A     | 226 | PRO  | 18.3 |
| 1   | D     | 98  | THR  | 18.2 |
| 1   | E     | 285 | GLN  | 18.0 |
| 1   | F     | 49  | GLY  | 17.7 |
| 1   | C     | 70  | PHE  | 17.6 |
| 1   | B     | 176 | TRP  | 17.5 |
| 1   | D     | 96  | ILE  | 17.5 |
| 1   | E     | 174 | LEU  | 17.3 |
| 1   | F     | 37  | LEU  | 17.3 |
| 1   | E     | 133 | LEU  | 17.2 |
| 1   | F     | 174 | LEU  | 17.2 |
| 1   | D     | 69  | THR  | 17.1 |
| 1   | C     | 195 | LEU  | 17.0 |
| 1   | E     | 75  | ASN  | 16.7 |
| 1   | E     | 195 | LEU  | 16.6 |
| 1   | E     | 68  | GLY  | 16.5 |
| 1   | F     | 224 | TYR  | 16.5 |
| 1   | D     | 77  | PRO  | 16.3 |
| 1   | D     | 226 | PRO  | 16.1 |
| 1   | E     | 194 | PHE  | 16.1 |
| 1   | E     | 81  | LEU  | 16.1 |
| 1   | C     | 185 | ILE  | 16.1 |
| 1   | C     | 266 | LEU  | 16.0 |
| 1   | D     | 143 | LEU  | 15.9 |
| 1   | E     | 158 | HIS  | 15.8 |
| 1   | C     | 181 | ASN  | 15.7 |
| 1   | E     | 268 | GLY  | 15.6 |
| 1   | F     | 94  | PHE  | 15.5 |
| 1   | D     | 118 | VAL  | 15.4 |
| 1   | A     | 174 | LEU  | 15.1 |
| 1   | C     | 121 | LEU  | 15.0 |
| 1   | A     | 170 | VAL  | 15.0 |
| 1   | B     | 67  | ASN  | 14.9 |
| 1   | B     | 185 | ILE  | 14.9 |
| 1   | A     | 233 | PHE  | 14.9 |
| 1   | C     | 18  | ASN  | 14.9 |
| 1   | E     | 215 | MET  | 14.8 |
| 1   | C     | 71  | PHE  | 14.8 |
| 1   | E     | 119 | ASN  | 14.7 |
| 1   | B     | 212 | PRO  | 14.6 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | F            | 74         | GLY         | 14.6        |
| 1          | B            | 250        | SER         | 14.6        |
| 1          | C            | 87         | LEU         | 14.5        |
| 1          | F            | 40         | ALA         | 14.5        |
| 1          | A            | 285        | GLN         | 14.5        |
| 1          | F            | 160        | ALA         | 14.5        |
| 1          | D            | 227        | GLY         | 14.4        |
| 1          | A            | 86         | HIS         | 14.4        |
| 1          | D            | 244        | LEU         | 14.4        |
| 1          | C            | 229        | LEU         | 14.3        |
| 1          | B            | 65         | MET         | 14.3        |
| 1          | F            | 113        | ARG         | 14.2        |
| 1          | A            | 189        | HIS         | 14.1        |
| 1          | E            | 201        | PRO         | 14.1        |
| 1          | F            | 153        | PHE         | 14.1        |
| 1          | C            | 255        | GLN         | 13.9        |
| 1          | C            | 88         | ASP         | 13.9        |
| 1          | A            | 168        | GLN         | 13.6        |
| 1          | C            | 136        | SER         | 13.6        |
| 1          | B            | 249        | ILE         | 13.6        |
| 1          | B            | 285        | GLN         | 13.4        |
| 1          | B            | 152        | VAL         | 13.4        |
| 1          | F            | 242        | PHE         | 13.3        |
| 1          | D            | 193        | ALA         | 13.2        |
| 1          | D            | 283        | VAL         | 13.2        |
| 1          | F            | 77         | PRO         | 13.2        |
| 1          | F            | 154        | ILE         | 13.1        |
| 1          | B            | 96         | ILE         | 13.1        |
| 1          | E            | 164        | LEU         | 13.0        |
| 1          | F            | 159        | GLY         | 13.0        |
| 1          | E            | 45         | PRO         | 13.0        |
| 1          | F            | 75         | ASN         | 12.9        |
| 1          | D            | 254        | PHE         | 12.9        |
| 1          | C            | 98         | THR         | 12.8        |
| 1          | E            | 134        | LYS         | 12.8        |
| 1          | C            | 106        | PHE         | 12.8        |
| 1          | C            | 117        | GLU         | 12.7        |
| 1          | C            | 6          | ASN         | 12.7        |
| 1          | B            | 106        | PHE         | 12.7        |
| 1          | D            | 94         | PHE         | 12.7        |
| 1          | E            | 24         | ALA         | 12.6        |
| 1          | A            | 15         | ALA         | 12.6        |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 65         | MET         | 12.6        |
| 1          | E            | 108        | TRP         | 12.6        |
| 1          | D            | 269        | ASN         | 12.5        |
| 1          | A            | 240        | ILE         | 12.5        |
| 1          | F            | 243        | GLU         | 12.5        |
| 1          | C            | 249        | ILE         | 12.4        |
| 1          | B            | 231        | TRP         | 12.4        |
| 1          | F            | 199        | ASP         | 12.3        |
| 1          | B            | 169        | GLU         | 12.3        |
| 1          | B            | 51         | TRP         | 12.3        |
| 1          | D            | 191        | PRO         | 12.3        |
| 1          | B            | 62         | TYR         | 12.3        |
| 1          | C            | 144        | GLY         | 12.3        |
| 1          | C            | 192        | ALA         | 12.2        |
| 1          | B            | 205        | GLY         | 12.2        |
| 1          | D            | 135        | LEU         | 12.1        |
| 1          | B            | 197        | VAL         | 12.0        |
| 1          | C            | 9          | HIS         | 12.0        |
| 1          | D            | 142        | ALA         | 12.0        |
| 1          | C            | 245        | LEU         | 12.0        |
| 1          | B            | 139        | ILE         | 12.0        |
| 1          | B            | 144        | GLY         | 11.9        |
| 1          | B            | 10         | PRO         | 11.9        |
| 1          | D            | 202        | LEU         | 11.9        |
| 1          | C            | 214        | GLU         | 11.9        |
| 1          | B            | 86         | HIS         | 11.8        |
| 1          | F            | 63         | LEU         | 11.8        |
| 1          | E            | 206        | TYR         | 11.7        |
| 1          | F            | 150        | ILE         | 11.7        |
| 1          | A            | 129        | PHE         | 11.7        |
| 1          | E            | 86         | HIS         | 11.7        |
