



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2017 – 12:45 AM EDT

PDB ID : 5BP4  
Title : Modifying region (DH-ER-KR) of a mycocerosic acid synthase-like (MAS-like) PKS  
Authors : Herbst, D.A.; Jakob, P.R.; Zaehring, F.; Maier, T.  
Deposited on : unknown  
Resolution : 3.75 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

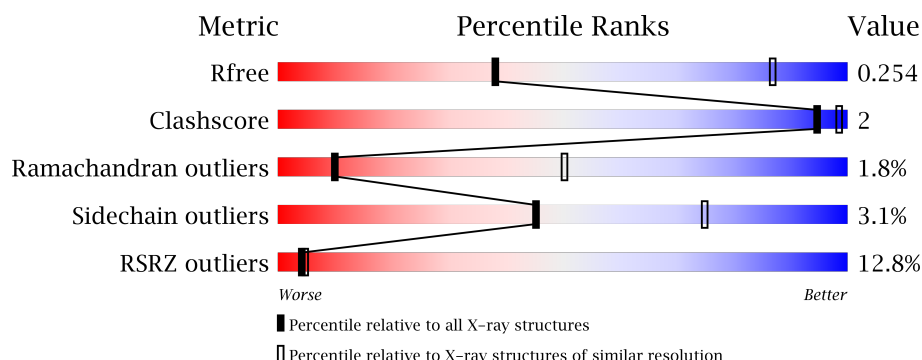
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1423 (4.02-3.50)                                      |
| Clashscore            | 112137                      | 1087 (4.00-3.52)                                      |
| Ramachandran outliers | 110173                      | 1047 (4.00-3.52)                                      |
| Sidechain outliers    | 110143                      | 1041 (4.00-3.52)                                      |
| RSRZ outliers         | 101464                      | 1011 (4.00-3.52)                                      |

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     | 1140   | <div> <div>10%</div> <div>88%</div> <div>8%</div> <div>••</div> </div> |
| 1   | B     | 1140   | <div> <div>4%</div> <div>89%</div> <div>7%</div> <div>••</div> </div>  |
| 1   | C     | 1140   | <div> <div>8%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>   |
| 1   | D     | 1140   | <div> <div>9%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>   |
| 1   | E     | 1140   | <div> <div>21%</div> <div>89%</div> <div>6%</div> <div>•</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 1140   |                  |
| 1   | G     | 1140   |                  |
| 1   | H     | 1140   |                  |
| 1   | I     | 1140   |                  |
| 1   | J     | 1140   |                  |
| 1   | K     | 1140   |                  |
| 1   | L     | 1140   |                  |
| 1   | M     | 1140   |                  |
| 1   | N     | 1140   |                  |
| 1   | O     | 1140   |                  |
| 1   | P     | 1140   |                  |
| 1   | Q     | 1140   |                  |
| 1   | R     | 1140   |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 262498 atoms, of which 129384 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 Mycocerosic acid synthase.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1102     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16283 | 5165 | 8038 | 1479 | 1576 | 25 |         |         |       |
| 1   | B     | 1102     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16283 | 5165 | 8038 | 1479 | 1576 | 25 |         |         |       |
| 1   | C     | 1102     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16283 | 5165 | 8038 | 1479 | 1576 | 25 |         |         |       |
| 1   | D     | 1102     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16283 | 5165 | 8038 | 1479 | 1576 | 25 |         |         |       |
| 1   | E     | 1089     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16094 | 5107 | 7945 | 1463 | 1555 | 24 |         |         |       |
| 1   | F     | 1093     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16142 | 5122 | 7965 | 1467 | 1564 | 24 |         |         |       |
| 1   | G     | 1088     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16079 | 5102 | 7939 | 1462 | 1552 | 24 |         |         |       |
| 1   | H     | 1097     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16195 | 5138 | 7991 | 1471 | 1571 | 24 |         |         |       |
| 1   | I     | 655      | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9680  | 3057 | 4801 | 872  | 935  | 15 |         |         |       |
| 1   | J     | 1089     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16094 | 5107 | 7945 | 1463 | 1555 | 24 |         |         |       |
| 1   | K     | 1089     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16094 | 5107 | 7945 | 1463 | 1555 | 24 |         |         |       |
| 1   | L     | 897      | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 13209 | 4199 | 6535 | 1183 | 1272 | 20 |         |         |       |
| 1   | M     | 1089     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16094 | 5107 | 7945 | 1463 | 1555 | 24 |         |         |       |
| 1   | N     | 1089     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16094 | 5107 | 7945 | 1463 | 1555 | 24 |         |         |       |
| 1   | O     | 633      | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9327  | 2950 | 4625 | 839  | 898  | 15 |         |         |       |
| 1   | P     | 1089     | Total | C    | H    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 16094 | 5107 | 7945 | 1463 | 1555 | 24 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | Q     | 608      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 8979  | 2846 | 4455 | 804 | 859 | 15 |         |         |       |
| 1   | R     | 637      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 9417  | 2980 | 4669 | 844 | 909 | 15 |         |         |       |

There are 54 discrepancies between the modelled and reference sequences:

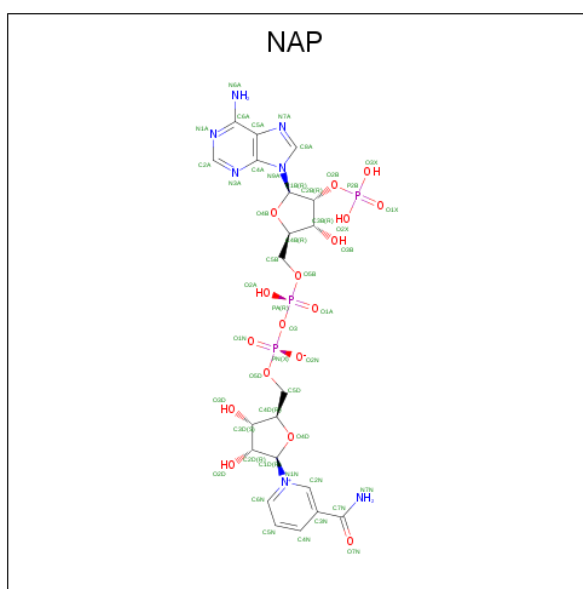
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| A     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| A     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| B     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| B     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| B     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| C     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| C     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| C     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| D     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| D     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| D     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| E     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| E     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| E     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| F     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| F     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| F     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| G     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| G     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| G     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| H     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| H     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| H     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| I     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| I     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| I     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| J     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| J     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| J     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| K     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| K     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| K     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| L     | 882     | SER      | -      | expression tag | UNP A0R1E8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| L     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| L     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| M     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| M     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| M     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| N     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| N     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| N     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| O     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| O     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| O     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| P     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| P     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| P     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| Q     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| Q     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| Q     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |
| R     | 882     | SER      | -      | expression tag | UNP A0R1E8 |
| R     | 883     | MET      | -      | expression tag | UNP A0R1E8 |
| R     | 2021    | GLN      | -      | expression tag | UNP A0R1E8 |

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|---------|
| 2   | A     | 1        | Total | C  | H  | N | O  | 0       | 0       |
|     |       |          | 73    | 21 | 25 | 7 | 17 |         |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 2   | A     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | B     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | B     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | C     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | C     | 1        | Total<br>42 | C<br>10 | H<br>11 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | E     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | G     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | G     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | H     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | H     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | I     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | J     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | J     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | K     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | K     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | L     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | M     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |

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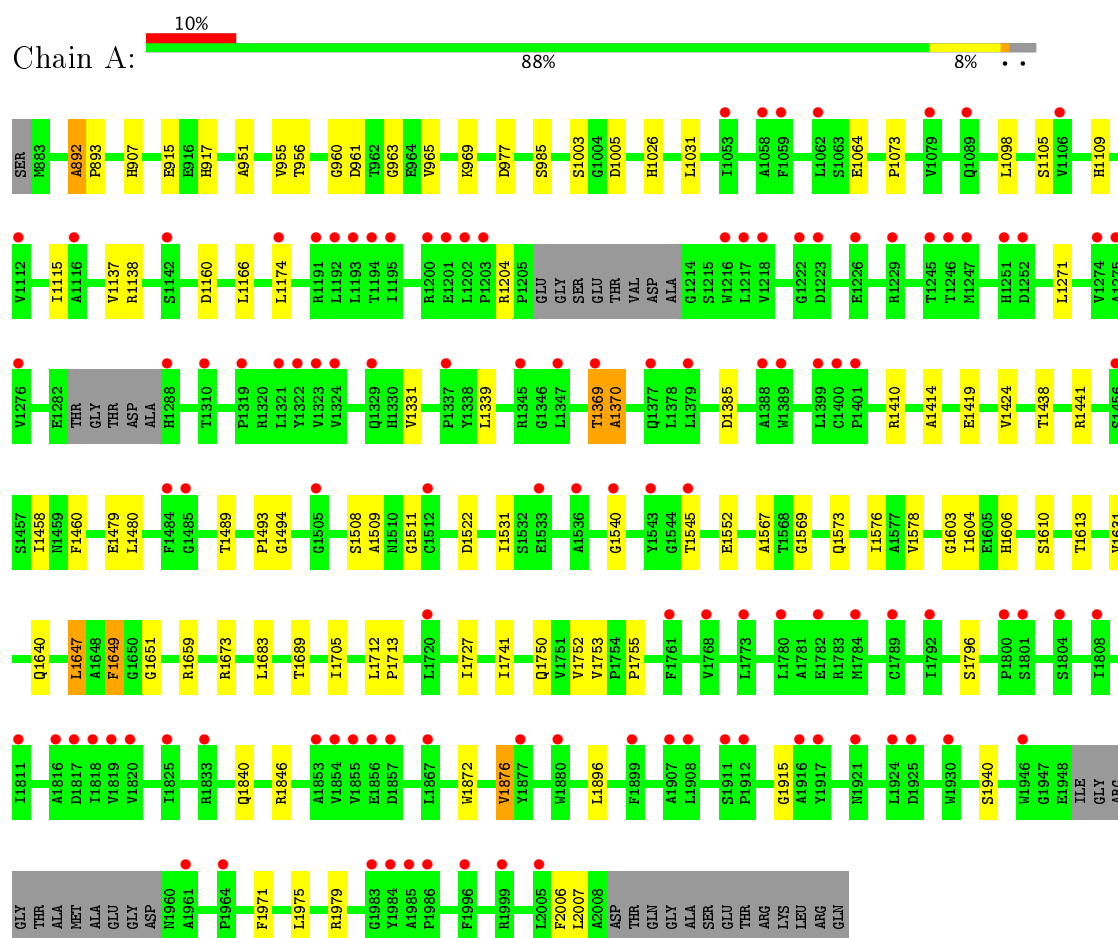
| Mol | Chain | Residues | Atoms       |         |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 2   | M     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | N     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | N     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | O     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | P     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | P     | 1        | Total<br>38 | C<br>10 | H<br>11 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 2   | Q     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | R     | 1        | Total<br>73 | C<br>21 | H<br>25 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |

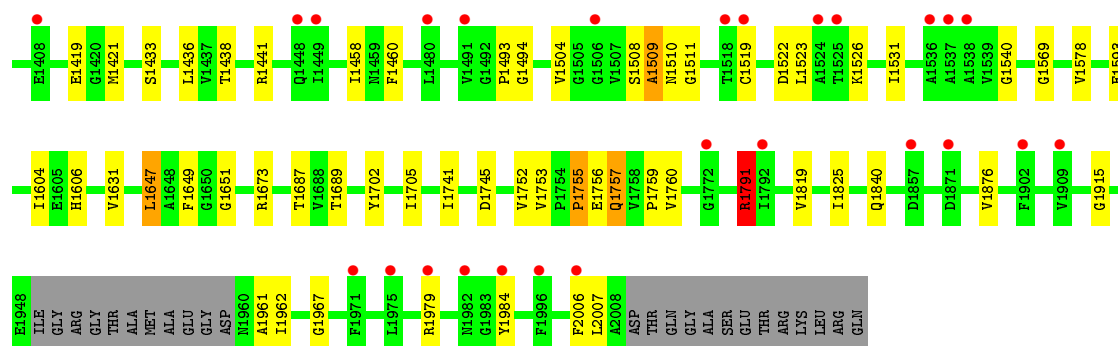


### 3 Residue-property plots

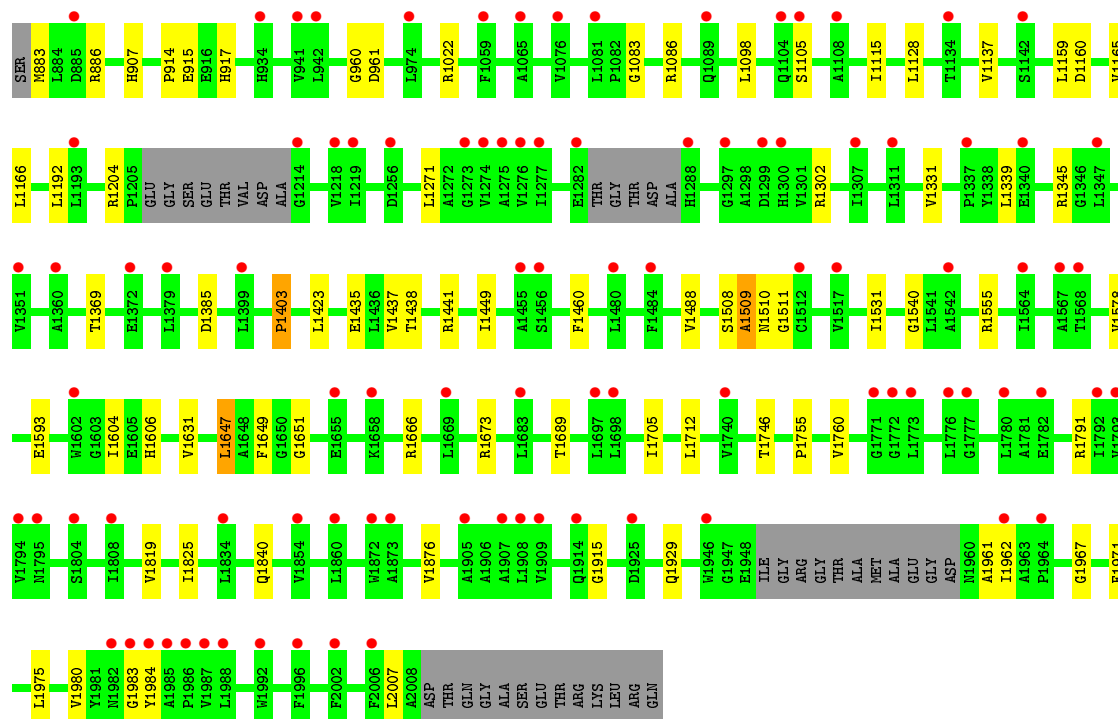
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Mycocerosic acid synthase

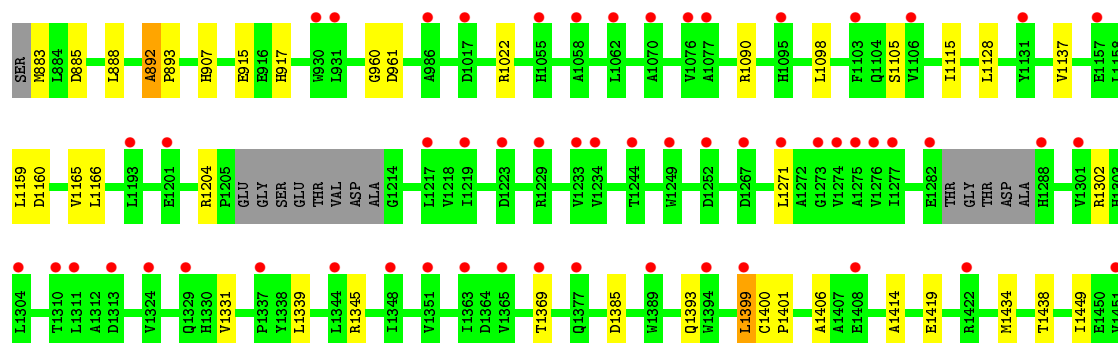
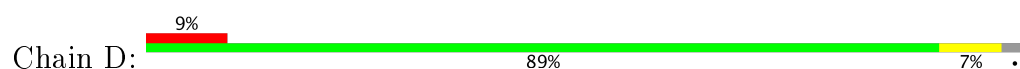


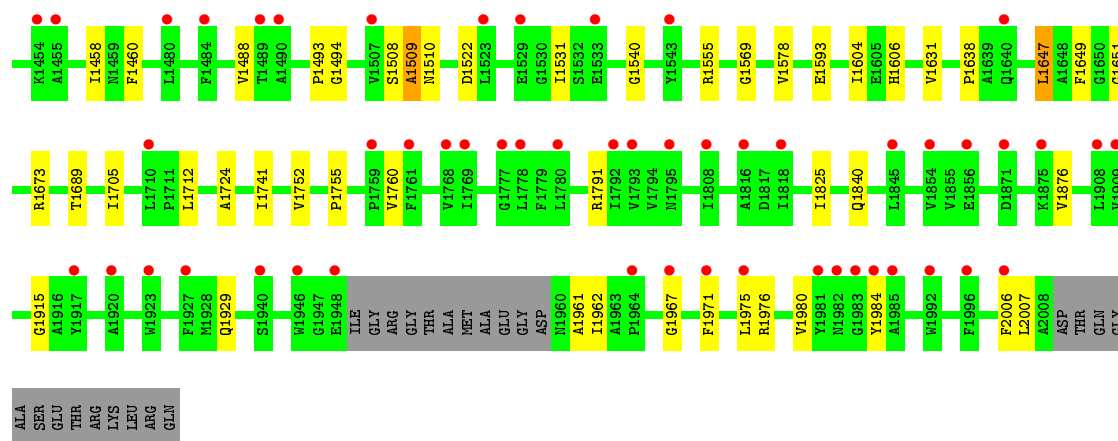


• Molecule 1: Mycocerosic acid synthase

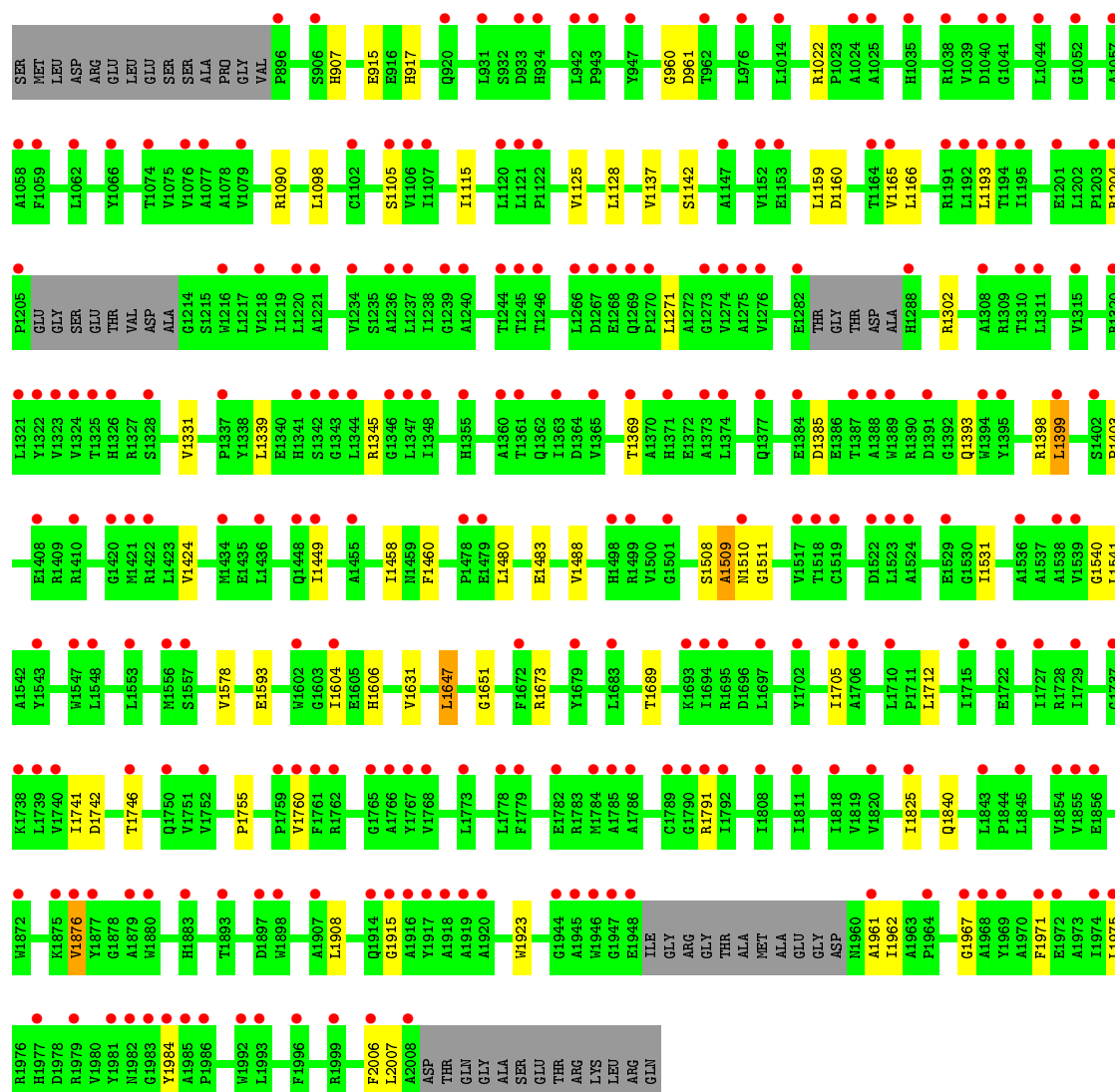


• Molecule 1: Mycocerosic acid synthase

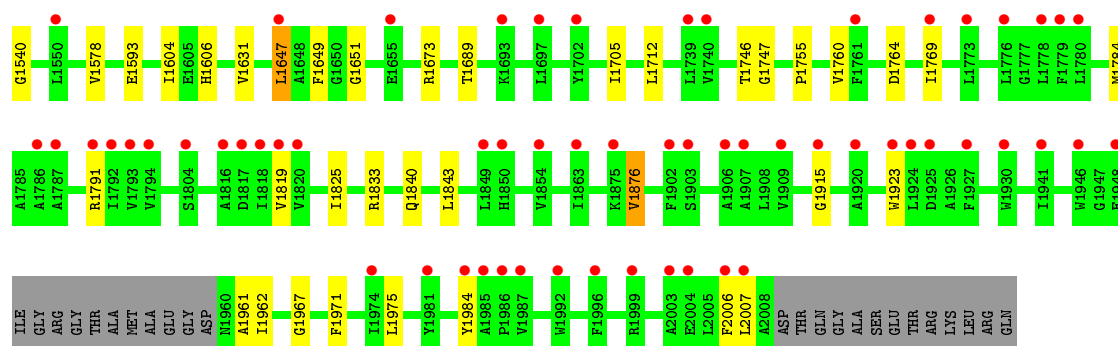




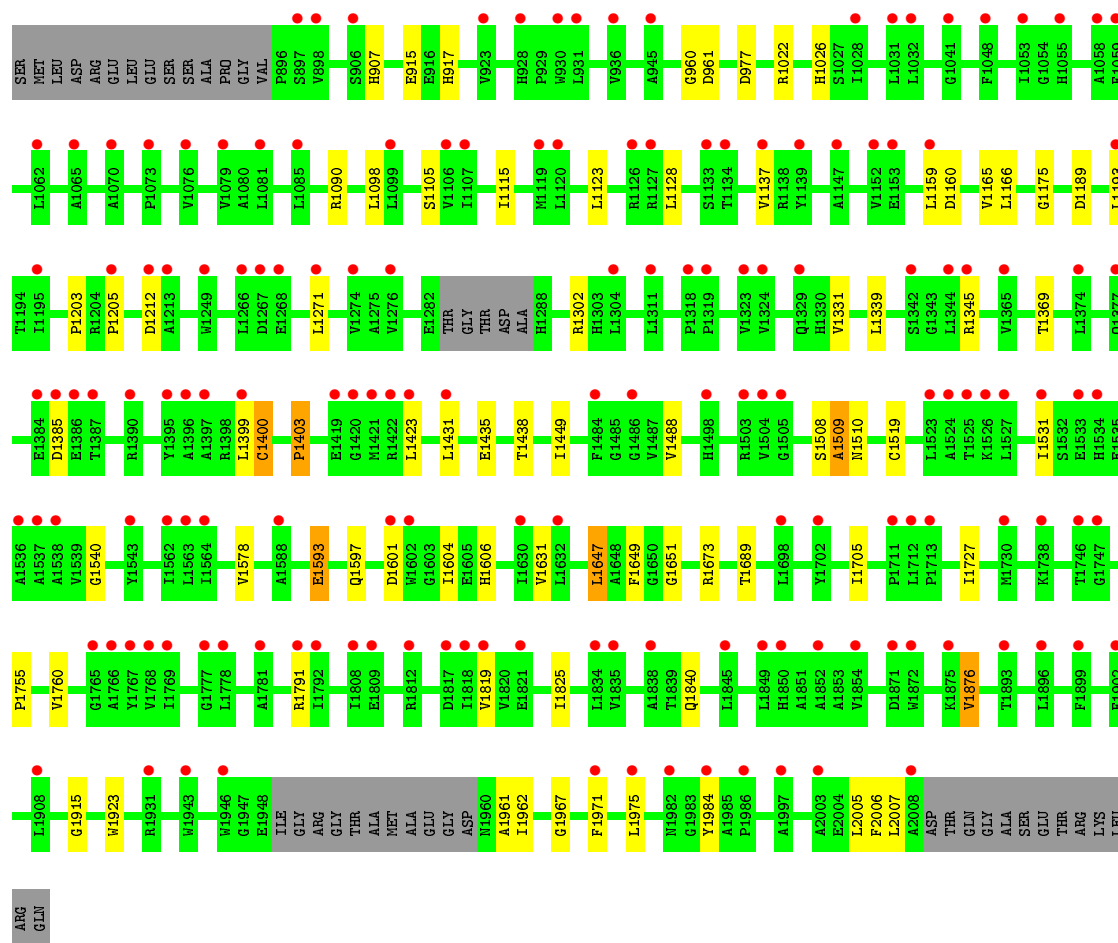
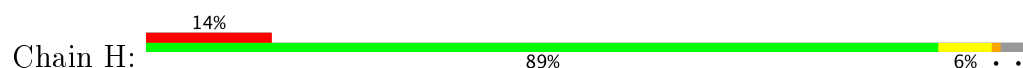
• Molecule 1: Mycocerosic acid synthase



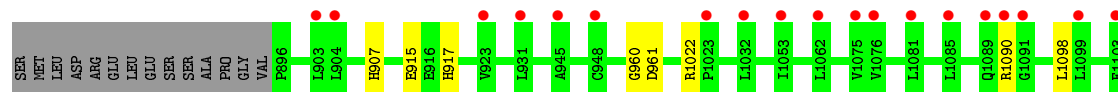




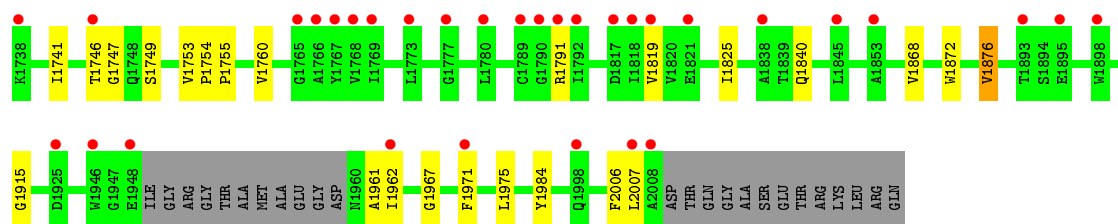
• Molecule 1: Mycocerosic acid synthase



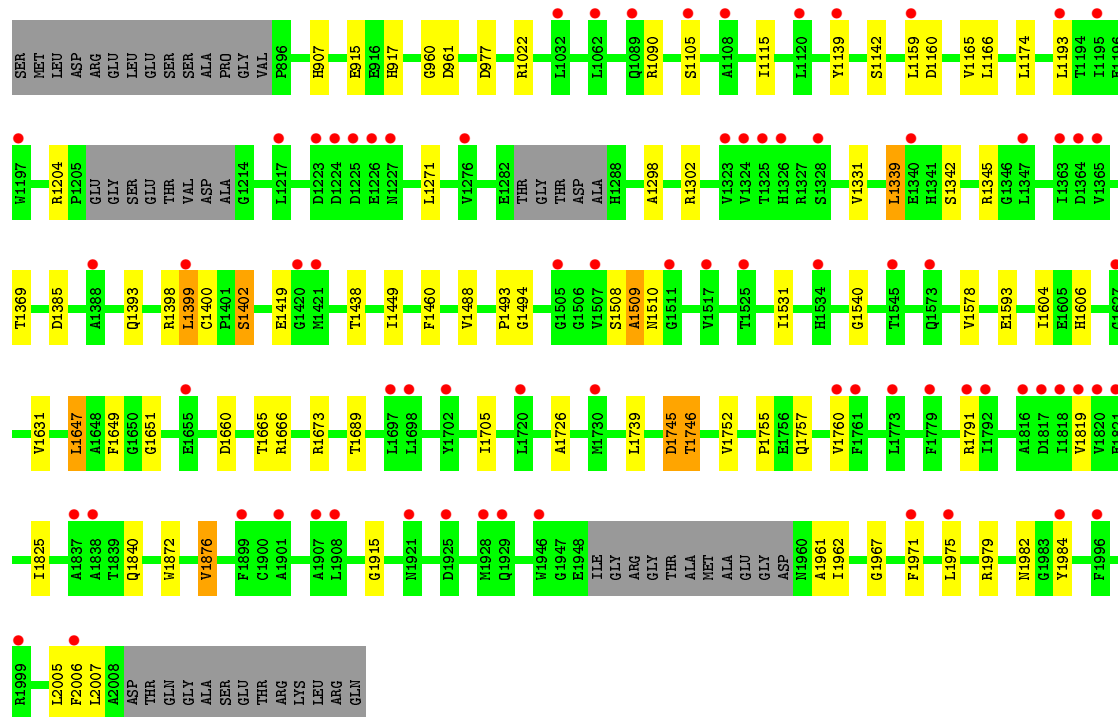
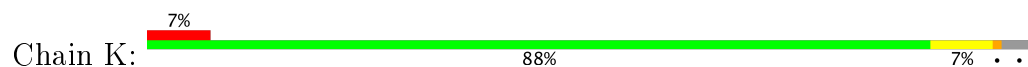
• Molecule 1: Mycocerosic acid synthase



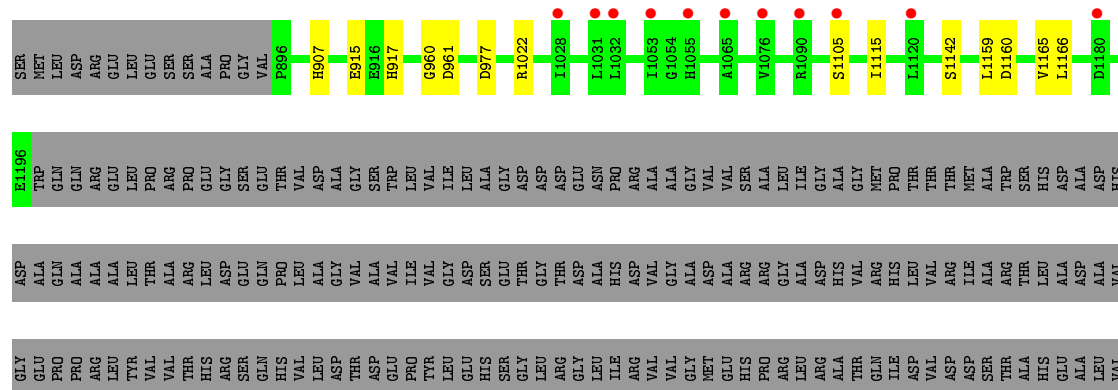
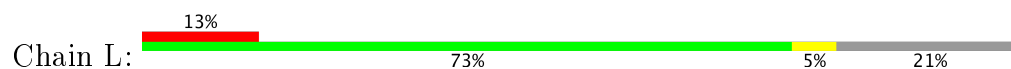




• Molecule 1: Mycocerosic acid synthase

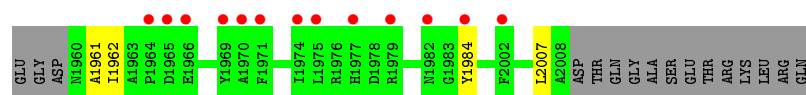


• Molecule 1: Mycocerosic acid synthase

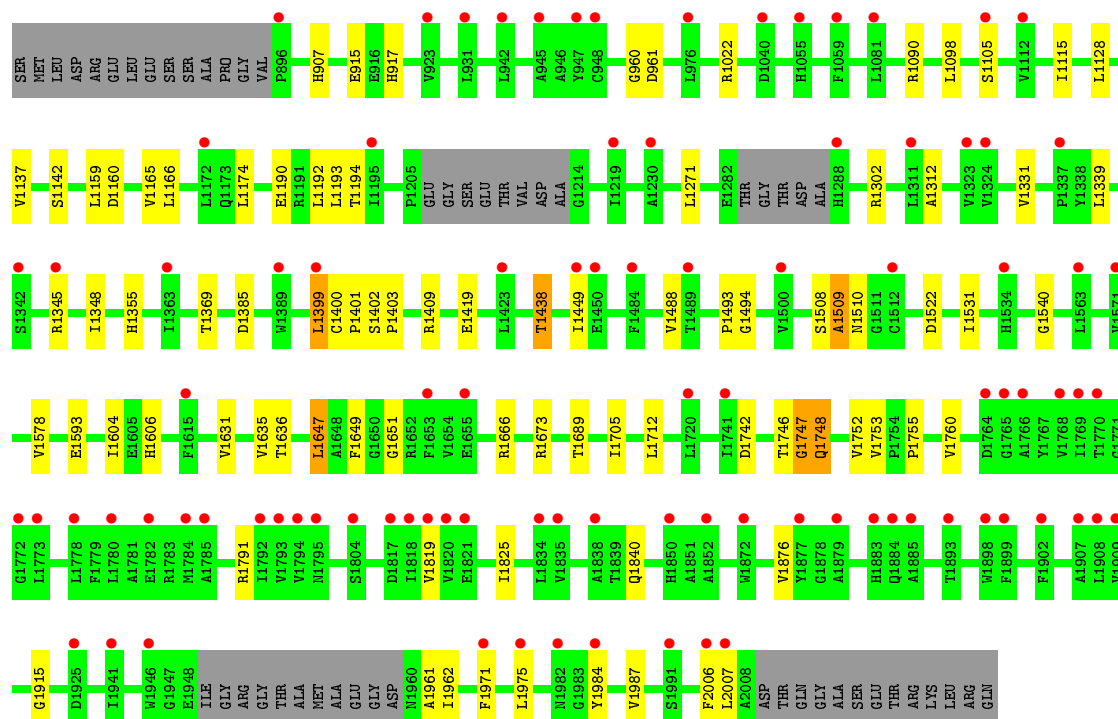
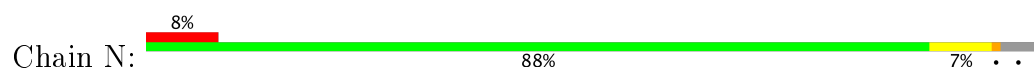




