



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 05:23 AM EDT

PDB ID : 5WKO  
Title : Crystal structure of antibody 27F3 recognizing the HA from A/California/04/2009 (H1N1) influenza virus  
Authors : Wilson, A.; Lang, S.; Zhu, X.  
Deposited on : 2017-07-25  
Resolution : 3.49 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

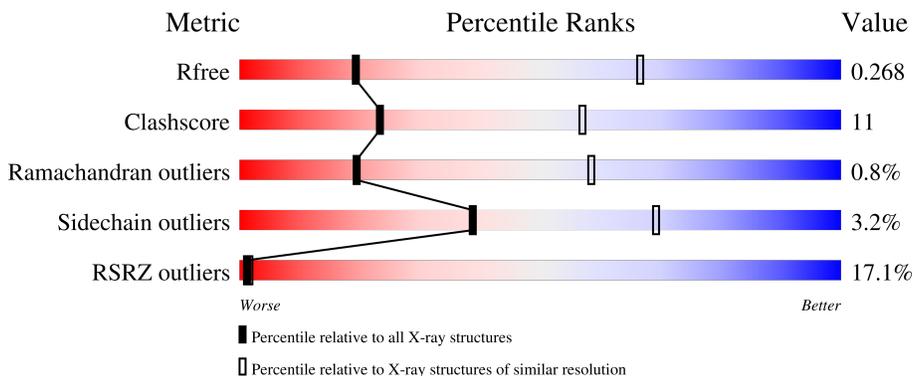
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1659 (3.60-3.40)                                      |
| Clashscore            | 141614                      | 1036 (3.58-3.42)                                      |
| Ramachandran outliers | 138981                      | 1005 (3.58-3.42)                                      |
| Sidechain outliers    | 138945                      | 1006 (3.58-3.42)                                      |
| RSRZ outliers         | 127900                      | 1559 (3.60-3.40)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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     | 225    | <br>6% 74% 21% 5%  |
| 1   | C     | 225    | <br>5% 70% 26% 5%  |
| 1   | E     | 225    | <br>4% 74% 23% 5%  |
| 1   | G     | 225    | <br>5% 70% 25% 5%  |
| 1   | I     | 225    | <br>15% 72% 25% 5% |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--------------------|
| 1   | K     | 225    | <br>6% 74% 23% .   |
| 2   | B     | 213    | <br>72% 23% ..     |
| 2   | D     | 213    | <br>68% 29% .      |
| 2   | F     | 213    | <br>78% 21% .      |
| 2   | H     | 213    | <br>75% 23% .      |
| 2   | J     | 213    | <br>2% 72% 25% ..  |
| 2   | L     | 213    | <br>76% 21% .      |
| 3   | M     | 331    | <br>44% 77% 20% .. |
| 3   | N     | 331    | <br>41% 81% 16% .. |
| 3   | O     | 331    | <br>50% 76% 21% .. |
| 3   | S     | 331    | <br>34% 79% 18% .. |
| 3   | T     | 331    | <br>34% 83% 13% .. |
| 3   | U     | 331    | <br>35% 79% 18% .. |
| 4   | P     | 177    | <br>6% 79% 20% .   |
| 4   | Q     | 177    | <br>6% 80% 17% .   |
| 4   | R     | 177    | <br>5% 76% 19% ..  |
| 4   | V     | 177    | <br>6% 80% 19% .   |
| 4   | W     | 177    | <br>7% 81% 15% ..  |
| 4   | X     | 177    | <br>6% 80% 16% ..  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 43322 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antibody 27F3 heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 1   | A     | 225      | 1675  | 1061 | 277 | 330 | 7 | 0       | 0       | 0     |
| 1   | C     | 225      | 1675  | 1061 | 277 | 330 | 7 | 0       | 0       | 0     |
| 1   | E     | 225      | 1675  | 1061 | 277 | 330 | 7 | 0       | 0       | 0     |
| 1   | G     | 225      | 1675  | 1061 | 277 | 330 | 7 | 0       | 0       | 0     |
| 1   | I     | 225      | 1675  | 1061 | 277 | 330 | 7 | 0       | 0       | 0     |
| 1   | K     | 225      | 1675  | 1061 | 277 | 330 | 7 | 0       | 0       | 0     |