| 1          | A            | 72         | SER         | 11.6        |
| 1          | D            | 130        | ARG         | 11.6        |
| 1          | F            | 35         | SER         | 11.6        |
| 1          | C            | 224        | TYR         | 11.6        |
| 1          | F            | 216        | ASP         | 11.6        |
| 1          | E            | 90         | ALA         | 11.5        |
| 1          | A            | 164        | LEU         | 11.5        |
| 1          | F            | 133        | LEU         | 11.5        |
| 1          | D            | 199        | ASP         | 11.4        |
| 1          | C            | 26         | SER         | 11.3        |
| 1          | B            | 135        | LEU         | 11.3        |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | D            | 75         | ASN         | 11.3        |
| 1          | E            | 9          | HIS         | 11.3        |
| 1          | B            | 224        | TYR         | 11.3        |
| 1          | C            | 89         | LYS         | 11.2        |
| 1          | D            | 223        | GLY         | 11.2        |
| 1          | E            | 10         | PRO         | 11.2        |
| 1          | C            | 275        | ALA         | 11.1        |
| 1          | E            | 222        | ILE         | 11.1        |
| 1          | D            | 107        | GLU         | 11.1        |
| 1          | E            | 62         | TYR         | 11.1        |
| 1          | A            | 113        | ARG         | 11.1        |
| 1          | F            | 62         | TYR         | 11.1        |
| 1          | A            | 38         | SER         | 11.0        |
| 1          | A            | 171        | LYS         | 11.0        |
| 1          | C            | 135        | LEU         | 11.0        |
| 1          | A            | 254        | PHE         | 11.0        |
| 1          | E            | 240        | ILE         | 11.0        |
| 1          | F            | 10         | PRO         | 11.0        |
| 1          | C            | 37         | LEU         | 10.9        |
| 1          | D            | 255        | GLN         | 10.9        |
| 1          | B            | 39         | GLY         | 10.9        |
| 1          | D            | 78         | VAL         | 10.9        |
| 1          | C            | 122        | TYR         | 10.9        |
| 1          | E            | 64         | MET         | 10.9        |
| 1          | B            | 216        | ASP         | 10.9        |
| 1          | B            | 30         | PHE         | 10.9        |
| 1          | A            | 154        | ILE         | 10.8        |
| 1          | D            | 146        | ASP         | 10.8        |
| 1          | F            | 270        | ALA         | 10.8        |
| 1          | D            | 54         | LEU         | 10.7        |
| 1          | A            | 161        | LEU         | 10.7        |
| 1          | D            | 147        | SER         | 10.7        |
| 1          | F            | 5          | MET         | 10.7        |
| 1          | D            | 42         | TYR         | 10.7        |
| 1          | E            | 57         | GLY         | 10.7        |
| 1          | F            | 12         | PRO         | 10.6        |
| 1          | D            | 279        | LEU         | 10.6        |
| 1          | D            | 127        | SER         | 10.6        |
| 1          | D            | 90         | ALA         | 10.6        |
| 1          | C            | 137        | ASP         | 10.5        |
| 1          | C            | 198        | GLY         | 10.5        |
| 1          | C            | 47         | GLN         | 10.5        |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 92  | PHE  | 10.4 |
| 1   | F     | 70  | PHE  | 10.4 |
| 1   | F     | 66  | ASP  | 10.4 |
| 1   | A     | 270 | ALA  | 10.4 |
| 1   | E     | 241 | GLY  | 10.3 |
| 1   | E     | 151 | GLY  | 10.3 |
| 1   | F     | 161 | LEU  | 10.3 |
| 1   | E     | 128 | SER  | 10.3 |
| 1   | E     | 139 | ILE  | 10.3 |
| 1   | D     | 99  | LEU  | 10.3 |
| 1   | F     | 121 | LEU  | 10.2 |
| 1   | F     | 73  | THR  | 10.2 |
| 1   | F     | 32  | ALA  | 10.2 |
| 1   | F     | 193 | ALA  | 10.2 |
| 1   | B     | 31  | THR  | 10.2 |
| 1   | D     | 138 | VAL  | 10.2 |
| 1   | C     | 208 | ILE  | 10.2 |
| 1   | B     | 108 | TRP  | 10.2 |
| 1   | E     | 42  | TYR  | 10.2 |
| 1   | D     | 35  | SER  | 10.1 |
| 1   | A     | 259 | MET  | 10.1 |
| 1   | A     | 97  | ALA  | 10.1 |
| 1   | D     | 216 | ASP  | 10.0 |
| 1   | B     | 183 | PHE  | 10.0 |
| 1   | F     | 142 | ALA  | 10.0 |
| 1   | A     | 176 | TRP  | 10.0 |
| 1   | F     | 219 | THR  | 10.0 |
| 1   | D     | 8   | LYS  | 9.9  |
| 1   | F     | 197 | VAL  | 9.9  |
| 1   | B     | 271 | LEU  | 9.9  |
| 1   | F     | 208 | ILE  | 9.9  |
| 1   | B     | 269 | ASN  | 9.9  |
| 1   | D     | 229 | LEU  | 9.9  |
| 1   | B     | 154 | ILE  | 9.9  |
| 1   | B     | 166 | ASP  | 9.9  |
| 1   | D     | 97  | ALA  | 9.9  |
| 1   | D     | 38  | SER  | 9.9  |
| 1   | A     | 18  | ASN  | 9.8  |
| 1   | A     | 7   | ASP  | 9.8  |
| 1   | B     | 6   | ASN  | 9.8  |
| 1   | E     | 203 | PHE  | 9.8  |
| 1   | F     | 97  | ALA  | 9.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | F            | 9          | HIS         | 9.8         |
| 1          | F            | 11         | THR         | 9.8         |
| 1          | B            | 194        | PHE         | 9.8         |
| 1          | D            | 210        | ALA         | 9.8         |
| 1          | C            | 164        | LEU         | 9.8         |
| 1          | E            | 94         | PHE         | 9.7         |
| 1          | E            | 88         | ASP         | 9.7         |
| 1          | F            | 106        | PHE         | 9.7         |
| 1          | F            | 170        | VAL         | 9.7         |
| 1          | B            | 222        | ILE         | 9.6         |
| 1          | B            | 5          | MET         | 9.6         |
| 1          | A            | 141        | THR         | 9.5         |
| 1          | A            | 21         | PHE         | 9.5         |
| 1          | F            | 96         | ILE         | 9.5         |
| 1          | B            | 219        | THR         | 9.5         |
| 1          | C            | 279        | LEU         | 9.5         |
| 1          | E            | 202        | LEU         | 9.5         |
| 1          | E            | 33         | SER         | 9.5         |
| 1          | E            | 136        | SER         | 9.4         |