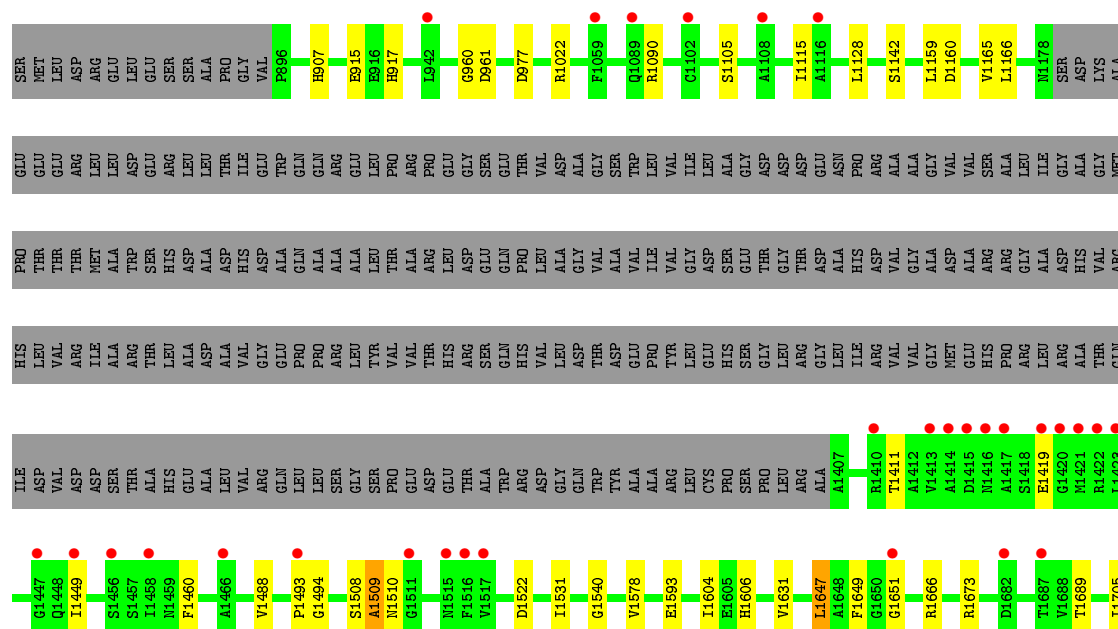


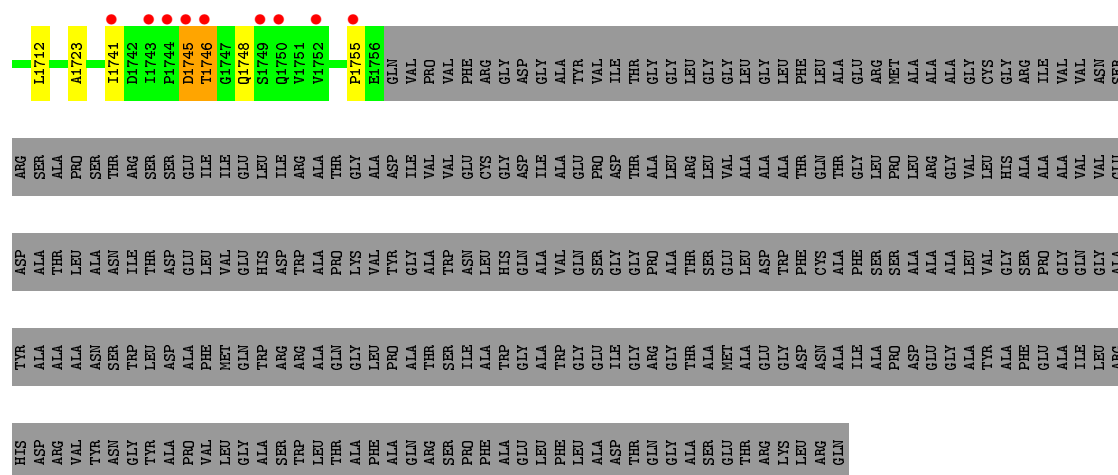


• Molecule 1: Mycocerosic acid synthase

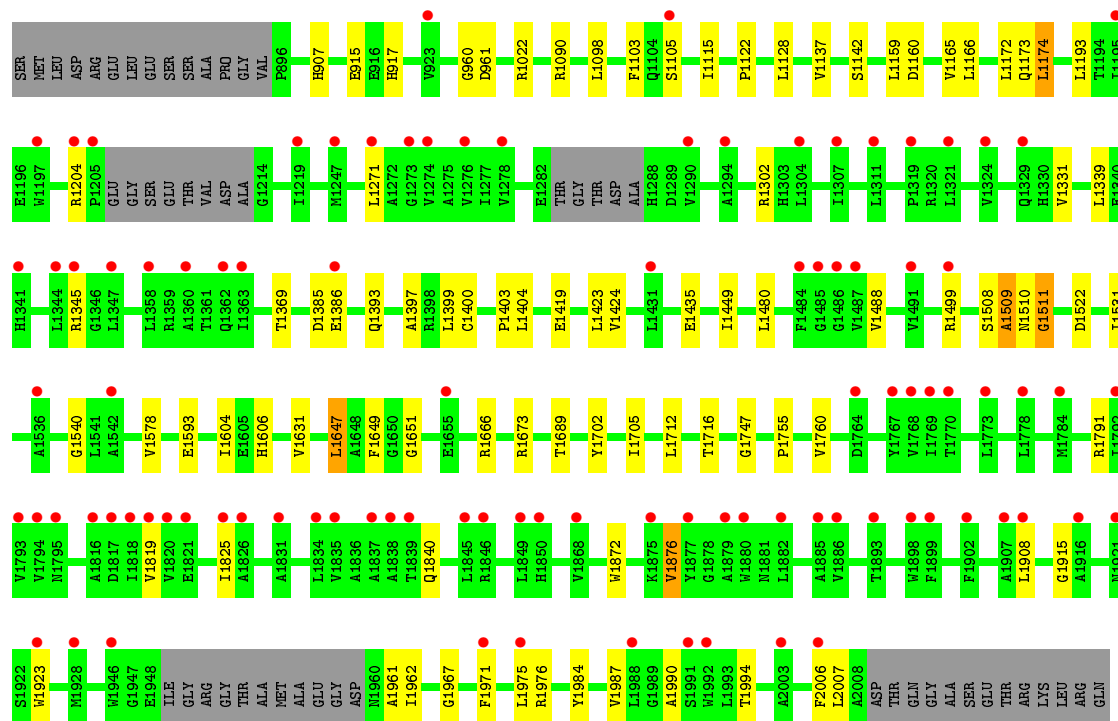
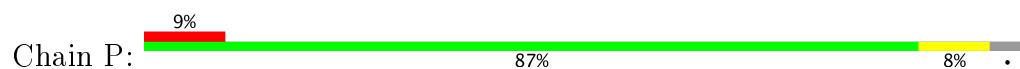


• Molecule 1: Mycocerosic acid synthase

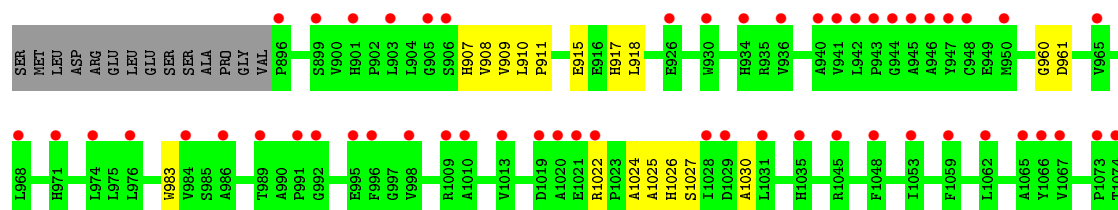


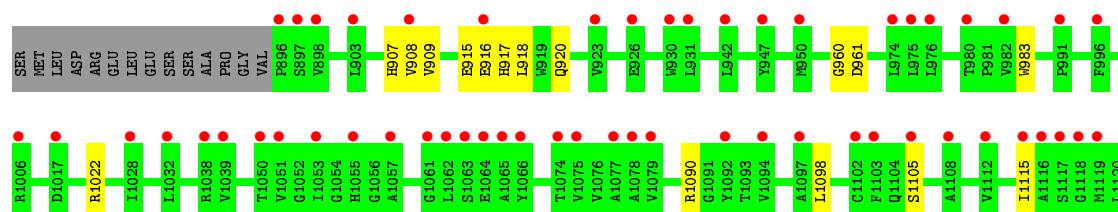


• Molecule 1: Mycocerosic acid synthase



• Molecule 1: Mycocerosic acid synthase







## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 151.38Å 190.37Å 270.84Å<br>95.58° 91.92° 103.65°            | Depositor        |
| Resolution (Å)  | 78.62 – 3.75<br>78.62 – 3.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (78.62-3.75)<br>95.4 (78.62-3.75)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.25  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.42 (at 3.78Å)   | Xtriage          |
| Refinement program  | BUSTER 2.10.2   | Depositor        |
| R, $R_{free}$   | 0.230 , 0.240<br>0.247 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2985 reflections (1.02%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 132.2   | Xtriage          |
| Anisotropy  | 0.073   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 132.5  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 262498  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 171.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAP

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     | 0.51         | 0/8420      | 0.65        | 0/11488         |
| 1   | B     | 0.45         | 0/8420      | 0.62        | 1/11488 (0.0%)  |
| 1   | C     | 0.41         | 0/8420      | 0.59        | 0/11488         |
| 1   | D     | 0.41         | 0/8420      | 0.59        | 0/11488         |
| 1   | E     | 0.40         | 0/8323      | 0.58        | 0/11356         |
| 1   | F     | 0.39         | 0/8351      | 0.58        | 0/11393         |
| 1   | G     | 0.42         | 0/8314      | 0.59        | 0/11344         |
| 1   | H     | 0.41         | 0/8379      | 0.59        | 0/11434         |
| 1   | I     | 0.40         | 0/4977      | 0.59        | 0/6783          |
| 1   | J     | 0.42         | 0/8323      | 0.59        | 0/11356         |
| 1   | K     | 0.44         | 0/8323      | 0.60        | 0/11356         |
| 1   | L     | 0.44         | 0/6815      | 0.61        | 0/9296          |
| 1   | M     | 0.40         | 0/8323      | 0.58        | 0/11356         |
| 1   | N     | 0.42         | 0/8323      | 0.61        | 0/11356         |
| 1   | O     | 0.44         | 0/4797      | 0.61        | 0/6540          |
| 1   | P     | 0.43         | 0/8323      | 0.60        | 0/11356         |
| 1   | Q     | 0.39         | 0/4617      | 0.58        | 0/6293          |
| 1   | R     | 0.40         | 0/4844      | 0.60        | 0/6602          |
| All | All   | 0.42         | 0/134712    | 0.60        | 1/183773 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 1   | B     | 1178 | ASN  | C-N-CA | 5.23 | 134.78      | 121.70   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 8245   | 8038     | 8072     | 32      | 0            |
| 1   | B     | 8245   | 8038     | 8072     | 33      | 0            |
| 1   | C     | 8245   | 8038     | 8072     | 22      | 1            |
| 1   | D     | 8245   | 8038     | 8072     | 26      | 0            |
| 1   | E     | 8149   | 7945     | 7979     | 23      | 0            |
| 1   | F     | 8177   | 7965     | 7999     | 27      | 0            |
| 1   | G     | 8140   | 7939     | 7973     | 23      | 0            |
| 1   | H     | 8204   | 7991     | 8025     | 35      | 0            |
| 1   | I     | 4879   | 4801     | 4822     | 12      | 0            |
| 1   | J     | 8149   | 7945     | 7979     | 30      | 1            |
| 1   | K     | 8149   | 7945     | 7979     | 30      | 0            |
| 1   | L     | 6674   | 6535     | 6560     | 19      | 0            |
| 1   | M     | 8149   | 7945     | 7979     | 19      | 0            |
| 1   | N     | 8149   | 7945     | 7979     | 24      | 0            |
| 1   | O     | 4702   | 4625     | 4646     | 14      | 0            |
| 1   | P     | 8149   | 7945     | 7979     | 28      | 0            |
| 1   | Q     | 4524   | 4455     | 4476     | 31      | 0            |
| 1   | R     | 4748   | 4669     | 4690     | 23      | 0            |
| 2   | A     | 75     | 36       | 36       | 2       | 0            |
| 2   | B     | 75     | 36       | 36       | 2       | 0            |
| 2   | C     | 79     | 36       | 36       | 1       | 0            |
| 2   | D     | 75     | 36       | 36       | 2       | 0            |
| 2   | E     | 48     | 25       | 25       | 1       | 0            |
| 2   | F     | 75     | 36       | 36       | 2       | 0            |
| 2   | G     | 75     | 36       | 36       | 0       | 0            |
| 2   | H     | 75     | 36       | 36       | 0       | 0            |
| 2   | I     | 48     | 25       | 25       | 1       | 0            |
| 2   | J     | 75     | 36       | 36       | 0       | 0            |
| 2   | K     | 75     | 36       | 36       | 2       | 0            |
| 2   | L     | 48     | 25       | 25       | 1       | 0            |
| 2   | M     | 75     | 36       | 36       | 0       | 0            |
| 2   | N     | 75     | 36       | 36       | 0       | 0            |
| 2   | O     | 48     | 25       | 25       | 1       | 0            |
| 2   | P     | 75     | 36       | 36       | 0       | 0            |
| 2   | Q     | 48     | 25       | 25       | 0       | 0            |
| 2   | R     | 48     | 25       | 25       | 0       | 0            |
| All | All   | 133114 | 129384   | 129935   | 406     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (406) 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:N:1348:ILE:CD1  | 1:N:1348:ILE:CG1  | 1.80                     | 1.59              |
| 1:Q:908:VAL:HG13  | 1:R:920:GLN:HB2   | 1.68                     | 0.75              |
| 1:N:1193:LEU:HD22 | 1:N:1399:LEU:HD22 | 1.70                     | 0.73              |
| 1:C:914:PRO:HD3   | 1:D:1638:PRO:HG3  | 1.71                     | 0.73              |
| 1:Q:909:VAL:O     | 1:R:983:TRP:NE1   | 2.21                     | 0.71              |
| 1:A:1098:LEU:HD21 | 1:A:1137:VAL:HG11 | 1.73                     | 0.71              |
| 1:A:1631:VAL:HG23 | 1:A:1647:LEU:HD23 | 1.73                     | 0.70              |
| 1:F:1050:THR:O    | 1:F:1988:LEU:HD22 | 1.92                     | 0.69              |
| 1:G:1962:ILE:HD12 | 1:G:1984:TYR:CE1  | 2.28                     | 0.69              |
| 1:L:1421:MET:HB2  | 1:L:1436:LEU:HD21 | 1.78                     | 0.65              |
| 1:K:1438:THR:HB   | 1:K:1752:VAL:HG11 | 1.81                     | 0.63              |
| 1:O:1649:PHE:CD1  | 1:P:1689:THR:HG21 | 2.33                     | 0.63              |
| 1:E:1689:THR:HG21 | 1:F:1649:PHE:CD1  | 2.34                     | 0.63              |
| 1:Q:909:VAL:HB    | 1:R:920:GLN:NE2   | 2.14                     | 0.63              |
| 1:Q:1507:VAL:HG23 | 1:Q:1698:LEU:HD11 | 1.80                     | 0.62              |
| 1:A:1567:ALA:HB1  | 1:A:1576:ILE:HD11 | 1.80                     | 0.62              |
| 1:A:1971:PHE:CZ   | 1:A:1975:LEU:HD11 | 2.35                     | 0.61              |
| 1:B:1421:MET:CE   | 1:B:1436:LEU:HD21 | 2.30                     | 0.61              |
| 1:H:1593:GLU:OE1  | 1:Q:1024:ALA:HB3  | 2.00                     | 0.61              |
| 1:Q:911:PRO:HD3   | 1:R:983:TRP:CD1   | 2.35                     | 0.61              |
| 1:Q:918:LEU:HD21  | 1:R:908:VAL:HG11  | 1.84                     | 0.60              |
| 1:B:1193:LEU:HD22 | 1:B:1399:LEU:HD11 | 1.85                     | 0.59              |
| 1:K:1666:ARG:HB3  | 1:L:1666:ARG:HB3  | 1.85                     | 0.59              |
| 1:E:1193:LEU:HD22 | 1:E:1399:LEU:HD22 | 1.84                     | 0.58              |
| 1:G:1421:MET:CE   | 1:G:1436:LEU:HD21 | 2.33                     | 0.58              |
| 1:H:1597:GLN:HG2  | 1:Q:1026:HIS:HA   | 1.84                     | 0.58              |
| 1:H:1193:LEU:HD22 | 1:H:1399:LEU:HD11 | 1.87                     | 0.57              |
| 1:M:1689:THR:HG21 | 1:N:1649:PHE:CD1  | 2.40                     | 0.57              |
| 1:J:1421:MET:CE   | 1:J:1436:LEU:HD21 | 2.35                     | 0.57              |
| 1:F:1791:ARG:CZ   | 1:F:1819:VAL:HG21 | 2.35                     | 0.56              |
| 1:Q:918:LEU:CD2   | 1:R:908:VAL:HG11  | 2.36                     | 0.56              |
| 1:A:892:ALA:HB3   | 1:A:893:PRO:HD3   | 1.87                     | 0.56              |
| 1:H:1601:ASP:HB3  | 1:Q:1030:ALA:HB3  | 1.88                     | 0.56              |
| 1:M:1962:ILE:HD12 | 1:M:1984:TYR:CE1  | 2.41                     | 0.56              |
| 1:Q:909:VAL:HB    | 1:R:920:GLN:HE22  | 1.71                     | 0.55              |
| 1:A:1689:THR:HG21 | 1:B:1649:PHE:CD1  | 2.41                     | 0.55              |
| 1:K:1649:PHE:CD1  | 1:L:1689:THR:HG21 | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1962:ILE:HD12 | 1:B:1984:TYR:CE1  | 2.43                     | 0.54              |
| 1:O:1689:THR:HG21 | 1:P:1649:PHE:CD1  | 2.43                     | 0.54              |
| 1:C:1649:PHE:CD1  | 1:D:1689:THR:HG21 | 2.42                     | 0.53              |
| 1:H:1601:ASP:HB3  | 1:Q:1030:ALA:CB   | 2.38                     | 0.53              |
| 1:D:1531:ILE:HG21 | 1:D:1705:ILE:HG23 | 1.90                     | 0.53              |
| 1:D:1962:ILE:HD12 | 1:D:1984:TYR:CE1  | 2.44                     | 0.53              |
| 1:B:892:ALA:HB3   | 1:B:893:PRO:CD    | 2.38                     | 0.53              |
| 1:A:1569:GLY:O    | 1:A:1573:GLN:HG3  | 2.09                     | 0.53              |
| 1:H:1531:ILE:HG21 | 1:H:1705:ILE:HG23 | 1.88                     | 0.53              |
| 1:H:1593:GLU:HB3  | 1:Q:1024:ALA:HB2  | 1.91                     | 0.52              |
| 1:L:1962:ILE:HD12 | 1:L:1984:TYR:CE1  | 2.44                     | 0.52              |
| 1:P:1399:LEU:HD21 | 1:P:1908:LEU:HD21 | 1.91                     | 0.52              |
| 1:C:907:HIS:HE2   | 1:C:917:HIS:HD1   | 1.57                     | 0.52              |
| 1:D:1929:GLN:HG2  | 1:D:1980:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:1438:THR:HB   | 1:A:1752:VAL:HG11 | 1.90                     | 0.52              |
| 1:M:1649:PHE:CD1  | 1:N:1689:THR:HG21 | 2.43                     | 0.52              |
| 1:D:1971:PHE:CZ   | 1:D:1975:LEU:HD11 | 2.45                     | 0.52              |
| 1:E:1962:ILE:HD12 | 1:E:1984:TYR:CE1  | 2.44                     | 0.52              |
| 1:J:1962:ILE:HD12 | 1:J:1984:TYR:CE1  | 2.45                     | 0.52              |
| 1:P:907:HIS:HE2   | 1:P:917:HIS:HD1   | 1.57                     | 0.52              |
| 1:B:1193:LEU:HD21 | 1:B:2006:PHE:CZ   | 2.45                     | 0.52              |
| 1:F:1962:ILE:HD12 | 1:F:1984:TYR:CE1  | 2.45                     | 0.52              |
| 1:H:1962:ILE:HD12 | 1:H:1984:TYR:CE1  | 2.44                     | 0.52              |
| 1:K:1631:VAL:HG23 | 1:K:1647:LEU:HD23 | 1.92                     | 0.51              |
| 1:K:1962:ILE:HD12 | 1:K:1984:TYR:CE1  | 2.45                     | 0.51              |
| 1:C:1962:ILE:HD12 | 1:C:1984:TYR:CE1  | 2.45                     | 0.51              |
| 1:F:1569:GLY:HA3  | 2:F:3001:NAP:O1A  | 2.11                     | 0.51              |
| 1:G:1971:PHE:CZ   | 1:G:1975:LEU:HD11 | 2.45                     | 0.51              |
| 1:E:1531:ILE:HG21 | 1:E:1705:ILE:HG23 | 1.93                     | 0.51              |
| 1:F:1421:MET:CE   | 1:F:1436:LEU:HD21 | 2.40                     | 0.51              |
| 1:M:907:HIS:HE2   | 1:M:917:HIS:HD1   | 1.58                     | 0.51              |
| 1:E:1971:PHE:CZ   | 1:E:1975:LEU:HD11 | 2.45                     | 0.51              |
| 1:R:907:HIS:HE2   | 1:R:917:HIS:HD1   | 1.59                     | 0.51              |
| 1:A:1073:PRO:HA   | 1:A:1109:HIS:HE2  | 1.76                     | 0.51              |
| 1:F:1971:PHE:CZ   | 1:F:1975:LEU:HD11 | 2.46                     | 0.51              |
| 1:G:1649:PHE:CD1  | 1:H:1689:THR:HG21 | 2.46                     | 0.51              |
| 1:I:907:HIS:HE2   | 1:I:917:HIS:HD1   | 1.59                     | 0.51              |
| 1:O:1631:VAL:HG23 | 1:O:1647:LEU:HD23 | 1.93                     | 0.51              |
| 1:G:1631:VAL:HG23 | 1:G:1647:LEU:HD23 | 1.93                     | 0.51              |
| 1:Q:1631:VAL:HG23 | 1:Q:1647:LEU:HD23 | 1.93                     | 0.51              |
| 1:I:1631:VAL:HG23 | 1:I:1647:LEU:HD23 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1569:GLY:HA3  | 2:B:3001:NAP:O1A  | 2.11                     | 0.50              |
| 1:E:1631:VAL:HG23 | 1:E:1647:LEU:HD23 | 1.93                     | 0.50              |
| 1:G:907:HIS:HE2   | 1:G:917:HIS:HD1   | 1.59                     | 0.50              |
| 1:R:1631:VAL:HG23 | 1:R:1647:LEU:HD23 | 1.94                     | 0.50              |
| 1:A:1531:ILE:HG21 | 1:A:1705:ILE:HG23 | 1.93                     | 0.50              |
| 1:A:1603:GLY:HA2  | 1:J:1029:ASP:HB2  | 1.92                     | 0.50              |
| 1:A:1441:ARG:NH2  | 1:A:1489:THR:HG21 | 2.26                     | 0.50              |
| 1:A:1458:ILE:HD11 | 1:A:1741:ILE:HD13 | 1.94                     | 0.50              |
| 1:D:1631:VAL:HG23 | 1:D:1647:LEU:HD23 | 1.94                     | 0.50              |
| 1:F:907:HIS:HE2   | 1:F:917:HIS:HD1   | 1.59                     | 0.50              |
| 1:H:1631:VAL:HG23 | 1:H:1647:LEU:HD23 | 1.93                     | 0.50              |
| 1:K:907:HIS:HE2   | 1:K:917:HIS:HD1   | 1.59                     | 0.50              |
| 1:O:907:HIS:HE2   | 1:O:917:HIS:HD1   | 1.59                     | 0.50              |
| 1:J:1193:LEU:HD21 | 1:J:2006:PHE:CZ   | 2.47                     | 0.50              |
| 1:N:1631:VAL:HG23 | 1:N:1647:LEU:HD23 | 1.93                     | 0.50              |
| 1:B:1339:LEU:HA   | 1:B:1342:SER:OG   | 2.12                     | 0.50              |
| 1:G:1193:LEU:HD21 | 1:G:2006:PHE:CZ   | 2.47                     | 0.50              |
| 1:H:907:HIS:HE2   | 1:H:917:HIS:HD1   | 1.60                     | 0.50              |
| 1:P:1480:LEU:O    | 1:P:1511:GLY:HA2  | 2.12                     | 0.50              |
| 1:P:1631:VAL:HG23 | 1:P:1647:LEU:HD23 | 1.93                     | 0.50              |
| 1:J:1753:VAL:O    | 1:J:1753:VAL:HG23 | 2.12                     | 0.50              |
| 1:N:1971:PHE:CZ   | 1:N:1975:LEU:HD11 | 2.47                     | 0.50              |
| 1:C:1971:PHE:CZ   | 1:C:1975:LEU:HD11 | 2.47                     | 0.50              |
| 1:K:1971:PHE:CZ   | 1:K:1975:LEU:HD11 | 2.46                     | 0.50              |
| 1:N:1438:THR:HB   | 1:N:1752:VAL:HG11 | 1.94                     | 0.50              |
| 1:B:1631:VAL:HG23 | 1:B:1647:LEU:HD23 | 1.93                     | 0.49              |
| 1:D:1399:LEU:HD13 | 1:D:2006:PHE:CZ   | 2.45                     | 0.49              |
| 1:F:1631:VAL:HG23 | 1:F:1647:LEU:HD23 | 1.93                     | 0.49              |
| 1:G:1531:ILE:HG21 | 1:G:1705:ILE:HG23 | 1.94                     | 0.49              |
| 1:J:907:HIS:HE2   | 1:J:917:HIS:HD1   | 1.59                     | 0.49              |
| 1:H:1193:LEU:HD21 | 1:H:2006:PHE:CZ   | 2.47                     | 0.49              |
| 1:K:1689:THR:HG21 | 1:L:1649:PHE:CD1  | 2.47                     | 0.49              |
| 1:L:1631:VAL:HG23 | 1:L:1647:LEU:HD23 | 1.93                     | 0.49              |
| 1:L:907:HIS:HE2   | 1:L:917:HIS:HD1   | 1.60                     | 0.49              |
| 1:Q:1449:ILE:HG23 | 1:Q:1488:VAL:HG13 | 1.93                     | 0.49              |
| 1:B:1458:ILE:HD11 | 1:B:1741:ILE:HD13 | 1.94                     | 0.49              |
| 1:K:1193:LEU:HD21 | 1:K:2006:PHE:CZ   | 2.48                     | 0.49              |
| 1:N:1531:ILE:HG21 | 1:N:1705:ILE:HG23 | 1.94                     | 0.49              |
| 1:F:1193:LEU:HD21 | 1:F:2006:PHE:CZ   | 2.47                     | 0.49              |
| 1:J:1531:ILE:HG21 | 1:J:1705:ILE:HG23 | 1.93                     | 0.49              |
| 1:C:1631:VAL:HG23 | 1:C:1647:LEU:HD23 | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:1971:PHE:CZ   | 1:J:1975:LEU:HD11 | 2.47                     | 0.49              |
| 1:M:1631:VAL:HG23 | 1:M:1647:LEU:HD23 | 1.93                     | 0.49              |
| 1:B:892:ALA:HB3   | 1:B:893:PRO:HD3   | 1.93                     | 0.49              |
| 1:B:907:HIS:HE2   | 1:B:917:HIS:HD1   | 1.60                     | 0.49              |
| 1:D:1460:PHE:CD1  | 2:D:3001:NAP:H52A | 2.46                     | 0.49              |
| 1:I:1649:PHE:CD1  | 1:J:1689:THR:HG21 | 2.48                     | 0.49              |
| 1:Q:907:HIS:HE2   | 1:Q:917:HIS:HD1   | 1.59                     | 0.49              |
| 1:J:1631:VAL:HG23 | 1:J:1647:LEU:HD23 | 1.93                     | 0.49              |
| 1:N:907:HIS:HE2   | 1:N:917:HIS:HD1   | 1.59                     | 0.49              |
| 1:B:1438:THR:HB   | 1:B:1752:VAL:HG11 | 1.95                     | 0.49              |
| 1:H:1601:ASP:OD2  | 1:Q:1027:SER:HB3  | 2.13                     | 0.49              |
| 1:P:1971:PHE:CZ   | 1:P:1975:LEU:HD11 | 2.47                     | 0.49              |
| 1:O:1531:ILE:HG21 | 1:O:1705:ILE:HG23 | 1.94                     | 0.49              |
| 1:E:907:HIS:HE2   | 1:E:917:HIS:HD1   | 1.60                     | 0.48              |
| 1:M:1531:ILE:HG21 | 1:M:1705:ILE:HG23 | 1.94                     | 0.48              |
| 1:B:1531:ILE:HG21 | 1:B:1705:ILE:HG23 | 1.95                     | 0.48              |
| 1:J:1189:ASP:HA   | 1:J:1403:PRO:HB3  | 1.95                     | 0.48              |
| 1:K:1531:ILE:HG21 | 1:K:1705:ILE:HG23 | 1.95                     | 0.48              |
| 1:D:1449:ILE:HG23 | 1:D:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:I:1449:ILE:HG23 | 1:I:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:I:1531:ILE:HG21 | 1:I:1705:ILE:HG23 | 1.94                     | 0.48              |
| 1:L:1531:ILE:HG21 | 1:L:1705:ILE:HG23 | 1.94                     | 0.48              |
| 1:M:1449:ILE:HG23 | 1:M:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:E:1193:LEU:HD21 | 1:E:2006:PHE:CZ   | 2.49                     | 0.48              |
| 1:A:1424:VAL:HA   | 1:A:1480:LEU:HD12 | 1.96                     | 0.48              |
| 1:C:1449:ILE:HG23 | 1:C:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:C:1531:ILE:HG21 | 1:C:1705:ILE:HG23 | 1.95                     | 0.48              |
| 1:C:1460:PHE:CD1  | 2:C:3001:NAP:H52A | 2.48                     | 0.48              |
| 1:N:1747:GLY:O    | 1:N:1748:GLN:C    | 2.50                     | 0.48              |
| 1:H:1431:LEU:HD21 | 1:H:1727:ILE:HG21 | 1.95                     | 0.48              |
| 1:Q:1538:ALA:HB2  | 1:Q:1740:VAL:CG2  | 2.43                     | 0.48              |
| 1:D:907:HIS:HE2   | 1:D:917:HIS:HD1   | 1.60                     | 0.48              |
| 1:E:1449:ILE:HG23 | 1:E:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:H:1189:ASP:HA   | 1:H:1403:PRO:HB3  | 1.94                     | 0.48              |
| 1:A:955:VAL:HG11  | 1:A:963:GLY:HA3   | 1.96                     | 0.48              |
| 1:I:1460:PHE:CD1  | 2:I:3001:NAP:H52A | 2.48                     | 0.48              |
| 1:N:1962:ILE:HD12 | 1:N:1984:TYR:CE1  | 2.49                     | 0.48              |
| 1:F:1449:ILE:HG23 | 1:F:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:R:1531:ILE:HG21 | 1:R:1705:ILE:HG23 | 1.94                     | 0.48              |
| 1:J:1431:LEU:HD21 | 1:J:1727:ILE:HG21 | 1.96                     | 0.48              |
| 1:K:1449:ILE:HG23 | 1:K:1488:VAL:HG13 | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:1449:ILE:HG23 | 1:P:1488:VAL:HG13 | 1.96                     | 0.48              |
| 1:G:1449:ILE:HG23 | 1:G:1488:VAL:HG13 | 1.96                     | 0.47              |
| 1:K:1402:SER:O    | 1:K:1979:ARG:NH2  | 2.46                     | 0.47              |
| 1:J:1410:ARG:O    | 1:J:1754:PRO:HD2  | 2.14                     | 0.47              |
| 1:N:1449:ILE:HG23 | 1:N:1488:VAL:HG13 | 1.96                     | 0.47              |
| 1:G:1689:THR:HG21 | 1:H:1649:PHE:CD1  | 2.50                     | 0.47              |
| 1:J:1421:MET:HE3  | 1:J:1436:LEU:HD21 | 1.96                     | 0.47              |
| 1:O:1449:ILE:HG23 | 1:O:1488:VAL:HG13 | 1.96                     | 0.47              |
| 1:R:1449:ILE:HG23 | 1:R:1488:VAL:HG13 | 1.96                     | 0.47              |
| 1:B:1504:VAL:HG12 | 1:B:1526:LYS:HA   | 1.97                     | 0.47              |
| 1:A:1441:ARG:HH22 | 1:A:1489:THR:HG21 | 1.80                     | 0.47              |
| 1:D:1160:ASP:HB3  | 1:D:1166:LEU:HD11 | 1.97                     | 0.47              |
| 1:C:886:ARG:NE    | 1:D:885:ASP:OD2   | 2.48                     | 0.47              |
| 1:J:1204:ARG:HB3  | 1:J:1205:PRO:HA   | 1.97                     | 0.47              |
| 1:Q:909:VAL:H     | 1:R:920:GLN:CD    | 2.18                     | 0.47              |
| 1:B:1193:LEU:HD21 | 1:B:2006:PHE:HZ   | 1.80                     | 0.47              |
| 1:R:916:GLU:OE2   | 1:R:1666:ARG:NH2  | 2.48                     | 0.46              |
| 1:B:1962:ILE:HD12 | 1:B:1984:TYR:CD1  | 2.50                     | 0.46              |
| 1:G:1962:ILE:HD12 | 1:G:1984:TYR:CD1  | 2.49                     | 0.46              |
| 1:O:1666:ARG:HB3  | 1:P:1666:ARG:HB3  | 1.97                     | 0.46              |
| 1:C:1791:ARG:CZ   | 1:C:1819:VAL:HG21 | 2.46                     | 0.46              |
| 1:L:1962:ILE:HD12 | 1:L:1984:TYR:CD1  | 2.50                     | 0.46              |
| 1:H:1449:ILE:HG23 | 1:H:1488:VAL:HG13 | 1.96                     | 0.46              |
| 1:C:1689:THR:HG21 | 1:D:1649:PHE:CD1  | 2.51                     | 0.46              |
| 1:J:1449:ILE:HG23 | 1:J:1488:VAL:HG13 | 1.97                     | 0.46              |
| 1:Q:911:PRO:HB3   | 1:R:983:TRP:CD2   | 2.51                     | 0.46              |
| 1:H:1193:LEU:HD22 | 1:H:1399:LEU:CD1  | 2.46                     | 0.46              |
| 1:E:1483:GLU:HB3  | 1:E:1541:LEU:HD13 | 1.98                     | 0.46              |
| 1:D:1962:ILE:HD12 | 1:D:1984:TYR:CD1  | 2.51                     | 0.46              |
| 1:O:1723:ALA:HB2  | 1:O:1741:ILE:HD11 | 1.98                     | 0.46              |
| 1:A:1569:GLY:HA3  | 2:A:3001:NAP:O1A  | 2.16                     | 0.46              |
| 1:F:1761:PHE:HB3  | 1:F:1789:CYS:SG   | 2.56                     | 0.45              |
| 1:B:1402:SER:O    | 1:B:1979:ARG:NH1  | 2.48                     | 0.45              |
| 1:B:1755:PRO:HD2  | 1:B:1757:GLN:HG3  | 1.97                     | 0.45              |
| 1:F:1962:ILE:HD12 | 1:F:1984:TYR:CD1  | 2.51                     | 0.45              |
| 1:G:1769:ILE:HD11 | 1:G:1784:MET:SD   | 2.56                     | 0.45              |
| 1:H:1160:ASP:HB3  | 1:H:1166:LEU:HD11 | 1.98                     | 0.45              |
| 1:N:1312:ALA:HB1  | 1:N:1355:HIS:CE1  | 2.51                     | 0.45              |
| 1:E:1399:LEU:HD21 | 1:E:1908:LEU:HD21 | 1.98                     | 0.45              |
| 1:M:1399:LEU:HD21 | 1:M:1908:LEU:HD11 | 1.98                     | 0.45              |
| 1:M:1421:MET:CE   | 1:M:1436:LEU:HD21 | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1160:ASP:HB3  | 1:B:1166:LEU:HD11 | 1.98                     | 0.45              |
| 1:B:1508:SER:O    | 1:B:1509:ALA:HB3  | 2.16                     | 0.45              |
| 1:J:1160:ASP:HB3  | 1:J:1166:LEU:HD11 | 1.98                     | 0.45              |
| 1:L:1160:ASP:HB3  | 1:L:1166:LEU:HD11 | 1.97                     | 0.45              |
| 1:M:1791:ARG:CZ   | 1:M:1819:VAL:HG21 | 2.46                     | 0.45              |
| 1:Q:1160:ASP:HB3  | 1:Q:1166:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:1962:ILE:HD12 | 1:E:1984:TYR:CD1  | 2.51                     | 0.45              |
| 1:J:1499:ARG:HD3  | 1:K:1139:TYR:OH   | 2.16                     | 0.45              |
| 1:K:1160:ASP:HB3  | 1:K:1166:LEU:HD11 | 1.98                     | 0.45              |
| 1:M:1493:PRO:HA   | 1:M:1494:GLY:HA2  | 1.86                     | 0.45              |
| 1:E:1458:ILE:HD11 | 1:E:1741:ILE:HD13 | 1.98                     | 0.45              |
| 1:F:1160:ASP:HB3  | 1:F:1166:LEU:HD11 | 1.99                     | 0.45              |
| 1:K:1193:LEU:HD22 | 1:K:1399:LEU:HD22 | 1.99                     | 0.45              |
| 1:O:1460:PHE:CD1  | 2:O:3001:NAP:H52A | 2.52                     | 0.45              |
| 1:O:1160:ASP:HB3  | 1:O:1166:LEU:HD11 | 1.99                     | 0.45              |
| 1:P:1160:ASP:HB3  | 1:P:1166:LEU:HD11 | 1.99                     | 0.45              |
| 1:P:1962:ILE:HD12 | 1:P:1984:TYR:CE2  | 2.52                     | 0.45              |
| 1:R:1756:GLU:HA   | 1:R:1757:GLN:C    | 2.37                     | 0.45              |
| 1:C:1192:LEU:HD12 | 1:C:1403:PRO:HB3  | 1.99                     | 0.45              |
| 1:E:1125:VAL:HG11 | 1:E:1128:LEU:HG   | 1.99                     | 0.44              |
| 1:F:1531:ILE:HG21 | 1:F:1705:ILE:HG23 | 1.98                     | 0.44              |
| 1:G:1193:LEU:HD21 | 1:G:2006:PHE:HZ   | 1.81                     | 0.44              |
| 1:H:1791:ARG:CZ   | 1:H:1819:VAL:HG21 | 2.47                     | 0.44              |
| 1:H:1962:ILE:HD12 | 1:H:1984:TYR:CD1  | 2.51                     | 0.44              |
| 1:K:1339:LEU:HA   | 1:K:1342:SER:OG   | 2.17                     | 0.44              |
| 1:P:1791:ARG:CZ   | 1:P:1819:VAL:HG21 | 2.46                     | 0.44              |
| 1:C:1962:ILE:HD12 | 1:C:1984:TYR:CD1  | 2.52                     | 0.44              |
| 1:N:1160:ASP:HB3  | 1:N:1166:LEU:HD11 | 1.98                     | 0.44              |
| 1:N:1752:VAL:HG12 | 1:N:1753:VAL:H    | 1.82                     | 0.44              |
| 1:N:1962:ILE:HD12 | 1:N:1984:TYR:CD1  | 2.52                     | 0.44              |
| 1:C:1160:ASP:HB3  | 1:C:1166:LEU:HD11 | 1.98                     | 0.44              |
| 1:D:1493:PRO:HA   | 1:D:1494:GLY:HA2  | 1.86                     | 0.44              |
| 1:J:1505:GLY:HA3  | 1:J:1527:LEU:HD21 | 1.99                     | 0.44              |
| 1:J:1791:ARG:CZ   | 1:J:1819:VAL:HG21 | 2.47                     | 0.44              |
| 1:E:1160:ASP:HB3  | 1:E:1166:LEU:HD11 | 1.98                     | 0.44              |
| 1:K:1962:ILE:HD12 | 1:K:1984:TYR:CD1  | 2.52                     | 0.44              |
| 1:L:1791:ARG:CZ   | 1:L:1819:VAL:HG21 | 2.47                     | 0.44              |
| 1:Q:910:LEU:HD22  | 1:R:918:LEU:HD21  | 2.00                     | 0.44              |
| 1:J:1962:ILE:HD12 | 1:J:1984:TYR:CD1  | 2.52                     | 0.44              |
| 1:K:1962:ILE:HD11 | 1:K:1967:GLY:CA   | 2.48                     | 0.44              |
| 1:L:1448:GLN:C    | 1:L:1449:ILE:HD12 | 2.37                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:1193:LEU:HD22 | 1:P:1399:LEU:HD22 | 1.99                     | 0.44              |
| 1:P:1962:ILE:HD12 | 1:P:1984:TYR:CD2  | 2.52                     | 0.44              |
| 1:G:1791:ARG:CZ   | 1:G:1819:VAL:HG21 | 2.48                     | 0.44              |
| 1:H:1193:LEU:HD21 | 1:H:2006:PHE:HZ   | 1.82                     | 0.44              |
| 1:K:1791:ARG:CZ   | 1:K:1819:VAL:HG21 | 2.48                     | 0.44              |
| 1:N:1791:ARG:CZ   | 1:N:1819:VAL:HG21 | 2.47                     | 0.44              |
| 1:P:1424:VAL:HA   | 1:P:1480:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:1649:PHE:CD1  | 1:B:1689:THR:HG21 | 2.53                     | 0.44              |
| 1:F:1962:ILE:HD11 | 1:F:1967:GLY:CA   | 2.48                     | 0.44              |
| 1:H:1962:ILE:HD11 | 1:H:1967:GLY:CA   | 2.48                     | 0.44              |
| 1:P:1962:ILE:HD11 | 1:P:1967:GLY:CA   | 2.48                     | 0.44              |
| 1:A:1026:HIS:HB3  | 1:A:1031:LEU:HD11 | 1.99                     | 0.44              |
| 1:R:1160:ASP:HB3  | 1:R:1166:LEU:HD11 | 1.98                     | 0.44              |
| 1:G:1160:ASP:HB3  | 1:G:1166:LEU:HD11 | 1.99                     | 0.44              |
| 1:L:1159:LEU:CD2  | 1:L:1165:VAL:HG22 | 2.48                     | 0.43              |
| 1:M:1160:ASP:HB3  | 1:M:1166:LEU:HD11 | 1.99                     | 0.43              |
| 1:M:1399:LEU:HD11 | 1:M:1908:LEU:HD21 | 2.00                     | 0.43              |
| 1:H:1593:GLU:HB3  | 1:Q:1024:ALA:CB   | 2.48                     | 0.43              |
| 1:I:1160:ASP:HB3  | 1:I:1166:LEU:HD11 | 1.99                     | 0.43              |
| 1:J:1386:GLU:HB3  | 1:J:1397:ALA:HB3  | 2.00                     | 0.43              |
| 1:K:1193:LEU:HD21 | 1:K:2006:PHE:HZ   | 1.82                     | 0.43              |
| 1:A:1369:THR:O    | 1:A:1370:ALA:HB3  | 2.18                     | 0.43              |
| 1:D:1962:ILE:HD11 | 1:D:1967:GLY:CA   | 2.48                     | 0.43              |
| 1:G:1962:ILE:HD11 | 1:G:1967:GLY:CA   | 2.48                     | 0.43              |
| 1:H:1971:PHE:CZ   | 1:H:1975:LEU:HD11 | 2.53                     | 0.43              |
| 1:A:1460:PHE:CD1  | 2:A:3001:NAP:H52A | 2.53                     | 0.43              |
| 1:B:1962:ILE:HD11 | 1:B:1967:GLY:CA   | 2.48                     | 0.43              |
| 1:E:1460:PHE:CD1  | 2:E:3001:NAP:H51A | 2.53                     | 0.43              |
| 1:J:1962:ILE:HD11 | 1:J:1967:GLY:CA   | 2.49                     | 0.43              |
| 1:M:1122:PRO:HA   | 1:M:1174:LEU:HD23 | 2.01                     | 0.43              |
| 1:F:1601:ASP:OD2  | 1:H:1026:HIS:HA   | 2.19                     | 0.43              |
| 1:C:1962:ILE:HD11 | 1:C:1967:GLY:CA   | 2.48                     | 0.43              |
| 1:E:1962:ILE:HD11 | 1:E:1967:GLY:CA   | 2.48                     | 0.43              |
| 1:C:1929:GLN:HG3  | 1:C:1980:VAL:HG11 | 2.01                     | 0.43              |
| 1:E:1159:LEU:CD2  | 1:E:1165:VAL:HG22 | 2.49                     | 0.43              |
| 1:L:1962:ILE:HD11 | 1:L:1967:GLY:CA   | 2.48                     | 0.43              |
| 1:Q:1159:LEU:CD2  | 1:Q:1165:VAL:HG22 | 2.49                     | 0.43              |
| 1:A:1545:THR:OG1  | 1:A:1683:LEU:HD22 | 2.19                     | 0.43              |
| 1:A:1752:VAL:HG12 | 1:A:1753:VAL:H    | 1.84                     | 0.43              |
| 1:C:1159:LEU:CD2  | 1:C:1165:VAL:HG22 | 2.49                     | 0.43              |
| 1:P:1531:ILE:HG21 | 1:P:1705:ILE:HG23 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1555:ARG:NH2  | 1:D:1555:ARG:NH2  | 2.66                     | 0.43              |
| 1:B:1193:LEU:HD22 | 1:B:1399:LEU:CD1  | 2.48                     | 0.42              |
| 1:F:1193:LEU:HD21 | 1:F:2006:PHE:HZ   | 1.82                     | 0.42              |
| 1:K:1745:ASP:O    | 1:K:1746:THR:O    | 2.38                     | 0.42              |
| 1:L:1449:ILE:HG23 | 1:L:1488:VAL:HG13 | 2.01                     | 0.42              |
| 1:R:1493:PRO:HA   | 1:R:1494:GLY:HA2  | 1.85                     | 0.42              |
| 1:A:1026:HIS:CB   | 1:A:1031:LEU:HD11 | 2.48                     | 0.42              |
| 1:D:1569:GLY:HA3  | 2:D:3001:NAP:O1A  | 2.18                     | 0.42              |
| 1:O:1159:LEU:CD2  | 1:O:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:F:1193:LEU:HD22 | 1:F:1399:LEU:HD11 | 2.01                     | 0.42              |
| 1:K:1460:PHE:CD1  | 2:K:3001:NAP:H52A | 2.54                     | 0.42              |
| 1:P:1159:LEU:CD2  | 1:P:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:B:1159:LEU:CD2  | 1:B:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:I:1159:LEU:CD2  | 1:I:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:H:1597:GLN:HG2  | 1:Q:1025:ALA:O    | 2.20                     | 0.42              |
| 1:J:1660:ASP:OD1  | 1:J:1665:THR:HG21 | 2.19                     | 0.42              |
| 1:K:1298:ALA:HB2  | 1:K:1872:TRP:NE1  | 2.34                     | 0.42              |
| 1:M:1159:LEU:CD2  | 1:M:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:D:1414:ALA:HB3  | 1:D:1752:VAL:HG21 | 2.01                     | 0.42              |
| 1:E:1098:LEU:HD21 | 1:E:1137:VAL:HG11 | 2.02                     | 0.42              |
| 1:G:1159:LEU:CD2  | 1:G:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:C:1423:LEU:HD12 | 1:C:1435:GLU:O    | 2.19                     | 0.42              |
| 1:F:1421:MET:HE3  | 1:F:1436:LEU:HD21 | 2.00                     | 0.42              |
| 1:K:1400:CYS:HB3  | 1:K:2005:LEU:HD12 | 2.02                     | 0.42              |
| 1:L:1436:LEU:HD23 | 1:L:1752:VAL:HG13 | 2.01                     | 0.42              |
| 1:F:1159:LEU:CD2  | 1:F:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:J:1159:LEU:CD2  | 1:J:1165:VAL:HG22 | 2.50                     | 0.42              |
| 1:K:1508:SER:O    | 1:K:1509:ALA:HB3  | 2.19                     | 0.42              |
| 1:F:1386:GLU:HB3  | 1:F:1397:ALA:HB3  | 2.01                     | 0.42              |
| 1:I:1689:THR:HG21 | 1:J:1649:PHE:CD1  | 2.55                     | 0.42              |
| 1:B:1523:LEU:HD22 | 1:B:1687:THR:HG23 | 2.02                     | 0.42              |
| 1:D:1159:LEU:CD2  | 1:D:1165:VAL:HG22 | 2.49                     | 0.42              |
| 1:F:1508:SER:O    | 1:F:1509:ALA:HB3  | 2.20                     | 0.42              |
| 1:K:1159:LEU:CD2  | 1:K:1165:VAL:HG22 | 2.50                     | 0.42              |
| 1:M:1900:CYS:SG   | 1:M:1901:ALA:N    | 2.93                     | 0.42              |
| 1:O:1508:SER:O    | 1:O:1509:ALA:HB3  | 2.20                     | 0.42              |
| 1:C:1098:LEU:HD21 | 1:C:1137:VAL:HG11 | 2.02                     | 0.41              |
| 1:D:1458:ILE:HD11 | 1:D:1741:ILE:HD13 | 2.02                     | 0.41              |
| 1:H:1159:LEU:CD2  | 1:H:1165:VAL:HG22 | 2.49                     | 0.41              |
| 1:H:1123:LEU:HD11 | 1:H:1175:GLY:O    | 2.19                     | 0.41              |
| 1:L:1508:SER:O    | 1:L:1509:ALA:HB3  | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:1876:VAL:HB   | 1:L:1923:TRP:CE3  | 2.55                     | 0.41              |
| 1:Q:1098:LEU:HD21 | 1:Q:1137:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:1414:ALA:HB3  | 1:A:1752:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:892:ALA:CB    | 1:D:893:PRO:CD    | 2.99                     | 0.41              |
| 1:G:1421:MET:HE3  | 1:G:1436:LEU:HD21 | 2.01                     | 0.41              |
| 1:G:1493:PRO:HA   | 1:G:1494:GLY:HA2  | 1.86                     | 0.41              |
| 1:I:1176:THR:HG21 | 1:I:1180:ASP:OD1  | 2.20                     | 0.41              |
| 1:A:1493:PRO:HA   | 1:A:1494:GLY:HA2  | 1.84                     | 0.41              |
| 1:J:1098:LEU:HD21 | 1:J:1137:VAL:HG11 | 2.03                     | 0.41              |
| 1:J:1302:ARG:HG3  | 1:J:1868:VAL:HG11 | 2.01                     | 0.41              |
| 1:A:1727:ILE:N    | 1:A:1727:ILE:HD13 | 2.36                     | 0.41              |
| 1:A:1846:ARG:HA   | 1:A:1896:LEU:HA   | 2.02                     | 0.41              |
| 1:F:1876:VAL:HB   | 1:F:1923:TRP:CE3  | 2.56                     | 0.41              |
| 1:N:1159:LEU:CD2  | 1:N:1165:VAL:HG22 | 2.50                     | 0.41              |
| 1:N:1635:VAL:HG22 | 1:N:1636:THR:H    | 1.85                     | 0.41              |
| 1:R:1159:LEU:CD2  | 1:R:1165:VAL:HG22 | 2.49                     | 0.41              |
| 1:B:1098:LEU:HD21 | 1:B:1137:VAL:HG11 | 2.03                     | 0.41              |
| 1:B:1493:PRO:HA   | 1:B:1494:GLY:HA2  | 1.85                     | 0.41              |
| 1:I:1098:LEU:HD21 | 1:I:1137:VAL:HG11 | 2.03                     | 0.41              |
| 1:M:1032:LEU:HD13 | 1:P:1499:ARG:HD2  | 2.02                     | 0.41              |
| 1:A:1872:TRP:NE1  | 1:A:1876:VAL:HG21 | 2.35                     | 0.41              |
| 1:B:1755:PRO:O    | 1:B:1756:GLU:OE1  | 2.39                     | 0.41              |
| 1:D:1098:LEU:HD21 | 1:D:1137:VAL:HG11 | 2.02                     | 0.41              |
| 1:E:1424:VAL:HA   | 1:E:1480:LEU:HD12 | 2.02                     | 0.41              |
| 1:F:1460:PHE:CD1  | 2:F:3001:NAP:H52A | 2.56                     | 0.41              |
| 1:H:1098:LEU:HD21 | 1:H:1137:VAL:HG11 | 2.02                     | 0.41              |
| 1:H:1876:VAL:HB   | 1:H:1923:TRP:CE3  | 2.56                     | 0.41              |
| 1:P:1386:GLU:HB3  | 1:P:1397:ALA:HB3  | 2.03                     | 0.41              |
| 1:A:951:ALA:HB1   | 1:A:965:VAL:HG11  | 2.02                     | 0.41              |
| 1:C:1508:SER:O    | 1:C:1509:ALA:HB3  | 2.21                     | 0.41              |
| 1:Q:1424:VAL:HA   | 1:Q:1480:LEU:HD12 | 2.03                     | 0.41              |
| 1:R:1508:SER:O    | 1:R:1509:ALA:HB3  | 2.21                     | 0.41              |
| 1:N:1098:LEU:HD21 | 1:N:1137:VAL:HG11 | 2.02                     | 0.41              |
| 1:N:1193:LEU:HD21 | 1:N:2006:PHE:CZ   | 2.56                     | 0.41              |
| 1:O:1493:PRO:HA   | 1:O:1494:GLY:HA2  | 1.86                     | 0.41              |
| 1:B:1791:ARG:CZ   | 1:B:1819:VAL:HG21 | 2.51                     | 0.41              |
| 1:G:1876:VAL:HB   | 1:G:1923:TRP:CE3  | 2.56                     | 0.41              |
| 1:J:1193:LEU:HD21 | 1:J:2006:PHE:HZ   | 1.84                     | 0.41              |
| 1:K:1872:TRP:NE1  | 1:K:1876:VAL:HG21 | 2.35                     | 0.41              |
| 1:L:1683:LEU:H    | 2:L:3001:NAP:H72N | 1.67                     | 0.41              |
| 1:M:1872:TRP:NE1  | 1:M:1876:VAL:HG21 | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:1872:TRP:NE1  | 1:P:1876:VAL:HG21 | 2.36                     | 0.41              |
| 1:Q:983:TRP:NE1   | 1:R:909:VAL:O     | 2.54                     | 0.41              |
| 1:B:1460:PHE:CD1  | 2:B:3001:NAP:H52A | 2.55                     | 0.41              |
| 1:D:1434:MET:CE   | 1:D:1724:ALA:HA   | 2.51                     | 0.41              |
| 1:F:1730:MET:CE   | 1:F:1739:LEU:HD22 | 2.51                     | 0.41              |
| 1:O:1745:ASP:O    | 1:O:1746:THR:C    | 2.60                     | 0.41              |
| 1:P:1876:VAL:HB   | 1:P:1923:TRP:CE3  | 2.56                     | 0.41              |
| 1:D:1508:SER:O    | 1:D:1509:ALA:HB3  | 2.21                     | 0.40              |
| 1:G:1764:ASP:C    | 1:G:1843:LEU:HD22 | 2.40                     | 0.40              |
| 1:H:1508:SER:O    | 1:H:1509:ALA:HB3  | 2.21                     | 0.40              |
| 2:K:3001:NAP:H4B  | 2:K:3001:NAP:O1A  | 2.19                     | 0.40              |
| 1:N:1493:PRO:HA   | 1:N:1494:GLY:HA2  | 1.86                     | 0.40              |
| 1:P:1122:PRO:HA   | 1:P:1174:LEU:HB3  | 2.02                     | 0.40              |
| 1:P:1508:SER:O    | 1:P:1509:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:1160:ASP:HB3  | 1:A:1166:LEU:HD11 | 2.03                     | 0.40              |
| 1:G:1098:LEU:HD21 | 1:G:1137:VAL:HG11 | 2.03                     | 0.40              |
| 1:H:1400:CYS:HB3  | 1:H:2005:LEU:HD22 | 2.03                     | 0.40              |
| 1:J:1872:TRP:NE1  | 1:J:1876:VAL:HG21 | 2.37                     | 0.40              |
| 1:K:1493:PRO:HA   | 1:K:1494:GLY:HA2  | 1.86                     | 0.40              |
| 1:K:1660:ASP:OD1  | 1:K:1665:THR:HG21 | 2.22                     | 0.40              |
| 1:N:1508:SER:O    | 1:N:1509:ALA:HB3  | 2.21                     | 0.40              |
| 1:H:1597:GLN:CG   | 1:Q:1026:HIS:HA   | 2.50                     | 0.40              |
| 1:Q:1493:PRO:HA   | 1:Q:1494:GLY:HA2  | 1.85                     | 0.40              |
| 1:Q:908:VAL:HG13  | 1:R:920:GLN:CB    | 2.46                     | 0.40              |
| 1:R:1098:LEU:HD21 | 1:R:1137:VAL:HG11 | 2.02                     | 0.40              |
| 1:B:1176:THR:O    | 1:B:1177:GLY:C    | 2.59                     | 0.40              |
| 1:E:1508:SER:O    | 1:E:1509:ALA:HB3  | 2.22                     | 0.40              |
| 1:G:1508:SER:O    | 1:G:1509:ALA:HB3  | 2.21                     | 0.40              |
| 1:H:1423:LEU:HD12 | 1:H:1435:GLU:O    | 2.22                     | 0.40              |
| 1:M:1666:ARG:HB3  | 1:N:1666:ARG:HB3  | 2.03                     | 0.40              |
| 1:P:1098:LEU:HD21 | 1:P:1137:VAL:HG11 | 2.03                     | 0.40              |
| 1:B:1531:ILE:HD11 | 1:B:1702:TYR:HB3  | 2.03                     | 0.40              |
| 1:E:1876:VAL:HB   | 1:E:1923:TRP:CE3  | 2.56                     | 0.40              |
| 1:F:1098:LEU:HD21 | 1:F:1137:VAL:HG11 | 2.02                     | 0.40              |
| 1:P:1103:PHE:CD1  | 1:P:1172:LEU:HD22 | 2.57                     | 0.40              |
| 1:P:1423:LEU:HD12 | 1:P:1435:GLU:O    | 2.21                     | 0.40              |
| 1:P:1531:ILE:HD11 | 1:P:1702:TYR:HB3  | 2.03                     | 0.40              |
| 1:A:907:HIS:NE2   | 1:A:917:HIS:ND1   | 2.69                     | 0.40              |
| 1:E:1193:LEU:HD21 | 1:E:2006:PHE:HZ   | 1.85                     | 0.40              |
| 1:I:1508:SER:O    | 1:I:1509:ALA:HB3  | 2.21                     | 0.40              |
| 1:K:1726:ALA:HB1  | 1:K:1739:LEU:HD23 | 2.04                     | 0.40              |