- Molecule 2 is a protein called Antibody 27F3 light chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 2   | B     | 213      | 1628  | 1020 | 275 | 329 | 4 | 0       | 0       | 0     |
| 2   | D     | 213      | 1628  | 1020 | 275 | 329 | 4 | 0       | 0       | 0     |
| 2   | F     | 213      | 1628  | 1020 | 275 | 329 | 4 | 0       | 0       | 0     |
| 2   | H     | 213      | 1628  | 1020 | 275 | 329 | 4 | 0       | 0       | 0     |
| 2   | J     | 213      | 1628  | 1020 | 275 | 329 | 4 | 0       | 0       | 0     |
| 2   | L     | 213      | 1628  | 1020 | 275 | 329 | 4 | 0       | 0       | 0     |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 76      | THR      | SER    | conflict | UNP Q9UL78 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 83      | PHE      | CYS    | conflict | UNP Q9UL78 |
| B     | 92      | VAL      | GLY    | conflict | UNP Q9UL78 |
| B     | 94      | THR      | SER    | conflict | UNP Q9UL78 |
| D     | 76      | THR      | SER    | conflict | UNP Q9UL78 |
| D     | 83      | PHE      | CYS    | conflict | UNP Q9UL78 |
| D     | 92      | VAL      | GLY    | conflict | UNP Q9UL78 |
| D     | 94      | THR      | SER    | conflict | UNP Q9UL78 |
| F     | 76      | THR      | SER    | conflict | UNP Q9UL78 |
| F     | 83      | PHE      | CYS    | conflict | UNP Q9UL78 |
| F     | 92      | VAL      | GLY    | conflict | UNP Q9UL78 |
| F     | 94      | THR      | SER    | conflict | UNP Q9UL78 |
| H     | 76      | THR      | SER    | conflict | UNP Q9UL78 |
| H     | 83      | PHE      | CYS    | conflict | UNP Q9UL78 |
| H     | 92      | VAL      | GLY    | conflict | UNP Q9UL78 |
| H     | 94      | THR      | SER    | conflict | UNP Q9UL78 |
| J     | 76      | THR      | SER    | conflict | UNP Q9UL78 |
| J     | 83      | PHE      | CYS    | conflict | UNP Q9UL78 |
| J     | 92      | VAL      | GLY    | conflict | UNP Q9UL78 |
| J     | 94      | THR      | SER    | conflict | UNP Q9UL78 |
| L     | 76      | THR      | SER    | conflict | UNP Q9UL78 |
| L     | 83      | PHE      | CYS    | conflict | UNP Q9UL78 |
| L     | 92      | VAL      | GLY    | conflict | UNP Q9UL78 |
| L     | 94      | THR      | SER    | conflict | UNP Q9UL78 |