| 1          | E            | 143        | LEU         | 9.4         |
| 1          | C            | 197        | VAL         | 9.4         |
| 1          | E            | 105        | LYS         | 9.4         |
| 1          | A            | 218        | GLN         | 9.4         |
| 1          | D            | 149        | TYR         | 9.4         |
| 1          | E            | 149        | TYR         | 9.3         |
| 1          | E            | 69         | THR         | 9.3         |
| 1          | E            | 226        | PRO         | 9.3         |
| 1          | E            | 71         | PHE         | 9.3         |
| 1          | D            | 6          | ASN         | 9.3         |
| 1          | F            | 245        | LEU         | 9.2         |
| 1          | C            | 212        | PRO         | 9.2         |
| 1          | A            | 53         | ILE         | 9.2         |
| 1          | B            | 55         | VAL         | 9.1         |
| 1          | C            | 11         | THR         | 9.1         |
| 1          | E            | 35         | SER         | 9.1         |
| 1          | E            | 231        | TRP         | 9.1         |
| 1          | A            | 245        | LEU         | 9.0         |
| 1          | D            | 133        | LEU         | 9.0         |
| 1          | D            | 220        | PRO         | 9.0         |
| 1          | F            | 68         | GLY         | 9.0         |
| 1          | A            | 212        | PRO         | 8.9         |
| 1          | F            | 234        | GLY         | 8.9         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | D            | 225        | MET         | 8.9         |
| 1          | D            | 228        | HIS         | 8.8         |
| 1          | A            | 279        | LEU         | 8.8         |
| 1          | E            | 265        | PRO         | 8.8         |
| 1          | E            | 130        | ARG         | 8.8         |
| 1          | F            | 259        | MET         | 8.8         |
| 1          | A            | 262        | GLY         | 8.8         |
| 1          | A            | 120        | GLY         | 8.7         |
| 1          | E            | 78         | VAL         | 8.7         |
| 1          | F            | 283        | VAL         | 8.7         |
| 1          | F            | 81         | LEU         | 8.7         |
| 1          | B            | 40         | ALA         | 8.6         |
| 1          | B            | 266        | LEU         | 8.6         |
| 1          | F            | 134        | LYS         | 8.6         |
| 1          | E            | 51         | TRP         | 8.6         |
| 1          | A            | 12         | PRO         | 8.6         |
| 1          | B            | 50         | ARG         | 8.6         |
| 1          | E            | 22         | PRO         | 8.6         |
| 1          | B            | 132        | PRO         | 8.6         |
| 1          | A            | 225        | MET         | 8.6         |
| 1          | F            | 211        | PHE         | 8.5         |
| 1          | E            | 237        | LEU         | 8.5         |
| 1          | D            | 126        | GLN         | 8.5         |
| 1          | F            | 85         | TYR         | 8.5         |
| 1          | B            | 162        | MET         | 8.5         |
| 1          | E            | 271        | LEU         | 8.5         |
| 1          | B            | 72         | SER         | 8.5         |
| 1          | E            | 46         | TYR         | 8.4         |
| 1          | D            | 207        | LYS         | 8.4         |
| 1          | F            | 8          | LYS         | 8.4         |
| 1          | D            | 51         | TRP         | 8.4         |
| 1          | C            | 196        | ALA         | 8.4         |
| 1          | B            | 156        | GLY         | 8.4         |
| 1          | D            | 76         | HIS         | 8.4         |
| 1          | C            | 153        | PHE         | 8.3         |
| 1          | C            | 124        | LYS         | 8.3         |
| 1          | A            | 222        | ILE         | 8.3         |
| 1          | B            | 122        | TYR         | 8.3         |
| 1          | E            | 145        | GLU         | 8.3         |
| 1          | B            | 129        | PHE         | 8.2         |
| 1          | F            | 218        | GLN         | 8.2         |
| 1          | E            | 53         | ILE         | 8.2         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 163 | GLY  | 8.1  |
| 1   | E     | 213 | ASP  | 8.1  |
| 1   | F     | 230 | THR  | 8.1  |
| 1   | C     | 148 | ASP  | 8.1  |
| 1   | F     | 135 | LEU  | 8.1  |
| 1   | F     | 44  | THR  | 8.1  |
| 1   | A     | 130 | ARG  | 8.1  |
| 1   | B     | 84  | MET  | 8.1  |
| 1   | B     | 280 | LEU  | 8.1  |
| 1   | D     | 211 | PHE  | 8.1  |
| 1   | B     | 276 | ALA  | 8.1  |
| 1   | F     | 233 | PHE  | 8.0  |
| 1   | E     | 6   | ASN  | 8.0  |
| 1   | C     | 41  | HIS  | 8.0  |
| 1   | D     | 184 | ILE  | 8.0  |
| 1   | D     | 217 | ALA  | 8.0  |
| 1   | C     | 56  | VAL  | 8.0  |
| 1   | D     | 219 | THR  | 8.0  |
| 1   | F     | 167 | SER  | 8.0  |
| 1   | A     | 112 | PRO  | 8.0  |
| 1   | F     | 261 | THR  | 7.9  |
| 1   | C     | 211 | PHE  | 7.9  |
| 1   | F     | 285 | GLN  | 7.9  |
| 1   | D     | 245 | LEU  | 7.9  |
| 1   | B     | 42  | TYR  | 7.9  |
| 1   | B     | 151 | GLY  | 7.9  |
| 1   | B     | 148 | ASP  | 7.9  |
| 1   | B     | 283 | VAL  | 7.9  |
| 1   | E     | 209 | VAL  | 7.8  |
| 1   | E     | 135 | LEU  | 7.8  |
| 1   | D     | 282 | GLU  | 7.8  |
| 1   | D     | 197 | VAL  | 7.8  |
| 1   | F     | 123 | SER  | 7.8  |
| 1   | F     | 14  | PRO  | 7.7  |
| 1   | A     | 83  | PRO  | 7.7  |
| 1   | B     | 110 | ALA  | 7.7  |
| 1   | B     | 237 | LEU  | 7.7  |
| 1   | A     | 84  | MET  | 7.7  |
| 1   | C     | 174 | LEU  | 7.7  |
| 1   | B     | 211 | PHE  | 7.7  |
| 1   | B     | 272 | GLY  | 7.7  |
| 1   | F     | 271 | LEU  | 7.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | B            | 66         | ASP         | 7.6         |
| 1          | A            | 105        | LYS         | 7.6         |
| 1          | F            | 215        | MET         | 7.6         |
| 1          | C            | 38         | SER         | 7.6         |
| 1          | E            | 127        | SER         | 7.6         |
| 1          | E            | 144        | GLY         | 7.6         |