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

| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:C:1083:GLY:HA2 | 1:J:1264:ALA:HB1[1_565] | 1.34                     | 0.26              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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     | 1094/1140 (96%)   | 995 (91%)   | 79 (7%)   | 20 (2%)  | 10          | 50 |
| 1   | B     | 1094/1140 (96%)   | 1002 (92%)  | 69 (6%)   | 23 (2%)  | 8           | 47 |
| 1   | C     | 1094/1140 (96%)   | 1002 (92%)  | 73 (7%)   | 19 (2%)  | 11          | 51 |
| 1   | D     | 1094/1140 (96%)   | 1001 (92%)  | 72 (7%)   | 21 (2%)  | 9           | 49 |
| 1   | E     | 1081/1140 (95%)   | 993 (92%)   | 68 (6%)   | 20 (2%)  | 9           | 49 |
| 1   | F     | 1085/1140 (95%)   | 995 (92%)   | 74 (7%)   | 16 (2%)  | 12          | 53 |
| 1   | G     | 1080/1140 (95%)   | 990 (92%)   | 72 (7%)   | 18 (2%)  | 11          | 51 |
| 1   | H     | 1091/1140 (96%)   | 996 (91%)   | 76 (7%)   | 19 (2%)  | 11          | 51 |
| 1   | I     | 651/1140 (57%)    | 601 (92%)   | 39 (6%)   | 11 (2%)  | 11          | 51 |
| 1   | J     | 1081/1140 (95%)   | 991 (92%)   | 68 (6%)   | 22 (2%)  | 9           | 49 |
| 1   | K     | 1081/1140 (95%)   | 990 (92%)   | 71 (7%)   | 20 (2%)  | 9           | 49 |
| 1   | L     | 891/1140 (78%)    | 815 (92%)   | 61 (7%)   | 15 (2%)  | 11          | 51 |
| 1   | M     | 1081/1140 (95%)   | 995 (92%)   | 71 (7%)   | 15 (1%)  | 13          | 54 |
| 1   | N     | 1081/1140 (95%)   | 982 (91%)   | 76 (7%)   | 23 (2%)  | 8           | 47 |
| 1   | O     | 629/1140 (55%)    | 580 (92%)   | 37 (6%)   | 12 (2%)  | 9           | 49 |
| 1   | P     | 1081/1140 (95%)   | 986 (91%)   | 72 (7%)   | 23 (2%)  | 8           | 47 |
| 1   | Q     | 604/1140 (53%)    | 562 (93%)   | 35 (6%)   | 7 (1%)   | 15          | 58 |
| 1   | R     | 633/1140 (56%)    | 582 (92%)   | 39 (6%)   | 12 (2%)  | 9           | 49 |
| All | All   | 17526/20520 (85%) | 16058 (92%) | 1152 (7%) | 316 (2%) | 10          | 50 |

All (316) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1755 | PRO  |
| 1   | B     | 892  | ALA  |
| 1   | B     | 1179 | SER  |
| 1   | C     | 1755 | PRO  |
| 1   | D     | 892  | ALA  |
| 1   | D     | 1755 | PRO  |
| 1   | E     | 1755 | PRO  |
| 1   | F     | 1755 | PRO  |
| 1   | G     | 1755 | PRO  |
| 1   | H     | 1403 | PRO  |
| 1   | H     | 1755 | PRO  |
| 1   | J     | 1403 | PRO  |
| 1   | K     | 1746 | THR  |
| 1   | K     | 1755 | PRO  |
| 1   | M     | 1755 | PRO  |
| 1   | N     | 1747 | GLY  |
| 1   | N     | 1748 | GLN  |
| 1   | N     | 1755 | PRO  |
| 1   | O     | 1746 | THR  |
| 1   | P     | 1404 | LEU  |
| 1   | P     | 1540 | GLY  |
| 1   | P     | 1755 | PRO  |
| 1   | A     | 892  | ALA  |
| 1   | A     | 915  | GLU  |
| 1   | A     | 960  | GLY  |
| 1   | A     | 1115 | ILE  |
| 1   | A     | 1339 | LEU  |
| 1   | A     | 1509 | ALA  |
| 1   | A     | 1651 | GLY  |
| 1   | A     | 1915 | GLY  |
| 1   | B     | 1177 | GLY  |
| 1   | B     | 1419 | GLU  |
| 1   | B     | 1540 | GLY  |
| 1   | B     | 1606 | HIS  |
| 1   | B     | 1651 | GLY  |
| 1   | B     | 1760 | VAL  |
| 1   | B     | 1840 | GLN  |
| 1   | B     | 1915 | GLY  |
| 1   | B     | 1961 | ALA  |
| 1   | C     | 1540 | GLY  |
| 1   | C     | 1606 | HIS  |
| 1   | C     | 1651 | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1840 | GLN  |
| 1   | C     | 1915 | GLY  |
| 1   | C     | 1961 | ALA  |
| 1   | D     | 1419 | GLU  |
| 1   | D     | 1540 | GLY  |
| 1   | D     | 1606 | HIS  |
| 1   | D     | 1651 | GLY  |
| 1   | D     | 1915 | GLY  |
| 1   | D     | 1961 | ALA  |
| 1   | E     | 1540 | GLY  |
| 1   | E     | 1606 | HIS  |
| 1   | E     | 1651 | GLY  |
| 1   | E     | 1915 | GLY  |
| 1   | E     | 1961 | ALA  |
| 1   | F     | 1540 | GLY  |
| 1   | F     | 1606 | HIS  |
| 1   | F     | 1651 | GLY  |
| 1   | F     | 1915 | GLY  |
| 1   | F     | 1961 | ALA  |
| 1   | G     | 1419 | GLU  |
| 1   | G     | 1540 | GLY  |
| 1   | G     | 1606 | HIS  |
| 1   | G     | 1651 | GLY  |
| 1   | G     | 1747 | GLY  |
| 1   | G     | 1915 | GLY  |
| 1   | G     | 1961 | ALA  |
| 1   | H     | 1540 | GLY  |
| 1   | H     | 1606 | HIS  |
| 1   | H     | 1651 | GLY  |
| 1   | H     | 1840 | GLN  |
| 1   | H     | 1915 | GLY  |
| 1   | H     | 1961 | ALA  |
| 1   | I     | 1540 | GLY  |
| 1   | I     | 1606 | HIS  |
| 1   | I     | 1651 | GLY  |
| 1   | J     | 1540 | GLY  |
| 1   | J     | 1606 | HIS  |
| 1   | J     | 1651 | GLY  |
| 1   | J     | 1746 | THR  |
| 1   | J     | 1755 | PRO  |
| 1   | J     | 1840 | GLN  |
| 1   | J     | 1915 | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 1961 | ALA  |
| 1   | K     | 1419 | GLU  |
| 1   | K     | 1540 | GLY  |
| 1   | K     | 1606 | HIS  |
| 1   | K     | 1651 | GLY  |
| 1   | K     | 1757 | GLN  |
| 1   | K     | 1840 | GLN  |
| 1   | K     | 1915 | GLY  |
| 1   | K     | 1961 | ALA  |
| 1   | L     | 1419 | GLU  |
| 1   | L     | 1540 | GLY  |
| 1   | L     | 1606 | HIS  |
| 1   | L     | 1651 | GLY  |
| 1   | L     | 1755 | PRO  |
| 1   | L     | 1840 | GLN  |
| 1   | L     | 1915 | GLY  |
| 1   | L     | 1961 | ALA  |
| 1   | M     | 1540 | GLY  |
| 1   | M     | 1606 | HIS  |
| 1   | M     | 1651 | GLY  |
| 1   | M     | 1840 | GLN  |
| 1   | M     | 1915 | GLY  |
| 1   | M     | 1961 | ALA  |
| 1   | N     | 1419 | GLU  |
| 1   | N     | 1540 | GLY  |
| 1   | N     | 1606 | HIS  |
| 1   | N     | 1651 | GLY  |
| 1   | N     | 1840 | GLN  |
| 1   | N     | 1915 | GLY  |
| 1   | N     | 1987 | VAL  |
| 1   | O     | 1540 | GLY  |
| 1   | O     | 1606 | HIS  |
| 1   | O     | 1651 | GLY  |
| 1   | O     | 1745 | ASP  |
| 1   | P     | 1419 | GLU  |
| 1   | P     | 1606 | HIS  |
| 1   | P     | 1651 | GLY  |
| 1   | P     | 1747 | GLY  |
| 1   | P     | 1840 | GLN  |
| 1   | P     | 1915 | GLY  |
| 1   | P     | 1961 | ALA  |
| 1   | P     | 1987 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | Q     | 1540 | GLY  |
| 1   | Q     | 1606 | HIS  |
| 1   | Q     | 1651 | GLY  |
| 1   | R     | 1540 | GLY  |
| 1   | R     | 1606 | HIS  |
| 1   | R     | 1651 | GLY  |
| 1   | A     | 1419 | GLU  |
| 1   | A     | 1540 | GLY  |
| 1   | A     | 1606 | HIS  |
| 1   | A     | 1840 | GLN  |
| 1   | B     | 1509 | ALA  |
| 1   | B     | 1755 | PRO  |
| 1   | C     | 1746 | THR  |
| 1   | D     | 1401 | PRO  |
| 1   | D     | 1840 | GLN  |
| 1   | E     | 1840 | GLN  |
| 1   | F     | 1419 | GLU  |
| 1   | G     | 1339 | LEU  |
| 1   | G     | 1746 | THR  |
| 1   | G     | 1840 | GLN  |
| 1   | H     | 1205 | PRO  |
| 1   | I     | 1419 | GLU  |
| 1   | J     | 1419 | GLU  |
| 1   | J     | 1747 | GLY  |
| 1   | K     | 1339 | LEU  |
| 1   | M     | 1419 | GLU  |
| 1   | N     | 1401 | PRO  |
| 1   | O     | 1419 | GLU  |
| 1   | P     | 1403 | PRO  |
| 1   | P     | 1990 | ALA  |
| 1   | R     | 1750 | GLN  |
| 1   | A     | 1369 | THR  |
| 1   | A     | 1649 | PHE  |
| 1   | B     | 915  | GLU  |
| 1   | B     | 960  | GLY  |
| 1   | B     | 1090 | ARG  |
| 1   | B     | 1339 | LEU  |
| 1   | C     | 915  | GLU  |
| 1   | C     | 960  | GLY  |
| 1   | C     | 1509 | ALA  |
| 1   | D     | 915  | GLU  |
| 1   | D     | 960  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1090 | ARG  |
| 1   | D     | 1509 | ALA  |
| 1   | D     | 1760 | VAL  |
| 1   | E     | 960  | GLY  |
| 1   | E     | 1090 | ARG  |
| 1   | E     | 1509 | ALA  |
| 1   | E     | 1746 | THR  |
| 1   | F     | 915  | GLU  |
| 1   | F     | 960  | GLY  |
| 1   | F     | 1090 | ARG  |
| 1   | F     | 1509 | ALA  |
| 1   | G     | 915  | GLU  |
| 1   | G     | 960  | GLY  |
| 1   | G     | 1090 | ARG  |
| 1   | G     | 1509 | ALA  |
| 1   | H     | 1090 | ARG  |
| 1   | H     | 1509 | ALA  |
| 1   | I     | 915  | GLU  |
| 1   | I     | 960  | GLY  |
| 1   | I     | 1090 | ARG  |
| 1   | I     | 1509 | ALA  |
| 1   | I     | 1754 | PRO  |
| 1   | J     | 915  | GLU  |
| 1   | J     | 960  | GLY  |
| 1   | J     | 1090 | ARG  |
| 1   | J     | 1509 | ALA  |
| 1   | K     | 915  | GLU  |
| 1   | K     | 960  | GLY  |
| 1   | K     | 1090 | ARG  |
| 1   | K     | 1509 | ALA  |
| 1   | K     | 1760 | VAL  |
| 1   | L     | 1509 | ALA  |
| 1   | M     | 915  | GLU  |
| 1   | M     | 1090 | ARG  |
| 1   | M     | 1509 | ALA  |
| 1   | N     | 915  | GLU  |
| 1   | N     | 1090 | ARG  |
| 1   | N     | 1509 | ALA  |
| 1   | N     | 1746 | THR  |
| 1   | N     | 1961 | ALA  |
| 1   | O     | 915  | GLU  |
| 1   | O     | 960  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | O     | 1090 | ARG  |
| 1   | O     | 1509 | ALA  |
| 1   | P     | 1090 | ARG  |
| 1   | P     | 1509 | ALA  |
| 1   | Q     | 915  | GLU  |
| 1   | Q     | 960  | GLY  |
| 1   | Q     | 1090 | ARG  |
| 1   | R     | 915  | GLU  |
| 1   | R     | 1090 | ARG  |
| 1   | R     | 1509 | ALA  |
| 1   | R     | 1748 | GLN  |
| 1   | A     | 1370 | ALA  |
| 1   | B     | 1115 | ILE  |
| 1   | B     | 1369 | THR  |
| 1   | B     | 1791 | ARG  |
| 1   | C     | 1115 | ILE  |
| 1   | C     | 1339 | LEU  |
| 1   | C     | 1369 | THR  |
| 1   | C     | 1403 | PRO  |
| 1   | D     | 1115 | ILE  |
| 1   | D     | 1339 | LEU  |
| 1   | D     | 1369 | THR  |
| 1   | D     | 1406 | ALA  |
| 1   | D     | 1791 | ARG  |
| 1   | E     | 915  | GLU  |
| 1   | E     | 1115 | ILE  |
| 1   | E     | 1339 | LEU  |
| 1   | E     | 1369 | THR  |
| 1   | E     | 1791 | ARG  |
| 1   | F     | 1115 | ILE  |
| 1   | F     | 1339 | LEU  |
| 1   | F     | 1369 | THR  |
| 1   | F     | 1791 | ARG  |
| 1   | G     | 1115 | ILE  |
| 1   | H     | 915  | GLU  |
| 1   | H     | 960  | GLY  |
| 1   | H     | 1115 | ILE  |
| 1   | H     | 1212 | ASP  |
| 1   | H     | 1339 | LEU  |
| 1   | H     | 1369 | THR  |
| 1   | I     | 1115 | ILE  |
| 1   | J     | 1115 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 1204 | ARG  |
| 1   | J     | 1339 | LEU  |
| 1   | J     | 1369 | THR  |
| 1   | K     | 1115 | ILE  |
| 1   | K     | 1369 | THR  |
| 1   | K     | 1745 | ASP  |
| 1   | L     | 915  | GLU  |
| 1   | L     | 1115 | ILE  |
| 1   | L     | 1746 | THR  |
| 1   | M     | 960  | GLY  |
| 1   | M     | 1115 | ILE  |
| 1   | M     | 1369 | THR  |
| 1   | N     | 960  | GLY  |
| 1   | N     | 1115 | ILE  |
| 1   | N     | 1339 | LEU  |
| 1   | N     | 1369 | THR  |
| 1   | N     | 1402 | SER  |
| 1   | O     | 1115 | ILE  |
| 1   | O     | 1755 | PRO  |
| 1   | P     | 915  | GLU  |
| 1   | P     | 960  | GLY  |
| 1   | P     | 1115 | ILE  |
| 1   | P     | 1339 | LEU  |
| 1   | P     | 1369 | THR  |
| 1   | Q     | 1115 | ILE  |
| 1   | R     | 960  | GLY  |
| 1   | R     | 1756 | GLU  |
| 1   | R     | 1758 | VAL  |
| 1   | A     | 1508 | SER  |
| 1   | B     | 1204 | ARG  |
| 1   | C     | 1511 | GLY  |
| 1   | E     | 1760 | VAL  |
| 1   | G     | 1369 | THR  |
| 1   | I     | 1177 | GLY  |
| 1   | J     | 1203 | PRO  |
| 1   | J     | 1760 | VAL  |
| 1   | L     | 960  | GLY  |
| 1   | L     | 1403 | PRO  |
| 1   | P     | 1760 | VAL  |
| 1   | R     | 1115 | ILE  |
| 1   | C     | 1760 | VAL  |
| 1   | E     | 1403 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1511 | GLY  |
| 1   | F     | 1760 | VAL  |
| 1   | G     | 1760 | VAL  |
| 1   | M     | 1760 | VAL  |
| 1   | A     | 1511 | GLY  |
| 1   | C     | 1204 | ARG  |
| 1   | D     | 1204 | ARG  |
| 1   | E     | 1204 | ARG  |
| 1   | H     | 1203 | PRO  |
| 1   | K     | 1204 | ARG  |
| 1   | P     | 1204 | ARG  |
| 1   | B     | 1759 | PRO  |
| 1   | C     | 1983 | GLY  |
| 1   | L     | 1747 | GLY  |
| 1   | N     | 1403 | PRO  |
| 1   | N     | 1760 | VAL  |
| 1   | A     | 1204 | ARG  |
| 1   | A     | 1713 | PRO  |
| 1   | B     | 1511 | GLY  |
| 1   | H     | 1760 | VAL  |
| 1   | J     | 1511 | GLY  |
| 1   | P     | 1511 | GLY  |