- Molecule 3 is a protein called Hemagglutinin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 3   | M     | 324      | 2529  | 1599 | 436 | 483 | 11 | 0       | 0       | 0     |
| 3   | N     | 323      | 2523  | 1596 | 435 | 481 | 11 | 0       | 0       | 0     |
| 3   | O     | 326      | 2544  | 1608 | 438 | 487 | 11 | 0       | 0       | 0     |
| 3   | S     | 324      | 2529  | 1599 | 436 | 483 | 11 | 0       | 0       | 0     |
| 3   | T     | 323      | 2523  | 1596 | 435 | 481 | 11 | 0       | 0       | 0     |
| 3   | U     | 326      | 2544  | 1608 | 438 | 487 | 11 | 0       | 0       | 0     |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| M     | 7       | ALA      | -      | expression tag | UNP C3W5S1 |
| M     | 8       | ASP      | -      | expression tag | UNP C3W5S1 |
| M     | 9       | PRO      | -      | expression tag | UNP C3W5S1 |
| M     | 10      | GLY      | -      | expression tag | UNP C3W5S1 |
| N     | 7       | ALA      | -      | expression tag | UNP C3W5S1 |
| N     | 8       | ASP      | -      | expression tag | UNP C3W5S1 |
| N     | 9       | PRO      | -      | expression tag | UNP C3W5S1 |
| N     | 10      | GLY      | -      | expression tag | UNP C3W5S1 |
| O     | 7       | ALA      | -      | expression tag | UNP C3W5S1 |
| O     | 8       | ASP      | -      | expression tag | UNP C3W5S1 |
| O     | 9       | PRO      | -      | expression tag | UNP C3W5S1 |
| O     | 10      | GLY      | -      | expression tag | UNP C3W5S1 |
| S     | 7       | ALA      | -      | expression tag | UNP C3W5S1 |
| S     | 8       | ASP      | -      | expression tag | UNP C3W5S1 |
| S     | 9       | PRO      | -      | expression tag | UNP C3W5S1 |
| S     | 10      | GLY      | -      | expression tag | UNP C3W5S1 |
| T     | 7       | ALA      | -      | expression tag | UNP C3W5S1 |
| T     | 8       | ASP      | -      | expression tag | UNP C3W5S1 |
| T     | 9       | PRO      | -      | expression tag | UNP C3W5S1 |
| T     | 10      | GLY      | -      | expression tag | UNP C3W5S1 |
| U     | 7       | ALA      | -      | expression tag | UNP C3W5S1 |
| U     | 8       | ASP      | -      | expression tag | UNP C3W5S1 |
| U     | 9       | PRO      | -      | expression tag | UNP C3W5S1 |
| U     | 10      | GLY      | -      | expression tag | UNP C3W5S1 |

- Molecule 4 is a protein called Hemagglutinin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | P     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 881 | 238 | 281 | 6 |         |         |       |
| 4   | Q     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1375  | 863 | 234 | 272 | 6 |         |         |       |
| 4   | R     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1375  | 863 | 234 | 272 | 6 |         |         |       |
| 4   | V     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 881 | 238 | 281 | 6 |         |         |       |
| 4   | W     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1375  | 863 | 234 | 272 | 6 |         |         |       |
| 4   | X     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1375  | 863 | 234 | 272 | 6 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

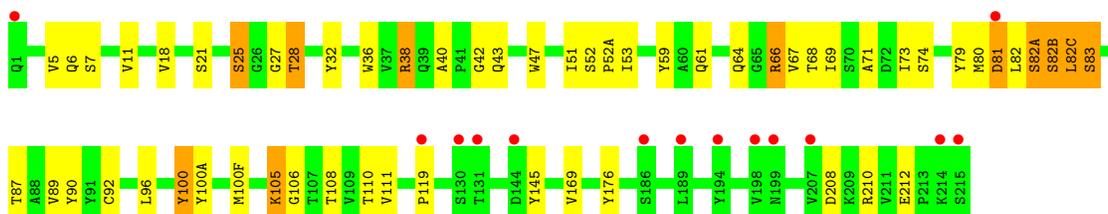
| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| P     | 47      | GLY      | GLU    | engineered mutation | UNP A0A023ZYH9 |
| P     | 175     | SER      | -      | expression tag      | UNP A0A023ZYH9 |
| P     | 176     | GLY      | -      | expression tag      | UNP A0A023ZYH9 |
| P     | 177     | ARG      | -      | expression tag      | UNP A0A023ZYH9 |
| Q     | 47      | GLY      | GLU    | engineered mutation | UNP A0A023ZYH9 |
| Q     | 175     | SER      | -      | expression tag      | UNP A0A023ZYH9 |
| Q     | 176     | GLY      | -      | expression tag      | UNP A0A023ZYH9 |
| Q     | 177     | ARG      | -      | expression tag      | UNP A0A023ZYH9 |
| R     | 47      | GLY      | GLU    | engineered mutation | UNP A0A023ZYH9 |
| R     | 175     | SER      | -      | expression tag      | UNP A0A023ZYH9 |
| R     | 176     | GLY      | -      | expression tag      | UNP A0A023ZYH9 |
| R     | 177     | ARG      | -      | expression tag      | UNP A0A023ZYH9 |
| V     | 47      | GLY      | GLU    | engineered mutation | UNP A0A023ZYH9 |
| V     | 175     | SER      | -      | expression tag      | UNP A0A023ZYH9 |
| V     | 176     | GLY      | -      | expression tag      | UNP A0A023ZYH9 |
| V     | 177     | ARG      | -      | expression tag      | UNP A0A023ZYH9 |
| W     | 47      | GLY      | GLU    | engineered mutation | UNP A0A023ZYH9 |
| W     | 175     | SER      | -      | expression tag      | UNP A0A023ZYH9 |
| W     | 176     | GLY      | -      | expression tag      | UNP A0A023ZYH9 |
| W     | 177     | ARG      | -      | expression tag      | UNP A0A023ZYH9 |
| X     | 47      | GLY      | GLU    | engineered mutation | UNP A0A023ZYH9 |
| X     | 175     | SER      | -      | expression tag      | UNP A0A023ZYH9 |
| X     | 176     | GLY      | -      | expression tag      | UNP A0A023ZYH9 |
| X     | 177     | ARG      | -      | expression tag      | UNP A0A023ZYH9 |