| 1          | F            | 149        | TYR         | 7.6         |
| 1          | F            | 223        | GLY         | 7.5         |
| 1          | C            | 244        | LEU         | 7.5         |
| 1          | C            | 7          | ASP         | 7.5         |
| 1          | E            | 160        | ALA         | 7.5         |
| 1          | F            | 214        | GLU         | 7.5         |
| 1          | F            | 78         | VAL         | 7.5         |
| 1          | D            | 257        | ARG         | 7.5         |
| 1          | B            | 209        | VAL         | 7.5         |
| 1          | D            | 170        | VAL         | 7.5         |
| 1          | B            | 94         | PHE         | 7.4         |
| 1          | E            | 63         | LEU         | 7.4         |
| 1          | E            | 283        | VAL         | 7.4         |
| 1          | E            | 141        | THR         | 7.4         |
| 1          | C            | 209        | VAL         | 7.4         |
| 1          | C            | 232        | LYS         | 7.4         |
| 1          | B            | 244        | LEU         | 7.4         |
| 1          | C            | 285        | GLN         | 7.4         |
| 1          | E            | 178        | MET         | 7.3         |
| 1          | E            | 180        | GLN         | 7.3         |
| 1          | F            | 146        | ASP         | 7.3         |
| 1          | E            | 39         | GLY         | 7.3         |
| 1          | F            | 280        | LEU         | 7.3         |
| 1          | B            | 57         | GLY         | 7.3         |
| 1          | A            | 99         | LEU         | 7.3         |
| 1          | D            | 249        | ILE         | 7.3         |
| 1          | F            | 6          | ASN         | 7.3         |
| 1          | D            | 21         | PHE         | 7.3         |
| 1          | E            | 216        | ASP         | 7.3         |
| 1          | B            | 255        | GLN         | 7.2         |
| 1          | A            | 280        | LEU         | 7.2         |
| 1          | C            | 46         | TYR         | 7.2         |
| 1          | D            | 209        | VAL         | 7.2         |
| 1          | D            | 14         | PRO         | 7.2         |
| 1          | A            | 140        | GLU         | 7.2         |
| 1          | C            | 140        | GLU         | 7.2         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 274 | LEU  | 7.1  |
| 1   | D     | 192 | ALA  | 7.1  |
| 1   | C     | 215 | MET  | 7.1  |
| 1   | F     | 182 | LYS  | 7.1  |
| 1   | B     | 133 | LEU  | 7.1  |
| 1   | C     | 282 | GLU  | 7.1  |
| 1   | B     | 203 | PHE  | 7.1  |
| 1   | F     | 89  | LYS  | 7.1  |
| 1   | A     | 114 | GLU  | 7.1  |
| 1   | D     | 48  | GLY  | 7.0  |
| 1   | D     | 46  | TYR  | 7.0  |
| 1   | E     | 267 | ALA  | 7.0  |
| 1   | A     | 231 | TRP  | 7.0  |
| 1   | E     | 155 | PRO  | 7.0  |
| 1   | E     | 122 | TYR  | 7.0  |
| 1   | B     | 14  | PRO  | 7.0  |
| 1   | E     | 252 | GLN  | 6.9  |
| 1   | A     | 124 | LYS  | 6.9  |
| 1   | F     | 253 | VAL  | 6.9  |
| 1   | C     | 271 | LEU  | 6.9  |
| 1   | D     | 87  | LEU  | 6.9  |
| 1   | C     | 81  | LEU  | 6.9  |
| 1   | C     | 113 | ARG  | 6.9  |
| 1   | C     | 129 | PHE  | 6.9  |
| 1   | A     | 24  | ALA  | 6.8  |
| 1   | E     | 138 | VAL  | 6.8  |
| 1   | D     | 188 | CYS  | 6.8  |
| 1   | A     | 221 | SER  | 6.8  |
| 1   | D     | 280 | LEU  | 6.8  |
| 1   | F     | 183 | PHE  | 6.8  |
| 1   | F     | 67  | ASN  | 6.8  |
| 1   | E     | 25  | TYR  | 6.8  |
| 1   | F     | 185 | ILE  | 6.8  |
| 1   | B     | 104 | VAL  | 6.8  |
| 1   | C     | 254 | PHE  | 6.8  |
| 1   | B     | 121 | LEU  | 6.8  |
| 1   | B     | 226 | PRO  | 6.8  |
| 1   | C     | 218 | GLN  | 6.8  |
| 1   | E     | 212 | PRO  | 6.8  |
| 1   | A     | 75  | ASN  | 6.7  |
| 1   | D     | 124 | LYS  | 6.7  |
| 1   | E     | 48  | GLY  | 6.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 25  | TYR  | 6.7  |
| 1   | F     | 132 | PRO  | 6.7  |
| 1   | B     | 21  | PHE  | 6.7  |
| 1   | A     | 194 | PHE  | 6.7  |
| 1   | F     | 88  | ASP  | 6.6  |
| 1   | F     | 213 | ASP  | 6.6  |
| 1   | F     | 258 | LYS  | 6.6  |
| 1   | A     | 217 | ALA  | 6.6  |
| 1   | E     | 197 | VAL  | 6.6  |
| 1   | C     | 45  | PRO  | 6.6  |
| 1   | F     | 201 | PRO  | 6.6  |
| 1   | B     | 19  | ALA  | 6.6  |
| 1   | F     | 237 | LEU  | 6.6  |
| 1   | F     | 76  | HIS  | 6.6  |
| 1   | D     | 187 | LEU  | 6.6  |
| 1   | A     | 71  | PHE  | 6.6  |
| 1   | A     | 143 | LEU  | 6.5  |
| 1   | A     | 219 | THR  | 6.5  |
| 1   | D     | 113 | ARG  | 6.5  |
| 1   | E     | 272 | GLY  | 6.5  |
| 1   | A     | 108 | TRP  | 6.5  |
| 1   | F     | 93  | SER  | 6.5  |
| 1   | B     | 243 | GLU  | 6.5  |
| 1   | A     | 210 | ALA  | 6.5  |
| 1   | D     | 264 | SER  | 6.4  |
| 1   | C     | 61  | ARG  | 6.4  |
| 1   | F     | 109 | TRP  | 6.4  |
| 1   | C     | 216 | ASP  | 6.4  |
| 1   | A     | 200 | ASP  | 6.4  |
| 1   | D     | 64  | MET  | 6.4  |
| 1   | F     | 254 | PHE  | 6.4  |
| 1   | E     | 173 | VAL  | 6.4  |
| 1   | D     | 68  | GLY  | 6.4  |
| 1   | B     | 267 | ALA  | 6.3  |
| 1   | C     | 84  | MET  | 6.3  |
| 1   | D     | 259 | MET  | 6.3  |
| 1   | E     | 189 | HIS  | 6.3  |
| 1   | A     | 36  | ASP  | 6.3  |
| 1   | E     | 228 | HIS  | 6.3  |
| 1   | E     | 60  | GLU  | 6.2  |
| 1   | F     | 202 | LEU  | 6.2  |
| 1   | A     | 102 | ASN  | 6.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 127 | SER  | 6.2  |
| 1   | C     | 39  | GLY  | 6.2  |
| 1   | D     | 57  | GLY  | 6.2  |
| 1   | D     | 157 | GLY  | 6.2  |
| 1   | C     | 200 | ASP  | 6.2  |
| 1   | A     | 180 | GLN  | 6.2  |
| 1   | A     | 44  | THR  | 6.2  |
| 1   | B     | 17  | ASP  | 6.2  |
| 1   | C     | 178 | MET  | 6.1  |
| 1   | F     | 198 | GLY  | 6.1  |
| 1   | E     | 183 | PHE  | 6.1  |
| 1   | A     | 198 | GLY  | 6.1  |
| 1   | A     | 167 | SER  | 6.1  |
| 1   | D     | 150 | ILE  | 6.1  |
| 1   | B     | 278 | ALA  | 6.1  |
| 1   | B     | 173 | VAL  | 6.1  |
| 1   | F     | 87  | LEU  | 6.1  |
| 1   | F     | 84  | MET  | 6.0  |
| 1   | E     | 161 | LEU  | 6.0  |
| 1   | B     | 265 | PRO  | 6.0  |
| 1   | B     | 47  | GLN  | 6.0  |
| 1   | C     | 50  | ARG  | 6.0  |
| 1   | D     | 153 | PHE  | 6.0  |
| 1   | A     | 110 | ALA  | 5.9  |
| 1   | E     | 110 | ALA  | 5.9  |
| 1   | A     | 192 | ALA  | 5.9  |
| 1   | E     | 61  | ARG  | 5.9  |
| 1   | B     | 248 | GLY  | 5.9  |