### 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     | 836/863 (97%) | 802 (96%) | 34 (4%)  | 35          | 69 |
| 1   | B     | 836/863 (97%) | 808 (97%) | 28 (3%)  | 43          | 74 |
| 1   | C     | 836/863 (97%) | 811 (97%) | 25 (3%)  | 46          | 75 |
| 1   | D     | 836/863 (97%) | 809 (97%) | 27 (3%)  | 44          | 74 |
| 1   | E     | 825/863 (96%) | 802 (97%) | 23 (3%)  | 49          | 76 |
| 1   | F     | 828/863 (96%) | 801 (97%) | 27 (3%)  | 43          | 74 |
| 1   | G     | 824/863 (96%) | 802 (97%) | 22 (3%)  | 50          | 77 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 1   | H     | 831/863 (96%)     | 809 (97%)   | 22 (3%)  | 51          | 78 |
| 1   | I     | 503/863 (58%)     | 487 (97%)   | 16 (3%)  | 44          | 74 |
| 1   | J     | 825/863 (96%)     | 795 (96%)   | 30 (4%)  | 40          | 72 |
| 1   | K     | 825/863 (96%)     | 800 (97%)   | 25 (3%)  | 46          | 75 |
| 1   | L     | 674/863 (78%)     | 653 (97%)   | 21 (3%)  | 45          | 75 |
| 1   | M     | 825/863 (96%)     | 803 (97%)   | 22 (3%)  | 50          | 77 |
| 1   | N     | 825/863 (96%)     | 795 (96%)   | 30 (4%)  | 40          | 72 |
| 1   | O     | 483/863 (56%)     | 467 (97%)   | 16 (3%)  | 43          | 74 |
| 1   | P     | 825/863 (96%)     | 796 (96%)   | 29 (4%)  | 41          | 73 |
| 1   | Q     | 464/863 (54%)     | 452 (97%)   | 12 (3%)  | 51          | 78 |
| 1   | R     | 490/863 (57%)     | 478 (98%)   | 12 (2%)  | 54          | 79 |
| All | All   | 13391/15534 (86%) | 12970 (97%) | 421 (3%) | 45          | 75 |

All (421) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 956  | THR  |
| 1   | A     | 961  | ASP  |
| 1   | A     | 969  | LYS  |
| 1   | A     | 977  | ASP  |
| 1   | A     | 985  | SER  |
| 1   | A     | 1003 | SER  |
| 1   | A     | 1005 | ASP  |
| 1   | A     | 1064 | GLU  |
| 1   | A     | 1105 | SER  |
| 1   | A     | 1138 | ARG  |
| 1   | A     | 1174 | LEU  |
| 1   | A     | 1271 | LEU  |
| 1   | A     | 1331 | VAL  |
| 1   | A     | 1385 | ASP  |
| 1   | A     | 1410 | ARG  |
| 1   | A     | 1479 | GLU  |
| 1   | A     | 1522 | ASP  |
| 1   | A     | 1552 | GLU  |
| 1   | A     | 1578 | VAL  |
| 1   | A     | 1604 | ILE  |
| 1   | A     | 1610 | SER  |
| 1   | A     | 1613 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1640 | GLN  |
| 1   | A     | 1647 | LEU  |
| 1   | A     | 1659 | ARG  |
| 1   | A     | 1673 | ARG  |
| 1   | A     | 1712 | LEU  |
| 1   | A     | 1750 | GLN  |
| 1   | A     | 1796 | SER  |
| 1   | A     | 1876 | VAL  |
| 1   | A     | 1940 | SER  |
| 1   | A     | 1979 | ARG  |
| 1   | A     | 2006 | PHE  |
| 1   | A     | 2007 | LEU  |
| 1   | B     | 961  | ASP  |
| 1   | B     | 1022 | ARG  |
| 1   | B     | 1105 | SER  |
| 1   | B     | 1142 | SER  |
| 1   | B     | 1271 | LEU  |
| 1   | B     | 1302 | ARG  |
| 1   | B     | 1331 | VAL  |
| 1   | B     | 1345 | ARG  |
| 1   | B     | 1385 | ASP  |
| 1   | B     | 1393 | GLN  |
| 1   | B     | 1402 | SER  |
| 1   | B     | 1433 | SER  |
| 1   | B     | 1441 | ARG  |
| 1   | B     | 1510 | ASN  |
| 1   | B     | 1519 | CYS  |
| 1   | B     | 1522 | ASP  |
| 1   | B     | 1578 | VAL  |
| 1   | B     | 1593 | GLU  |
| 1   | B     | 1604 | ILE  |
| 1   | B     | 1647 | LEU  |
| 1   | B     | 1673 | ARG  |
| 1   | B     | 1745 | ASP  |
| 1   | B     | 1753 | VAL  |
| 1   | B     | 1757 | GLN  |
| 1   | B     | 1791 | ARG  |
| 1   | B     | 1825 | ILE  |
| 1   | B     | 1876 | VAL  |
| 1   | B     | 2007 | LEU  |
| 1   | C     | 883  | MET  |
| 1   | C     | 961  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1022 | ARG  |
| 1   | C     | 1086 | ARG  |
| 1   | C     | 1105 | SER  |
| 1   | C     | 1128 | LEU  |
| 1   | C     | 1271 | LEU  |
| 1   | C     | 1302 | ARG  |
| 1   | C     | 1331 | VAL  |
| 1   | C     | 1345 | ARG  |
| 1   | C     | 1385 | ASP  |
| 1   | C     | 1437 | VAL  |
| 1   | C     | 1438 | THR  |
| 1   | C     | 1441 | ARG  |
| 1   | C     | 1510 | ASN  |
| 1   | C     | 1578 | VAL  |
| 1   | C     | 1593 | GLU  |
| 1   | C     | 1604 | ILE  |
| 1   | C     | 1647 | LEU  |
| 1   | C     | 1666 | ARG  |
| 1   | C     | 1673 | ARG  |
| 1   | C     | 1712 | LEU  |
| 1   | C     | 1825 | ILE  |
| 1   | C     | 1876 | VAL  |
| 1   | C     | 2007 | LEU  |
| 1   | D     | 883  | MET  |
| 1   | D     | 888  | LEU  |
| 1   | D     | 961  | ASP  |
| 1   | D     | 1022 | ARG  |
| 1   | D     | 1105 | SER  |
| 1   | D     | 1128 | LEU  |
| 1   | D     | 1271 | LEU  |
| 1   | D     | 1302 | ARG  |
| 1   | D     | 1331 | VAL  |
| 1   | D     | 1345 | ARG  |
| 1   | D     | 1385 | ASP  |
| 1   | D     | 1393 | GLN  |
| 1   | D     | 1399 | LEU  |
| 1   | D     | 1400 | CYS  |
| 1   | D     | 1438 | THR  |
| 1   | D     | 1510 | ASN  |
| 1   | D     | 1522 | ASP  |
| 1   | D     | 1578 | VAL  |
| 1   | D     | 1593 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1604 | ILE  |
| 1   | D     | 1647 | LEU  |
| 1   | D     | 1673 | ARG  |
| 1   | D     | 1712 | LEU  |
| 1   | D     | 1825 | ILE  |
| 1   | D     | 1876 | VAL  |
| 1   | D     | 1976 | ARG  |
| 1   | D     | 2007 | LEU  |
| 1   | E     | 961  | ASP  |
| 1   | E     | 1022 | ARG  |
| 1   | E     | 1105 | SER  |
| 1   | E     | 1142 | SER  |
| 1   | E     | 1271 | LEU  |
| 1   | E     | 1302 | ARG  |
| 1   | E     | 1331 | VAL  |
| 1   | E     | 1345 | ARG  |
| 1   | E     | 1385 | ASP  |
| 1   | E     | 1393 | GLN  |
| 1   | E     | 1398 | ARG  |
| 1   | E     | 1399 | LEU  |
| 1   | E     | 1510 | ASN  |
| 1   | E     | 1578 | VAL  |
| 1   | E     | 1593 | GLU  |
| 1   | E     | 1604 | ILE  |
| 1   | E     | 1647 | LEU  |
| 1   | E     | 1673 | ARG  |
| 1   | E     | 1712 | LEU  |
| 1   | E     | 1742 | ASP  |
| 1   | E     | 1825 | ILE  |
| 1   | E     | 1876 | VAL  |
| 1   | E     | 2007 | LEU  |
| 1   | F     | 961  | ASP  |
| 1   | F     | 977  | ASP  |
| 1   | F     | 1022 | ARG  |
| 1   | F     | 1105 | SER  |
| 1   | F     | 1128 | LEU  |
| 1   | F     | 1142 | SER  |
| 1   | F     | 1170 | MET  |
| 1   | F     | 1271 | LEU  |
| 1   | F     | 1302 | ARG  |
| 1   | F     | 1331 | VAL  |
| 1   | F     | 1345 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 1385 | ASP  |
| 1   | F     | 1393 | GLN  |
| 1   | F     | 1398 | ARG  |
| 1   | F     | 1438 | THR  |
| 1   | F     | 1510 | ASN  |
| 1   | F     | 1522 | ASP  |
| 1   | F     | 1578 | VAL  |
| 1   | F     | 1593 | GLU  |
| 1   | F     | 1604 | ILE  |
| 1   | F     | 1647 | LEU  |
| 1   | F     | 1673 | ARG  |
| 1   | F     | 1712 | LEU  |
| 1   | F     | 1748 | GLN  |
| 1   | F     | 1825 | ILE  |
| 1   | F     | 1876 | VAL  |
| 1   | F     | 2007 | LEU  |
| 1   | G     | 961  | ASP  |
| 1   | G     | 1022 | ARG  |
| 1   | G     | 1105 | SER  |
| 1   | G     | 1128 | LEU  |
| 1   | G     | 1271 | LEU  |
| 1   | G     | 1302 | ARG  |
| 1   | G     | 1331 | VAL  |
| 1   | G     | 1345 | ARG  |
| 1   | G     | 1385 | ASP  |
| 1   | G     | 1438 | THR  |
| 1   | G     | 1510 | ASN  |
| 1   | G     | 1522 | ASP  |
| 1   | G     | 1578 | VAL  |
| 1   | G     | 1593 | GLU  |
| 1   | G     | 1604 | ILE  |
| 1   | G     | 1647 | LEU  |
| 1   | G     | 1673 | ARG  |
| 1   | G     | 1712 | LEU  |
| 1   | G     | 1825 | ILE  |
| 1   | G     | 1833 | ARG  |
| 1   | G     | 1876 | VAL  |
| 1   | G     | 2007 | LEU  |
| 1   | H     | 961  | ASP  |
| 1   | H     | 977  | ASP  |
| 1   | H     | 1022 | ARG  |
| 1   | H     | 1105 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 1128 | LEU  |
| 1   | H     | 1271 | LEU  |
| 1   | H     | 1302 | ARG  |
| 1   | H     | 1331 | VAL  |
| 1   | H     | 1345 | ARG  |
| 1   | H     | 1385 | ASP  |
| 1   | H     | 1400 | CYS  |
| 1   | H     | 1438 | THR  |
| 1   | H     | 1510 | ASN  |
| 1   | H     | 1519 | CYS  |
| 1   | H     | 1578 | VAL  |
| 1   | H     | 1593 | GLU  |
| 1   | H     | 1604 | ILE  |
| 1   | H     | 1647 | LEU  |
| 1   | H     | 1673 | ARG  |
| 1   | H     | 1825 | ILE  |
| 1   | H     | 1876 | VAL  |
| 1   | H     | 2007 | LEU  |
| 1   | I     | 961  | ASP  |
| 1   | I     | 1022 | ARG  |
| 1   | I     | 1105 | SER  |
| 1   | I     | 1128 | LEU  |
| 1   | I     | 1142 | SER  |
| 1   | I     | 1438 | THR  |
| 1   | I     | 1510 | ASN  |
| 1   | I     | 1522 | ASP  |
| 1   | I     | 1578 | VAL  |
| 1   | I     | 1593 | GLU  |
| 1   | I     | 1604 | ILE  |
| 1   | I     | 1647 | LEU  |
| 1   | I     | 1673 | ARG  |
| 1   | I     | 1712 | LEU  |
| 1   | I     | 1746 | THR  |
| 1   | I     | 1750 | GLN  |
| 1   | J     | 961  | ASP  |
| 1   | J     | 977  | ASP  |
| 1   | J     | 1006 | ARG  |
| 1   | J     | 1022 | ARG  |
| 1   | J     | 1105 | SER  |
| 1   | J     | 1128 | LEU  |
| 1   | J     | 1271 | LEU  |
| 1   | J     | 1302 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 1331 | VAL  |
| 1   | J     | 1345 | ARG  |
| 1   | J     | 1385 | ASP  |
| 1   | J     | 1393 | GLN  |
| 1   | J     | 1400 | CYS  |
| 1   | J     | 1405 | ARG  |
| 1   | J     | 1409 | ARG  |
| 1   | J     | 1427 | ASN  |
| 1   | J     | 1510 | ASN  |
| 1   | J     | 1522 | ASP  |
| 1   | J     | 1525 | THR  |
| 1   | J     | 1578 | VAL  |
| 1   | J     | 1593 | GLU  |
| 1   | J     | 1604 | ILE  |
| 1   | J     | 1647 | LEU  |
| 1   | J     | 1673 | ARG  |
| 1   | J     | 1712 | LEU  |
| 1   | J     | 1741 | ILE  |
| 1   | J     | 1749 | SER  |
| 1   | J     | 1825 | ILE  |
| 1   | J     | 1876 | VAL  |
| 1   | J     | 2007 | LEU  |
| 1   | K     | 961  | ASP  |
| 1   | K     | 977  | ASP  |
| 1   | K     | 1022 | ARG  |
| 1   | K     | 1105 | SER  |
| 1   | K     | 1142 | SER  |
| 1   | K     | 1174 | LEU  |
| 1   | K     | 1271 | LEU  |
| 1   | K     | 1302 | ARG  |
| 1   | K     | 1331 | VAL  |
| 1   | K     | 1345 | ARG  |
| 1   | K     | 1385 | ASP  |
| 1   | K     | 1393 | GLN  |
| 1   | K     | 1398 | ARG  |
| 1   | K     | 1399 | LEU  |
| 1   | K     | 1402 | SER  |
| 1   | K     | 1510 | ASN  |
| 1   | K     | 1578 | VAL  |
| 1   | K     | 1593 | GLU  |
| 1   | K     | 1604 | ILE  |
| 1   | K     | 1647 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K     | 1673 | ARG  |
| 1   | K     | 1825 | ILE  |
| 1   | K     | 1876 | VAL  |
| 1   | K     | 1982 | ASN  |
| 1   | K     | 2007 | LEU  |
| 1   | L     | 961  | ASP  |
| 1   | L     | 977  | ASP  |
| 1   | L     | 1022 | ARG  |
| 1   | L     | 1105 | SER  |
| 1   | L     | 1142 | SER  |
| 1   | L     | 1409 | ARG  |
| 1   | L     | 1435 | GLU  |
| 1   | L     | 1436 | LEU  |
| 1   | L     | 1510 | ASN  |
| 1   | L     | 1522 | ASP  |
| 1   | L     | 1525 | THR  |
| 1   | L     | 1578 | VAL  |
| 1   | L     | 1593 | GLU  |
| 1   | L     | 1604 | ILE  |
| 1   | L     | 1647 | LEU  |
| 1   | L     | 1673 | ARG  |
| 1   | L     | 1712 | LEU  |
| 1   | L     | 1741 | ILE  |
| 1   | L     | 1825 | ILE  |
| 1   | L     | 1876 | VAL  |
| 1   | L     | 2007 | LEU  |
| 1   | M     | 961  | ASP  |
| 1   | M     | 977  | ASP  |
| 1   | M     | 1022 | ARG  |
| 1   | M     | 1105 | SER  |
| 1   | M     | 1128 | LEU  |
| 1   | M     | 1142 | SER  |
| 1   | M     | 1271 | LEU  |
| 1   | M     | 1302 | ARG  |
| 1   | M     | 1331 | VAL  |
| 1   | M     | 1345 | ARG  |
| 1   | M     | 1385 | ASP  |
| 1   | M     | 1393 | GLN  |
| 1   | M     | 1510 | ASN  |
| 1   | M     | 1522 | ASP  |
| 1   | M     | 1578 | VAL  |
| 1   | M     | 1593 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | M     | 1604 | ILE  |
| 1   | M     | 1647 | LEU  |
| 1   | M     | 1673 | ARG  |
| 1   | M     | 1825 | ILE  |
| 1   | M     | 1876 | VAL  |
| 1   | M     | 2007 | LEU  |
| 1   | N     | 961  | ASP  |
| 1   | N     | 1022 | ARG  |
| 1   | N     | 1105 | SER  |
| 1   | N     | 1128 | LEU  |
| 1   | N     | 1142 | SER  |
| 1   | N     | 1174 | LEU  |
| 1   | N     | 1190 | GLU  |
| 1   | N     | 1192 | LEU  |
| 1   | N     | 1194 | THR  |
| 1   | N     | 1271 | LEU  |
| 1   | N     | 1302 | ARG  |
| 1   | N     | 1331 | VAL  |
| 1   | N     | 1345 | ARG  |
| 1   | N     | 1385 | ASP  |
| 1   | N     | 1399 | LEU  |
| 1   | N     | 1400 | CYS  |
| 1   | N     | 1409 | ARG  |
| 1   | N     | 1438 | THR  |
| 1   | N     | 1510 | ASN  |
| 1   | N     | 1522 | ASP  |
| 1   | N     | 1578 | VAL  |
| 1   | N     | 1593 | GLU  |
| 1   | N     | 1604 | ILE  |
| 1   | N     | 1647 | LEU  |
| 1   | N     | 1673 | ARG  |
| 1   | N     | 1712 | LEU  |
| 1   | N     | 1742 | ASP  |
| 1   | N     | 1825 | ILE  |
| 1   | N     | 1876 | VAL  |
| 1   | N     | 2007 | LEU  |
| 1   | O     | 961  | ASP  |
| 1   | O     | 977  | ASP  |
| 1   | O     | 1022 | ARG  |
| 1   | O     | 1105 | SER  |
| 1   | O     | 1128 | LEU  |
| 1   | O     | 1142 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | O     | 1411 | THR  |
| 1   | O     | 1510 | ASN  |
| 1   | O     | 1522 | ASP  |
| 1   | O     | 1578 | VAL  |
| 1   | O     | 1593 | GLU  |
| 1   | O     | 1604 | ILE  |
| 1   | O     | 1647 | LEU  |
| 1   | O     | 1673 | ARG  |
| 1   | O     | 1712 | LEU  |
| 1   | O     | 1748 | GLN  |
| 1   | P     | 961  | ASP  |
| 1   | P     | 1022 | ARG  |
| 1   | P     | 1105 | SER  |
| 1   | P     | 1128 | LEU  |
| 1   | P     | 1142 | SER  |
| 1   | P     | 1173 | GLN  |
| 1   | P     | 1174 | LEU  |
| 1   | P     | 1271 | LEU  |
| 1   | P     | 1302 | ARG  |
| 1   | P     | 1331 | VAL  |
| 1   | P     | 1345 | ARG  |
| 1   | P     | 1385 | ASP  |
| 1   | P     | 1393 | GLN  |
| 1   | P     | 1400 | CYS  |
| 1   | P     | 1510 | ASN  |
| 1   | P     | 1522 | ASP  |
| 1   | P     | 1578 | VAL  |
| 1   | P     | 1593 | GLU  |
| 1   | P     | 1604 | ILE  |
| 1   | P     | 1647 | LEU  |
| 1   | P     | 1673 | ARG  |
| 1   | P     | 1712 | LEU  |
| 1   | P     | 1716 | THR  |
| 1   | P     | 1825 | ILE  |
| 1   | P     | 1876 | VAL  |
| 1   | P     | 1976 | ARG  |
| 1   | P     | 1994 | THR  |
| 1   | P     | 2006 | PHE  |
| 1   | P     | 2007 | LEU  |
| 1   | Q     | 961  | ASP  |
| 1   | Q     | 1022 | ARG  |
| 1   | Q     | 1105 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | Q     | 1128 | LEU  |
| 1   | Q     | 1142 | SER  |
| 1   | Q     | 1510 | ASN  |
| 1   | Q     | 1578 | VAL  |
| 1   | Q     | 1593 | GLU  |
| 1   | Q     | 1604 | ILE  |
| 1   | Q     | 1647 | LEU  |
| 1   | Q     | 1673 | ARG  |
| 1   | Q     | 1712 | LEU  |
| 1   | R     | 961  | ASP  |
| 1   | R     | 1022 | ARG  |
| 1   | R     | 1105 | SER  |
| 1   | R     | 1128 | LEU  |
| 1   | R     | 1510 | ASN  |
| 1   | R     | 1533 | GLU  |
| 1   | R     | 1578 | VAL  |
| 1   | R     | 1593 | GLU  |
| 1   | R     | 1604 | ILE  |
| 1   | R     | 1647 | LEU  |
| 1   | R     | 1673 | ARG  |
| 1   | R     | 1712 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1416 | ASN  |
| 1   | B     | 1633 | ASN  |
| 1   | C     | 1459 | ASN  |
| 1   | C     | 1633 | ASN  |
| 1   | D     | 1459 | ASN  |
| 1   | D     | 1633 | ASN  |
| 1   | E     | 1633 | ASN  |
| 1   | F     | 1459 | ASN  |
| 1   | F     | 1633 | ASN  |
| 1   | G     | 1459 | ASN  |
| 1   | G     | 1633 | ASN  |
| 1   | H     | 1459 | ASN  |
| 1   | H     | 1597 | GLN  |
| 1   | H     | 1633 | ASN  |
| 1   | I     | 1633 | ASN  |
| 1   | J     | 1459 | ASN  |
| 1   | J     | 1633 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K     | 1459 | ASN  |
| 1   | K     | 1633 | ASN  |
| 1   | K     | 1735 | HIS  |
| 1   | L     | 1633 | ASN  |
| 1   | M     | 1633 | ASN  |
| 1   | N     | 1459 | ASN  |
| 1   | O     | 1633 | ASN  |
| 1   | P     | 1633 | ASN  |
| 1   | Q     | 1633 | ASN  |
| 1   | R     | 1633 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

30 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   | NAP  | A     | 3001 | -    | 44,52,52     | 0.75 | 0           | 51,80,80    | 0.79 | 0           |
| 2   | NAP  | A     | 3002 | -    | 25,29,52     | 0.68 | 0           | 32,45,80    | 1.06 | 1 (3%)      |
| 2   | NAP  | B     | 3001 | -    | 44,52,52     | 0.83 | 2 (4%)      | 51,80,80    | 0.98 | 2 (3%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAP  | B     | 3002 | -    | 25,29,52     | 0.78 | 0        | 32,45,80    | 1.31 | 3 (9%)   |
| 2   | NAP  | C     | 3001 | -    | 44,52,52     | 0.71 | 1 (2%)   | 51,80,80    | 0.70 | 0        |
| 2   | NAP  | C     | 3002 | -    | 28,33,52     | 0.72 | 0        | 32,52,80    | 0.95 | 2 (6%)   |
| 2   | NAP  | D     | 3001 | -    | 44,52,52     | 0.64 | 1 (2%)   | 51,80,80    | 0.86 | 0        |
| 2   | NAP  | D     | 3002 | -    | 25,29,52     | 0.71 | 0        | 32,45,80    | 1.19 | 4 (12%)  |
| 2   | NAP  | E     | 3001 | -    | 44,52,52     | 0.69 | 2 (4%)   | 51,80,80    | 0.76 | 2 (3%)   |
| 2   | NAP  | F     | 3001 | -    | 44,52,52     | 0.81 | 2 (4%)   | 51,80,80    | 0.86 | 1 (1%)   |
| 2   | NAP  | F     | 3002 | -    | 25,29,52     | 0.70 | 0        | 32,45,80    | 1.17 | 3 (9%)   |
| 2   | NAP  | G     | 3001 | -    | 44,52,52     | 0.59 | 0        | 51,80,80    | 0.75 | 1 (1%)   |
| 2   | NAP  | G     | 3002 | -    | 25,29,52     | 0.66 | 0        | 32,45,80    | 1.19 | 2 (6%)   |
| 2   | NAP  | H     | 3001 | -    | 44,52,52     | 0.63 | 0        | 51,80,80    | 0.68 | 0        |
| 2   | NAP  | H     | 3002 | -    | 25,29,52     | 0.71 | 0        | 32,45,80    | 1.15 | 5 (15%)  |
| 2   | NAP  | I     | 3001 | -    | 44,52,52     | 0.64 | 0        | 51,80,80    | 0.58 | 0        |
| 2   | NAP  | J     | 3001 | -    | 44,52,52     | 0.62 | 1 (2%)   | 51,80,80    | 0.79 | 1 (1%)   |
| 2   | NAP  | J     | 3002 | -    | 25,29,52     | 0.76 | 0        | 32,45,80    | 1.14 | 2 (6%)   |
| 2   | NAP  | K     | 3001 | -    | 44,52,52     | 0.88 | 2 (4%)   | 51,80,80    | 0.94 | 2 (3%)   |
| 2   | NAP  | K     | 3002 | -    | 25,29,52     | 0.62 | 0        | 32,45,80    | 1.26 | 4 (12%)  |
| 2   | NAP  | L     | 3001 | -    | 44,52,52     | 0.82 | 1 (2%)   | 51,80,80    | 0.87 | 1 (1%)   |
| 2   | NAP  | M     | 3001 | -    | 44,52,52     | 0.83 | 2 (4%)   | 51,80,80    | 0.74 | 0        |
| 2   | NAP  | M     | 3002 | -    | 25,29,52     | 0.86 | 1 (4%)   | 32,45,80    | 1.06 | 2 (6%)   |
| 2   | NAP  | N     | 3001 | -    | 44,52,52     | 0.74 | 1 (2%)   | 51,80,80    | 0.71 | 1 (1%)   |
| 2   | NAP  | N     | 3002 | -    | 25,29,52     | 0.84 | 1 (4%)   | 32,45,80    | 1.36 | 2 (6%)   |
| 2   | NAP  | O     | 3001 | -    | 44,52,52     | 0.86 | 1 (2%)   | 51,80,80    | 0.85 | 0        |
| 2   | NAP  | P     | 3001 | -    | 44,52,52     | 0.70 | 1 (2%)   | 51,80,80    | 0.70 | 0        |
| 2   | NAP  | P     | 3002 | -    | 25,29,52     | 0.72 | 0        | 32,45,80    | 1.21 | 4 (12%)  |
| 2   | NAP  | Q     | 3001 | -    | 44,52,52     | 0.63 | 0        | 51,80,80    | 0.98 | 3 (5%)   |
| 2   | NAP  | R     | 3001 | -    | 44,52,52     | 0.54 | 0        | 51,80,80    | 0.62 | 1 (1%)   |

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   | NAP  | A     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | A     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | B     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | NAP  | B     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | C     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | C     | 3002 | -    | -       | 0/17/37/67 | 0/3/3/5 |
| 2   | NAP  | D     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | D     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | E     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | F     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | F     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | G     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | G     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | H     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | H     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | I     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | J     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | J     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | K     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | K     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | L     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | M     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | M     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | N     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | N     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | O     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | P     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | P     | 3002 | -    | -       | 0/11/31/67 | 0/3/3/5 |
| 2   | NAP  | Q     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |
| 2   | NAP  | R     | 3001 | -    | -       | 0/27/67/67 | 0/5/5/5 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 3001 | NAP  | O4D-C1D | -3.16 | 1.36        | 1.41     |
| 2   | N     | 3001 | NAP  | O4D-C1D | -3.07 | 1.37        | 1.41     |
| 2   | K     | 3001 | NAP  | O7N-C7N | -2.94 | 1.18        | 1.24     |
| 2   | M     | 3001 | NAP  | O4D-C1D | -2.89 | 1.37        | 1.41     |
| 2   | M     | 3001 | NAP  | C7N-N7N | -2.88 | 1.27        | 1.33     |
| 2   | E     | 3001 | NAP  | P2B-O1X | -2.26 | 1.43        | 1.50     |
| 2   | D     | 3001 | NAP  | C2D-C1D | 2.03  | 1.56        | 1.53     |
| 2   | B     | 3001 | NAP  | C2D-C1D | 2.04  | 1.56        | 1.53     |
| 2   | E     | 3001 | NAP  | C2D-C1D | 2.05  | 1.56        | 1.53     |
| 2   | P     | 3001 | NAP  | P2B-O1X | 2.07  | 1.57        | 1.50     |
| 2   | F     | 3001 | NAP  | C2D-C1D | 2.38  | 1.57        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | C     | 3001 | NAP  | C2D-C1D | 2.38 | 1.57        | 1.53     |
| 2   | J     | 3001 | NAP  | C2D-C1D | 2.44 | 1.57        | 1.53     |
| 2   | F     | 3001 | NAP  | C3N-C7N | 2.72 | 1.54        | 1.50     |
| 2   | M     | 3002 | NAP  | PA-O1A  | 2.84 | 1.60        | 1.50     |
| 2   | N     | 3002 | NAP  | PA-O1A  | 2.85 | 1.60        | 1.50     |
| 2   | K     | 3001 | NAP  | C2D-C1D | 3.20 | 1.58        | 1.53     |
| 2   | O     | 3001 | NAP  | P2B-O1X | 3.46 | 1.62        | 1.50     |
| 2   | L     | 3001 | NAP  | P2B-O1X | 3.52 | 1.62        | 1.50     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | N     | 3002 | NAP  | O2B-P2B-O1X | -4.24 | 92.64       | 109.26   |
| 2   | F     | 3001 | NAP  | C4D-O4D-C1D | -3.96 | 105.55      | 109.77   |
| 2   | B     | 3002 | NAP  | O5B-PA-O1A  | -3.80 | 95.83       | 106.47   |
| 2   | K     | 3001 | NAP  | O2A-PA-O5B  | -3.78 | 90.31       | 108.14   |
| 2   | P     | 3002 | NAP  | O2B-P2B-O1X | -3.45 | 95.72       | 109.26   |
| 2   | K     | 3002 | NAP  | O2A-PA-O5B  | -3.00 | 98.75       | 106.73   |
| 2   | J     | 3002 | NAP  | O3-PA-O5B   | -2.90 | 99.01       | 106.73   |
| 2   | Q     | 3001 | NAP  | C4B-O4B-C1B | -2.87 | 106.72      | 109.77   |
| 2   | H     | 3002 | NAP  | O5B-PA-O1A  | -2.77 | 98.70       | 106.47   |
| 2   | F     | 3002 | NAP  | O3-PA-O5B   | -2.72 | 99.51       | 106.73   |
| 2   | L     | 3001 | NAP  | O2A-PA-O5B  | -2.64 | 95.66       | 108.14   |
| 2   | B     | 3002 | NAP  | O3-PA-O5B   | -2.61 | 99.77       | 106.73   |
| 2   | D     | 3002 | NAP  | O2X-P2B-O2B | -2.54 | 94.45       | 106.00   |
| 2   | A     | 3002 | NAP  | O3-PA-O5B   | -2.53 | 100.00      | 106.73   |
| 2   | Q     | 3001 | NAP  | O2D-C2D-C1D | -2.40 | 104.10      | 111.61   |
| 2   | D     | 3002 | NAP  | O3-PA-O5B   | -2.37 | 100.41      | 106.73   |
| 2   | G     | 3002 | NAP  | O2X-P2B-O2B | -2.35 | 95.31       | 106.00   |
| 2   | K     | 3002 | NAP  | O2X-P2B-O2B | -2.35 | 95.31       | 106.00   |
| 2   | K     | 3002 | NAP  | O3-PA-O5B   | -2.34 | 100.49      | 106.73   |
| 2   | M     | 3002 | NAP  | O2B-P2B-O1X | -2.28 | 100.33      | 109.26   |
| 2   | N     | 3001 | NAP  | O3X-P2B-O2B | -2.26 | 95.72       | 106.00   |
| 2   | F     | 3002 | NAP  | O2X-P2B-O2B | -2.25 | 95.78       | 106.00   |
| 2   | P     | 3002 | NAP  | O3-PA-O5B   | -2.22 | 100.83      | 106.73   |
| 2   | C     | 3002 | NAP  | O2X-P2B-O2B | -2.20 | 96.01       | 106.00   |
| 2   | F     | 3002 | NAP  | O2A-PA-O5B  | -2.16 | 100.99      | 106.73   |
| 2   | E     | 3001 | NAP  | O2D-C2D-C1D | -2.04 | 105.24      | 111.61   |
| 2   | R     | 3001 | NAP  | O2A-PA-O5B  | -2.03 | 98.55       | 108.14   |
| 2   | K     | 3001 | NAP  | O3X-P2B-O2B | -2.02 | 96.81       | 106.00   |
| 2   | H     | 3002 | NAP  | O2X-P2B-O2B | -2.01 | 96.85       | 106.00   |
| 2   | G     | 3001 | NAP  | O2D-C2D-C1D | -2.01 | 105.33      | 111.61   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | J     | 3002 | NAP  | O2X-P2B-O2B | -2.00 | 96.89       | 106.00   |
| 2   | P     | 3002 | NAP  | PA-O5B-C5B  | 2.00  | 123.81      | 118.30   |
| 2   | K     | 3002 | NAP  | PA-O5B-C5B  | 2.03  | 123.88      | 118.30   |
| 2   | B     | 3001 | NAP  | O3D-C3D-C2D | 2.03  | 118.33      | 111.83   |
| 2   | P     | 3002 | NAP  | O3-PA-O2A   | 2.03  | 115.82      | 107.61   |
| 2   | B     | 3002 | NAP  | O3-PA-O2A   | 2.10  | 116.09      | 107.61   |
| 2   | J     | 3001 | NAP  | O2D-C2D-C3D | 2.13  | 118.64      | 111.83   |
| 2   | C     | 3002 | NAP  | O2N-PN-O1N  | 2.14  | 118.86      | 110.50   |
| 2   | H     | 3002 | NAP  | O3-PA-O2A   | 2.15  | 116.28      | 107.61   |
| 2   | H     | 3002 | NAP  | O2A-PA-O5B  | 2.21  | 112.60      | 106.73   |
| 2   | D     | 3002 | NAP  | PA-O5B-C5B  | 2.24  | 124.47      | 118.30   |
| 2   | H     | 3002 | NAP  | PA-O5B-C5B  | 2.26  | 124.53      | 118.30   |
| 2   | E     | 3001 | NAP  | C4D-O4D-C1D | 2.37  | 112.29      | 109.77   |
| 2   | N     | 3002 | NAP  | PA-O5B-C5B  | 2.41  | 124.92      | 118.30   |
| 2   | M     | 3002 | NAP  | PA-O5B-C5B  | 2.42  | 124.97      | 118.30   |
| 2   | D     | 3002 | NAP  | O3-PA-O2A   | 2.44  | 117.45      | 107.61   |
| 2   | G     | 3002 | NAP  | PA-O5B-C5B  | 2.58  | 125.40      | 118.30   |
| 2   | B     | 3001 | NAP  | C4D-O4D-C1D | 3.40  | 113.39      | 109.77   |
| 2   | Q     | 3001 | NAP  | C4D-O4D-C1D | 4.28  | 114.33      | 109.77   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 3001 | NAP  | 2       | 0            |
| 2   | B     | 3001 | NAP  | 2       | 0            |
| 2   | C     | 3001 | NAP  | 1       | 0            |
| 2   | D     | 3001 | NAP  | 2       | 0            |
| 2   | E     | 3001 | NAP  | 1       | 0            |
| 2   | F     | 3001 | NAP  | 2       | 0            |
| 2   | I     | 3001 | NAP  | 1       | 0            |
| 2   | K     | 3001 | NAP  | 2       | 0            |
| 2   | L     | 3001 | NAP  | 1       | 0            |
| 2   | O     | 3001 | NAP  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 1   | A     | 1102/1140 (96%)   | 0.77   | 114 (10%) 7 7  | 84, 166, 265, 278     | 0     |
| 1   | B     | 1102/1140 (96%)   | 0.61   | 51 (4%) 33 27  | 85, 136, 221, 240     | 0     |
| 1   | C     | 1102/1140 (96%)   | 0.66   | 96 (8%) 11 9   | 89, 162, 233, 261     | 0     |
| 1   | D     | 1102/1140 (96%)   | 0.70   | 108 (9%) 8 7   | 92, 173, 262, 282     | 0     |
| 1   | E     | 1089/1140 (95%)   | 1.14   | 243 (22%) 1 1  | 127, 204, 264, 278    | 0     |
| 1   | F     | 1093/1140 (95%)   | 0.97   | 187 (17%) 2 2  | 125, 193, 236, 259    | 0     |
| 1   | G     | 1088/1140 (95%)   | 0.82   | 156 (14%) 3 4  | 108, 174, 224, 261    | 0     |
| 1   | H     | 1097/1140 (96%)   | 0.85   | 160 (14%) 3 3  | 113, 180, 220, 255    | 0     |
| 1   | I     | 655/1140 (57%)    | 0.80   | 66 (10%) 8 7   | 96, 167, 220, 254     | 0     |
| 1   | J     | 1089/1140 (95%)   | 0.68   | 82 (7%) 15 12  | 95, 166, 213, 252     | 0     |
| 1   | K     | 1089/1140 (95%)   | 0.68   | 76 (6%) 17 13  | 85, 138, 187, 226     | 0     |
| 1   | L     | 897/1140 (78%)    | 1.13   | 148 (16%) 2 3  | 81, 145, 244, 264     | 0     |
| 1   | M     | 1089/1140 (95%)   | 1.06   | 207 (19%) 1 2  | 111, 175, 239, 265    | 0     |
| 1   | N     | 1089/1140 (95%)   | 0.66   | 94 (8%) 11 9   | 107, 157, 205, 254    | 0     |
| 1   | O     | 633/1140 (55%)    | 0.69   | 39 (6%) 21 16  | 84, 131, 183, 222     | 0     |
| 1   | P     | 1089/1140 (95%)   | 0.72   | 97 (8%) 10 8   | 85, 150, 211, 247     | 0     |
| 1   | Q     | 608/1140 (53%)    | 1.75   | 200 (32%) 0 1  | 180, 229, 263, 279    | 0     |
| 1   | R     | 637/1140 (55%)    | 1.10   | 140 (21%) 1 1  | 158, 210, 247, 266    | 0     |
| All | All   | 17650/20520 (86%) | 0.85   | 2264 (12%) 4 5 | 81, 170, 243, 282     | 0     |