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

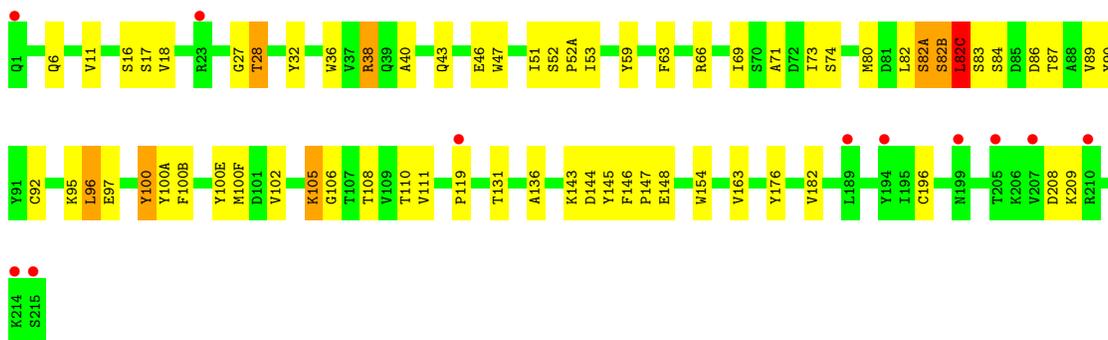
- Molecule 1: Antibody 27F3 heavy chain

Chain A: 



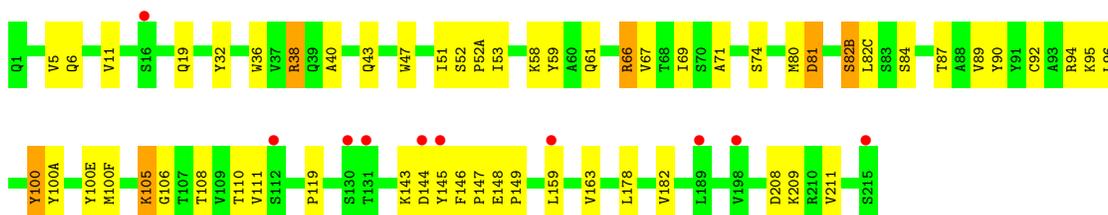
- Molecule 1: Antibody 27F3 heavy chain

Chain C: 