| 1   | C     | 283 | VAL  | 5.9  |
| 1   | B     | 184 | ILE  | 5.9  |
| 1   | B     | 61  | ARG  | 5.8  |
| 1   | F     | 86  | HIS  | 5.8  |
| 1   | F     | 22  | PRO  | 5.8  |
| 1   | E     | 254 | PHE  | 5.8  |
| 1   | A     | 202 | LEU  | 5.8  |
| 1   | A     | 98  | THR  | 5.8  |
| 1   | A     | 178 | MET  | 5.8  |
| 1   | F     | 82  | LEU  | 5.8  |
| 1   | F     | 7   | ASP  | 5.8  |
| 1   | E     | 67  | ASN  | 5.8  |
| 1   | A     | 244 | LEU  | 5.8  |
| 1   | F     | 264 | SER  | 5.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 109 | TRP  | 5.8  |
| 1   | F     | 100 | SER  | 5.7  |
| 1   | E     | 233 | PHE  | 5.7  |
| 1   | A     | 193 | ALA  | 5.7  |
| 1   | F     | 136 | SER  | 5.7  |
| 1   | A     | 199 | ASP  | 5.7  |
| 1   | B     | 15  | ALA  | 5.7  |
| 1   | F     | 92  | PHE  | 5.7  |
| 1   | E     | 238 | GLN  | 5.6  |
| 1   | A     | 276 | ALA  | 5.6  |
| 1   | B     | 111 | MET  | 5.6  |
| 1   | F     | 138 | VAL  | 5.6  |
| 1   | C     | 35  | SER  | 5.6  |
| 1   | D     | 65  | MET  | 5.6  |
| 1   | F     | 162 | MET  | 5.6  |
| 1   | C     | 42  | TYR  | 5.5  |
| 1   | E     | 169 | GLU  | 5.5  |
| 1   | A     | 27  | LEU  | 5.5  |
| 1   | F     | 207 | LYS  | 5.5  |
| 1   | F     | 47  | GLN  | 5.5  |
| 1   | F     | 225 | MET  | 5.5  |
| 1   | D     | 270 | ALA  | 5.5  |
| 1   | A     | 30  | PHE  | 5.5  |
| 1   | A     | 92  | PHE  | 5.5  |
| 1   | B     | 69  | THR  | 5.5  |
| 1   | E     | 191 | PRO  | 5.5  |
| 1   | C     | 258 | LYS  | 5.5  |
| 1   | B     | 118 | VAL  | 5.5  |
| 1   | A     | 237 | LEU  | 5.4  |
| 1   | E     | 16  | GLU  | 5.4  |
| 1   | C     | 238 | GLN  | 5.4  |
| 1   | B     | 202 | LEU  | 5.4  |
| 1   | C     | 34  | LYS  | 5.4  |
| 1   | A     | 158 | HIS  | 5.4  |
| 1   | D     | 93  | SER  | 5.4  |
| 1   | B     | 77  | PRO  | 5.4  |
| 1   | D     | 177 | ALA  | 5.3  |
| 1   | D     | 121 | LEU  | 5.3  |
| 1   | A     | 119 | ASN  | 5.3  |
| 1   | A     | 195 | LEU  | 5.3  |
| 1   | A     | 50  | ARG  | 5.3  |
| 1   | C     | 69  | THR  | 5.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 277 | LYS  | 5.3  |
| 1   | A     | 238 | GLN  | 5.3  |
| 1   | F     | 20  | PHE  | 5.3  |
| 1   | C     | 25  | TYR  | 5.2  |
| 1   | F     | 131 | GLN  | 5.2  |
| 1   | F     | 279 | LEU  | 5.2  |
| 1   | A     | 145 | GLU  | 5.2  |
| 1   | D     | 284 | GLU  | 5.2  |
| 1   | C     | 206 | TYR  | 5.2  |
| 1   | A     | 179 | LYS  | 5.2  |
| 1   | C     | 32  | ALA  | 5.2  |
| 1   | F     | 45  | PRO  | 5.2  |
| 1   | B     | 140 | GLU  | 5.1  |
| 1   | E     | 187 | LEU  | 5.1  |
| 1   | F     | 101 | GLY  | 5.1  |
| 1   | E     | 185 | ILE  | 5.1  |
| 1   | D     | 246 | ASN  | 5.1  |
| 1   | F     | 130 | ARG  | 5.1  |
| 1   | C     | 170 | VAL  | 5.1  |
| 1   | C     | 146 | ASP  | 5.1  |
| 1   | C     | 63  | LEU  | 5.1  |
| 1   | A     | 8   | LYS  | 5.1  |
| 1   | C     | 102 | ASN  | 5.1  |
| 1   | B     | 141 | THR  | 5.1  |
| 1   | D     | 49  | GLY  | 5.1  |
| 1   | E     | 31  | THR  | 5.0  |
| 1   | E     | 80  | THR  | 5.0  |
| 1   | F     | 118 | VAL  | 5.0  |
| 1   | D     | 250 | SER  | 5.0  |
| 1   | A     | 204 | ALA  | 5.0  |
| 1   | F     | 232 | LYS  | 5.0  |
| 1   | C     | 103 | PRO  | 5.0  |
| 1   | A     | 93  | SER  | 5.0  |
| 1   | A     | 122 | TYR  | 5.0  |
| 1   | C     | 10  | PRO  | 5.0  |
| 1   | E     | 246 | ASN  | 5.0  |
| 1   | A     | 87  | LEU  | 5.0  |
| 1   | C     | 259 | MET  | 5.0  |
| 1   | A     | 150 | ILE  | 5.0  |
| 1   | B     | 252 | GLN  | 5.0  |
| 1   | C     | 24  | ALA  | 4.9  |
| 1   | C     | 48  | GLY  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 52  | LYS  | 4.9  |
| 1   | F     | 108 | TRP  | 4.9  |
| 1   | D     | 240 | ILE  | 4.9  |
| 1   | E     | 11  | THR  | 4.9  |
| 1   | A     | 236 | GLN  | 4.9  |
| 1   | B     | 134 | LYS  | 4.9  |
| 1   | E     | 218 | GLN  | 4.9  |
| 1   | F     | 51  | TRP  | 4.9  |
| 1   | C     | 120 | GLY  | 4.9  |
| 1   | B     | 206 | TYR  | 4.9  |
| 1   | C     | 114 | GLU  | 4.9  |
| 1   | A     | 252 | GLN  | 4.8  |
| 1   | E     | 232 | LYS  | 4.8  |
| 1   | B     | 87  | LEU  | 4.8  |
| 1   | D     | 122 | TYR  | 4.8  |
| 1   | D     | 238 | GLN  | 4.8  |
| 1   | F     | 80  | THR  | 4.8  |
| 1   | C     | 92  | PHE  | 4.8  |
| 1   | A     | 227 | GLY  | 4.8  |
| 1   | F     | 116 | GLN  | 4.8  |
| 1   | B     | 71  | PHE  | 4.8  |
| 1   | B     | 145 | GLU  | 4.8  |
| 1   | A     | 96  | ILE  | 4.8  |
| 1   | F     | 59  | ASP  | 4.8  |
| 1   | B     | 235 | GLU  | 4.8  |
| 1   | D     | 237 | LEU  | 4.8  |
| 1   | C     | 109 | TRP  | 4.8  |
| 1   | D     | 183 | PHE  | 4.7  |
| 1   | A     | 261 | THR  | 4.7  |
| 1   | B     | 200 | ASP  | 4.7  |
| 1   | C     | 65  | MET  | 4.7  |
| 1   | C     | 31  | THR  | 4.7  |
| 1   | F     | 110 | ALA  | 4.7  |
| 1   | A     | 55  | VAL  | 4.7  |
| 1   | E     | 79  | GLU  | 4.7  |
| 1   | F     | 65  | MET  | 4.7  |
| 1   | A     | 134 | LYS  | 4.7  |
| 1   | D     | 208 | ILE  | 4.7  |
| 1   | E     | 280 | LEU  | 4.7  |
| 1   | F     | 196 | ALA  | 4.7  |
| 1   | B     | 223 | GLY  | 4.7  |
| 1   | C     | 190 | GLY  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 47  | GLN  | 4.7  |
| 1   | F     | 235 | GLU  | 4.7  |
| 1   | C     | 51  | TRP  | 4.7  |
| 1   | C     | 64  | MET  | 4.7  |
| 1   | A     | 203 | PHE  | 4.6  |
| 1   | D     | 179 | LYS  | 4.6  |
| 1   | D     | 37  | LEU  | 4.6  |
| 1   | A     | 117 | GLU  | 4.6  |
| 1   | C     | 118 | VAL  | 4.6  |
| 1   | F     | 99  | LEU  | 4.6  |
| 1   | C     | 33  | SER  | 4.6  |
| 1   | B     | 220 | PRO  | 4.6  |
| 1   | C     | 274 | LEU  | 4.6  |
| 1   | F     | 141 | THR  | 4.6  |
| 1   | E     | 50  | ARG  | 4.6  |
| 1   | E     | 8   | LYS  | 4.5  |
| 1   | A     | 62  | TYR  | 4.5  |
| 1   | C     | 94  | PHE  | 4.5  |
| 1   | C     | 203 | PHE  | 4.5  |
| 1   | A     | 224 | TYR  | 4.5  |
| 1   | C     | 142 | ALA  | 4.5  |
| 1   | B     | 254 | PHE  | 4.5  |
| 1   | C     | 78  | VAL  | 4.5  |
| 1   | E     | 13  | ASP  | 4.5  |
| 1   | F     | 95  | ASP  | 4.5  |
| 1   | A     | 60  | GLU  | 4.5  |
| 1   | D     | 176 | TRP  | 4.5  |
| 1   | A     | 85  | TYR  | 4.5  |
| 1   | C     | 226 | PRO  | 4.5  |
| 1   | E     | 18  | ASN  | 4.4  |
| 1   | B     | 174 | LEU  | 4.4  |
| 1   | E     | 38  | SER  | 4.4  |
| 1   | E     | 82  | LEU  | 4.4  |
| 1   | D     | 189 | HIS  | 4.4  |
| 1   | A     | 278 | ALA  | 4.4  |
| 1   | F     | 240 | ILE  | 4.4  |
| 1   | C     | 188 | CYS  | 4.4  |
| 1   | D     | 43  | PRO  | 4.4  |
| 1   | A     | 187 | LEU  | 4.4  |
| 1   | D     | 260 | LEU  | 4.4  |
| 1   | A     | 5   | MET  | 4.4  |
| 1   | A     | 121 | LEU  | 4.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 7   | ASP  | 4.4  |