All (2264) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1074 | THR  | 18.2 |
| 1   | L     | 1871 | ASP  | 17.4 |
| 1   | Q     | 1073 | PRO  | 13.6 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 943  | PRO  | 13.1 |
| 1   | Q     | 942  | LEU  | 12.8 |
| 1   | M     | 1794 | VAL  | 12.6 |
| 1   | L     | 1947 | GLY  | 11.9 |
| 1   | L     | 1879 | ALA  | 11.4 |
| 1   | Q     | 1123 | LEU  | 11.2 |
| 1   | M     | 1799 | ALA  | 10.7 |
| 1   | L     | 1818 | ILE  | 10.4 |
| 1   | L     | 1948 | GLU  | 10.3 |
| 1   | M     | 1224 | ASP  | 9.3  |
| 1   | Q     | 946  | ALA  | 9.2  |
| 1   | M     | 1795 | ASN  | 9.1  |
| 1   | L     | 1768 | VAL  | 8.8  |
| 1   | E     | 1761 | PHE  | 8.7  |
| 1   | M     | 1773 | LEU  | 8.6  |
| 1   | A     | 1856 | GLU  | 8.6  |
| 1   | A     | 1275 | ALA  | 8.4  |
| 1   | Q     | 1152 | VAL  | 8.3  |
| 1   | L     | 1838 | ALA  | 8.2  |
| 1   | A     | 1274 | VAL  | 8.0  |
| 1   | A     | 1217 | LEU  | 7.9  |
| 1   | Q     | 1513 | TRP  | 7.8  |
| 1   | L     | 1769 | ILE  | 7.8  |
| 1   | L     | 1967 | GLY  | 7.7  |
| 1   | L     | 1792 | ILE  | 7.6  |
| 1   | M     | 1821 | GLU  | 7.6  |
| 1   | Q     | 1423 | LEU  | 7.5  |
| 1   | L     | 1850 | HIS  | 7.4  |
| 1   | F     | 1506 | GLY  | 7.4  |
| 1   | E     | 1983 | GLY  | 7.2  |
| 1   | L     | 1793 | VAL  | 7.2  |
| 1   | E     | 1982 | ASN  | 7.1  |
| 1   | E     | 1274 | VAL  | 7.1  |
| 1   | L     | 1856 | GLU  | 6.9  |
| 1   | E     | 1395 | TYR  | 6.9  |
| 1   | D     | 1948 | GLU  | 6.9  |
| 1   | F     | 1655 | GLU  | 6.9  |
| 1   | C     | 1983 | GLY  | 6.8  |
| 1   | Q     | 1588 | ALA  | 6.8  |
| 1   | Q     | 1717 | HIS  | 6.8  |
| 1   | Q     | 1683 | LEU  | 6.8  |
| 1   | E     | 1498 | HIS  | 6.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | L     | 1968 | ALA  | 6.8  |
| 1   | L     | 1880 | TRP  | 6.8  |
| 1   | E     | 1275 | ALA  | 6.7  |
| 1   | M     | 1280 | ASP  | 6.6  |
| 1   | A     | 1986 | PRO  | 6.5  |
| 1   | L     | 1964 | PRO  | 6.5  |
| 1   | Q     | 1107 | ILE  | 6.5  |
| 1   | L     | 1985 | ALA  | 6.5  |
| 1   | L     | 1887 | GLN  | 6.5  |
| 1   | A     | 1192 | LEU  | 6.5  |
| 1   | Q     | 1496 | THR  | 6.4  |
| 1   | L     | 1989 | GLY  | 6.4  |
| 1   | E     | 1388 | ALA  | 6.4  |
| 1   | K     | 1420 | GLY  | 6.4  |
| 1   | A     | 1288 | HIS  | 6.4  |
| 1   | L     | 2002 | PHE  | 6.4  |
| 1   | Q     | 1119 | MET  | 6.4  |
| 1   | A     | 1323 | VAL  | 6.3  |
| 1   | E     | 1192 | LEU  | 6.2  |
| 1   | M     | 1796 | SER  | 6.2  |
| 1   | E     | 1321 | LEU  | 6.2  |
| 1   | L     | 1771 | GLY  | 6.2  |
| 1   | M     | 1792 | ILE  | 6.2  |
| 1   | Q     | 945  | ALA  | 6.1  |
| 1   | L     | 1851 | ALA  | 6.1  |
| 1   | Q     | 944  | GLY  | 6.1  |
| 1   | M     | 1223 | ASP  | 6.1  |
| 1   | R     | 1739 | LEU  | 6.1  |
| 1   | B     | 1217 | LEU  | 6.1  |
| 1   | L     | 1780 | LEU  | 6.0  |
| 1   | Q     | 1174 | LEU  | 6.0  |
| 1   | E     | 1767 | TYR  | 6.0  |
| 1   | L     | 1942 | ALA  | 6.0  |
| 1   | M     | 1886 | VAL  | 6.0  |
| 1   | D     | 1533 | GLU  | 6.0  |
| 1   | F     | 1710 | LEU  | 6.0  |
| 1   | F     | 1505 | GLY  | 5.9  |
| 1   | M     | 1820 | VAL  | 5.9  |
| 1   | A     | 1984 | TYR  | 5.9  |
| 1   | F     | 1483 | GLU  | 5.9  |
| 1   | L     | 1770 | THR  | 5.9  |
| 1   | A     | 1818 | ILE  | 5.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | R     | 1736 | THR  | 5.9  |
| 1   | A     | 1276 | VAL  | 5.9  |
| 1   | A     | 1321 | LEU  | 5.9  |
| 1   | E     | 1310 | THR  | 5.9  |
| 1   | G     | 1399 | LEU  | 5.9  |
| 1   | Q     | 1104 | GLN  | 5.8  |
| 1   | L     | 1946 | TRP  | 5.8  |
| 1   | Q     | 1067 | VAL  | 5.8  |
| 1   | Q     | 1108 | ALA  | 5.8  |
| 1   | G     | 1773 | LEU  | 5.8  |
| 1   | Q     | 1102 | CYS  | 5.8  |
| 1   | L     | 1794 | VAL  | 5.7  |
| 1   | L     | 1812 | ARG  | 5.7  |
| 1   | Q     | 1175 | GLY  | 5.7  |
| 1   | Q     | 1075 | VAL  | 5.7  |
| 1   | E     | 1518 | THR  | 5.7  |
| 1   | E     | 1920 | ALA  | 5.6  |
| 1   | B     | 1996 | PHE  | 5.6  |
| 1   | E     | 1917 | TYR  | 5.6  |
| 1   | P     | 1818 | ILE  | 5.6  |
| 1   | C     | 1984 | TYR  | 5.6  |
| 1   | Q     | 1128 | LEU  | 5.6  |
| 1   | L     | 1802 | THR  | 5.6  |
| 1   | E     | 942  | LEU  | 5.6  |
| 1   | Q     | 1113 | GLN  | 5.5  |
| 1   | D     | 1274 | VAL  | 5.5  |
| 1   | D     | 1984 | TYR  | 5.5  |
| 1   | L     | 1962 | ILE  | 5.5  |
| 1   | F     | 1447 | GLY  | 5.5  |
| 1   | Q     | 1129 | ARG  | 5.5  |
| 1   | K     | 1227 | ASN  | 5.5  |
| 1   | P     | 1486 | GLY  | 5.4  |
| 1   | Q     | 1165 | VAL  | 5.4  |
| 1   | E     | 1246 | THR  | 5.4  |
| 1   | Q     | 1172 | LEU  | 5.4  |
| 1   | A     | 1337 | PRO  | 5.4  |
| 1   | Q     | 1124 | GLY  | 5.4  |
| 1   | H     | 1588 | ALA  | 5.4  |
| 1   | E     | 943  | PRO  | 5.4  |
| 1   | N     | 1288 | HIS  | 5.4  |
| 1   | R     | 1660 | ASP  | 5.4  |
| 1   | Q     | 940  | ALA  | 5.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1151 | GLY  | 5.3  |
| 1   | M     | 1822 | CYS  | 5.3  |
| 1   | C     | 1275 | ALA  | 5.3  |
| 1   | D     | 1983 | GLY  | 5.3  |
| 1   | R     | 1523 | LEU  | 5.3  |
| 1   | G     | 1925 | ASP  | 5.3  |
| 1   | L     | 1883 | HIS  | 5.3  |
| 1   | Q     | 1021 | GLU  | 5.3  |
| 1   | G     | 1902 | PHE  | 5.3  |
| 1   | N     | 1773 | LEU  | 5.3  |
| 1   | G     | 2006 | PHE  | 5.3  |
| 1   | R     | 1050 | THR  | 5.2  |
| 1   | O     | 1745 | ASP  | 5.2  |
| 1   | M     | 1798 | SER  | 5.2  |
| 1   | A     | 1985 | ALA  | 5.2  |
| 1   | Q     | 1122 | PRO  | 5.2  |
| 1   | L     | 1784 | MET  | 5.2  |
| 1   | C     | 1792 | ILE  | 5.2  |
| 1   | Q     | 1029 | ASP  | 5.2  |
| 1   | E     | 1322 | TYR  | 5.2  |
| 1   | Q     | 941  | VAL  | 5.2  |
| 1   | D     | 1277 | ILE  | 5.1  |
| 1   | E     | 1276 | VAL  | 5.1  |
| 1   | L     | 1971 | PHE  | 5.1  |
| 1   | M     | 1761 | PHE  | 5.1  |
| 1   | M     | 1737 | GLY  | 5.1  |
| 1   | M     | 1226 | GLU  | 5.1  |
| 1   | J     | 1792 | ILE  | 5.1  |
| 1   | M     | 1857 | ASP  | 5.0  |
| 1   | Q     | 1130 | ALA  | 5.0  |
| 1   | L     | 1845 | LEU  | 5.0  |
| 1   | Q     | 947  | TYR  | 5.0  |
| 1   | H     | 1525 | THR  | 5.0  |
| 1   | C     | 1218 | VAL  | 5.0  |
| 1   | R     | 1079 | VAL  | 5.0  |
| 1   | L     | 1944 | GLY  | 5.0  |
| 1   | M     | 1750 | GLN  | 4.9  |
| 1   | L     | 2003 | ALA  | 4.9  |
| 1   | L     | 1925 | ASP  | 4.9  |
| 1   | F     | 1105 | SER  | 4.9  |
| 1   | E     | 1529 | GLU  | 4.9  |
| 1   | F     | 1773 | LEU  | 4.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1084 | PRO  | 4.9  |
| 1   | M     | 1863 | ILE  | 4.9  |
| 1   | M     | 1883 | HIS  | 4.9  |
| 1   | B     | 1218 | VAL  | 4.9  |
| 1   | M     | 1408 | GLU  | 4.9  |
| 1   | R     | 1533 | GLU  | 4.9  |
| 1   | H     | 1531 | ILE  | 4.8  |
| 1   | E     | 1342 | SER  | 4.8  |
| 1   | G     | 1337 | PRO  | 4.8  |
| 1   | Q     | 1493 | PRO  | 4.8  |
| 1   | C     | 1274 | VAL  | 4.8  |
| 1   | E     | 1968 | ALA  | 4.8  |
| 1   | F     | 1907 | ALA  | 4.8  |
| 1   | L     | 1882 | LEU  | 4.8  |
| 1   | F     | 1161 | ALA  | 4.8  |
| 1   | M     | 1966 | GLU  | 4.8  |
| 1   | E     | 1947 | GLY  | 4.8  |
| 1   | F     | 1984 | TYR  | 4.8  |
| 1   | Q     | 1521 | ALA  | 4.8  |
| 1   | E     | 1348 | ILE  | 4.8  |
| 1   | M     | 1825 | ILE  | 4.7  |
| 1   | L     | 1782 | GLU  | 4.7  |
| 1   | E     | 1738 | LYS  | 4.7  |
| 1   | F     | 1792 | ILE  | 4.7  |
| 1   | H     | 1505 | GLY  | 4.7  |
| 1   | L     | 1927 | PHE  | 4.7  |
| 1   | Q     | 1103 | PHE  | 4.7  |
| 1   | Q     | 1076 | VAL  | 4.7  |
| 1   | E     | 1058 | ALA  | 4.7  |
| 1   | F     | 1482 | SER  | 4.7  |
| 1   | Q     | 1473 | PHE  | 4.7  |
| 1   | Q     | 1466 | ALA  | 4.7  |
| 1   | H     | 1602 | TRP  | 4.7  |
| 1   | M     | 1979 | ARG  | 4.7  |
| 1   | A     | 1399 | LEU  | 4.7  |
| 1   | E     | 1539 | VAL  | 4.7  |
| 1   | F     | 1986 | PRO  | 4.7  |
| 1   | I     | 1142 | SER  | 4.7  |
| 1   | Q     | 1470 | CYS  | 4.7  |
| 1   | L     | 1799 | ALA  | 4.7  |
| 1   | M     | 1856 | GLU  | 4.7  |
| 1   | L     | 1870 | HIS  | 4.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 1120 | LEU  | 4.7  |
| 1   | G     | 1362 | GLN  | 4.7  |
| 1   | I     | 1062 | LEU  | 4.6  |
| 1   | F     | 1647 | LEU  | 4.6  |
| 1   | L     | 2008 | ALA  | 4.6  |
| 1   | A     | 1792 | ILE  | 4.6  |
| 1   | M     | 1875 | LYS  | 4.6  |
| 1   | H     | 1396 | ALA  | 4.6  |
| 1   | E     | 896  | PRO  | 4.6  |
| 1   | D     | 1193 | LEU  | 4.6  |
| 1   | O     | 1750 | GLN  | 4.6  |
| 1   | R     | 1191 | ARG  | 4.6  |
| 1   | L     | 1878 | GLY  | 4.5  |
| 1   | Q     | 1512 | CYS  | 4.5  |
| 1   | G     | 1279 | GLY  | 4.5  |
| 1   | E     | 1421 | MET  | 4.5  |
| 1   | A     | 1246 | THR  | 4.5  |
| 1   | E     | 1269 | GLN  | 4.5  |
| 1   | F     | 1152 | VAL  | 4.5  |
| 1   | N     | 1850 | HIS  | 4.5  |
| 1   | C     | 1089 | GLN  | 4.5  |
| 1   | E     | 1387 | THR  | 4.5  |
| 1   | M     | 1374 | LEU  | 4.5  |
| 1   | I     | 1482 | SER  | 4.5  |
| 1   | Q     | 1449 | ILE  | 4.5  |
| 1   | E     | 1203 | PRO  | 4.5  |
| 1   | L     | 1781 | ALA  | 4.5  |
| 1   | Q     | 1491 | VAL  | 4.5  |
| 1   | Q     | 1434 | MET  | 4.5  |
| 1   | G     | 1274 | VAL  | 4.5  |
| 1   | R     | 1039 | VAL  | 4.5  |
| 1   | M     | 1902 | PHE  | 4.5  |
| 1   | A     | 1322 | TYR  | 4.5  |
| 1   | G     | 1903 | SER  | 4.5  |
| 1   | R     | 1051 | VAL  | 4.5  |
| 1   | C     | 1772 | GLY  | 4.4  |
| 1   | Q     | 1142 | SER  | 4.4  |
| 1   | P     | 1816 | ALA  | 4.4  |
| 1   | H     | 1386 | GLU  | 4.4  |
| 1   | R     | 903  | LEU  | 4.4  |
| 1   | M     | 1195 | ILE  | 4.4  |
| 1   | I     | 1089 | GLN  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1498 | HIS  | 4.4  |
| 1   | L     | 2006 | PHE  | 4.4  |
| 1   | A     | 1400 | CYS  | 4.4  |
| 1   | I     | 1505 | GLY  | 4.4  |
| 1   | M     | 1899 | PHE  | 4.4  |
| 1   | P     | 1825 | ILE  | 4.4  |
| 1   | M     | 1772 | GLY  | 4.4  |
| 1   | F     | 1996 | PHE  | 4.4  |
| 1   | H     | 1778 | LEU  | 4.4  |
| 1   | L     | 1779 | PHE  | 4.4  |
| 1   | R     | 1524 | ALA  | 4.4  |
| 1   | M     | 1295 | ARG  | 4.4  |
| 1   | G     | 1498 | HIS  | 4.4  |
| 1   | G     | 1999 | ARG  | 4.4  |
| 1   | D     | 1909 | VAL  | 4.4  |
| 1   | Q     | 1010 | ALA  | 4.4  |
| 1   | E     | 1992 | TRP  | 4.3  |
| 1   | R     | 1065 | ALA  | 4.3  |
| 1   | R     | 1053 | ILE  | 4.3  |
| 1   | N     | 1984 | TYR  | 4.3  |
| 1   | B     | 1449 | ILE  | 4.3  |
| 1   | G     | 1195 | ILE  | 4.3  |
| 1   | G     | 1108 | ALA  | 4.3  |
| 1   | H     | 1397 | ALA  | 4.3  |
| 1   | P     | 1329 | GLN  | 4.3  |
| 1   | E     | 1059 | PHE  | 4.3  |
| 1   | D     | 1982 | ASN  | 4.3  |
| 1   | J     | 1845 | LEU  | 4.3  |
| 1   | P     | 1835 | VAL  | 4.3  |
| 1   | M     | 1225 | ASP  | 4.3  |
| 1   | P     | 1992 | TRP  | 4.3  |
| 1   | E     | 1789 | CYS  | 4.3  |
| 1   | M     | 1898 | TRP  | 4.3  |
| 1   | H     | 1055 | HIS  | 4.3  |
| 1   | B     | 1219 | ILE  | 4.3  |
| 1   | H     | 1792 | ILE  | 4.3  |
| 1   | M     | 1871 | ASP  | 4.2  |
| 1   | E     | 1343 | GLY  | 4.2  |
| 1   | F     | 1107 | ILE  | 4.2  |
| 1   | Q     | 1739 | LEU  | 4.2  |
| 1   | Q     | 1694 | ILE  | 4.2  |
| 1   | G     | 1996 | PHE  | 4.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1739 | LEU  | 4.2  |
| 1   | F     | 2006 | PHE  | 4.2  |
| 1   | M     | 1868 | VAL  | 4.2  |
| 1   | E     | 1194 | THR  | 4.2  |
| 1   | M     | 1759 | PRO  | 4.2  |
| 1   | E     | 1919 | ALA  | 4.2  |
| 1   | E     | 1543 | TYR  | 4.2  |
| 1   | A     | 1800 | PRO  | 4.2  |
| 1   | D     | 1282 | GLU  | 4.2  |
| 1   | F     | 1074 | THR  | 4.2  |
| 1   | O     | 1421 | MET  | 4.2  |
| 1   | F     | 1456 | SER  | 4.2  |
| 1   | F     | 1705 | ILE  | 4.2  |
| 1   | F     | 1507 | VAL  | 4.2  |
| 1   | G     | 1032 | LEU  | 4.1  |
| 1   | F     | 1971 | PHE  | 4.1  |
| 1   | E     | 1399 | LEU  | 4.1  |
| 1   | F     | 1941 | ILE  | 4.1  |
| 1   | H     | 1139 | TYR  | 4.1  |
| 1   | E     | 1282 | GLU  | 4.1  |
| 1   | F     | 1909 | VAL  | 4.1  |
| 1   | H     | 1147 | ALA  | 4.1  |
| 1   | F     | 1104 | GLN  | 4.1  |
| 1   | M     | 1947 | GLY  | 4.1  |
| 1   | M     | 1896 | LEU  | 4.1  |
| 1   | H     | 2003 | ALA  | 4.1  |
| 1   | Q     | 1065 | ALA  | 4.1  |
| 1   | F     | 1160 | ASP  | 4.1  |
| 1   | J     | 1746 | THR  | 4.1  |
| 1   | R     | 1683 | LEU  | 4.1  |
| 1   | J     | 1386 | GLU  | 4.1  |
| 1   | L     | 1872 | TRP  | 4.1  |
| 1   | G     | 1193 | LEU  | 4.1  |
| 1   | Q     | 950  | MET  | 4.1  |
| 1   | Q     | 1009 | ARG  | 4.1  |
| 1   | P     | 1991 | SER  | 4.1  |
| 1   | G     | 1374 | LEU  | 4.1  |
| 1   | A     | 1854 | VAL  | 4.1  |
| 1   | L     | 1884 | GLN  | 4.1  |
| 1   | C     | 1219 | ILE  | 4.1  |
| 1   | N     | 1793 | VAL  | 4.1  |
| 1   | L     | 1789 | CYS  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | L     | 1795 | ASN  | 4.1  |
| 1   | H     | 1946 | TRP  | 4.1  |
| 1   | L     | 1820 | VAL  | 4.1  |
| 1   | H     | 923  | VAL  | 4.1  |
| 1   | A     | 1964 | PRO  | 4.0  |
| 1   | R     | 1190 | GLU  | 4.0  |
| 1   | A     | 1218 | VAL  | 4.0  |
| 1   | Q     | 1066 | TYR  | 4.0  |
| 1   | G     | 2003 | ALA  | 4.0  |
| 1   | A     | 1247 | MET  | 4.0  |
| 1   | H     | 1767 | TYR  | 4.0  |
| 1   | I     | 1081 | LEU  | 4.0  |
| 1   | L     | 1764 | ASP  | 4.0  |
| 1   | Q     | 1143 | ARG  | 4.0  |
| 1   | P     | 1882 | LEU  | 4.0  |
| 1   | M     | 1893 | THR  | 4.0  |
| 1   | Q     | 1696 | ASP  | 4.0  |
| 1   | E     | 1786 | ALA  | 4.0  |
| 1   | M     | 1344 | LEU  | 4.0  |
| 1   | Q     | 974  | LEU  | 4.0  |
| 1   | M     | 1767 | TYR  | 4.0  |
| 1   | R     | 1119 | MET  | 4.0  |
| 1   | Q     | 1440 | GLU  | 4.0  |
| 1   | L     | 1984 | TYR  | 4.0  |
| 1   | E     | 1374 | LEU  | 4.0  |
| 1   | H     | 898  | VAL  | 4.0  |
| 1   | Q     | 1497 | THR  | 4.0  |
| 1   | F     | 1273 | GLY  | 4.0  |
| 1   | A     | 1203 | PRO  | 4.0  |
| 1   | F     | 1702 | TYR  | 4.0  |
| 1   | F     | 1735 | HIS  | 4.0  |
| 1   | G     | 1205 | PRO  | 4.0  |
| 1   | H     | 1106 | VAL  | 4.0  |
| 1   | I     | 1737 | GLY  | 4.0  |
| 1   | E     | 1972 | GLU  | 3.9  |
| 1   | O     | 1414 | ALA  | 4.0  |
| 1   | E     | 1369 | THR  | 3.9  |
| 1   | F     | 1065 | ALA  | 3.9  |
| 1   | A     | 1202 | LEU  | 3.9  |
| 1   | C     | 2006 | PHE  | 3.9  |
| 1   | M     | 1964 | PRO  | 3.9  |
| 1   | M     | 1946 | TRP  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | L     | 1977 | HIS  | 3.9  |
| 1   | Q     | 934  | HIS  | 3.9  |
| 1   | M     | 1880 | TRP  | 3.9  |
| 1   | Q     | 1654 | VAL  | 3.9  |
| 1   | C     | 1777 | GLY  | 3.9  |
| 1   | F     | 1055 | HIS  | 3.9  |
| 1   | J     | 1153 | GLU  | 3.9  |
| 1   | R     | 1506 | GLY  | 3.9  |
| 1   | Q     | 1173 | GLN  | 3.9  |
| 1   | A     | 1324 | VAL  | 3.9  |
| 1   | E     | 1759 | PRO  | 3.9  |
| 1   | G     | 1268 | GLU  | 3.9  |
| 1   | G     | 1218 | VAL  | 3.9  |
| 1   | H     | 1533 | GLU  | 3.9  |
| 1   | Q     | 1702 | TYR  | 3.9  |
| 1   | E     | 1785 | ALA  | 3.9  |
| 1   | E     | 1760 | VAL  | 3.9  |
| 1   | E     | 1524 | ALA  | 3.9  |
| 1   | D     | 1324 | VAL  | 3.9  |
| 1   | G     | 1058 | ALA  | 3.9  |
| 1   | J     | 1789 | CYS  | 3.9  |
| 1   | Q     | 1059 | PHE  | 3.9  |
| 1   | Q     | 1471 | PRO  | 3.8  |
| 1   | F     | 1675 | ASN  | 3.8  |
| 1   | A     | 1195 | ILE  | 3.8  |
| 1   | R     | 1654 | VAL  | 3.8  |
| 1   | N     | 1907 | ALA  | 3.8  |
| 1   | Q     | 1062 | LEU  | 3.8  |
| 1   | Q     | 1571 | VAL  | 3.8  |
| 1   | H     | 1081 | LEU  | 3.8  |
| 1   | L     | 1901 | ALA  | 3.8  |
| 1   | L     | 1961 | ALA  | 3.8  |
| 1   | E     | 1245 | THR  | 3.8  |
| 1   | F     | 1743 | ILE  | 3.8  |
| 1   | Q     | 1540 | GLY  | 3.8  |
| 1   | E     | 1907 | ALA  | 3.8  |
| 1   | F     | 1247 | MET  | 3.8  |
| 1   | N     | 1768 | VAL  | 3.8  |
| 1   | N     | 1769 | ILE  | 3.8  |
| 1   | R     | 1465 | VAL  | 3.8  |
| 1   | E     | 1323 | VAL  | 3.8  |
| 1   | E     | 1766 | ALA  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 1394 | TRP  | 3.8  |
| 1   | G     | 1152 | VAL  | 3.8  |
| 1   | I     | 1497 | THR  | 3.8  |
| 1   | F     | 1294 | ALA  | 3.8  |
| 1   | F     | 1053 | ILE  | 3.8  |
| 1   | G     | 1301 | VAL  | 3.8  |
| 1   | H     | 1808 | ILE  | 3.8  |
| 1   | R     | 1737 | GLY  | 3.8  |
| 1   | A     | 1880 | TRP  | 3.8  |
| 1   | P     | 1817 | ASP  | 3.8  |
| 1   | G     | 1278 | VAL  | 3.7  |
| 1   | H     | 1399 | LEU  | 3.7  |
| 1   | G     | 1818 | ILE  | 3.7  |
| 1   | H     | 1562 | ILE  | 3.7  |
| 1   | H     | 1702 | TYR  | 3.7  |
| 1   | F     | 1079 | VAL  | 3.7  |
| 1   | A     | 1319 | PRO  | 3.7  |
| 1   | A     | 1855 | VAL  | 3.7  |
| 1   | G     | 1076 | VAL  | 3.7  |
| 1   | E     | 1325 | THR  | 3.7  |
| 1   | N     | 1818 | ILE  | 3.7  |
| 1   | N     | 1764 | ASP  | 3.7  |
| 1   | E     | 1066 | TYR  | 3.7  |
| 1   | L     | 1839 | THR  | 3.7  |
| 1   | H     | 1504 | VAL  | 3.7  |
| 1   | P     | 1975 | LEU  | 3.7  |
| 1   | Q     | 1112 | VAL  | 3.7  |
| 1   | E     | 1984 | TYR  | 3.7  |
| 1   | E     | 1792 | ILE  | 3.7  |
| 1   | F     | 1077 | ALA  | 3.7  |
| 1   | F     | 1340 | GLU  | 3.7  |
| 1   | C     | 1214 | GLY  | 3.7  |
| 1   | Q     | 1114 | ASN  | 3.7  |
| 1   | Q     | 1436 | LEU  | 3.7  |
| 1   | P     | 1837 | ALA  | 3.7  |
| 1   | E     | 1315 | VAL  | 3.7  |
| 1   | E     | 1074 | THR  | 3.7  |
| 1   | E     | 906  | SER  | 3.7  |
| 1   | L     | 2005 | LEU  | 3.7  |
| 1   | R     | 1655 | GLU  | 3.7  |
| 1   | F     | 1386 | GLU  | 3.7  |
| 1   | K     | 1773 | LEU  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 1777 | GLY  | 3.7  |
| 1   | E     | 1479 | GLU  | 3.7  |
| 1   | M     | 1855 | VAL  | 3.7  |
| 1   | E     | 1519 | CYS  | 3.6  |
| 1   | A     | 1877 | TYR  | 3.6  |
| 1   | F     | 1385 | ASP  | 3.6  |
| 1   | E     | 1076 | VAL  | 3.6  |
| 1   | F     | 1098 | LEU  | 3.6  |
| 1   | N     | 1794 | VAL  | 3.6  |
| 1   | N     | 1899 | PHE  | 3.6  |
| 1   | F     | 1626 | TYR  | 3.6  |
| 1   | R     | 1640 | GLN  | 3.6  |
| 1   | G     | 1275 | ALA  | 3.6  |
| 1   | Q     | 1085 | LEU  | 3.6  |
| 1   | I     | 1085 | LEU  | 3.6  |
| 1   | A     | 1329 | GLN  | 3.6  |
| 1   | N     | 1534 | HIS  | 3.6  |
| 1   | F     | 1633 | ASN  | 3.6  |
| 1   | Q     | 1698 | LEU  | 3.6  |
| 1   | A     | 1780 | LEU  | 3.6  |
| 1   | G     | 1109 | HIS  | 3.6  |
| 1   | P     | 1834 | LEU  | 3.6  |
| 1   | H     | 1107 | ILE  | 3.6  |
| 1   | H     | 1212 | ASP  | 3.6  |
| 1   | M     | 1969 | TYR  | 3.6  |
| 1   | J     | 1105 | SER  | 3.6  |
| 1   | M     | 1325 | THR  | 3.6  |
| 1   | B     | 1984 | TYR  | 3.6  |
| 1   | Q     | 1718 | TYR  | 3.6  |
| 1   | L     | 1849 | LEU  | 3.6  |
| 1   | P     | 2006 | PHE  | 3.6  |
| 1   | L     | 1028 | ILE  | 3.6  |
| 1   | Q     | 1589 | THR  | 3.6  |
| 1   | M     | 1222 | GLY  | 3.6  |
| 1   | H     | 1563 | LEU  | 3.6  |
| 1   | M     | 1323 | VAL  | 3.6  |
| 1   | P     | 1271 | LEU  | 3.6  |
| 1   | P     | 1845 | LEU  | 3.6  |
| 1   | R     | 1632 | LEU  | 3.6  |
| 1   | M     | 1907 | ALA  | 3.6  |
| 1   | E     | 1946 | TRP  | 3.6  |
| 1   | F     | 1384 | GLU  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | O     | 1744 | PRO  | 3.6  |
| 1   | R     | 1462 | ASP  | 3.6  |
| 1   | M     | 1402 | SER  | 3.6  |
| 1   | R     | 1498 | HIS  | 3.6  |
| 1   | E     | 1697 | LEU  | 3.6  |
| 1   | E     | 1204 | ARG  | 3.6  |
| 1   | E     | 1918 | ALA  | 3.6  |
| 1   | E     | 1363 | ILE  | 3.6  |
| 1   | L     | 1811 | ILE  | 3.6  |
| 1   | A     | 1216 | TRP  | 3.6  |
| 1   | G     | 1323 | VAL  | 3.6  |
| 1   | C     | 1773 | LEU  | 3.6  |
| 1   | C     | 1996 | PHE  | 3.6  |
| 1   | E     | 1975 | LEU  | 3.6  |
| 1   | R     | 1505 | GLY  | 3.6  |
| 1   | A     | 1194 | THR  | 3.6  |
| 1   | M     | 1440 | GLU  | 3.6  |
| 1   | F     | 1288 | HIS  | 3.6  |
| 1   | F     | 1060 | ALA  | 3.6  |
| 1   | O     | 1089 | GLN  | 3.6  |
| 1   | H     | 1971 | PHE  | 3.6  |
| 1   | Q     | 1527 | LEU  | 3.6  |
| 1   | R     | 976  | LEU  | 3.6  |
| 1   | E     | 1221 | ALA  | 3.5  |
| 1   | M     | 1769 | ILE  | 3.5  |
| 1   | C     | 1311 | LEU  | 3.5  |
| 1   | I     | 1091 | GLY  | 3.5  |
| 1   | M     | 1776 | LEU  | 3.5  |
| 1   | M     | 1943 | TRP  | 3.5  |
| 1   | I     | 1090 | ARG  | 3.5  |
| 1   | I     | 1471 | PRO  | 3.5  |
| 1   | J     | 1767 | TYR  | 3.5  |
| 1   | M     | 1194 | THR  | 3.5  |
| 1   | C     | 1986 | PRO  | 3.5  |
| 1   | Q     | 1121 | LEU  | 3.5  |
| 1   | M     | 1297 | GLY  | 3.5  |
| 1   | Q     | 1028 | ILE  | 3.5  |
| 1   | G     | 1239 | GLY  | 3.5  |
| 1   | E     | 1845 | LEU  | 3.5  |
| 1   | H     | 1053 | ILE  | 3.5  |
| 1   | J     | 2007 | LEU  | 3.5  |
| 1   | R     | 1189 | ASP  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 1768 | VAL  | 3.5  |
| 1   | L     | 1746 | THR  | 3.5  |
| 1   | L     | 1808 | ILE  | 3.5  |
| 1   | E     | 1436 | LEU  | 3.5  |
| 1   | G     | 1277 | ILE  | 3.5  |
| 1   | I     | 1504 | VAL  | 3.5  |
| 1   | G     | 2007 | LEU  | 3.5  |
| 1   | E     | 1420 | GLY  | 3.5  |
| 1   | D     | 1106 | VAL  | 3.5  |
| 1   | E     | 1971 | PHE  | 3.5  |
| 1   | F     | 1769 | ILE  | 3.5  |
| 1   | H     | 1818 | ILE  | 3.5  |
| 1   | F     | 1648 | ALA  | 3.5  |
| 1   | M     | 1816 | ALA  | 3.5  |
| 1   | R     | 1078 | ALA  | 3.5  |
| 1   | O     | 1447 | GLY  | 3.5  |
| 1   | Q     | 948  | CYS  | 3.5  |
| 1   | E     | 1195 | ILE  | 3.5  |
| 1   | D     | 1985 | ALA  | 3.5  |
| 1   | Q     | 1481 | GLY  | 3.5  |
| 1   | B     | 1220 | LEU  | 3.5  |
| 1   | H     | 931  | LEU  | 3.5  |
| 1   | I     | 1513 | TRP  | 3.5  |
| 1   | P     | 1795 | ASN  | 3.5  |
| 1   | D     | 1344 | LEU  | 3.5  |
| 1   | F     | 1946 | TRP  | 3.5  |
| 1   | H     | 2008 | ALA  | 3.5  |
| 1   | A     | 1401 | PRO  | 3.5  |
| 1   | E     | 1205 | PRO  | 3.5  |
| 1   | H     | 1319 | PRO  | 3.5  |
| 1   | R     | 991  | PRO  | 3.5  |
| 1   | A     | 1223 | ASP  | 3.5  |
| 1   | E     | 1784 | MET  | 3.5  |
| 1   | P     | 1820 | VAL  | 3.5  |
| 1   | Q     | 1500 | VAL  | 3.5  |