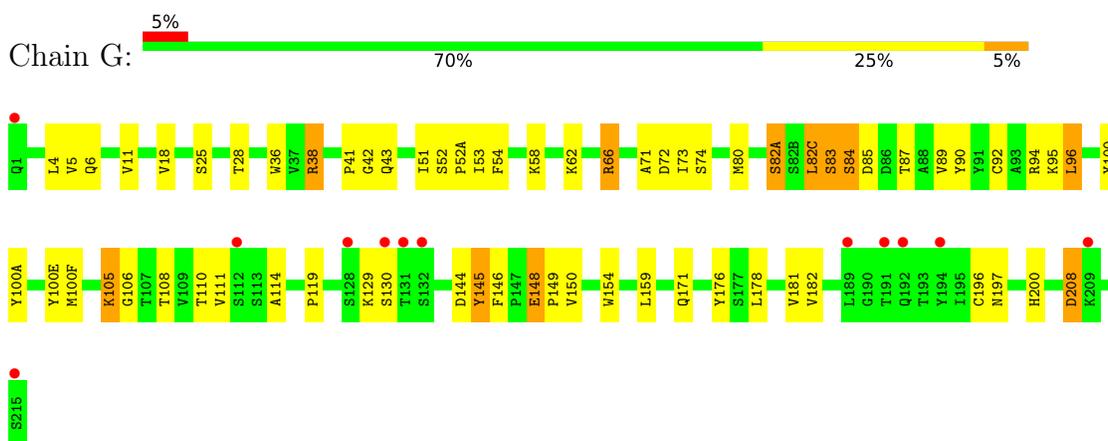


- Molecule 1: Antibody 27F3 heavy chain

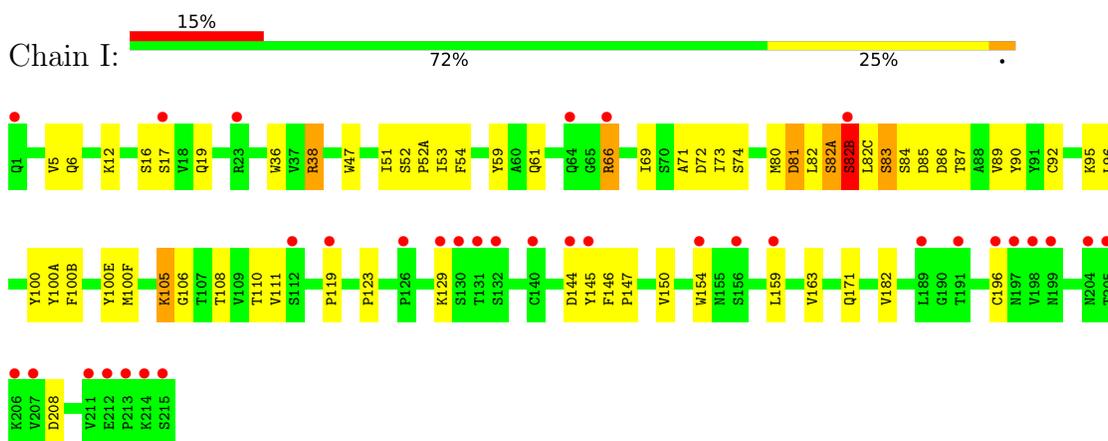
Chain E: 