| 1   | F     | 247 | THR  | 4.4  |
| 1   | C     | 49  | GLY  | 4.4  |
| 1   | B     | 20  | PHE  | 4.3  |
| 1   | A     | 66  | ASP  | 4.3  |
| 1   | A     | 115 | ASP  | 4.3  |
| 1   | A     | 173 | VAL  | 4.3  |
| 1   | D     | 224 | TYR  | 4.3  |
| 1   | B     | 284 | GLU  | 4.3  |
| 1   | D     | 16  | GLU  | 4.3  |
| 1   | F     | 30  | PHE  | 4.3  |
| 1   | E     | 162 | MET  | 4.3  |
| 1   | A     | 54  | LEU  | 4.3  |
| 1   | E     | 112 | PRO  | 4.3  |
| 1   | F     | 172 | ALA  | 4.3  |
| 1   | C     | 207 | LYS  | 4.3  |
| 1   | B     | 90  | ALA  | 4.3  |
| 1   | E     | 84  | MET  | 4.3  |
| 1   | A     | 81  | LEU  | 4.3  |
| 1   | A     | 45  | PRO  | 4.3  |
| 1   | B     | 29  | GLN  | 4.2  |
| 1   | F     | 61  | ARG  | 4.2  |
| 1   | E     | 125 | TYR  | 4.2  |
| 1   | F     | 158 | HIS  | 4.2  |
| 1   | D     | 151 | GLY  | 4.2  |
| 1   | D     | 261 | THR  | 4.2  |
| 1   | B     | 242 | PHE  | 4.2  |
| 1   | B     | 277 | LYS  | 4.2  |
| 1   | D     | 166 | ASP  | 4.2  |
| 1   | C     | 99  | LEU  | 4.2  |
| 1   | D     | 58  | ALA  | 4.2  |
| 1   | D     | 85  | TYR  | 4.2  |
| 1   | D     | 7   | ASP  | 4.2  |
| 1   | C     | 240 | ILE  | 4.2  |
| 1   | C     | 171 | LYS  | 4.2  |
| 1   | C     | 189 | HIS  | 4.2  |
| 1   | E     | 85  | TYR  | 4.2  |
| 1   | C     | 112 | PRO  | 4.2  |
| 1   | E     | 220 | PRO  | 4.2  |
| 1   | A     | 29  | GLN  | 4.1  |
| 1   | F     | 102 | ASN  | 4.1  |
| 1   | A     | 201 | PRO  | 4.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 63  | LEU  | 4.1  |
| 1   | B     | 91  | GLY  | 4.1  |
| 1   | F     | 52  | LYS  | 4.1  |
| 1   | B     | 234 | GLY  | 4.1  |
| 1   | C     | 19  | ALA  | 4.1  |
| 1   | D     | 129 | PHE  | 4.1  |
| 1   | B     | 70  | PHE  | 4.1  |
| 1   | B     | 241 | GLY  | 4.1  |
| 1   | D     | 72  | SER  | 4.1  |
| 1   | F     | 129 | PHE  | 4.1  |
| 1   | D     | 164 | LEU  | 4.1  |
| 1   | F     | 122 | TYR  | 4.1  |
| 1   | F     | 38  | SER  | 4.1  |
| 1   | C     | 82  | LEU  | 4.1  |
| 1   | E     | 205 | GLY  | 4.0  |
| 1   | A     | 184 | ILE  | 4.0  |
| 1   | E     | 27  | LEU  | 4.0  |
| 1   | F     | 276 | ALA  | 4.0  |
| 1   | A     | 128 | SER  | 4.0  |
| 1   | D     | 106 | PHE  | 4.0  |
| 1   | C     | 260 | LEU  | 4.0  |
| 1   | A     | 186 | SER  | 4.0  |
| 1   | A     | 275 | ALA  | 4.0  |
| 1   | C     | 236 | GLN  | 4.0  |
| 1   | E     | 20  | PHE  | 4.0  |
| 1   | A     | 9   | HIS  | 4.0  |
| 1   | C     | 105 | LYS  | 4.0  |
| 1   | D     | 273 | GLN  | 4.0  |
| 1   | D     | 173 | VAL  | 3.9  |
| 1   | E     | 170 | VAL  | 3.9  |
| 1   | D     | 53  | ILE  | 3.9  |
| 1   | C     | 263 | ASP  | 3.9  |
| 1   | A     | 196 | ALA  | 3.9  |
| 1   | B     | 258 | LYS  | 3.9  |
| 1   | B     | 170 | VAL  | 3.9  |
| 1   | E     | 104 | VAL  | 3.9  |
| 1   | A     | 234 | GLY  | 3.9  |
| 1   | F     | 144 | GLY  | 3.9  |
| 1   | E     | 249 | ILE  | 3.9  |
| 1   | C     | 247 | THR  | 3.9  |
| 1   | F     | 176 | TRP  | 3.9  |
| 1   | C     | 222 | ILE  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 172 | ALA  | 3.9  |
| 1   | E     | 193 | ALA  | 3.9  |
| 1   | F     | 140 | GLU  | 3.9  |
| 1   | F     | 173 | VAL  | 3.9  |
| 1   | C     | 27  | LEU  | 3.9  |
| 1   | E     | 54  | LEU  | 3.9  |
| 1   | D     | 67  | ASN  | 3.9  |
| 1   | E     | 29  | GLN  | 3.9  |
| 1   | B     | 32  | ALA  | 3.9  |
| 1   | E     | 248 | GLY  | 3.9  |
| 1   | F     | 148 | ASP  | 3.9  |
| 1   | C     | 125 | TYR  | 3.9  |
| 1   | D     | 82  | LEU  | 3.9  |
| 1   | B     | 201 | PRO  | 3.8  |
| 1   | B     | 126 | GLN  | 3.8  |
| 1   | A     | 153 | PHE  | 3.8  |
| 1   | D     | 152 | VAL  | 3.8  |
| 1   | B     | 178 | MET  | 3.8  |
| 1   | F     | 15  | ALA  | 3.8  |
| 1   | B     | 175 | GLN  | 3.8  |
| 1   | B     | 274 | LEU  | 3.8  |
| 1   | F     | 206 | TYR  | 3.8  |
| 1   | F     | 203 | PHE  | 3.8  |
| 1   | B     | 240 | ILE  | 3.8  |
| 1   | C     | 156 | GLY  | 3.8  |
| 1   | B     | 119 | ASN  | 3.8  |
| 1   | F     | 266 | LEU  | 3.8  |
| 1   | A     | 20  | PHE  | 3.8  |
| 1   | D     | 56  | VAL  | 3.8  |
| 1   | C     | 281 | ALA  | 3.8  |
| 1   | D     | 11  | THR  | 3.8  |
| 1   | E     | 177 | ALA  | 3.8  |
| 1   | C     | 157 | GLY  | 3.8  |
| 1   | D     | 60  | GLU  | 3.8  |
| 1   | B     | 191 | PRO  | 3.7  |
| 1   | F     | 98  | THR  | 3.7  |
| 1   | F     | 124 | LYS  | 3.7  |
| 1   | D     | 285 | GLN  | 3.7  |
| 1   | B     | 48  | GLY  | 3.7  |
| 1   | E     | 74  | GLY  | 3.7  |
| 1   | D     | 32  | ALA  | 3.7  |
| 1   | B     | 245 | LEU  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 22  | PRO  | 3.7  |
| 1   | C     | 225 | MET  | 3.7  |
| 1   | E     | 5   | MET  | 3.7  |
| 1   | A     | 26  | SER  | 3.7  |
| 1   | D     | 18  | ASN  | 3.7  |
| 1   | E     | 99  | LEU  | 3.7  |
| 1   | A     | 209 | VAL  | 3.7  |
| 1   | E     | 12  | PRO  | 3.7  |
| 1   | A     | 177 | ALA  | 3.6  |
| 1   | B     | 41  | HIS  | 3.6  |
| 1   | E     | 253 | VAL  | 3.6  |
| 1   | A     | 10  | PRO  | 3.6  |
| 1   | C     | 176 | TRP  | 3.6  |
| 1   | E     | 166 | ASP  | 3.6  |
| 1   | E     | 72  | SER  | 3.6  |
| 1   | A     | 64  | MET  | 3.6  |
| 1   | D     | 156 | GLY  | 3.6  |
| 1   | D     | 165 | PRO  | 3.6  |
| 1   | F     | 13  | ASP  | 3.6  |
| 1   | C     | 213 | ASP  | 3.6  |
| 1   | B     | 82  | LEU  | 3.6  |
| 1   | A     | 28  | SER  | 3.6  |
| 1   | C     | 242 | PHE  | 3.6  |
| 1   | C     | 16  | GLU  | 3.6  |
| 1   | B     | 26  | SER  | 3.5  |
| 1   | E     | 217 | ALA  | 3.5  |
| 1   | A     | 155 | PRO  | 3.5  |
| 1   | A     | 185 | ILE  | 3.5  |
| 1   | A     | 136 | SER  | 3.5  |
| 1   | A     | 260 | LEU  | 3.5  |
| 1   | E     | 255 | GLN  | 3.5  |
| 1   | E     | 281 | ALA  | 3.5  |
| 1   | F     | 48  | GLY  | 3.5  |
| 1   | F     | 163 | GLY  | 3.5  |
| 1   | D     | 253 | VAL  | 3.5  |
| 1   | F     | 222 | ILE  | 3.5  |
| 1   | A     | 16  | GLU  | 3.5  |
| 1   | A     | 42  | TYR  | 3.5  |
| 1   | A     | 11  | THR  | 3.5  |
| 1   | C     | 248 | GLY  | 3.5  |
| 1   | F     | 188 | CYS  | 3.5  |
| 1   | F     | 72  | SER  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 37  | LEU  | 3.5  |
| 1   | E     | 95  | ASP  | 3.5  |
| 1   | D     | 86  | HIS  | 3.5  |
| 1   | C     | 233 | PHE  | 3.5  |
| 1   | A     | 6   | ASN  | 3.4  |
| 1   | E     | 251 | GLY  | 3.4  |
| 1   | F     | 189 | HIS  | 3.4  |
| 1   | B     | 147 | SER  | 3.4  |
| 1   | C     | 53  | ILE  | 3.4  |
| 1   | C     | 150 | ILE  | 3.4  |
| 1   | E     | 115 | ASP  | 3.4  |
| 1   | C     | 201 | PRO  | 3.4  |
| 1   | D     | 200 | ASP  | 3.4  |
| 1   | E     | 36  | ASP  | 3.4  |
| 1   | F     | 103 | PRO  | 3.4  |