| 1   | G     | 1120 | LEU  | 3.5  |
| 1   | D     | 1759 | PRO  | 3.5  |
| 1   | H     | 1070 | ALA  | 3.5  |
| 1   | M     | 1294 | ALA  | 3.5  |
| 1   | F     | 1902 | PHE  | 3.5  |
| 1   | G     | 1793 | VAL  | 3.5  |
| 1   | G     | 1820 | VAL  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1076 | VAL  | 3.5  |
| 1   | A     | 1825 | ILE  | 3.4  |
| 1   | R     | 1074 | THR  | 3.4  |
| 1   | E     | 1695 | ARG  | 3.4  |
| 1   | M     | 1330 | HIS  | 3.4  |
| 1   | A     | 1200 | ARG  | 3.4  |
| 1   | G     | 1372 | GLU  | 3.4  |
| 1   | P     | 1773 | LEU  | 3.4  |
| 1   | Q     | 1498 | HIS  | 3.4  |
| 1   | I     | 1512 | CYS  | 3.4  |
| 1   | P     | 1794 | VAL  | 3.4  |
| 1   | R     | 1529 | GLU  | 3.4  |
| 1   | C     | 1909 | VAL  | 3.4  |
| 1   | I     | 1141 | LEU  | 3.4  |
| 1   | M     | 1845 | LEU  | 3.4  |
| 1   | J     | 1147 | ALA  | 3.4  |
| 1   | F     | 1908 | LEU  | 3.4  |
| 1   | P     | 1778 | LEU  | 3.4  |
| 1   | R     | 1627 | GLY  | 3.4  |
| 1   | E     | 1729 | ILE  | 3.4  |
| 1   | K     | 1820 | VAL  | 3.4  |
| 1   | L     | 1824 | ASP  | 3.4  |
| 1   | Q     | 1508 | SER  | 3.4  |
| 1   | L     | 1986 | PRO  | 3.4  |
| 1   | R     | 1419 | GLU  | 3.4  |
| 1   | D     | 1816 | ALA  | 3.4  |
| 1   | E     | 1402 | SER  | 3.4  |
| 1   | G     | 1197 | TRP  | 3.4  |
| 1   | L     | 1874 | PRO  | 3.4  |
| 1   | D     | 1854 | VAL  | 3.4  |
| 1   | E     | 1985 | ALA  | 3.4  |
| 1   | J     | 1791 | ARG  | 3.4  |
| 1   | M     | 1385 | ASP  | 3.4  |
| 1   | L     | 1868 | VAL  | 3.4  |
| 1   | G     | 1360 | ALA  | 3.4  |
| 1   | D     | 1818 | ILE  | 3.4  |
| 1   | E     | 1341 | HIS  | 3.4  |
| 1   | C     | 1795 | ASN  | 3.4  |
| 1   | M     | 1936 | LEU  | 3.4  |
| 1   | E     | 1746 | THR  | 3.4  |
| 1   | Q     | 1681 | VAL  | 3.4  |
| 1   | I     | 1498 | HIS  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1221 | ALA  | 3.4  |
| 1   | N     | 1821 | GLU  | 3.4  |
| 1   | R     | 1485 | GLY  | 3.4  |
| 1   | L     | 1791 | ARG  | 3.4  |
| 1   | F     | 1337 | PRO  | 3.4  |
| 1   | G     | 1169 | ALA  | 3.4  |
| 1   | E     | 962  | THR  | 3.3  |
| 1   | M     | 1921 | ASN  | 3.3  |
| 1   | G     | 1850 | HIS  | 3.3  |
| 1   | E     | 1517 | VAL  | 3.3  |
| 1   | C     | 974  | LEU  | 3.3  |
| 1   | F     | 1028 | ILE  | 3.3  |
| 1   | L     | 1798 | SER  | 3.3  |
| 1   | N     | 1817 | ASP  | 3.3  |
| 1   | H     | 1845 | LEU  | 3.3  |
| 1   | Q     | 998  | VAL  | 3.3  |
| 1   | E     | 1273 | GLY  | 3.3  |
| 1   | N     | 923  | VAL  | 3.3  |
| 1   | L     | 1983 | GLY  | 3.3  |
| 1   | M     | 1306 | ARG  | 3.3  |
| 1   | M     | 1970 | ALA  | 3.3  |
| 1   | Q     | 1543 | TYR  | 3.3  |
| 1   | M     | 1934 | GLN  | 3.3  |
| 1   | A     | 1804 | SER  | 3.3  |
| 1   | G     | 1223 | ASP  | 3.3  |
| 1   | H     | 1738 | LYS  | 3.3  |
| 1   | L     | 1827 | GLU  | 3.3  |
| 1   | L     | 1981 | TYR  | 3.3  |
| 1   | O     | 1417 | ALA  | 3.3  |
| 1   | Q     | 1643 | GLY  | 3.3  |
| 1   | I     | 1053 | ILE  | 3.3  |
| 1   | G     | 1924 | LEU  | 3.3  |
| 1   | M     | 1849 | LEU  | 3.3  |
| 1   | P     | 1946 | TRP  | 3.3  |
| 1   | P     | 1879 | ALA  | 3.3  |
| 1   | G     | 1739 | LEU  | 3.3  |
| 1   | H     | 1387 | THR  | 3.3  |
| 1   | M     | 1870 | HIS  | 3.3  |
| 1   | E     | 1880 | TRP  | 3.3  |
| 1   | D     | 1365 | VAL  | 3.3  |
| 1   | F     | 1653 | PHE  | 3.3  |
| 1   | R     | 1152 | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1524 | ALA  | 3.3  |
| 1   | E     | 1216 | TRP  | 3.3  |
| 1   | Q     | 996  | PHE  | 3.3  |
| 1   | E     | 1986 | PRO  | 3.3  |
| 1   | J     | 2008 | ALA  | 3.3  |
| 1   | L     | 1834 | LEU  | 3.3  |
| 1   | N     | 1975 | LEU  | 3.3  |
| 1   | M     | 948  | CYS  | 3.3  |
| 1   | G     | 1794 | VAL  | 3.3  |
| 1   | J     | 1817 | ASP  | 3.3  |
| 1   | L     | 1908 | LEU  | 3.3  |
| 1   | R     | 1117 | SER  | 3.3  |
| 1   | A     | 1345 | ARG  | 3.2  |
| 1   | D     | 1267 | ASP  | 3.2  |
| 1   | E     | 1041 | GLY  | 3.2  |
| 1   | F     | 1983 | GLY  | 3.2  |
| 1   | R     | 1633 | ASN  | 3.2  |
| 1   | G     | 1987 | VAL  | 3.2  |
| 1   | H     | 1819 | VAL  | 3.2  |
| 1   | M     | 1848 | VAL  | 3.2  |
| 1   | M     | 1784 | MET  | 3.2  |
| 1   | G     | 1792 | ILE  | 3.2  |
| 1   | P     | 1793 | VAL  | 3.2  |
| 1   | F     | 1631 | VAL  | 3.2  |
| 1   | E     | 1762 | ARG  | 3.2  |
| 1   | A     | 1484 | PHE  | 3.2  |
| 1   | M     | 1331 | VAL  | 3.2  |
| 1   | A     | 1924 | LEU  | 3.2  |
| 1   | G     | 1992 | TRP  | 3.2  |
| 1   | P     | 1204 | ARG  | 3.2  |
| 1   | F     | 1455 | ALA  | 3.2  |
| 1   | K     | 1702 | TYR  | 3.2  |
| 1   | K     | 1925 | ASP  | 3.2  |
| 1   | R     | 942  | LEU  | 3.2  |
| 1   | R     | 1726 | ALA  | 3.2  |
| 1   | C     | 1288 | HIS  | 3.2  |
| 1   | R     | 1062 | LEU  | 3.2  |
| 1   | R     | 1720 | LEU  | 3.2  |
| 1   | G     | 1946 | TRP  | 3.2  |
| 1   | R     | 897  | SER  | 3.2  |
| 1   | A     | 1310 | THR  | 3.2  |
| 1   | P     | 1792 | ILE  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | R     | 1658 | LYS  | 3.2  |
| 1   | M     | 1229 | ARG  | 3.2  |
| 1   | A     | 1916 | ALA  | 3.2  |
| 1   | L     | 1970 | ALA  | 3.2  |
| 1   | P     | 1838 | ALA  | 3.2  |
| 1   | Q     | 896  | PRO  | 3.2  |
| 1   | R     | 1480 | LEU  | 3.2  |
| 1   | P     | 1768 | VAL  | 3.2  |
| 1   | R     | 1075 | VAL  | 3.2  |
| 1   | E     | 1782 | GLU  | 3.2  |
| 1   | G     | 1357 | ARG  | 3.2  |
| 1   | M     | 1328 | SER  | 3.2  |
| 1   | D     | 1971 | PHE  | 3.2  |
| 1   | M     | 1290 | VAL  | 3.2  |
| 1   | E     | 1193 | LEU  | 3.2  |
| 1   | J     | 1853 | ALA  | 3.2  |
| 1   | L     | 1943 | TRP  | 3.2  |
| 1   | O     | 1420 | GLY  | 3.2  |
| 1   | E     | 1499 | ARG  | 3.2  |
| 1   | G     | 1373 | ALA  | 3.2  |
| 1   | G     | 1769 | ILE  | 3.2  |
| 1   | H     | 1423 | LEU  | 3.2  |
| 1   | G     | 1267 | ASP  | 3.2  |
| 1   | R     | 1723 | ALA  | 3.2  |
| 1   | F     | 1709 | THR  | 3.2  |
| 1   | E     | 1981 | TYR  | 3.2  |
| 1   | R     | 1730 | MET  | 3.2  |
| 1   | R     | 1066 | TYR  | 3.1  |
| 1   | H     | 1712 | LEU  | 3.1  |
| 1   | M     | 1770 | THR  | 3.1  |
| 1   | P     | 1319 | PRO  | 3.1  |
| 1   | E     | 1604 | ILE  | 3.1  |
| 1   | F     | 1536 | ALA  | 3.1  |
| 1   | Q     | 976  | LEU  | 3.1  |
| 1   | A     | 1817 | ASP  | 3.1  |
| 1   | N     | 1512 | CYS  | 3.1  |
| 1   | Q     | 1745 | ASP  | 3.1  |
| 1   | F     | 1738 | LYS  | 3.1  |
| 1   | D     | 1233 | VAL  | 3.1  |
| 1   | M     | 1927 | PHE  | 3.1  |
| 1   | D     | 1389 | TRP  | 3.1  |
| 1   | F     | 1573 | GLN  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1059 | PHE  | 3.1  |
| 1   | N     | 1819 | VAL  | 3.1  |
| 1   | N     | 1946 | TRP  | 3.1  |
| 1   | Q     | 1692 | GLN  | 3.1  |
| 1   | R     | 1038 | ARG  | 3.1  |
| 1   | E     | 1522 | ASP  | 3.1  |
| 1   | H     | 1523 | LEU  | 3.1  |
| 1   | P     | 1484 | PHE  | 3.1  |
| 1   | K     | 1089 | GLN  | 3.1  |
| 1   | E     | 1790 | GLY  | 3.1  |
| 1   | F     | 1108 | ALA  | 3.1  |
| 1   | M     | 1771 | GLY  | 3.1  |
| 1   | K     | 1421 | MET  | 3.1  |
| 1   | Q     | 965  | VAL  | 3.1  |
| 1   | C     | 1081 | LEU  | 3.1  |
| 1   | Q     | 991  | PRO  | 3.1  |
| 1   | Q     | 1096 | PRO  | 3.1  |
| 1   | Q     | 1098 | LEU  | 3.1  |
| 1   | R     | 1454 | LYS  | 3.1  |
| 1   | B     | 2006 | PHE  | 3.1  |
| 1   | Q     | 1484 | PHE  | 3.1  |
| 1   | F     | 1513 | TRP  | 3.1  |
| 1   | F     | 1457 | SER  | 3.1  |
| 1   | P     | 1769 | ILE  | 3.1  |
| 1   | Q     | 1020 | ALA  | 3.1  |
| 1   | L     | 1437 | VAL  | 3.1  |
| 1   | E     | 1408 | GLU  | 3.1  |
| 1   | F     | 1480 | LEU  | 3.1  |
| 1   | A     | 1058 | ALA  | 3.1  |
| 1   | F     | 1059 | PHE  | 3.1  |
| 1   | L     | 1903 | SER  | 3.1  |
| 1   | M     | 1116 | ALA  | 3.1  |
| 1   | G     | 1791 | ARG  | 3.1  |
| 1   | D     | 1856 | GLU  | 3.1  |
| 1   | M     | 1948 | GLU  | 3.1  |
| 1   | F     | 1486 | GLY  | 3.1  |
| 1   | M     | 1749 | SER  | 3.1  |
| 1   | D     | 1923 | TRP  | 3.1  |
| 1   | F     | 1081 | LEU  | 3.1  |
| 1   | L     | 1886 | VAL  | 3.1  |
| 1   | L     | 1120 | LEU  | 3.1  |
| 1   | M     | 1778 | LEU  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1028 | ILE  | 3.1  |
| 1   | M     | 1851 | ALA  | 3.1  |
| 1   | P     | 1907 | ALA  | 3.1  |
| 1   | G     | 1311 | LEU  | 3.1  |
| 1   | L     | 1896 | LEU  | 3.1  |
| 1   | A     | 1816 | ALA  | 3.0  |
| 1   | C     | 1273 | GLY  | 3.0  |
| 1   | F     | 1097 | ALA  | 3.0  |
| 1   | L     | 1997 | ALA  | 3.0  |
| 1   | E     | 1536 | ALA  | 3.0  |
| 1   | F     | 1073 | PRO  | 3.0  |
| 1   | F     | 1914 | GLN  | 3.0  |
| 1   | A     | 2005 | LEU  | 3.0  |
| 1   | E     | 1722 | GLU  | 3.0  |
| 1   | K     | 1761 | PHE  | 3.0  |
| 1   | P     | 1850 | HIS  | 3.0  |
| 1   | C     | 1351 | VAL  | 3.0  |
| 1   | G     | 1235 | SER  | 3.0  |
| 1   | I     | 1411 | THR  | 3.0  |
| 1   | J     | 1154 | ALA  | 3.0  |
| 1   | M     | 1416 | ASN  | 3.0  |
| 1   | P     | 1290 | VAL  | 3.0  |
| 1   | H     | 1324 | VAL  | 3.0  |
| 1   | H     | 1854 | VAL  | 3.0  |
| 1   | L     | 1076 | VAL  | 3.0  |
| 1   | J     | 1538 | ALA  | 3.0  |
| 1   | D     | 1761 | PHE  | 3.0  |
| 1   | F     | 1138 | ARG  | 3.0  |
| 1   | C     | 1992 | TRP  | 3.0  |
| 1   | H     | 1058 | ALA  | 3.0  |
| 1   | H     | 1524 | ALA  | 3.0  |
| 1   | N     | 1399 | LEU  | 3.0  |
| 1   | O     | 1456 | SER  | 3.0  |
| 1   | I     | 1421 | MET  | 3.0  |
| 1   | M     | 1874 | PRO  | 3.0  |
| 1   | N     | 1500 | VAL  | 3.0  |
| 1   | Q     | 1147 | ALA  | 3.0  |
| 1   | D     | 1996 | PHE  | 3.0  |
| 1   | G     | 1361 | THR  | 3.0  |
| 1   | Q     | 1570 | GLY  | 3.0  |
| 1   | L     | 1090 | ARG  | 3.0  |
| 1   | D     | 1276 | VAL  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1137 | VAL  | 3.0  |
| 1   | P     | 1875 | LYS  | 3.0  |
| 1   | R     | 1115 | ILE  | 3.0  |
| 1   | E     | 1236 | ALA  | 3.0  |
| 1   | J     | 1563 | LEU  | 3.0  |
| 1   | N     | 945  | ALA  | 3.0  |
| 1   | E     | 1361 | THR  | 3.0  |
| 1   | F     | 1504 | VAL  | 3.0  |
| 1   | B     | 1216 | TRP  | 3.0  |
| 1   | G     | 1523 | LEU  | 3.0  |
| 1   | E     | 1883 | HIS  | 3.0  |
| 1   | E     | 1979 | ARG  | 3.0  |
| 1   | H     | 1791 | ARG  | 3.0  |
| 1   | O     | 1422 | ARG  | 3.0  |
| 1   | O     | 1511 | GLY  | 3.0  |
| 1   | P     | 1971 | PHE  | 3.0  |
| 1   | H     | 1893 | THR  | 3.0  |
| 1   | E     | 1964 | PRO  | 3.0  |
| 1   | H     | 1766 | ALA  | 3.0  |
| 1   | J     | 1946 | TRP  | 3.0  |
| 1   | M     | 1931 | ARG  | 3.0  |
| 1   | R     | 1116 | ALA  | 3.0  |
| 1   | H     | 936  | VAL  | 3.0  |
| 1   | I     | 1185 | GLU  | 3.0  |
| 1   | L     | 1511 | GLY  | 3.0  |
| 1   | E     | 1876 | VAL  | 3.0  |
| 1   | F     | 1522 | ASP  | 3.0  |
| 1   | Q     | 1495 | VAL  | 3.0  |
| 1   | R     | 1504 | VAL  | 3.0  |
| 1   | H     | 1875 | LYS  | 3.0  |
| 1   | K     | 1325 | THR  | 3.0  |
| 1   | N     | 1450 | GLU  | 3.0  |
| 1   | P     | 1821 | GLU  | 3.0  |
| 1   | G     | 1915 | GLY  | 3.0  |
| 1   | R     | 1653 | PHE  | 3.0  |
| 1   | P     | 1868 | VAL  | 3.0  |
| 1   | O     | 1515 | ASN  | 3.0  |
| 1   | D     | 1451 | VAL  | 3.0  |
| 1   | J     | 1318 | PRO  | 3.0  |
| 1   | M     | 1909 | VAL  | 3.0  |
| 1   | H     | 1384 | GLU  | 3.0  |
| 1   | C     | 1276 | VAL  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1557 | SER  | 2.9  |
| 1   | E     | 1854 | VAL  | 2.9  |
| 1   | J     | 1317 | GLU  | 2.9  |
| 1   | K     | 1399 | LEU  | 2.9  |
| 1   | Q     | 968  | LEU  | 2.9  |
| 1   | C     | 1065 | ALA  | 2.9  |
| 1   | E     | 1360 | ALA  | 2.9  |
| 1   | E     | 1944 | GLY  | 2.9  |
| 1   | F     | 1698 | LEU  | 2.9  |
| 1   | F     | 1746 | THR  | 2.9  |
| 1   | R     | 896  | PRO  | 2.9  |
| 1   | B     | 1337 | PRO  | 2.9  |
| 1   | F     | 1064 | GLU  | 2.9  |
| 1   | N     | 1571 | VAL  | 2.9  |
| 1   | R     | 1681 | VAL  | 2.9  |
| 1   | M     | 1843 | LEU  | 2.9  |
| 1   | Q     | 995  | GLU  | 2.9  |
| 1   | G     | 1363 | ILE  | 2.9  |
| 1   | D     | 1229 | ARG  | 2.9  |
| 1   | L     | 1881 | ASN  | 2.9  |
| 1   | M     | 1120 | LEU  | 2.9  |
| 1   | R     | 1682 | ASP  | 2.9  |
| 1   | I     | 1075 | VAL  | 2.9  |
| 1   | J     | 1818 | ILE  | 2.9  |
| 1   | K     | 1505 | GLY  | 2.9  |
| 1   | D     | 1845 | LEU  | 2.9  |
| 1   | M     | 1762 | ARG  | 2.9  |
| 1   | M     | 1872 | TRP  | 2.9  |
| 1   | F     | 1109 | HIS  | 2.9  |
| 1   | M     | 1977 | HIS  | 2.9  |
| 1   | M     | 1982 | ASN  | 2.9  |
| 1   | M     | 1911 | SER  | 2.9  |
| 1   | H     | 1543 | TYR  | 2.9  |
| 1   | C     | 1360 | ALA  | 2.9  |
| 1   | E     | 1705 | ILE  | 2.9  |
| 1   | G     | 1219 | ILE  | 2.9  |
| 1   | I     | 1108 | ALA  | 2.9  |
| 1   | J     | 1525 | THR  | 2.9  |
| 1   | C     | 1347 | LEU  | 2.9  |
| 1   | A     | 1059 | PHE  | 2.9  |
| 1   | H     | 1850 | HIS  | 2.9  |
| 1   | K     | 1838 | ALA  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1091 | GLY  | 2.9  |
| 1   | R     | 1659 | ARG  | 2.9  |
| 1   | E     | 1377 | GLN  | 2.9  |
| 1   | F     | 1484 | PHE  | 2.9  |
| 1   | C     | 934  | HIS  | 2.9  |
| 1   | D     | 1363 | ILE  | 2.9  |
| 1   | E     | 1040 | ASP  | 2.9  |
| 1   | F     | 2003 | ALA  | 2.9  |
| 1   | I     | 1422 | ARG  | 2.9  |
| 1   | K     | 1818 | ILE  | 2.9  |
| 1   | N     | 931  | LEU  | 2.9  |
| 1   | D     | 1377 | GLN  | 2.9  |
| 1   | O     | 1746 | THR  | 2.9  |
| 1   | E     | 1147 | ALA  | 2.9  |
| 1   | F     | 1221 | ALA  | 2.9  |
| 1   | F     | 1409 | ARG  | 2.9  |
| 1   | F     | 1523 | LEU  | 2.9  |
| 1   | G     | 1816 | ALA  | 2.9  |
| 1   | K     | 1792 | ILE  | 2.9  |
| 1   | Q     | 1542 | ALA  | 2.9  |
| 1   | F     | 1454 | LYS  | 2.9  |
| 1   | F     | 1578 | VAL  | 2.9  |
| 1   | H     | 1730 | MET  | 2.9  |
| 1   | D     | 1219 | ILE  | 2.9  |
| 1   | E     | 1765 | GLY  | 2.9  |
| 1   | M     | 1800 | PRO  | 2.9  |
| 1   | M     | 1975 | LEU  | 2.9  |
| 1   | H     | 1419 | GLU  | 2.9  |
| 1   | H     | 1698 | LEU  | 2.9  |
| 1   | N     | 1765 | GLY  | 2.9  |
| 1   | A     | 1925 | ASP  | 2.9  |
| 1   | J     | 1768 | VAL  | 2.9  |
| 1   | H     | 1503 | ARG  | 2.9  |
| 1   | M     | 1917 | TYR  | 2.9  |
| 1   | D     | 2006 | PHE  | 2.9  |
| 1   | H     | 1902 | PHE  | 2.9  |
| 1   | Q     | 1157 | GLU  | 2.9  |
| 1   | B     | 1792 | ILE  | 2.9  |
| 1   | K     | 1139 | TYR  | 2.9  |
| 1   | K     | 1217 | LEU  | 2.9  |
| 1   | J     | 1777 | GLY  | 2.9  |
| 1   | M     | 1852 | ALA  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1099 | LEU  | 2.9  |
| 1   | F     | 1451 | VAL  | 2.9  |
| 1   | B     | 1288 | HIS  | 2.9  |
| 1   | D     | 1946 | TRP  | 2.9  |
| 1   | Q     | 906  | SER  | 2.9  |
| 1   | A     | 1193 | LEU  | 2.9  |
| 1   | C     | 1193 | LEU  | 2.9  |
| 1   | D     | 1792 | ILE  | 2.9  |
| 1   | H     | 1329 | GLN  | 2.9  |
| 1   | L     | 1860 | LEU  | 2.9  |
| 1   | M     | 1227 | ASN  | 2.9  |
| 1   | M     | 1884 | GLN  | 2.9  |
| 1   | Q     | 1167 | LEU  | 2.9  |
| 1   | H     | 1065 | ALA  | 2.8  |
| 1   | E     | 1602 | TRP  | 2.8  |
| 1   | H     | 1205 | PRO  | 2.8  |
| 1   | D     | 1055 | HIS  | 2.8  |
| 1   | E     | 1373 | ALA  | 2.8  |
| 1   | M     | 1076 | VAL  | 2.8  |
| 1   | A     | 1533 | GLU  | 2.8  |
| 1   | G     | 1128 | LEU  | 2.8  |
| 1   | H     | 1769 | ILE  | 2.8  |
| 1   | I     | 1128 | LEU  | 2.8  |
| 1   | G     | 1116 | ALA  | 2.8  |
| 1   | H     | 1747 | GLY  | 2.8  |
| 1   | M     | 1169 | ALA  | 2.8  |
| 1   | G     | 1385 | ASP  | 2.8  |
| 1   | G     | 1092 | TYR  | 2.8  |
| 1   | G     | 1927 | PHE  | 2.8  |
| 1   | M     | 1399 | LEU  | 2.8  |
| 1   | F     | 1218 | VAL  | 2.8  |
| 1   | F     | 1781 | ALA  | 2.8  |
| 1   | G     | 1909 | VAL  | 2.8  |
| 1   | R     | 1094 | VAL  | 2.8  |
| 1   | J     | 1408 | GLU  | 2.8  |
| 1   | O     | 1419 | GLU  | 2.8  |
| 1   | R     | 1017 | ASP  | 2.8  |
| 1   | K     | 1347 | LEU  | 2.8  |
| 1   | A     | 1112 | VAL  | 2.8  |
| 1   | J     | 986  | ALA  | 2.8  |
| 1   | R     | 1165 | VAL  | 2.8  |
| 1   | J     | 1371 | HIS  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 1871 | ASP  | 2.8  |
| 1   | J     | 1773 | LEU  | 2.8  |
| 1   | M     | 1745 | ASP  | 2.8  |
| 1   | R     | 1134 | THR  | 2.8  |
| 1   | H     | 1127 | ARG  | 2.8  |
| 1   | R     | 1154 | ALA  | 2.8  |
| 1   | E     | 1977 | HIS  | 2.8  |
| 1   | K     | 1105 | SER  | 2.8  |
| 1   | N     | 1991 | SER  | 2.8  |
| 1   | C     | 1399 | LEU  | 2.8  |
| 1   | I     | 903  | LEU  | 2.8  |
| 1   | K     | 1226 | GLU  | 2.8  |
| 1   | Q     | 1019 | ASP  | 2.8  |
| 1   | E     | 1855 | VAL  | 2.8  |
| 1   | G     | 1276 | VAL  | 2.8  |
| 1   | E     | 1191 | ARG  | 2.8  |
| 1   | E     | 1548 | LEU  | 2.8  |
| 1   | K     | 1326 | HIS  | 2.8  |
| 1   | K     | 1698 | LEU  | 2.8  |
| 1   | P     | 1219 | ILE  | 2.8  |
| 1   | R     | 1137 | VAL  | 2.8  |
| 1   | L     | 1486 | GLY  | 2.8  |
| 1   | A     | 1761 | PHE  | 2.8  |
| 1   | E     | 1999 | ARG  | 2.8  |
| 1   | D     | 986  | ALA  | 2.8  |
| 1   | Q     | 1582 | ALA  | 2.8  |
| 1   | G     | 1347 | LEU  | 2.8  |
| 1   | L     | 1899 | PHE  | 2.8  |
| 1   | Q     | 1480 | LEU  | 2.8  |
| 1   | F     | 1538 | ALA  | 2.8  |
| 1   | K     | 1907 | ALA  | 2.8  |
| 1   | M     | 1938 | ALA  | 2.8  |
| 1   | L     | 1031 | LEU  | 2.8  |
| 1   | N     | 976  | LEU  | 2.8  |
| 1   | A     | 1768 | VAL  | 2.8  |
| 1   | E     | 1893 | THR  | 2.8  |
| 1   | F     | 1449 | ILE  | 2.8  |
| 1   | F     | 1116 | ALA  | 2.8  |
| 1   | R     | 931  | LEU  | 2.8  |
| 1   | R     | 1158 | LEU  | 2.8  |
| 1   | D     | 1768 | VAL  | 2.8  |
| 1   | D     | 1808 | ILE  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1740 | VAL  | 2.8  |
| 1   | M     | 1914 | GLN  | 2.8  |
| 1   | F     | 1534 | HIS  | 2.8  |
| 1   | J     | 1838 | ALA  | 2.8  |
| 1   | E     | 1365 | VAL  | 2.8  |
| 1   | K     | 1195 | ILE  | 2.8  |
| 1   | L     | 1893 | THR  | 2.8  |
| 1   | E     | 1996 | PHE  | 2.8  |
| 1   | P     | 1341 | HIS  | 2.8  |
| 1   | K     | 1276 | VAL  | 2.8  |
| 1   | L     | 1828 | PRO  | 2.8  |
| 1   | M     | 1301 | VAL  | 2.8  |
| 1   | P     | 1386 | GLU  | 2.8  |
| 1   | J     | 1893 | THR  | 2.8  |
| 1   | H     | 1534 | HIS  | 2.7  |
| 1   | P     | 1899 | PHE  | 2.8  |
| 1   | R     | 1669 | LEU  | 2.8  |
| 1   | A     | 1226 | GLU  | 2.7  |
| 1   | I     | 1507 | VAL  | 2.7  |
| 1   | M     | 1937 | PRO  | 2.7  |
| 1   | A     | 1867 | LEU  | 2.7  |
| 1   | H     | 1849 | LEU  | 2.7  |
| 1   | M     | 1924 | LEU  | 2.7  |
| 1   | P     | 1294 | ALA  | 2.7  |
| 1   | A     | 1999 | ARG  | 2.7  |
| 1   | F     | 1219 | ILE  | 2.7  |
| 1   | G     | 1804 | SER  | 2.7  |
| 1   | L     | 1498 | HIS  | 2.7  |
| 1   | L     | 1819 | VAL  | 2.7  |
| 1   | I     | 1754 | PRO  | 2.7  |
| 1   | F     | 1078 | ALA  | 2.7  |
| 1   | H     | 1041 | GLY  | 2.7  |
| 1   | H     | 1872 | TRP  | 2.7  |
| 1   | I     | 1163 | GLY  | 2.7  |
| 1   | J     | 996  | PHE  | 2.7  |
| 1   | M     | 1918 | ALA  | 2.7  |
| 1   | O     | 1415 | ASP  | 2.7  |
| 1   | Q     | 1120 | LEU  | 2.7  |
| 1   | L     | 1876 | VAL  | 2.7  |
| 1   | L     | 1800 | PRO  | 2.7  |
| 1   | M     | 1326 | HIS  | 2.7  |
| 1   | N     | 1655 | GLU  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | M     | 1984 | TYR  | 2.7  |
| 1   | A     | 1222 | GLY  | 2.7  |
| 1   | A     | 1853 | ALA  | 2.7  |
| 1   | F     | 1360 | ALA  | 2.7  |
| 1   | G     | 1907 | ALA  | 2.7  |
| 1   | A     | 1079 | VAL  | 2.7  |
| 1   | A     | 1820 | VAL  | 2.7  |
| 1   | G     | 1920 | ALA  | 2.7  |
| 1   | N     | 1741 | ILE  | 2.7  |
| 1   | Q     | 1106 | VAL  | 2.7  |
| 1   | Q     | 1422 | ARG  | 2.7  |
| 1   | J     | 1531 | ILE  | 2.7  |
| 1   | A     | 1899 | PHE  | 2.7  |
| 1   | C     | 1780 | LEU  | 2.7  |
| 1   | N     | 2006 | PHE  | 2.7  |
| 1   | F     | 1540 | GLY  | 2.7  |
| 1   | D     | 1981 | TYR  | 2.7  |
| 1   | F     | 1095 | HIS  | 2.7  |
| 1   | H     | 1031 | LEU  | 2.7  |
| 1   | H     | 1711 | PRO  | 2.7  |
| 1   | M     | 970  | PHE  | 2.7  |
| 1   | N     | 1877 | TYR  | 2.7  |
| 1   | Q     | 903  | LEU  | 2.7  |
| 1   | A     | 1907 | ALA  | 2.7  |
| 1   | E     | 2008 | ALA  | 2.7  |
| 1   | F     | 1274 | VAL  | 2.7  |
| 1   | R     | 1118 | GLY  | 2.7  |
| 1   | E     | 1120 | LEU  | 2.7  |
| 1   | H     | 1484 | PHE  | 2.7  |
| 1   | K     | 1975 | LEU  | 2.7  |
| 1   | B     | 1518 | THR  | 2.7  |
| 1   | D     | 1077 | ALA  | 2.7  |
| 1   | D     | 1490 | ALA  | 2.7  |
| 1   | G     | 1325 | THR  | 2.7  |
| 1   | I     | 1147 | ALA  | 2.7  |
| 1   | M     | 1197 | TRP  | 2.7  |
| 1   | F     | 1730 | MET  | 2.7  |
| 1   | J     | 1059 | PHE  | 2.7  |
| 1   | L     | 2004 | GLU  | 2.7  |
| 1   | G     | 1321 | LEU  | 2.7  |
| 1   | P     | 1849 | LEU  | 2.7  |
| 1   | D     | 1793 | VAL  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1768 | VAL  | 2.7  |
| 1   | O     | 1449 | ILE  | 2.7  |
| 1   | Q     | 1472 | SER  | 2.7  |
| 1   | L     | 1923 | TRP  | 2.7  |
| 1   | H     | 1304 | LEU  | 2.7  |
| 1   | I     | 1436 | LEU  | 2.7  |
| 1   | L     | 2007 | LEU  | 2.7  |
| 1   | Q     | 1166 | LEU  | 2.7  |
| 1   | A     | 1388 | ALA  | 2.7  |
| 1   | E     | 934  | HIS  | 2.7  |
| 1   | E     | 1948 | GLU  | 2.7  |
| 1   | F     | 1632 | LEU  | 2.7  |
| 1   | G     | 1031 | LEU  | 2.7  |
| 1   | J     | 1821 | GLU  | 2.7  |
| 1   | H     | 1323 | VAL  | 2.7  |
| 1   | L     | 1854 | VAL  | 2.7  |
| 1   | M     | 1279 | GLY  | 2.7  |
| 1   | E     | 1105 | SER  | 2.7  |
| 1   | F     | 1096 | PRO  | 2.7  |
| 1   | R     | 1097 | ALA  | 2.7  |
| 1   | Q     | 1117 | SER  | 2.7  |
| 1   | A     | 1833 | ARG  | 2.7  |
| 1   | H     | 1099 | LEU  | 2.7  |
| 1   | H     | 1975 | LEU  | 2.7  |
| 1   | L     | 1867 | LEU  | 2.7  |
| 1   | R     | 1431 | LEU  | 2.7  |
| 1   | R     | 1460 | PHE  | 2.7  |
| 1   | O     | 1413 | VAL  | 2.7  |
| 1   | R     | 947  | TYR  | 2.7  |
| 1   | A     | 1540 | GLY  | 2.7  |
| 1   | E     | 1974 | ILE  | 2.7  |
| 1   | Q     | 986  | ALA  | 2.7  |
| 1   | Q     | 1522 | ASP  | 2.7  |
| 1   | H     | 1896 | LEU  | 2.7  |