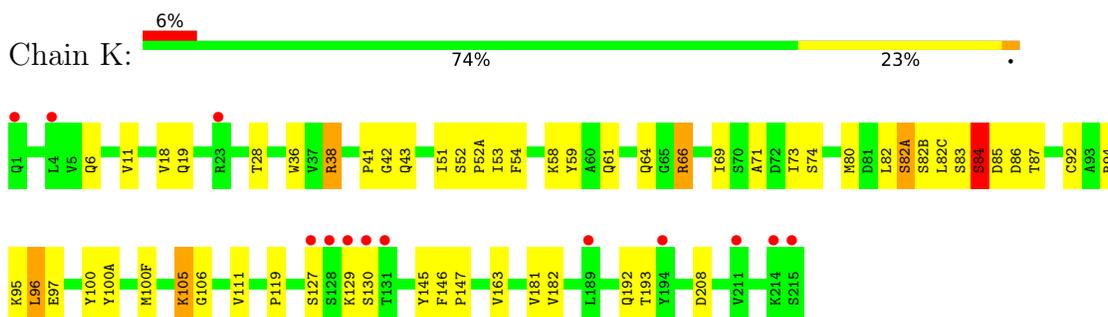
- Molecule 1: Antibody 27F3 heavy chain



- Molecule 1: Antibody 27F3 heavy chain



- Molecule 1: Antibody 27F3 heavy chain



- Molecule 2: Antibody 27F3 light chain



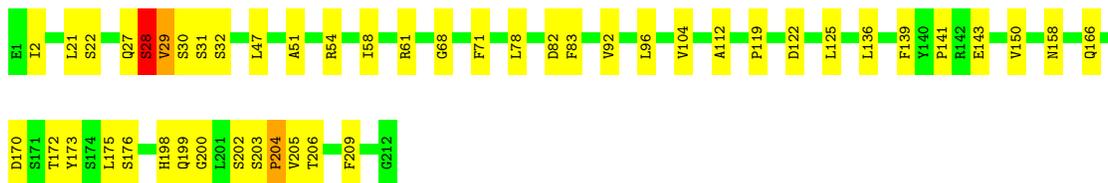
- Molecule 2: Antibody 27F3 light chain

Chain D:  68% 29%



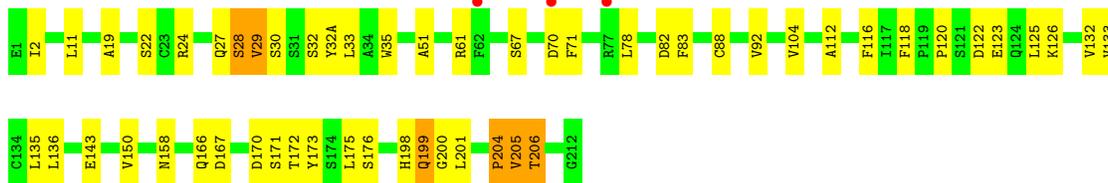