| 1   | B     | 101 | GLY  | 3.4  |
| 1   | A     | 132 | PRO  | 3.4  |
| 1   | E     | 121 | LEU  | 3.4  |
| 1   | C     | 36  | ASP  | 3.4  |
| 1   | E     | 168 | GLN  | 3.4  |
| 1   | C     | 12  | PRO  | 3.4  |
| 1   | C     | 101 | GLY  | 3.4  |
| 1   | B     | 46  | TYR  | 3.4  |
| 1   | E     | 154 | ILE  | 3.4  |
| 1   | D     | 174 | LEU  | 3.4  |
| 1   | D     | 34  | LYS  | 3.4  |
| 1   | B     | 239 | ALA  | 3.4  |
| 1   | F     | 79  | GLU  | 3.4  |
| 1   | C     | 187 | LEU  | 3.3  |
| 1   | C     | 204 | ALA  | 3.3  |
| 1   | E     | 181 | ASN  | 3.3  |
| 1   | B     | 186 | SER  | 3.3  |
| 1   | D     | 123 | SER  | 3.3  |
| 1   | D     | 104 | VAL  | 3.3  |
| 1   | F     | 209 | VAL  | 3.3  |
| 1   | B     | 80  | THR  | 3.3  |
| 1   | B     | 172 | ALA  | 3.3  |
| 1   | D     | 120 | GLY  | 3.3  |
| 1   | F     | 180 | GLN  | 3.3  |
| 1   | A     | 46  | TYR  | 3.3  |
| 1   | D     | 114 | GLU  | 3.3  |
| 1   | A     | 220 | PRO  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 262 | GLY  | 3.3  |
| 1   | E     | 165 | PRO  | 3.3  |
| 1   | D     | 31  | THR  | 3.2  |
| 1   | F     | 277 | LYS  | 3.2  |
| 1   | B     | 164 | LEU  | 3.2  |
| 1   | D     | 25  | TYR  | 3.2  |
| 1   | E     | 176 | TRP  | 3.2  |
| 1   | D     | 204 | ALA  | 3.2  |
| 1   | C     | 13  | ASP  | 3.2  |
| 1   | F     | 71  | PHE  | 3.2  |
| 1   | A     | 103 | PRO  | 3.2  |
| 1   | B     | 34  | LYS  | 3.2  |
| 1   | F     | 90  | ALA  | 3.2  |
| 1   | D     | 19  | ALA  | 3.2  |
| 1   | B     | 163 | GLY  | 3.2  |
| 1   | E     | 21  | PHE  | 3.2  |
| 1   | B     | 230 | THR  | 3.2  |
| 1   | A     | 253 | VAL  | 3.2  |
| 1   | C     | 199 | ASP  | 3.2  |
| 1   | E     | 118 | VAL  | 3.2  |
| 1   | E     | 200 | ASP  | 3.2  |
| 1   | E     | 270 | ALA  | 3.2  |
| 1   | B     | 9   | HIS  | 3.2  |
| 1   | B     | 221 | SER  | 3.2  |
| 1   | C     | 270 | ALA  | 3.1  |
| 1   | D     | 9   | HIS  | 3.1  |
| 1   | D     | 66  | ASP  | 3.1  |
| 1   | E     | 150 | ILE  | 3.1  |
| 1   | D     | 239 | ALA  | 3.1  |
| 1   | A     | 197 | VAL  | 3.1  |
| 1   | B     | 64  | MET  | 3.1  |
| 1   | C     | 30  | PHE  | 3.1  |
| 1   | E     | 279 | LEU  | 3.1  |
| 1   | E     | 34  | LYS  | 3.1  |
| 1   | E     | 142 | ALA  | 3.1  |
| 1   | D     | 115 | ASP  | 3.1  |
| 1   | D     | 233 | PHE  | 3.1  |
| 1   | A     | 272 | GLY  | 3.1  |
| 1   | E     | 91  | GLY  | 3.1  |
| 1   | B     | 8   | LYS  | 3.1  |
| 1   | A     | 73  | THR  | 3.1  |
| 1   | D     | 17  | ASP  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 42  | TYR  | 3.1  |
| 1   | B     | 127 | SER  | 3.1  |
| 1   | B     | 73  | THR  | 3.1  |
| 1   | A     | 127 | SER  | 3.1  |
| 1   | B     | 79  | GLU  | 3.1  |
| 1   | A     | 248 | GLY  | 3.1  |
| 1   | C     | 21  | PHE  | 3.0  |
| 1   | B     | 256 | ASP  | 3.0  |
| 1   | E     | 30  | PHE  | 3.0  |
| 1   | E     | 207 | LYS  | 3.0  |
| 1   | F     | 117 | GLU  | 3.0  |
| 1   | E     | 196 | ALA  | 3.0  |
| 1   | D     | 277 | LYS  | 3.0  |
| 1   | E     | 211 | PHE  | 3.0  |
| 1   | C     | 96  | ILE  | 3.0  |
| 1   | D     | 52  | LYS  | 3.0  |
| 1   | C     | 223 | GLY  | 3.0  |
| 1   | B     | 153 | PHE  | 3.0  |
| 1   | F     | 151 | GLY  | 3.0  |
| 1   | A     | 78  | VAL  | 3.0  |
| 1   | F     | 64  | MET  | 3.0  |
| 1   | C     | 20  | PHE  | 3.0  |
| 1   | C     | 183 | PHE  | 3.0  |
| 1   | B     | 282 | GLU  | 3.0  |
| 1   | C     | 107 | GLU  | 3.0  |
| 1   | A     | 126 | GLN  | 3.0  |
| 1   | C     | 269 | ASN  | 3.0  |
| 1   | B     | 37  | LEU  | 2.9  |
| 1   | D     | 27  | LEU  | 2.9  |
| 1   | E     | 126 | GLN  | 2.9  |
| 1   | F     | 175 | GLN  | 2.9  |
| 1   | F     | 114 | GLU  | 2.9  |
| 1   | B     | 225 | MET  | 2.9  |
| 1   | E     | 117 | GLU  | 2.9  |
| 1   | F     | 31  | THR  | 2.9  |
| 1   | E     | 97  | ALA  | 2.9  |
| 1   | F     | 27  | LEU  | 2.9  |
| 1   | A     | 52  | LYS  | 2.9  |
| 1   | A     | 273 | GLN  | 2.9  |
| 1   | E     | 230 | THR  | 2.9  |
| 1   | F     | 24  | ALA  | 2.9  |
| 1   | F     | 43  | PRO  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 151 | GLY  | 2.9  |
| 1   | E     | 227 | GLY  | 2.9  |
| 1   | C     | 221 | SER  | 2.9  |
| 1   | D     | 195 | LEU  | 2.9  |
| 1   | E     | 276 | ALA  | 2.9  |
| 1   | E     | 146 | ASP  | 2.9  |
| 1   | E     | 147 | SER  | 2.9  |
| 1   | B     | 187 | LEU  | 2.9  |
| 1   | B     | 215 | MET  | 2.9  |
| 1   | C     | 169 | GLU  | 2.9  |
| 1   | D     | 169 | GLU  | 2.9  |
| 1   | C     | 116 | GLN  | 2.9  |
| 1   | D     | 196 | ALA  | 2.9  |
| 1   | D     | 267 | ALA  | 2.9  |
| 1   | A     | 146 | ASP  | 2.9  |
| 1   | C     | 95  | ASP  | 2.9  |
| 1   | F     | 155 | PRO  | 2.9  |
| 1   | E     | 96  | ILE  | 2.9  |
| 1   | C     | 202 | LEU  | 2.8  |
| 1   | C     | 237 | LEU  | 2.8  |
| 1   | D     | 102 | ASN  | 2.8  |
| 1   | A     | 63  | LEU  | 2.8  |
| 1   | D     | 134 | LYS  | 2.8  |
| 1   | D     | 140 | GLU  | 2.8  |
| 1   | F     | 229 | LEU  | 2.8  |
| 1   | D     | 61  | ARG  | 2.8  |
| 1   | D     | 171 | LYS  | 2.8  |
| 1   | E     | 47  | GLN  | 2.8  |
| 1   | B     | 115 | ASP  | 2.8  |
| 1   | D     | 271 | LEU  | 2.8  |
| 1   | D     | 274 | LEU  | 2.8  |
| 1   | B     | 116 | GLN  | 2.8  |
| 1   | C     | 97  | ALA  | 2.8  |
| 1   | A     | 250 | SER  | 2.8  |
| 1   | F     | 28  | SER  | 2.8  |
| 1   | A     | 95  | ASP  | 2.8  |
| 1   | F     | 238 | GLN  | 2.8  |
| 1   | D     | 268 | GLY  | 2.8  |
| 1   | F     | 190 | GLY  | 2.8  |
| 1   | B     | 92  | PHE  | 2.8  |
| 1   | A     | 258 | LYS  | 2.8  |
| 1   | F     | 187 | LEU  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 55  | VAL  | 2.7  |
| 1   | E     | 129 | PHE  | 2.7  |
| 1   | A     | 17  | ASP  | 2.7  |
| 1   | E     | 28  | SER  | 2.7  |
| 1   | F     | 36  | ASP  | 2.7  |
| 1   | E     | 284 | GLU  | 2.7  |
| 1   | A     | 249 | ILE  | 2.7  |
| 1   | A     | 268 | GLY  | 2.7  |
| 1   | D     | 119 | ASN  | 2.7  |
| 1   | E     | 73  | THR  | 2.7  |
| 1   | D     | 145 | GLU  | 2.7  |
| 1   | B     | 204 | ALA  | 2.7  |
| 1   | C     | 145 | GLU  | 2.7  |
| 1   | A     | 165 | PRO  | 2.7  |
| 1   | B     | 179 | LYS  | 2.7  |
| 1   | E     | 179 | LYS  | 2.7  |
| 1   | D     | 160 | ALA  | 2.7  |
| 1   | E     | 120 | GLY  | 2.7  |
| 1   | E     | 269 | ASN  | 2.7  |
| 1   | A     | 191 | PRO  | 2.7  |
| 1   | D     | 28  | SER  | 2.7  |
| 1   | A     | 235 | GLU  | 2.7  |
| 1   | E     | 219 | THR  | 2.7  |
| 1   | C     | 252 | GLN  | 2.7  |
| 1   | B     | 150 | ILE  | 2.6  |
| 1   | D     | 71  | PHE  | 2.6  |
| 1   | F     | 244 | LEU  | 2.6  |
| 1   | D     | 234 | GLY  | 2.6  |
| 1   | E     | 152 | VAL  | 2.6  |