| 1   | R     | 1697 | LEU  | 2.7  |
| 1   | K     | 1507 | VAL  | 2.7  |
| 1   | K     | 1573 | GLN  | 2.7  |
| 1   | G     | 1308 | ALA  | 2.7  |
| 1   | Q     | 1101 | ALA  | 2.7  |
| 1   | B     | 1971 | PHE  | 2.7  |
| 1   | G     | 1127 | ARG  | 2.7  |
| 1   | K     | 1999 | ARG  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | L     | 1817 | ASP  | 2.7  |
| 1   | Q     | 1695 | ARG  | 2.7  |
| 1   | K     | 1517 | VAL  | 2.7  |
| 1   | P     | 1274 | VAL  | 2.7  |
| 1   | F     | 1795 | ASN  | 2.7  |
| 1   | M     | 1108 | ALA  | 2.7  |
| 1   | A     | 1389 | TRP  | 2.7  |
| 1   | G     | 1480 | LEU  | 2.7  |
| 1   | G     | 1550 | LEU  | 2.7  |
| 1   | N     | 1971 | PHE  | 2.7  |
| 1   | B     | 1408 | GLU  | 2.7  |
| 1   | G     | 1986 | PRO  | 2.7  |
| 1   | N     | 1337 | PRO  | 2.7  |
| 1   | P     | 1898 | TRP  | 2.7  |
| 1   | E     | 1434 | MET  | 2.7  |
| 1   | E     | 1556 | MET  | 2.7  |
| 1   | A     | 1369 | THR  | 2.7  |
| 1   | D     | 1288 | HIS  | 2.7  |
| 1   | E     | 1969 | TYR  | 2.7  |
| 1   | K     | 1324 | VAL  | 2.7  |
| 1   | G     | 1941 | ILE  | 2.7  |
| 1   | L     | 1816 | ALA  | 2.7  |
| 1   | I     | 1076 | VAL  | 2.6  |
| 1   | J     | 1819 | VAL  | 2.6  |
| 1   | D     | 1252 | ASP  | 2.6  |
| 1   | C     | 1860 | LEU  | 2.6  |
| 1   | D     | 1271 | LEU  | 2.6  |
| 1   | R     | 975  | LEU  | 2.6  |
| 1   | F     | 1039 | VAL  | 2.6  |
| 1   | G     | 1740 | VAL  | 2.6  |
| 1   | H     | 1152 | VAL  | 2.6  |
| 1   | A     | 1505 | GLY  | 2.6  |
| 1   | E     | 1916 | ALA  | 2.6  |
| 1   | M     | 1369 | THR  | 2.6  |
| 1   | P     | 1311 | LEU  | 2.6  |
| 1   | Q     | 1134 | THR  | 2.6  |
| 1   | G     | 1854 | VAL  | 2.6  |
| 1   | M     | 1793 | VAL  | 2.6  |
| 1   | N     | 1941 | ILE  | 2.6  |
| 1   | P     | 1195 | ILE  | 2.6  |
| 1   | R     | 1727 | ILE  | 2.6  |
| 1   | Q     | 1022 | ARG  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1149 | SER  | 2.6  |
| 1   | N     | 1872 | TRP  | 2.6  |
| 1   | Q     | 1465 | VAL  | 2.6  |
| 1   | A     | 1808 | ILE  | 2.6  |
| 1   | B     | 1277 | ILE  | 2.6  |
| 1   | F     | 1319 | PRO  | 2.6  |
| 1   | H     | 1899 | PHE  | 2.6  |
| 1   | H     | 1527 | LEU  | 2.6  |
| 1   | H     | 1817 | ASP  | 2.6  |
| 1   | D     | 1234 | VAL  | 2.6  |
| 1   | P     | 1276 | VAL  | 2.6  |
| 1   | Q     | 1539 | VAL  | 2.6  |
| 1   | C     | 1946 | TRP  | 2.6  |
| 1   | D     | 1249 | TRP  | 2.6  |
| 1   | R     | 1108 | ALA  | 2.6  |
| 1   | A     | 1917 | TYR  | 2.6  |
| 1   | G     | 1533 | GLU  | 2.6  |
| 1   | Q     | 1519 | CYS  | 2.6  |
| 1   | R     | 1602 | TRP  | 2.6  |
| 1   | E     | 1107 | ILE  | 2.6  |
| 1   | H     | 1048 | PHE  | 2.6  |
| 1   | H     | 1390 | ARG  | 2.6  |
| 1   | M     | 1932 | ARG  | 2.6  |
| 1   | Q     | 1653 | PHE  | 2.6  |
| 1   | E     | 1014 | LEU  | 2.6  |
| 1   | F     | 1156 | LEU  | 2.6  |
| 1   | R     | 1667 | LEU  | 2.6  |
| 1   | K     | 1929 | GLN  | 2.6  |
| 1   | P     | 1886 | VAL  | 2.6  |
| 1   | L     | 1930 | TRP  | 2.6  |
| 1   | Q     | 1587 | TYR  | 2.6  |
| 1   | E     | 1270 | PRO  | 2.6  |
| 1   | F     | 1521 | ALA  | 2.6  |
| 1   | H     | 945  | ALA  | 2.6  |
| 1   | J     | 1766 | ALA  | 2.6  |
| 1   | C     | 1740 | VAL  | 2.6  |
| 1   | M     | 1768 | VAL  | 2.6  |
| 1   | R     | 1740 | VAL  | 2.6  |
| 1   | K     | 1363 | ILE  | 2.6  |
| 1   | Q     | 1035 | HIS  | 2.6  |
| 1   | Q     | 1131 | TYR  | 2.6  |
| 1   | G     | 1194 | THR  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | G     | 1090 | ARG  | 2.6  |
| 1   | H     | 1267 | ASP  | 2.6  |
| 1   | H     | 1374 | LEU  | 2.6  |
| 1   | L     | 1857 | ASP  | 2.6  |
| 1   | C     | 1964 | PRO  | 2.6  |
| 1   | H     | 1781 | ALA  | 2.6  |
| 1   | M     | 1351 | VAL  | 2.6  |
| 1   | C     | 1655 | GLU  | 2.6  |
| 1   | C     | 1105 | SER  | 2.6  |
| 1   | E     | 1347 | LEU  | 2.6  |
| 1   | G     | 1085 | LEU  | 2.6  |
| 1   | K     | 1120 | LEU  | 2.6  |
| 1   | D     | 1017 | ASP  | 2.6  |
| 1   | D     | 1076 | VAL  | 2.6  |
| 1   | F     | 1485 | GLY  | 2.6  |
| 1   | I     | 923  | VAL  | 2.6  |
| 1   | F     | 1399 | LEU  | 2.6  |
| 1   | H     | 1564 | ILE  | 2.6  |
| 1   | Q     | 1667 | LEU  | 2.6  |
| 1   | D     | 1275 | ALA  | 2.6  |
| 1   | C     | 1908 | LEU  | 2.6  |
| 1   | E     | 1683 | LEU  | 2.6  |
| 1   | N     | 1884 | GLN  | 2.6  |
| 1   | H     | 1835 | VAL  | 2.6  |
| 1   | L     | 1852 | ALA  | 2.6  |
| 1   | P     | 1273 | GLY  | 2.6  |
| 1   | D     | 1908 | LEU  | 2.6  |
| 1   | F     | 1172 | LEU  | 2.6  |
| 1   | P     | 1655 | GLU  | 2.6  |
| 1   | A     | 1106 | VAL  | 2.6  |
| 1   | M     | 1766 | ALA  | 2.6  |
| 1   | R     | 1186 | ARG  | 2.6  |
| 1   | B     | 885  | ASP  | 2.6  |
| 1   | M     | 896  | PRO  | 2.6  |
| 1   | P     | 1324 | VAL  | 2.6  |
| 1   | P     | 1362 | GLN  | 2.6  |
| 1   | N     | 1852 | ALA  | 2.6  |
| 1   | Q     | 1097 | ALA  | 2.6  |
| 1   | N     | 1804 | SER  | 2.6  |
| 1   | O     | 1410 | ARG  | 2.6  |
| 1   | R     | 1503 | ARG  | 2.6  |
| 1   | E     | 1391 | ASP  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | G     | 1217 | LEU  | 2.5  |
| 1   | J     | 1925 | ASP  | 2.5  |
| 1   | M     | 1341 | HIS  | 2.5  |
| 1   | M     | 1850 | HIS  | 2.5  |
| 1   | N     | 1782 | GLU  | 2.5  |
| 1   | N     | 1834 | LEU  | 2.5  |
| 1   | F     | 1094 | VAL  | 2.5  |
| 1   | H     | 930  | TRP  | 2.5  |
| 1   | Q     | 1687 | THR  | 2.5  |
| 1   | H     | 1812 | ARG  | 2.5  |
| 1   | P     | 1542 | ALA  | 2.5  |
| 1   | C     | 1142 | SER  | 2.5  |
| 1   | L     | 1902 | PHE  | 2.5  |
| 1   | D     | 1523 | LEU  | 2.5  |
| 1   | F     | 1311 | LEU  | 2.5  |
| 1   | F     | 1251 | HIS  | 2.5  |
| 1   | H     | 1126 | ARG  | 2.5  |
| 1   | E     | 2006 | PHE  | 2.5  |
| 1   | M     | 1818 | ILE  | 2.5  |
| 1   | F     | 1701 | VAL  | 2.5  |
| 1   | E     | 1371 | HIS  | 2.5  |
| 1   | E     | 1779 | PHE  | 2.5  |
| 1   | L     | 1875 | LYS  | 2.5  |
| 1   | M     | 1779 | PHE  | 2.5  |
| 1   | E     | 1311 | LEU  | 2.5  |
| 1   | K     | 1821 | GLU  | 2.5  |
| 1   | N     | 1784 | MET  | 2.5  |
| 1   | A     | 1789 | CYS  | 2.5  |
| 1   | Q     | 1426 | ARG  | 2.5  |
| 1   | B     | 1538 | ALA  | 2.5  |
| 1   | Q     | 1447 | GLY  | 2.5  |
| 1   | F     | 1834 | LEU  | 2.5  |
| 1   | J     | 1387 | THR  | 2.5  |
| 1   | M     | 1128 | LEU  | 2.5  |
| 1   | P     | 1767 | TYR  | 2.5  |
| 1   | R     | 1131 | TYR  | 2.5  |
| 1   | A     | 1191 | ARG  | 2.5  |
| 1   | C     | 1872 | TRP  | 2.5  |
| 1   | L     | 1763 | GLY  | 2.5  |
| 1   | L     | 1873 | ALA  | 2.5  |
| 1   | R     | 1061 | GLY  | 2.5  |
| 1   | C     | 1776 | LEU  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1962 | ILE  | 2.5  |
| 1   | M     | 1925 | ASP  | 2.5  |
| 1   | Q     | 1644 | LEU  | 2.5  |
| 1   | D     | 1489 | THR  | 2.5  |
| 1   | D     | 1940 | SER  | 2.5  |
| 1   | F     | 1405 | ARG  | 2.5  |
| 1   | R     | 1064 | GLU  | 2.5  |
| 1   | K     | 2006 | PHE  | 2.5  |
| 1   | L     | 1963 | ALA  | 2.5  |
| 1   | F     | 1519 | CYS  | 2.5  |
| 1   | M     | 1789 | CYS  | 2.5  |
| 1   | F     | 1868 | VAL  | 2.5  |
| 1   | Q     | 1427 | ASN  | 2.5  |
| 1   | R     | 1753 | VAL  | 2.5  |
| 1   | P     | 1902 | PHE  | 2.5  |
| 1   | A     | 1946 | TRP  | 2.5  |
| 1   | D     | 1769 | ILE  | 2.5  |
| 1   | E     | 1778 | LEU  | 2.5  |
| 1   | J     | 1669 | LEU  | 2.5  |
| 1   | L     | 1858 | ALA  | 2.5  |
| 1   | I     | 1107 | ILE  | 2.5  |
| 1   | M     | 1974 | ILE  | 2.5  |
| 1   | N     | 1792 | ILE  | 2.5  |
| 1   | P     | 1988 | LEU  | 2.5  |
| 1   | F     | 933  | ASP  | 2.5  |
| 1   | H     | 1153 | GLU  | 2.5  |
| 1   | J     | 1155 | ASP  | 2.5  |
| 1   | A     | 1784 | MET  | 2.5  |
| 1   | D     | 1310 | THR  | 2.5  |
| 1   | E     | 1244 | THR  | 2.5  |
| 1   | F     | 1561 | LYS  | 2.5  |
| 1   | A     | 1983 | GLY  | 2.5  |
| 1   | E     | 1706 | ALA  | 2.5  |
| 1   | I     | 1480 | LEU  | 2.5  |
| 1   | J     | 1397 | ALA  | 2.5  |
| 1   | J     | 1790 | GLY  | 2.5  |
| 1   | F     | 1032 | LEU  | 2.5  |
| 1   | R     | 1121 | LEU  | 2.5  |
| 1   | G     | 1819 | VAL  | 2.5  |
| 1   | I     | 1448 | GLN  | 2.5  |
| 1   | K     | 1791 | ARG  | 2.5  |
| 1   | M     | 1196 | GLU  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1141 | LEU  | 2.5  |
| 1   | G     | 1298 | ALA  | 2.5  |
| 1   | F     | 1165 | VAL  | 2.5  |
| 1   | G     | 1974 | ILE  | 2.5  |
| 1   | H     | 1120 | LEU  | 2.5  |
| 1   | M     | 1823 | GLY  | 2.5  |
| 1   | N     | 1230 | ALA  | 2.5  |
| 1   | P     | 1360 | ALA  | 2.5  |
| 1   | O     | 1517 | VAL  | 2.5  |
| 1   | H     | 1931 | ARG  | 2.5  |
| 1   | I     | 1516 | PHE  | 2.5  |
| 1   | Q     | 1048 | PHE  | 2.5  |
| 1   | B     | 1772 | GLY  | 2.5  |
| 1   | D     | 1062 | LEU  | 2.5  |
| 1   | E     | 1449 | ILE  | 2.5  |
| 1   | F     | 1793 | VAL  | 2.5  |
| 1   | G     | 1863 | ILE  | 2.5  |
| 1   | L     | 1053 | ILE  | 2.5  |
| 1   | G     | 1110 | PRO  | 2.5  |
| 1   | M     | 998  | VAL  | 2.5  |
| 1   | K     | 1899 | PHE  | 2.5  |
| 1   | K     | 1984 | TYR  | 2.5  |
| 1   | Q     | 1658 | LYS  | 2.5  |
| 1   | C     | 1480 | LEU  | 2.5  |
| 1   | E     | 1344 | LEU  | 2.5  |
| 1   | F     | 1789 | CYS  | 2.5  |
| 1   | C     | 1602 | TRP  | 2.5  |
| 1   | G     | 1227 | ASN  | 2.5  |
| 1   | N     | 1324 | VAL  | 2.5  |
| 1   | D     | 1640 | GLN  | 2.5  |
| 1   | H     | 1193 | LEU  | 2.5  |
| 1   | D     | 1301 | VAL  | 2.5  |
| 1   | F     | 1808 | ILE  | 2.5  |
| 1   | O     | 1116 | ALA  | 2.5  |
| 1   | F     | 1943 | TRP  | 2.5  |
| 1   | H     | 1943 | TRP  | 2.5  |
| 1   | M     | 1965 | ASP  | 2.5  |
| 1   | R     | 1531 | ILE  | 2.5  |
| 1   | A     | 1245 | THR  | 2.5  |
| 1   | F     | 1533 | GLU  | 2.5  |
| 1   | E     | 976  | LEU  | 2.5  |
| 1   | F     | 1119 | MET  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 1068 | ALA  | 2.5  |
| 1   | H     | 1997 | ALA  | 2.5  |
| 1   | M     | 1777 | GLY  | 2.5  |
| 1   | O     | 1755 | PRO  | 2.5  |
| 1   | M     | 950  | MET  | 2.5  |
| 1   | N     | 1311 | LEU  | 2.5  |
| 1   | D     | 1920 | ALA  | 2.5  |
| 1   | G     | 1375 | VAL  | 2.5  |
| 1   | B     | 1857 | ASP  | 2.4  |
| 1   | E     | 1201 | GLU  | 2.4  |
| 1   | L     | 1965 | ASP  | 2.4  |
| 1   | L     | 1969 | TYR  | 2.4  |
| 1   | H     | 897  | SER  | 2.4  |
| 1   | B     | 1537 | ALA  | 2.4  |
| 1   | B     | 1519 | CYS  | 2.4  |
| 1   | C     | 1484 | PHE  | 2.4  |
| 1   | R     | 1055 | HIS  | 2.4  |
| 1   | G     | 1062 | LEU  | 2.4  |
| 1   | G     | 1655 | GLU  | 2.4  |
| 1   | L     | 1939 | THR  | 2.4  |
| 1   | C     | 1307 | ILE  | 2.4  |
| 1   | M     | 1758 | VAL  | 2.4  |
| 1   | P     | 923  | VAL  | 2.4  |
| 1   | D     | 1201 | GLU  | 2.4  |
| 1   | I     | 1710 | LEU  | 2.4  |
| 1   | Q     | 1646 | LEU  | 2.4  |
| 1   | R     | 926  | GLU  | 2.4  |
| 1   | R     | 1153 | GLU  | 2.4  |
| 1   | E     | 1079 | VAL  | 2.4  |
| 1   | E     | 1750 | GLN  | 2.4  |
| 1   | C     | 1985 | ALA  | 2.4  |
| 1   | E     | 1024 | ALA  | 2.4  |
| 1   | F     | 1576 | ILE  | 2.4  |
| 1   | C     | 1794 | VAL  | 2.4  |
| 1   | E     | 1288 | HIS  | 2.4  |
| 1   | I     | 1431 | LEU  | 2.4  |
| 1   | K     | 1323 | VAL  | 2.4  |
| 1   | P     | 1499 | ARG  | 2.4  |
| 1   | E     | 1337 | PRO  | 2.4  |
| 1   | F     | 1458 | ILE  | 2.4  |
| 1   | H     | 1713 | PRO  | 2.4  |
| 1   | L     | 1941 | ILE  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 2002 | PHE  | 2.4  |
| 1   | M     | 1672 | PHE  | 2.4  |
| 1   | P     | 1921 | ASN  | 2.4  |
| 1   | D     | 1095 | HIS  | 2.4  |
| 1   | E     | 1818 | ILE  | 2.4  |
| 1   | B     | 1108 | ALA  | 2.4  |
| 1   | M     | 1916 | ALA  | 2.4  |
| 1   | L     | 1994 | THR  | 2.4  |
| 1   | O     | 1682 | ASP  | 2.4  |
| 1   | C     | 1658 | LYS  | 2.4  |
| 1   | H     | 1431 | LEU  | 2.4  |
| 1   | N     | 1795 | ASN  | 2.4  |
| 1   | Q     | 1632 | LEU  | 2.4  |
| 1   | Q     | 1669 | LEU  | 2.4  |
| 1   | A     | 1536 | ALA  | 2.4  |
| 1   | C     | 1771 | GLY  | 2.4  |
| 1   | I     | 1519 | CYS  | 2.4  |
| 1   | M     | 1337 | PRO  | 2.4  |
| 1   | B     | 1311 | LEU  | 2.4  |
| 1   | C     | 1925 | ASP  | 2.4  |
| 1   | H     | 1526 | LYS  | 2.4  |
| 1   | I     | 1660 | ASP  | 2.4  |
| 1   | K     | 1062 | LEU  | 2.4  |
| 1   | K     | 1224 | ASP  | 2.4  |
| 1   | M     | 1897 | ASP  | 2.4  |
| 1   | M     | 1296 | ARG  | 2.4  |
| 1   | Q     | 989  | THR  | 2.4  |
| 1   | Q     | 1125 | VAL  | 2.4  |
| 1   | R     | 1636 | THR  | 2.4  |
| 1   | D     | 1484 | PHE  | 2.4  |
| 1   | F     | 1080 | ALA  | 2.4  |
| 1   | J     | 1998 | GLN  | 2.4  |
| 1   | C     | 1834 | LEU  | 2.4  |
| 1   | G     | 1379 | LEU  | 2.4  |
| 1   | A     | 1142 | SER  | 2.4  |
| 1   | B     | 1075 | VAL  | 2.4  |
| 1   | G     | 1984 | TYR  | 2.4  |
| 1   | I     | 1106 | VAL  | 2.4  |
| 1   | M     | 1304 | LEU  | 2.4  |
| 1   | P     | 1877 | TYR  | 2.4  |
| 1   | R     | 1631 | VAL  | 2.4  |
| 1   | F     | 1586 | ILE  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | K     | 1511 | GLY  | 2.4  |
| 1   | N     | 1982 | ASN  | 2.4  |
| 1   | I     | 1565 | HIS  | 2.4  |
| 1   | M     | 1455 | ALA  | 2.4  |
| 1   | R     | 1077 | ALA  | 2.4  |
| 1   | D     | 1964 | PRO  | 2.4  |
| 1   | E     | 1266 | LEU  | 2.4  |
| 1   | E     | 1875 | LYS  | 2.4  |
| 1   | F     | 1453 | VAL  | 2.4  |
| 1   | H     | 1062 | LEU  | 2.4  |
| 1   | H     | 1365 | VAL  | 2.4  |
| 1   | M     | 1780 | LEU  | 2.4  |
| 1   | N     | 1389 | TRP  | 2.4  |
| 1   | R     | 1543 | TYR  | 2.4  |
| 1   | A     | 1053 | ILE  | 2.4  |
| 1   | M     | 1421 | MET  | 2.4  |
| 1   | G     | 1906 | ALA  | 2.4  |
| 1   | E     | 1062 | LEU  | 2.4  |
| 1   | F     | 1750 | GLN  | 2.4  |
| 1   | G     | 968  | LEU  | 2.4  |
| 1   | G     | 1351 | VAL  | 2.4  |
| 1   | H     | 1276 | VAL  | 2.4  |
| 1   | K     | 1908 | LEU  | 2.4  |
| 1   | C     | 1782 | GLU  | 2.4  |
| 1   | P     | 1880 | TRP  | 2.4  |
| 1   | A     | 1911 | SER  | 2.4  |
| 1   | N     | 1040 | ASP  | 2.4  |
| 1   | N     | 1105 | SER  | 2.4  |
| 1   | Q     | 1656 | ILE  | 2.4  |
| 1   | Q     | 1672 | PHE  | 2.4  |
| 1   | E     | 1077 | ALA  | 2.4  |
| 1   | L     | 1567 | ALA  | 2.4  |
| 1   | E     | 1106 | VAL  | 2.4  |
| 1   | L     | 1843 | LEU  | 2.4  |
| 1   | M     | 1400 | CYS  | 2.4  |
| 1   | D     | 1313 | ASP  | 2.4  |
| 1   | N     | 1785 | ALA  | 2.4  |
| 1   | N     | 1925 | ASP  | 2.4  |
| 1   | Q     | 1485 | GLY  | 2.4  |
| 1   | D     | 1304 | LEU  | 2.4  |
| 1   | F     | 1882 | LEU  | 2.4  |
| 1   | G     | 954  | ALA  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1213 | ALA  | 2.4  |
| 1   | A     | 1930 | TRP  | 2.4  |
| 1   | C     | 1277 | ILE  | 2.4  |
| 1   | R     | 1103 | PHE  | 2.4  |
| 1   | F     | 1625 | GLY  | 2.4  |
| 1   | B     | 1304 | LEU  | 2.4  |
| 1   | E     | 1523 | LEU  | 2.4  |
| 1   | G     | 1776 | LEU  | 2.4  |
| 1   | B     | 1363 | ILE  | 2.4  |
| 1   | E     | 1448 | GLN  | 2.4  |
| 1   | G     | 1875 | LYS  | 2.4  |
| 1   | E     | 1239 | GLY  | 2.4  |
| 1   | I     | 948  | CYS  | 2.4  |
| 1   | J     | 1454 | LYS  | 2.4  |
| 1   | C     | 1907 | ALA  | 2.4  |
| 1   | C     | 1987 | VAL  | 2.4  |
| 1   | F     | 903  | LEU  | 2.4  |
| 1   | G     | 1075 | VAL  | 2.4  |
| 1   | J     | 1379 | LEU  | 2.4  |
| 1   | P     | 1536 | ALA  | 2.4  |
| 1   | L     | 1897 | ASP  | 2.4  |
| 1   | E     | 1715 | ILE  | 2.4  |
| 1   | E     | 1727 | ILE  | 2.4  |
| 1   | A     | 1485 | GLY  | 2.4  |
| 1   | A     | 1512 | CYS  | 2.4  |
| 1   | E     | 1035 | HIS  | 2.4  |
| 1   | B     | 1975 | LEU  | 2.4  |
| 1   | J     | 1311 | LEU  | 2.4  |
| 1   | J     | 1765 | GLY  | 2.4  |
| 1   | M     | 1747 | GLY  | 2.4  |
| 1   | G     | 1324 | VAL  | 2.4  |
| 1   | P     | 1885 | ALA  | 2.4  |
| 1   | B     | 1871 | ASP  | 2.4  |
| 1   | N     | 1902 | PHE  | 2.4  |
| 1   | Q     | 1435 | GLU  | 2.3  |
| 1   | R     | 1564 | ILE  | 2.3  |
| 1   | R     | 1586 | ILE  | 2.3  |
| 1   | D     | 1455 | ALA  | 2.3  |
| 1   | E     | 1538 | ALA  | 2.3  |
| 1   | F     | 1076 | VAL  | 2.3  |
| 1   | Q     | 1612 | THR  | 2.3  |
| 1   | H     | 1318 | PRO  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1455 | ALA  | 2.3  |
| 1   | E     | 1752 | VAL  | 2.3  |
| 1   | F     | 1075 | VAL  | 2.3  |
| 1   | K     | 1819 | VAL  | 2.3  |
| 1   | L     | 1447 | GLY  | 2.3  |
| 1   | M     | 1202 | LEU  | 2.3  |
| 1   | Q     | 1730 | MET  | 2.3  |
| 1   | Q     | 1740 | VAL  | 2.3  |
| 1   | R     | 1057 | ALA  | 2.3  |
| 1   | E     | 1877 | TYR  | 2.3  |
| 1   | M     | 1168 | SER  | 2.3  |
| 1   | K     | 1730 | MET  | 2.3  |
| 1   | K     | 1946 | TRP  | 2.3  |
| 1   | E     | 1057 | ALA  | 2.3  |
| 1   | F     | 1654 | VAL  | 2.3  |
| 1   | L     | 1750 | GLN  | 2.3  |
| 1   | Q     | 1720 | LEU  | 2.3  |
| 1   | M     | 1373 | ALA  | 2.3  |
| 1   | M     | 1945 | ALA  | 2.3  |
| 1   | A     | 1921 | ASN  | 2.3  |
| 1   | G     | 1779 | PHE  | 2.3  |
| 1   | B     | 1142 | SER  | 2.3  |
| 1   | C     | 1988 | LEU  | 2.3  |
| 1   | D     | 931  | LEU  | 2.3  |
| 1   | D     | 1337 | PRO  | 2.3  |
| 1   | E     | 1267 | ASP  | 2.3  |
| 1   | E     | 1897 | ASP  | 2.3  |
| 1   | F     | 1570 | GLY  | 2.3  |
| 1   | L     | 1436 | LEU  | 2.3  |
| 1   | P     | 1784 | MET  | 2.3  |
| 1   | Q     | 1701 | VAL  | 2.3  |
| 1   | D     | 1070 | ALA  | 2.3  |
| 1   | P     | 2003 | ALA  | 2.3  |
| 1   | C     | 1282 | GLU  | 2.3  |
| 1   | G     | 1849 | LEU  | 2.3  |
| 1   | N     | 1835 | VAL  | 2.3  |
| 1   | R     | 1635 | VAL  | 2.3  |
| 1   | E     | 1308 | ALA  | 2.3  |
| 1   | E     | 1326 | HIS  | 2.3  |
| 1   | P     | 1846 | ARG  | 2.3  |
| 1   | G     | 1778 | LEU  | 2.3  |
| 1   | E     | 1346 | GLY  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1872 | TRP  | 2.3  |
| 1   | G     | 1693 | LYS  | 2.3  |
| 1   | G     | 1930 | TRP  | 2.3  |
| 1   | M     | 1511 | GLY  | 2.3  |
| 1   | O     | 1466 | ALA  | 2.3  |
| 1   | Q     | 1623 | THR  | 2.3  |
| 1   | A     | 1174 | LEU  | 2.3  |
| 1   | Q     | 1158 | LEU  | 2.3  |
| 1   | Q     | 930  | TRP  | 2.3  |
| 1   | D     | 1103 | PHE  | 2.3  |
| 1   | E     | 920  | GLN  | 2.3  |
| 1   | E     | 1879 | ALA  | 2.3  |
| 1   | M     | 1906 | ALA  | 2.3  |
| 1   | D     | 1871 | ASP  | 2.3  |
| 1   | P     | 1893 | THR  | 2.3  |
| 1   | C     | 1379 | LEU  | 2.3  |
| 1   | G     | 1780 | LEU  | 2.3  |
| 1   | H     | 1079 | VAL  | 2.3  |
| 1   | K     | 1032 | LEU  | 2.3  |
| 1   | M     | 1102 | CYS  | 2.3  |
| 1   | Q     | 971  | HIS  | 2.3  |
| 1   | M     | 1928 | MET  | 2.3  |
| 1   | Q     | 992  | GLY  | 2.3  |
| 1   | E     | 1240 | ALA  | 2.3  |
| 1   | G     | 1059 | PHE  | 2.3  |
| 1   | O     | 1416 | ASN  | 2.3  |
| 1   | G     | 1329 | GLN  | 2.3  |
| 1   | O     | 1749 | SER  | 2.3  |
| 1   | R     | 1006 | ARG  | 2.3  |
| 1   | K     | 1365 | VAL  | 2.3  |
| 1   | L     | 1975 | LEU  | 2.3  |
| 1   | F     | 950  | MET  | 2.3  |
| 1   | F     | 1942 | ALA  | 2.3  |
| 1   | M     | 1971 | PHE  | 2.3  |
| 1   | C     | 1808 | ILE  | 2.3  |
| 1   | C     | 1982 | ASN  | 2.3  |
| 1   | J     | 1962 | ILE  | 2.3  |
| 1   | G     | 1981 | TYR  | 2.3  |
| 1   | B     | 1252 | ASP  | 2.3  |
| 1   | B     | 1909 | VAL  | 2.3  |
| 1   | E     | 1820 | VAL  | 2.3  |
| 1   | R     | 1517 | VAL  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | K     | 1928 | MET  | 2.3  |
| 1   | Q     | 1627 | GLY  | 2.3  |
| 1   | E     | 1394 | TRP  | 2.3  |
| 1   | E     | 1811 | ILE  | 2.3  |
| 1   | D     | 1311 | LEU  | 2.3  |
| 1   | E     | 1152 | VAL  | 2.3  |
| 1   | F     | 1988 | LEU  | 2.3  |
| 1   | H     | 1085 | LEU  | 2.3  |
| 1   | K     | 1720 | LEU  | 2.3  |
| 1   | L     | 1032 | LEU  | 2.3  |
| 1   | L     | 1934 | GLN  | 2.3  |
| 1   | M     | 1096 | PRO  | 2.3  |
| 1   | M     | 1104 | GLN  | 2.3  |
| 1   | O     | 942  | LEU  | 2.3  |
| 1   | R     | 1527 | LEU  | 2.3  |
| 1   | R     | 1738 | LYS  | 2.3  |
| 1   | D     | 1422 | ARG  | 2.3  |
| 1   | D     | 1348 | ILE  | 2.3  |
| 1   | N     | 1195 | ILE  | 2.3  |
| 1   | P     | 1307 | ILE  | 2.3  |
| 1   | E     | 1773 | LEU  | 2.3  |
| 1   | H     | 1908 | LEU  | 2.3  |
| 1   | R     | 1759 | PRO  | 2.3  |
| 1   | A     | 1252 | ASP  | 2.3  |
| 1   | H     | 1119 | MET  | 2.3  |
| 1   | Q     | 1686 | MET  | 2.3  |
| 1   | L     | 1863 | ILE  | 2.3  |
| 1   | F     | 1158 | LEU  | 2.3  |
| 1   | G     | 1066 | TYR  | 2.3  |
| 1   | I     | 1032 | LEU  | 2.3  |
| 1   | B     | 1902 | PHE  | 2.3  |
| 1   | H     | 906  | SER  | 2.3  |
| 1   | H     | 1268 | GLU  | 2.3  |
| 1   | N     | 1484 | PHE  | 2.3  |
| 1   | G     | 1080 | ALA  | 2.3  |
| 1   | J     | 1108 | ALA  | 2.3  |
| 1   | J     | 1738 | LYS  | 2.3  |
| 1   | P     | 1197 | TRP  | 2.3  |
| 1   | B     | 1379 | LEU  | 2.3  |
| 1   | G     | 1647 | LEU  | 2.3  |
| 1   | M     | 1860 | LEU  | 2.3  |
| 1   | P     | 1839 | THR  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | R     | 1092 | TYR  | 2.3  |
| 1   | A     | 1201 | GLU  | 2.3  |
| 1   | H     | 1073 | PRO  | 2.3  |
| 1   | G     | 1241 | GLY  | 2.3  |
| 1   | H     | 1422 | ARG  | 2.3  |
| 1   | H     | 1986 | PRO  | 2.3  |
| 1   | L     | 1966 | GLU  | 2.3  |
| 1   | Q     | 1045 | ARG  | 2.3  |
| 1   | L     | 1421 | MET  | 2.3  |
| 1   | A     | 1908 | LEU  | 2.3  |
| 1   | H     | 1134 | THR  | 2.3  |
| 1   | I     | 1120 | LEU  | 2.3  |
| 1   | J     | 1307 | ILE  | 2.3  |
| 1   | I     | 1419 | GLU  | 2.2  |
| 1   | N     | 1653 | PHE  | 2.3  |
| 1   | Q     | 926  | GLU  | 2.2  |
| 1   | J     | 1003 | SER  | 2.2  |
| 1   | M     | 1804 | SER  | 2.2  |
| 1   | Q     | 905  | GLY  | 2.2  |
| 1   | Q     | 1482 | SER  | 2.2  |
| 1   | C     | 1108 | ALA  | 2.2  |
| 1   | D     | 1351 | VAL  | 2.2  |
| 1   | F     | 1872 | TRP  | 2.2  |
| 1   | G     | 1158 | LEU  | 2.2  |
| 1   | G     | 1531 | ILE  | 2.2  |
| 1   | H     | 1271 | LEU  | 2.2  |
| 1   | K     | 1197 | TRP  | 2.2  |
| 1   | L     | 1921 | ASN  | 2.2  |
| 1   | M     | 1879 | ALA  | 2.2  |
| 1   | O     | 1752 | VAL  | 2.2  |
| 1   | Q     | 1013 | VAL  | 2.2  |
| 1   | Q     | 1431 | LEU  | 2.2  |