• Molecule 2: Antibody 27F3 light chain

Chain F:  78% 21%



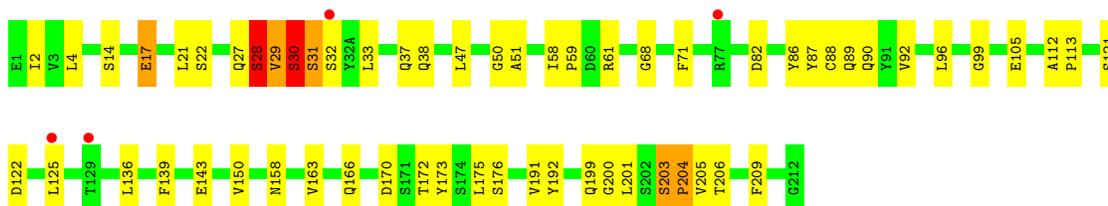
• Molecule 2: Antibody 27F3 light chain

Chain H:  75% 23%



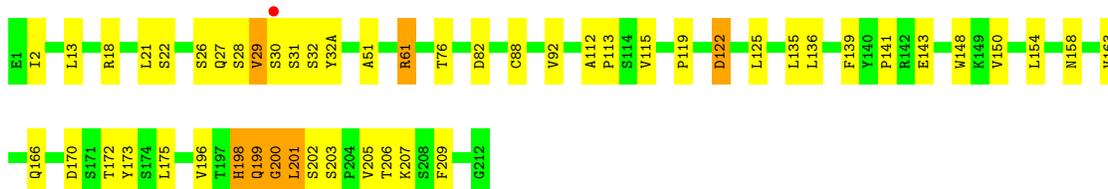
• Molecule 2: Antibody 27F3 light chain

Chain J:  72% 25%

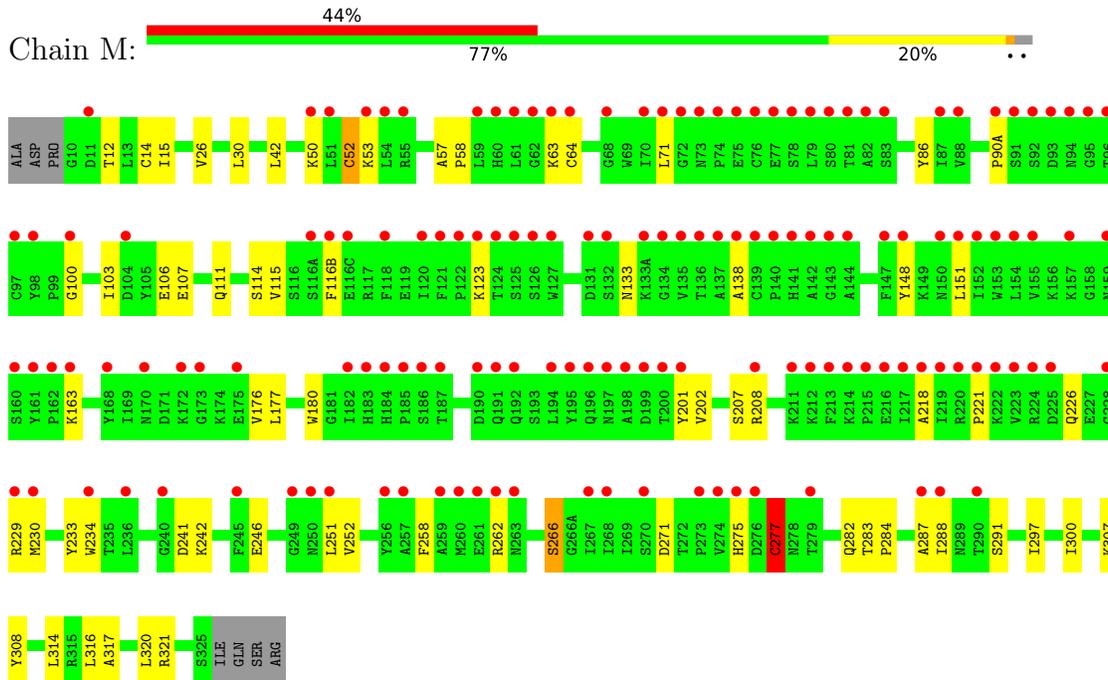