| 1   | A     | 37  | LEU  | 2.6  |
| 1   | A     | 31  | THR  | 2.6  |
| 1   | D     | 55  | VAL  | 2.6  |
| 1   | F     | 192 | ALA  | 2.6  |
| 1   | C     | 127 | SER  | 2.6  |
| 1   | D     | 198 | GLY  | 2.6  |
| 1   | F     | 50  | ARG  | 2.6  |
| 1   | D     | 206 | TYR  | 2.6  |
| 1   | E     | 258 | LYS  | 2.6  |
| 1   | D     | 242 | PHE  | 2.6  |
| 1   | D     | 36  | ASP  | 2.6  |
| 1   | C     | 141 | THR  | 2.6  |
| 1   | B     | 259 | MET  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 214 | GLU  | 2.6  |
| 1   | C     | 239 | ALA  | 2.6  |
| 1   | C     | 173 | VAL  | 2.5  |
| 1   | C     | 128 | SER  | 2.5  |
| 1   | C     | 100 | SER  | 2.5  |
| 1   | F     | 33  | SER  | 2.5  |
| 1   | A     | 43  | PRO  | 2.5  |
| 1   | C     | 219 | THR  | 2.5  |
| 1   | C     | 261 | THR  | 2.5  |
| 1   | D     | 185 | ILE  | 2.5  |
| 1   | E     | 32  | ALA  | 2.5  |
| 1   | E     | 242 | PHE  | 2.5  |
| 1   | B     | 190 | GLY  | 2.5  |
| 1   | E     | 101 | GLY  | 2.5  |
| 1   | A     | 265 | PRO  | 2.5  |
| 1   | B     | 177 | ALA  | 2.5  |
| 1   | C     | 250 | SER  | 2.5  |
| 1   | B     | 138 | VAL  | 2.5  |
| 1   | C     | 14  | PRO  | 2.5  |
| 1   | E     | 229 | LEU  | 2.5  |
| 1   | A     | 162 | MET  | 2.5  |
| 1   | A     | 207 | LYS  | 2.5  |
| 1   | F     | 204 | ALA  | 2.5  |
| 1   | D     | 155 | PRO  | 2.5  |
| 1   | C     | 152 | VAL  | 2.5  |
| 1   | D     | 45  | PRO  | 2.5  |
| 1   | A     | 76  | HIS  | 2.5  |
| 1   | E     | 83  | PRO  | 2.4  |
| 1   | D     | 84  | MET  | 2.4  |
| 1   | C     | 28  | SER  | 2.4  |
| 1   | E     | 19  | ALA  | 2.4  |
| 1   | E     | 224 | TYR  | 2.4  |
| 1   | F     | 278 | ALA  | 2.4  |
| 1   | E     | 70  | PHE  | 2.4  |
| 1   | D     | 22  | PRO  | 2.4  |
| 1   | E     | 198 | GLY  | 2.4  |
| 1   | B     | 233 | PHE  | 2.4  |
| 1   | F     | 16  | GLU  | 2.4  |
| 1   | F     | 191 | PRO  | 2.4  |
| 1   | F     | 220 | PRO  | 2.4  |
| 1   | D     | 41  | HIS  | 2.4  |
| 1   | E     | 76  | HIS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 74  | GLY  | 2.4  |
| 1   | E     | 223 | GLY  | 2.4  |
| 1   | A     | 80  | THR  | 2.4  |
| 1   | C     | 166 | ASP  | 2.4  |
| 1   | B     | 236 | GLN  | 2.4  |
| 1   | B     | 263 | ASP  | 2.4  |
| 1   | B     | 112 | PRO  | 2.4  |
| 1   | F     | 228 | HIS  | 2.4  |
| 1   | B     | 124 | LYS  | 2.4  |
| 1   | A     | 111 | MET  | 2.4  |
| 1   | B     | 189 | HIS  | 2.4  |
| 1   | A     | 138 | VAL  | 2.4  |
| 1   | A     | 166 | ASP  | 2.4  |
| 1   | A     | 266 | LEU  | 2.4  |
| 1   | B     | 78  | VAL  | 2.4  |
| 1   | A     | 239 | ALA  | 2.4  |
| 1   | C     | 276 | ALA  | 2.4  |
| 1   | D     | 110 | ALA  | 2.4  |
| 1   | A     | 109 | TRP  | 2.3  |
| 1   | B     | 18  | ASN  | 2.3  |
| 1   | C     | 265 | PRO  | 2.3  |
| 1   | B     | 99  | LEU  | 2.3  |
| 1   | D     | 80  | THR  | 2.3  |
| 1   | C     | 194 | PHE  | 2.3  |
| 1   | E     | 153 | PHE  | 2.3  |
| 1   | C     | 80  | THR  | 2.3  |
| 1   | D     | 276 | ALA  | 2.3  |
| 1   | F     | 120 | GLY  | 2.3  |
| 1   | E     | 277 | LYS  | 2.3  |
| 1   | D     | 186 | SER  | 2.3  |
| 1   | A     | 39  | GLY  | 2.3  |
| 1   | C     | 273 | GLN  | 2.3  |
| 1   | D     | 203 | PHE  | 2.3  |
| 1   | B     | 85  | TYR  | 2.3  |
| 1   | A     | 19  | ALA  | 2.3  |
| 1   | A     | 77  | PRO  | 2.3  |
| 1   | C     | 139 | ILE  | 2.3  |
| 1   | F     | 83  | PRO  | 2.3  |
| 1   | B     | 117 | GLU  | 2.3  |
| 1   | F     | 181 | ASN  | 2.3  |
| 1   | A     | 59  | ASP  | 2.3  |
| 1   | C     | 256 | ASP  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 182 | LYS  | 2.3  |
| 1   | C     | 111 | MET  | 2.3  |
| 1   | A     | 229 | LEU  | 2.3  |
| 1   | E     | 59  | ASP  | 2.3  |
| 1   | D     | 108 | TRP  | 2.3  |
| 1   | E     | 109 | TRP  | 2.3  |
| 1   | C     | 172 | ALA  | 2.2  |
| 1   | A     | 214 | GLU  | 2.2  |
| 1   | C     | 180 | GLN  | 2.2  |
| 1   | D     | 178 | MET  | 2.2  |
| 1   | E     | 100 | SER  | 2.2  |
| 1   | F     | 186 | SER  | 2.2  |
| 1   | A     | 49  | GLY  | 2.2  |
| 1   | A     | 163 | GLY  | 2.2  |
| 1   | D     | 201 | PRO  | 2.2  |
| 1   | C     | 108 | TRP  | 2.2  |
| 1   | A     | 147 | SER  | 2.2  |
| 1   | E     | 23  | SER  | 2.2  |
| 1   | A     | 133 | LEU  | 2.2  |
| 1   | D     | 182 | LYS  | 2.2  |
| 1   | A     | 255 | GLN  | 2.2  |
| 1   | B     | 192 | ALA  | 2.2  |
| 1   | E     | 192 | ALA  | 2.2  |
| 1   | D     | 59  | ASP  | 2.2  |
| 1   | F     | 166 | ASP  | 2.2  |
| 1   | E     | 26  | SER  | 2.2  |
| 1   | B     | 149 | TYR  | 2.2  |
| 1   | E     | 89  | LYS  | 2.2  |
| 1   | F     | 267 | ALA  | 2.2  |
| 1   | E     | 208 | ILE  | 2.2  |
| 1   | C     | 60  | GLU  | 2.2  |
| 1   | C     | 246 | ASN  | 2.2  |
| 1   | E     | 148 | ASP  | 2.2  |
| 1   | C     | 264 | SER  | 2.2  |
| 1   | F     | 273 | GLN  | 2.2  |
| 1   | F     | 171 | LYS  | 2.2  |
| 1   | A     | 281 | ALA  | 2.1  |
| 1   | F     | 54  | LEU  | 2.1  |
| 1   | C     | 220 | PRO  | 2.1  |
| 1   | F     | 165 | PRO  | 2.1  |
| 1   | A     | 142 | ALA  | 2.1  |
| 1   | B     | 257 | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 92  | PHE  | 2.1  |
| 1   | B     | 168 | GLN  | 2.1  |
| 1   | C     | 23  | SER  | 2.1  |
| 1   | F     | 231 | TRP  | 2.1  |
| 1   | B     | 208 | ILE  | 2.1  |
| 1   | E     | 124 | LYS  | 2.1  |
| 1   | E     | 266 | LEU  | 2.1  |
| 1   | F     | 23  | SER  | 2.1  |
| 1   | A     | 139 | ILE  | 2.1  |
| 1   | F     | 91  | GLY  | 2.1  |
| 1   | D     | 95  | ASP  | 2.1  |
| 1   | E     | 65  | MET  | 2.1  |
| 1   | D     | 136 | SER  | 2.1  |
| 1   | B     | 146 | ASP  | 2.0  |
| 1   | F     | 115 | ASP  | 2.0  |
| 1   | F     | 126 | GLN  | 2.0  |
| 1   | B     | 160 | ALA  | 2.0  |
| 1   | C     | 57  | GLY  | 2.0  |
| 1   | F     | 256 | ASP  | 2.0  |
| 1   | B     | 93  | SER  | 2.0  |
| 1   | E     | 199 | ASP  | 2.0  |
| 1   | D     | 266 | LEU  | 2.0  |
| 1   | A     | 232 | LYS  | 2.0  |
| 1   | B     | 246 | ASN  | 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-------|-----------------------------|-------|
| 2   | MPD  | B     | 5001 | 8/8   | 0.16  | 2.58 | 10.57 | 53,54,55,55                 | 0     |
| 2   | MPD  | F     | 301  | 8/8   | 0.44  | 1.67 | 2.89  | 63,64,65,65                 | 0     |
| 2   | MPD  | B     | 5002 | 8/8   | -0.03 | 1.06 | 2.82  | 49,50,52,54                 | 0     |
| 2   | MPD  | A     | 301  | 8/8   | 0.51  | 1.35 | 0.66  | 51,52,53,54                 | 0     |
| 2   | MPD  | D     | 301  | 8/8   | 0.29  | 0.72 | 0.66  | 58,59,60,60                 | 0     |
| 2   | MPD  | E     | 301  | 8/8   | 0.63  | 0.40 | 0.26  | 53,56,57,60                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.