| 1   | R     | 1656 | ILE  | 2.2  |
| 1   | D     | 1543 | TYR  | 2.2  |
| 1   | M     | 1543 | TYR  | 2.2  |
| 1   | A     | 1229 | ARG  | 2.2  |
| 1   | J     | 1895 | GLU  | 2.2  |
| 1   | M     | 1362 | GLN  | 2.2  |
| 1   | M     | 1847 | GLY  | 2.2  |
| 1   | E     | 1825 | ILE  | 2.2  |
| 1   | E     | 1547 | TRP  | 2.2  |
| 1   | H     | 1032 | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1159 | LEU  | 2.2  |
| 1   | H     | 1630 | ILE  | 2.2  |
| 1   | M     | 945  | ALA  | 2.2  |
| 1   | N     | 1838 | ALA  | 2.2  |
| 1   | B     | 1979 | ARG  | 2.2  |
| 1   | C     | 1059 | PHE  | 2.2  |
| 1   | I     | 1103 | PHE  | 2.2  |
| 1   | N     | 1059 | PHE  | 2.2  |
| 1   | N     | 1345 | ARG  | 2.2  |
| 1   | B     | 1525 | THR  | 2.2  |
| 1   | L     | 1790 | GLY  | 2.2  |
| 1   | C     | 1512 | CYS  | 2.2  |
| 1   | F     | 1067 | VAL  | 2.2  |
| 1   | F     | 1301 | VAL  | 2.2  |
| 1   | F     | 1906 | ALA  | 2.2  |
| 1   | L     | 1848 | VAL  | 2.2  |
| 1   | M     | 976  | LEU  | 2.2  |
| 1   | R     | 1680 | ALA  | 2.2  |
| 1   | M     | 1923 | TRP  | 2.2  |
| 1   | B     | 1129 | ARG  | 2.2  |
| 1   | E     | 1510 | ASN  | 2.2  |
| 1   | L     | 1960 | ASN  | 2.2  |
| 1   | E     | 1553 | LEU  | 2.2  |
| 1   | F     | 1062 | LEU  | 2.2  |
| 1   | H     | 1537 | ALA  | 2.2  |
| 1   | K     | 1816 | ALA  | 2.2  |
| 1   | N     | 1563 | LEU  | 2.2  |
| 1   | P     | 1205 | PRO  | 2.2  |
| 1   | R     | 974  | LEU  | 2.2  |
| 1   | H     | 1342 | SER  | 2.2  |
| 1   | R     | 1514 | SER  | 2.2  |
| 1   | C     | 1567 | ALA  | 2.2  |
| 1   | D     | 1369 | THR  | 2.2  |
| 1   | D     | 1780 | LEU  | 2.2  |
| 1   | F     | 1488 | VAL  | 2.2  |
| 1   | F     | 1545 | THR  | 2.2  |
| 1   | G     | 1817 | ASP  | 2.2  |
| 1   | L     | 1772 | GLY  | 2.2  |
| 1   | O     | 1458 | ILE  | 2.2  |
| 1   | O     | 1741 | ILE  | 2.2  |
| 1   | Q     | 1640 | GLN  | 2.2  |
| 1   | E     | 1702 | TYR  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1738 | LYS  | 2.2  |
| 1   | R     | 1063 | SER  | 2.2  |
| 1   | H     | 1311 | LEU  | 2.2  |
| 1   | C     | 1873 | ALA  | 2.2  |
| 1   | D     | 1058 | ALA  | 2.2  |
| 1   | E     | 1694 | ILE  | 2.2  |
| 1   | M     | 1790 | GLY  | 2.2  |
| 1   | Q     | 1564 | ILE  | 2.2  |
| 1   | A     | 1912 | PRO  | 2.2  |
| 1   | R     | 980  | THR  | 2.2  |
| 1   | G     | 1322 | TYR  | 2.2  |
| 1   | K     | 1328 | SER  | 2.2  |
| 1   | L     | 1105 | SER  | 2.2  |
| 1   | R     | 1140 | CYS  | 2.2  |
| 1   | D     | 1710 | LEU  | 2.2  |
| 1   | G     | 1527 | LEU  | 2.2  |
| 1   | N     | 1172 | LEU  | 2.2  |
| 1   | P     | 1908 | LEU  | 2.2  |
| 1   | R     | 1112 | VAL  | 2.2  |
| 1   | C     | 1905 | ALA  | 2.2  |
| 1   | C     | 1914 | GLN  | 2.2  |
| 1   | H     | 1838 | ALA  | 2.2  |
| 1   | C     | 1568 | THR  | 2.2  |
| 1   | H     | 1385 | ASP  | 2.2  |
| 1   | J     | 1244 | THR  | 2.2  |
| 1   | L     | 1738 | LYS  | 2.2  |
| 1   | Q     | 1528 | PRO  | 2.2  |
| 1   | B     | 1506 | GLY  | 2.2  |
| 1   | E     | 931  | LEU  | 2.2  |
| 1   | F     | 1541 | LEU  | 2.2  |
| 1   | F     | 1818 | ILE  | 2.2  |
| 1   | G     | 1273 | GLY  | 2.2  |
| 1   | I     | 1099 | LEU  | 2.2  |
| 1   | J     | 1324 | VAL  | 2.2  |
| 1   | L     | 1974 | ILE  | 2.2  |
| 1   | Q     | 1494 | GLY  | 2.2  |
| 1   | D     | 1875 | LYS  | 2.2  |
| 1   | E     | 1320 | ARG  | 2.2  |
| 1   | M     | 1129 | ARG  | 2.2  |
| 1   | P     | 1345 | ARG  | 2.2  |
| 1   | A     | 1857 | ASP  | 2.2  |
| 1   | E     | 1478 | PRO  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1871 | ASP  | 2.2  |
| 1   | J     | 1066 | TYR  | 2.2  |
| 1   | P     | 1770 | THR  | 2.2  |
| 1   | A     | 1782 | GLU  | 2.2  |
| 1   | G     | 1088 | GLY  | 2.2  |
| 1   | H     | 1821 | GLU  | 2.2  |
| 1   | J     | 1533 | GLU  | 2.2  |
| 1   | K     | 1193 | LEU  | 2.2  |
| 1   | N     | 2007 | LEU  | 2.2  |
| 1   | P     | 1278 | VAL  | 2.2  |
| 1   | R     | 1102 | CYS  | 2.2  |
| 1   | R     | 1105 | SER  | 2.2  |
| 1   | E     | 1945 | ALA  | 2.2  |
| 1   | M     | 1920 | ALA  | 2.2  |
| 1   | C     | 885  | ASP  | 2.2  |
| 1   | J     | 1319 | PRO  | 2.2  |
| 1   | E     | 1121 | LEU  | 2.2  |
| 1   | E     | 1220 | LEU  | 2.2  |
| 1   | G     | 1157 | GLU  | 2.2  |
| 1   | K     | 1225 | ASP  | 2.2  |
| 1   | M     | 1736 | THR  | 2.2  |
| 1   | M     | 1817 | ASP  | 2.2  |
| 1   | Q     | 1568 | THR  | 2.2  |
| 1   | K     | 1627 | GLY  | 2.2  |
| 1   | M     | 1118 | GLY  | 2.2  |
| 1   | R     | 1499 | ARG  | 2.2  |
| 1   | G     | 1786 | ALA  | 2.2  |
| 1   | Q     | 1509 | ALA  | 2.2  |
| 1   | D     | 1917 | TYR  | 2.2  |
| 1   | G     | 1089 | GLN  | 2.2  |
| 1   | C     | 941  | VAL  | 2.2  |
| 1   | E     | 1993 | LEU  | 2.2  |
| 1   | F     | 1962 | ILE  | 2.2  |
| 1   | G     | 1079 | VAL  | 2.2  |
| 1   | I     | 931  | LEU  | 2.2  |
| 1   | J     | 1631 | VAL  | 2.2  |
| 1   | K     | 1364 | ASP  | 2.2  |
| 1   | O     | 1423 | LEU  | 2.2  |
| 1   | R     | 923  | VAL  | 2.2  |
| 1   | N     | 1615 | PHE  | 2.2  |
| 1   | N     | 1772 | GLY  | 2.2  |
| 1   | O     | 1108 | ALA  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | P     | 1928 | MET  | 2.2  |
| 1   | Q     | 1433 | SER  | 2.2  |
| 1   | C     | 1337 | PRO  | 2.2  |
| 1   | E     | 1710 | LEU  | 2.2  |
| 1   | E     | 1808 | ILE  | 2.2  |
| 1   | H     | 1809 | GLU  | 2.2  |
| 1   | J     | 1374 | LEU  | 2.2  |
| 1   | I     | 1469 | ARG  | 2.2  |
| 1   | J     | 1495 | VAL  | 2.2  |
| 1   | G     | 1341 | HIS  | 2.2  |
| 1   | H     | 1746 | THR  | 2.2  |
| 1   | M     | 1783 | ARG  | 2.2  |
| 1   | N     | 1363 | ILE  | 2.2  |
| 1   | A     | 1801 | SER  | 2.2  |
| 1   | C     | 1542 | ALA  | 2.2  |
| 1   | E     | 1328 | SER  | 2.2  |
| 1   | H     | 1852 | ALA  | 2.2  |
| 1   | I     | 945  | ALA  | 2.2  |
| 1   | L     | 1055 | HIS  | 2.2  |
| 1   | M     | 1105 | SER  | 2.2  |
| 1   | M     | 1873 | ALA  | 2.2  |
| 1   | E     | 1218 | VAL  | 2.2  |
| 1   | E     | 1422 | ARG  | 2.2  |
| 1   | E     | 1898 | TRP  | 2.2  |
| 1   | D     | 1157 | GLU  | 2.2  |
| 1   | F     | 1295 | ARG  | 2.2  |
| 1   | Q     | 1437 | VAL  | 2.2  |
| 1   | F     | 1048 | PHE  | 2.2  |
| 1   | F     | 1061 | GLY  | 2.2  |
| 1   | G     | 1082 | PRO  | 2.2  |
| 1   | I     | 1564 | ILE  | 2.2  |
| 1   | B     | 1524 | ALA  | 2.2  |
| 1   | D     | 1244 | THR  | 2.2  |
| 1   | E     | 1164 | THR  | 2.2  |
| 1   | K     | 1108 | ALA  | 2.2  |
| 1   | L     | 1853 | ALA  | 2.2  |
| 1   | P     | 1105 | SER  | 2.2  |
| 1   | Q     | 1078 | ALA  | 2.2  |
| 1   | D     | 1992 | TRP  | 2.2  |
| 1   | H     | 1377 | GLN  | 2.2  |
| 1   | K     | 1760 | VAL  | 2.2  |
| 1   | Q     | 1031 | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | Q     | 1079 | VAL  | 2.2  |
| 1   | C     | 1340 | GLU  | 2.2  |
| 1   | E     | 1967 | GLY  | 2.2  |
| 1   | K     | 1655 | GLU  | 2.2  |
| 1   | N     | 896  | PRO  | 2.2  |
| 1   | B     | 1982 | ASN  | 2.2  |
| 1   | A     | 1456 | SER  | 2.2  |
| 1   | A     | 1545 | THR  | 2.2  |
| 1   | E     | 1455 | ALA  | 2.2  |
| 1   | G     | 1074 | THR  | 2.2  |
| 1   | G     | 1497 | THR  | 2.2  |
| 1   | R     | 1567 | ALA  | 2.2  |
| 1   | R     | 1568 | THR  | 2.2  |
| 1   | E     | 1044 | LEU  | 2.2  |
| 1   | A     | 1811 | ILE  | 2.2  |
| 1   | F     | 1022 | ARG  | 2.2  |
| 1   | H     | 1344 | LEU  | 2.2  |
| 1   | I     | 1165 | VAL  | 2.2  |
| 1   | N     | 1423 | LEU  | 2.2  |
| 1   | R     | 982  | VAL  | 2.2  |
| 1   | M     | 1483 | GLU  | 2.2  |
| 1   | P     | 1363 | ILE  | 2.2  |
| 1   | R     | 1562 | ILE  | 2.2  |
| 1   | O     | 1651 | GLY  | 2.1  |
| 1   | R     | 1421 | MET  | 2.1  |
| 1   | B     | 1262 | LEU  | 2.1  |
| 1   | F     | 1867 | LEU  | 2.1  |
| 1   | I     | 1683 | LEU  | 2.1  |
| 1   | E     | 1856 | GLU  | 2.1  |
| 1   | F     | 1880 | TRP  | 2.1  |
| 1   | M     | 2002 | PHE  | 2.1  |
| 1   | R     | 1028 | ILE  | 2.1  |
| 1   | F     | 1627 | GLY  | 2.1  |
| 1   | G     | 1151 | GLY  | 2.1  |
| 1   | L     | 1540 | GLY  | 2.1  |
| 1   | E     | 1025 | ALA  | 2.1  |
| 1   | H     | 1538 | ALA  | 2.1  |
| 1   | P     | 1247 | MET  | 2.1  |
| 1   | A     | 1773 | LEU  | 2.1  |
| 1   | B     | 1480 | LEU  | 2.1  |
| 1   | E     | 1237 | LEU  | 2.1  |
| 1   | E     | 1355 | HIS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | J     | 1423 | LEU  | 2.1  |
| 1   | M     | 1095 | HIS  | 2.1  |
| 1   | Q     | 936  | VAL  | 2.1  |
| 1   | A     | 1089 | GLN  | 2.1  |
| 1   | C     | 1104 | GLN  | 2.1  |
| 1   | F     | 1992 | TRP  | 2.1  |
| 1   | D     | 1967 | GLY  | 2.1  |
| 1   | E     | 1268 | GLU  | 2.1  |
| 1   | Q     | 1053 | ILE  | 2.1  |
| 1   | Q     | 1505 | GLY  | 2.1  |
| 1   | R     | 1639 | ALA  | 2.1  |
| 1   | G     | 1517 | VAL  | 2.1  |
| 1   | G     | 1697 | LEU  | 2.1  |
| 1   | H     | 1632 | LEU  | 2.1  |
| 1   | I     | 904  | LEU  | 2.1  |
| 1   | P     | 1487 | VAL  | 2.1  |
| 1   | Q     | 901  | HIS  | 2.1  |
| 1   | R     | 996  | PHE  | 2.1  |
| 1   | E     | 1153 | GLU  | 2.1  |
| 1   | E     | 1384 | GLU  | 2.1  |
| 1   | I     | 1189 | ASP  | 2.1  |
| 1   | I     | 1682 | ASP  | 2.1  |
| 1   | M     | 1389 | TRP  | 2.1  |
| 1   | C     | 1517 | VAL  | 2.1  |
| 1   | F     | 1357 | ARG  | 2.1  |
| 1   | M     | 1644 | LEU  | 2.1  |
| 1   | C     | 1456 | SER  | 2.1  |
| 1   | H     | 1765 | GLY  | 2.1  |
| 1   | L     | 1180 | ASP  | 2.1  |
| 1   | M     | 1190 | GLU  | 2.1  |
| 1   | N     | 1898 | TRP  | 2.1  |
| 1   | A     | 1720 | LEU  | 2.1  |
| 1   | A     | 1961 | ALA  | 2.1  |
| 1   | D     | 1975 | LEU  | 2.1  |
| 1   | H     | 1834 | LEU  | 2.1  |
| 1   | N     | 1820 | VAL  | 2.1  |
| 1   | M     | 1395 | TYR  | 2.1  |
| 1   | I     | 1741 | ILE  | 2.1  |
| 1   | N     | 1449 | ILE  | 2.1  |
| 1   | E     | 1915 | GLY  | 2.1  |
| 1   | G     | 1923 | TRP  | 2.1  |
| 1   | A     | 1347 | LEU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1076 | VAL  | 2.1  |
| 1   | C     | 1299 | ASP  | 2.1  |
| 1   | C     | 1698 | LEU  | 2.1  |
| 1   | D     | 1480 | LEU  | 2.1  |
| 1   | G     | 1787 | ALA  | 2.1  |
| 1   | I     | 1514 | SER  | 2.1  |
| 1   | I     | 1166 | LEU  | 2.1  |
| 1   | J     | 942  | LEU  | 2.1  |
| 1   | K     | 1388 | ALA  | 2.1  |
| 1   | M     | 942  | LEU  | 2.1  |
| 1   | N     | 1780 | LEU  | 2.1  |
| 1   | R     | 1032 | LEU  | 2.1  |
| 1   | R     | 1507 | VAL  | 2.1  |
| 1   | J     | 1769 | ILE  | 2.1  |
| 1   | E     | 1389 | TRP  | 2.1  |
| 1   | Q     | 1655 | GLU  | 2.1  |
| 1   | A     | 1062 | LEU  | 2.1  |
| 1   | A     | 1819 | VAL  | 2.1  |
| 1   | B     | 1134 | THR  | 2.1  |
| 1   | C     | 1683 | LEU  | 2.1  |
| 1   | D     | 1217 | LEU  | 2.1  |
| 1   | F     | 1281 | SER  | 2.1  |
| 1   | H     | 1133 | SER  | 2.1  |
| 1   | H     | 1266 | LEU  | 2.1  |
| 1   | J     | 1274 | VAL  | 2.1  |
| 1   | M     | 1760 | VAL  | 2.1  |
| 1   | N     | 1879 | ALA  | 2.1  |
| 1   | N     | 1893 | THR  | 2.1  |
| 1   | Q     | 984  | VAL  | 2.1  |
| 1   | D     | 1795 | ASN  | 2.1  |
| 1   | E     | 1052 | GLY  | 2.1  |
| 1   | F     | 1739 | LEU  | 2.1  |
| 1   | G     | 1304 | LEU  | 2.1  |
| 1   | P     | 1358 | LEU  | 2.1  |
| 1   | P     | 1831 | ALA  | 2.1  |
| 1   | C     | 1256 | ASP  | 2.1  |
| 1   | J     | 1971 | PHE  | 2.1  |
| 1   | K     | 1525 | THR  | 2.1  |
| 1   | D     | 1454 | LYS  | 2.1  |
| 1   | E     | 1324 | VAL  | 2.1  |
| 1   | R     | 908  | VAL  | 2.1  |
| 1   | K     | 1534 | HIS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1122 | PRO  | 2.1  |
| 1   | H     | 1601 | ASP  | 2.1  |
| 1   | J     | 1017 | ASP  | 2.1  |
| 1   | J     | 1028 | ILE  | 2.1  |
| 1   | M     | 1941 | ILE  | 2.1  |
| 1   | C     | 1372 | GLU  | 2.1  |
| 1   | G     | 2004 | GLU  | 2.1  |
| 1   | H     | 1777 | GLY  | 2.1  |
| 1   | J     | 1948 | GLU  | 2.1  |
| 1   | K     | 1159 | LEU  | 2.1  |
| 1   | K     | 1996 | PHE  | 2.1  |
| 1   | L     | 1065 | ALA  | 2.1  |
| 1   | P     | 1304 | LEU  | 2.1  |
| 1   | P     | 1344 | LEU  | 2.1  |
| 1   | P     | 1347 | LEU  | 2.1  |
| 1   | Q     | 1541 | LEU  | 2.1  |
| 1   | O     | 1516 | PHE  | 2.1  |
| 1   | J     | 1195 | ILE  | 2.1  |
| 1   | N     | 1055 | HIS  | 2.1  |
| 1   | F     | 1134 | THR  | 2.1  |
| 1   | E     | 1165 | VAL  | 2.1  |
| 1   | G     | 908  | VAL  | 2.1  |
| 1   | J     | 1647 | LEU  | 2.1  |
| 1   | K     | 1779 | PHE  | 2.1  |
| 1   | K     | 1971 | PHE  | 2.1  |
| 1   | R     | 950  | MET  | 2.1  |
| 1   | A     | 1251 | HIS  | 2.1  |
| 1   | C     | 1804 | SER  | 2.1  |
| 1   | F     | 1566 | SER  | 2.1  |
| 1   | Q     | 899  | SER  | 2.1  |
| 1   | Q     | 1514 | SER  | 2.1  |
| 1   | B     | 1076 | VAL  | 2.1  |
| 1   | E     | 1737 | GLY  | 2.1  |
| 1   | M     | 1217 | LEU  | 2.1  |
| 1   | N     | 942  | LEU  | 2.1  |
| 1   | O     | 1687 | THR  | 2.1  |
| 1   | P     | 1819 | VAL  | 2.1  |
| 1   | R     | 1172 | LEU  | 2.1  |
| 1   | H     | 1536 | ALA  | 2.1  |
| 1   | H     | 1982 | ASN  | 2.1  |
| 1   | M     | 1360 | ALA  | 2.1  |
| 1   | E     | 947  | TYR  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | G     | 1702 | TYR  | 2.1  |
| 1   | H     | 1195 | ILE  | 2.1  |
| 1   | J     | 1090 | ARG  | 2.1  |
| 1   | C     | 1297 | GLY  | 2.1  |
| 1   | D     | 1399 | LEU  | 2.1  |
| 1   | E     | 1843 | LEU  | 2.1  |
| 1   | H     | 1274 | VAL  | 2.1  |
| 1   | J     | 1152 | VAL  | 2.1  |
| 1   | M     | 1165 | VAL  | 2.1  |
| 1   | M     | 1392 | GLY  | 2.1  |
| 1   | M     | 1740 | VAL  | 2.1  |
| 1   | M     | 1882 | LEU  | 2.1  |
| 1   | R     | 898  | VAL  | 2.1  |
| 1   | O     | 1102 | CYS  | 2.1  |
| 1   | F     | 1531 | ILE  | 2.1  |
| 1   | B     | 1448 | GLN  | 2.1  |
| 1   | M     | 1929 | GLN  | 2.1  |
| 1   | C     | 942  | LEU  | 2.1  |
| 1   | D     | 1408 | GLU  | 2.1  |
| 1   | E     | 1234 | VAL  | 2.1  |
| 1   | I     | 1653 | PHE  | 2.1  |
| 1   | J     | 1205 | PRO  | 2.1  |
| 1   | K     | 1340 | GLU  | 2.1  |
| 1   | M     | 1375 | VAL  | 2.1  |
| 1   | N     | 1720 | LEU  | 2.1  |
| 1   | P     | 1491 | VAL  | 2.1  |
| 1   | R     | 1539 | VAL  | 2.1  |
| 1   | A     | 1996 | PHE  | 2.1  |
| 1   | I     | 1023 | PRO  | 2.1  |
| 1   | D     | 930  | TRP  | 2.1  |
| 1   | F     | 1293 | ASP  | 2.1  |
| 1   | F     | 1938 | ALA  | 2.1  |
| 1   | H     | 1249 | TRP  | 2.1  |
| 1   | P     | 1916 | ALA  | 2.1  |
| 1   | H     | 1984 | TYR  | 2.1  |
| 1   | N     | 947  | TYR  | 2.1  |
| 1   | A     | 1379 | LEU  | 2.1  |
| 1   | E     | 1501 | GLY  | 2.1  |
| 1   | F     | 1271 | LEU  | 2.1  |
| 1   | F     | 1843 | LEU  | 2.1  |
| 1   | M     | 944  | GLY  | 2.1  |
| 1   | N     | 1081 | LEU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | R     | 916  | GLU  | 2.1  |
| 1   | J     | 1055 | HIS  | 2.0  |
| 1   | A     | 1543 | TYR  | 2.0  |
| 1   | E     | 1102 | CYS  | 2.0  |
| 1   | G     | 1307 | ILE  | 2.0  |
| 1   | I     | 1619 | ILE  | 2.0  |
| 1   | O     | 1743 | ILE  | 2.0  |
| 1   | C     | 1697 | LEU  | 2.0  |
| 1   | F     | 1794 | VAL  | 2.0  |
| 1   | G     | 1339 | LEU  | 2.0  |
| 1   | I     | 1423 | LEU  | 2.0  |
| 1   | J     | 1504 | VAL  | 2.0  |
| 1   | L     | 1632 | LEU  | 2.0  |
| 1   | L     | 1987 | VAL  | 2.0  |
| 1   | M     | 1156 | LEU  | 2.0  |
| 1   | N     | 1112 | VAL  | 2.0  |
| 1   | P     | 1431 | LEU  | 2.0  |
| 1   | R     | 1447 | GLY  | 2.0  |
| 1   | A     | 1116 | ALA  | 2.0  |
| 1   | C     | 1564 | ILE  | 2.0  |
| 1   | E     | 1961 | ALA  | 2.0  |
| 1   | G     | 1249 | TRP  | 2.0  |
| 1   | J     | 1249 | TRP  | 2.0  |
| 1   | M     | 1930 | TRP  | 2.0  |
| 1   | H     | 1345 | ARG  | 2.0  |
| 1   | C     | 1854 | VAL  | 2.0  |
| 1   | D     | 1223 | ASP  | 2.0  |
| 1   | M     | 1074 | THR  | 2.0  |
| 1   | N     | 1770 | THR  | 2.0  |
| 1   | D     | 1507 | VAL  | 2.0  |
| 1   | F     | 988  | VAL  | 2.0  |
| 1   | R     | 1628 | VAL  | 2.0  |
| 1   | C     | 2002 | PHE  | 2.0  |
| 1   | D     | 1529 | GLU  | 2.0  |
| 1   | E     | 1693 | LYS  | 2.0  |
| 1   | G     | 1761 | PHE  | 2.0  |
| 1   | H     | 1420 | GLY  | 2.0  |
| 1   | B     | 1536 | ALA  | 2.0  |
| 1   | E     | 1038 | ARG  | 2.0  |
| 1   | E     | 1679 | TYR  | 2.0  |
| 1   | E     | 1791 | ARG  | 2.0  |
| 1   | F     | 1092 | TYR  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 1679 | TYR  | 2.0  |
| 1   | H     | 928  | HIS  | 2.0  |
| 1   | H     | 1421 | MET  | 2.0  |
| 1   | L     | 1945 | ALA  | 2.0  |
| 1   | N     | 1766 | ALA  | 2.0  |
| 1   | O     | 1493 | PRO  | 2.0  |
| 1   | J     | 1076 | VAL  | 2.0  |
| 1   | K     | 1545 | THR  | 2.0  |
| 1   | K     | 1817 | ASP  | 2.0  |
| 1   | N     | 1489 | THR  | 2.0  |
| 1   | N     | 1909 | VAL  | 2.0  |
| 1   | D     | 1927 | PHE  | 2.0  |
| 1   | P     | 1764 | ASP  | 2.0  |
| 1   | A     | 1377 | GLN  | 2.0  |
| 1   | E     | 1914 | GLN  | 2.0  |
| 1   | F     | 991  | PRO  | 2.0  |
| 1   | C     | 1300 | HIS  | 2.0  |
| 1   | H     | 1395 | TYR  | 2.0  |
| 1   | L     | 1898 | TRP  | 2.0  |
| 1   | N     | 1342 | SER  | 2.0  |
| 1   | R     | 1528 | PRO  | 2.0  |
| 1   | N     | 1908 | LEU  | 2.0  |
| 1   | C     | 1134 | THR  | 2.0  |
| 1   | E     | 933  | ASP  | 2.0  |
| 1   | J     | 1630 | ILE  | 2.0  |
| 1   | K     | 1901 | ALA  | 2.0  |
| 1   | Q     | 1584 | ALA  | 2.0  |
| 1   | B     | 1380 | SER  | 2.0  |
| 1   | B     | 1491 | VAL  | 2.0  |
| 1   | J     | 1218 | VAL  | 2.0  |
| 1   | J     | 1780 | LEU  | 2.0  |
| 1   | N     | 1778 | LEU  | 2.0  |
| 1   | Q     | 1453 | VAL  | 2.0  |
| 1   | F     | 1678 | PHE  | 2.0  |
| 1   | Q     | 1456 | SER  | 2.0  |
| 1   | H     | 1486 | GLY  | 2.0  |
| 1   | D     | 1329 | GLN  | 2.0  |
| 1   | G     | 1985 | ALA  | 2.0  |
| 1   | M     | 1414 | ALA  | 2.0  |
| 1   | P     | 1826 | ALA  | 2.0  |
| 1   | B     | 1128 | LEU  | 2.0  |
| 1   | C     | 1669 | LEU  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 1778 | LEU  | 2.0  |
| 1   | E     | 1768 | VAL  | 2.0  |
| 1   | E     | 1672 | PHE  | 2.0  |
| 1   | F     | 1192 | LEU  | 2.0  |
| 1   | K     | 1697 | LEU  | 2.0  |
| 1   | K     | 1921 | ASN  | 2.0  |
| 1   | M     | 1032 | LEU  | 2.0  |
| 1   | M     | 1513 | TRP  | 2.0  |
| 1   | P     | 1321 | LEU  | 2.0  |
| 1   | R     | 1615 | PHE  | 2.0  |
| 1   | G     | 1340 | GLU  | 2.0  |
| 1   | G     | 1483 | GLU  | 2.0  |
| 1   | G     | 1377 | GLN  | 2.0  |
| 1   | K     | 1223 | ASP  | 2.0  |
| 1   | K     | 1837 | ALA  | 2.0  |
| 1   | N     | 948  | CYS  | 2.0  |
| 1   | N     | 1219 | ILE  | 2.0  |
| 1   | N     | 1885 | ALA  | 2.0  |
| 1   | Q     | 1560 | ASP  | 2.0  |
| 1   | C     | 1793 | VAL  | 2.0  |
| 1   | D     | 1131 | TYR  | 2.0  |
| 1   | I     | 1477 | LEU  | 2.0  |
| 1   | J     | 1898 | TRP  | 2.0  |
| 1   | N     | 1323 | VAL  | 2.0  |
| 1   | P     | 1923 | TRP  | 2.0  |
| 1   | R     | 930  | TRP  | 2.0  |
| 1   | O     | 1059 | PHE  | 2.0  |
| 1   | D     | 1273 | GLY  | 2.0  |
| 1   | E     | 1410 | ARG  | 2.0  |
| 1   | G     | 1095 | HIS  | 2.0  |
| 1   | G     | 1948 | GLU  | 2.0  |
| 1   | M     | 1498 | HIS  | 2.0  |
| 1   | N     | 1883 | HIS  | 2.0  |
| 1   | P     | 1485 | GLY  | 2.0  |
| 1   | Q     | 1457 | SER  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 2   | NAP  | L     | 3001 | 48/48 | 0.91 | 0.37 | -0.03 | 110,118,130,134            | 0     |
| 2   | NAP  | M     | 3001 | 48/48 | 0.89 | 0.36 | -0.13 | 132,144,158,161            | 0     |
| 2   | NAP  | A     | 3001 | 48/48 | 0.92 | 0.35 | -0.14 | 104,124,136,137            | 0     |
| 2   | NAP  | E     | 3001 | 48/48 | 0.82 | 0.34 | -0.21 | 181,193,197,198            | 0     |
| 2   | NAP  | K     | 3002 | 27/48 | 0.75 | 0.31 | -0.21 | 135,151,159,161            | 0     |
| 2   | NAP  | J     | 3002 | 27/48 | 0.68 | 0.30 | -0.23 | 166,169,175,176            | 0     |
| 2   | NAP  | B     | 3001 | 48/48 | 0.92 | 0.34 | -0.25 | 103,111,127,129            | 0     |
| 2   | NAP  | P     | 3001 | 48/48 | 0.93 | 0.33 | -0.31 | 106,124,132,136            | 0     |
| 2   | NAP  | N     | 3001 | 48/48 | 0.89 | 0.32 | -0.33 | 141,152,175,175            | 0     |
| 2   | NAP  | Q     | 3001 | 48/48 | 0.61 | 0.40 | -0.33 | 222,225,232,235            | 0     |
| 2   | NAP  | K     | 3001 | 48/48 | 0.94 | 0.34 | -0.35 | 109,123,141,145            | 0     |
| 2   | NAP  | O     | 3001 | 48/48 | 0.92 | 0.35 | -0.36 | 101,113,135,138            | 0     |
| 2   | NAP  | H     | 3001 | 48/48 | 0.85 | 0.32 | -0.38 | 129,146,170,171            | 0     |
| 2   | NAP  | D     | 3002 | 27/48 | 0.68 | 0.28 | -0.38 | 193,197,199,199            | 0     |
| 2   | NAP  | D     | 3001 | 48/48 | 0.90 | 0.31 | -0.39 | 114,124,138,139            | 0     |
| 2   | NAP  | H     | 3002 | 27/48 | 0.64 | 0.30 | -0.46 | 179,187,190,190            | 0     |
| 2   | NAP  | F     | 3002 | 27/48 | 0.67 | 0.28 | -0.47 | 164,168,171,171            | 0     |
| 2   | NAP  | G     | 3001 | 48/48 | 0.90 | 0.31 | -0.48 | 117,132,158,158            | 0     |
| 2   | NAP  | I     | 3001 | 48/48 | 0.87 | 0.33 | -0.49 | 133,144,150,151            | 0     |
| 2   | NAP  | B     | 3002 | 27/48 | 0.78 | 0.29 | -0.53 | 120,134,148,148            | 0     |
| 2   | NAP  | C     | 3001 | 48/48 | 0.91 | 0.33 | -0.55 | 110,132,150,153            | 0     |
| 2   | NAP  | F     | 3001 | 48/48 | 0.85 | 0.33 | -0.58 | 165,176,183,184            | 0     |
| 2   | NAP  | J     | 3001 | 48/48 | 0.92 | 0.30 | -0.66 | 115,126,149,153            | 0     |
| 2   | NAP  | G     | 3002 | 27/48 | 0.70 | 0.20 | -0.67 | 195,201,205,205            | 0     |
| 2   | NAP  | A     | 3002 | 27/48 | 0.61 | 0.26 | -0.69 | 229,235,241,242            | 0     |
| 2   | NAP  | C     | 3002 | 31/48 | 0.73 | 0.27 | -0.71 | 141,162,203,205            | 0     |
| 2   | NAP  | N     | 3002 | 27/48 | 0.58 | 0.25 | -0.79 | 156,165,181,182            | 0     |
| 2   | NAP  | R     | 3001 | 48/48 | 0.77 | 0.23 | -0.96 | 210,221,233,234            | 0     |
| 2   | NAP  | P     | 3002 | 27/48 | 0.61 | 0.21 | -1.12 | 191,203,209,210            | 0     |
| 2   | NAP  | M     | 3002 | 27/48 | 0.54 | 0.28 | -1.38 | 233,235,240,240            | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.