• Molecule 2: Antibody 27F3 light chain

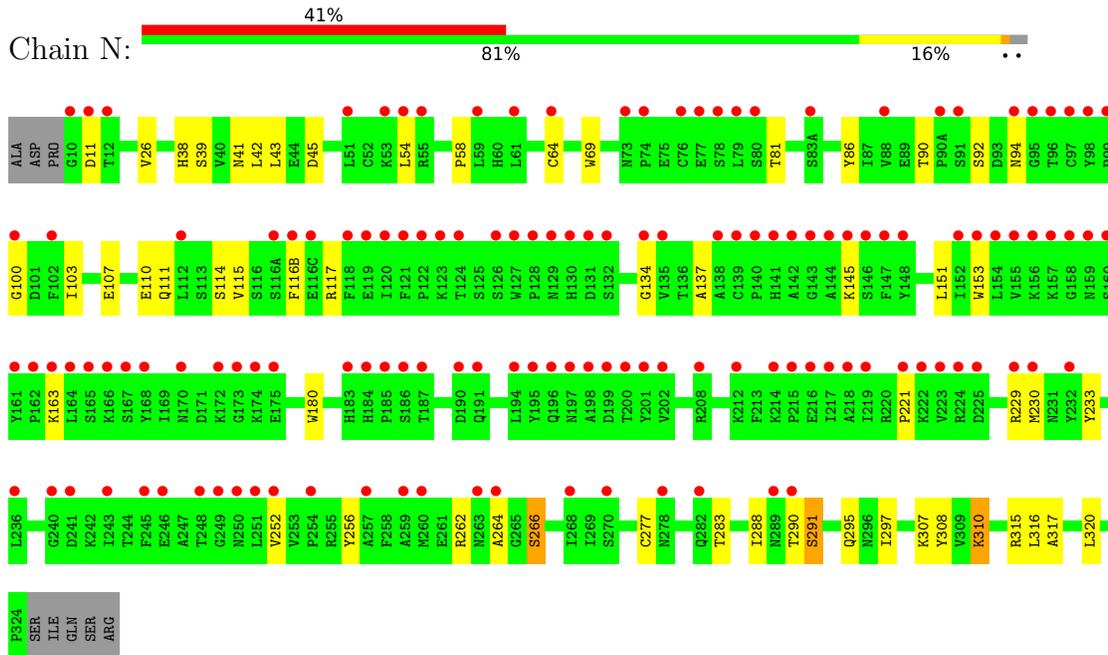
Chain L:  76% 21%



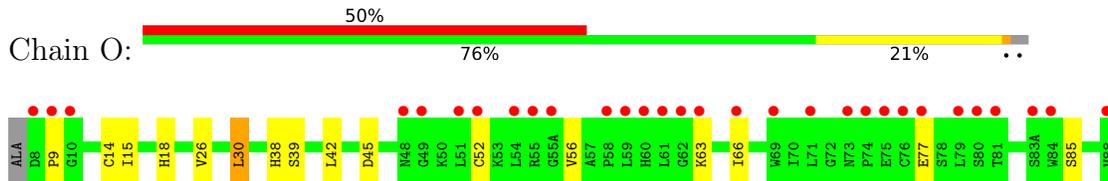
• Molecule 3: Hemagglutinin

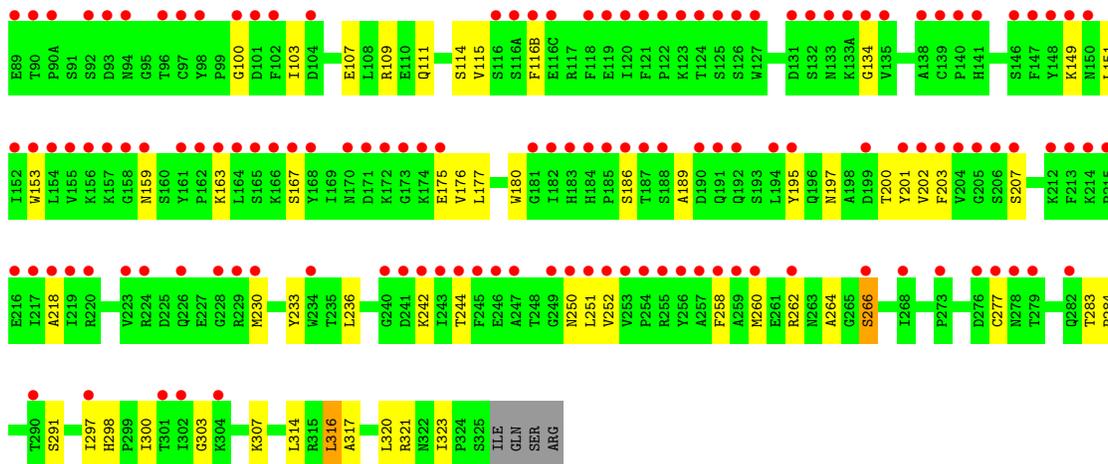


• Molecule 3: Hemagglutinin

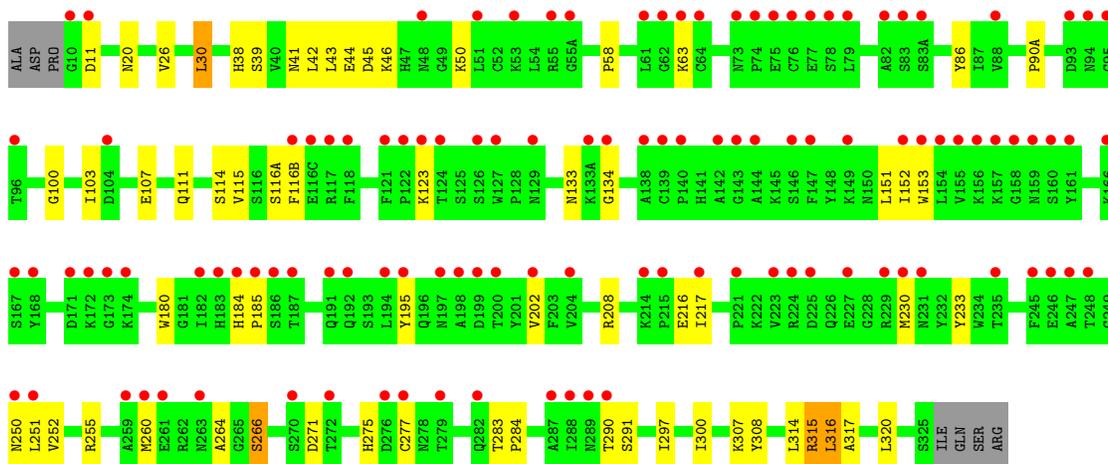
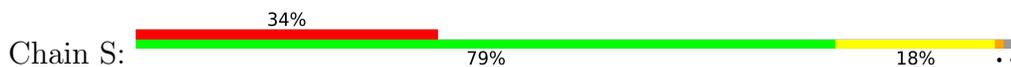


• Molecule 3: Hemagglutinin

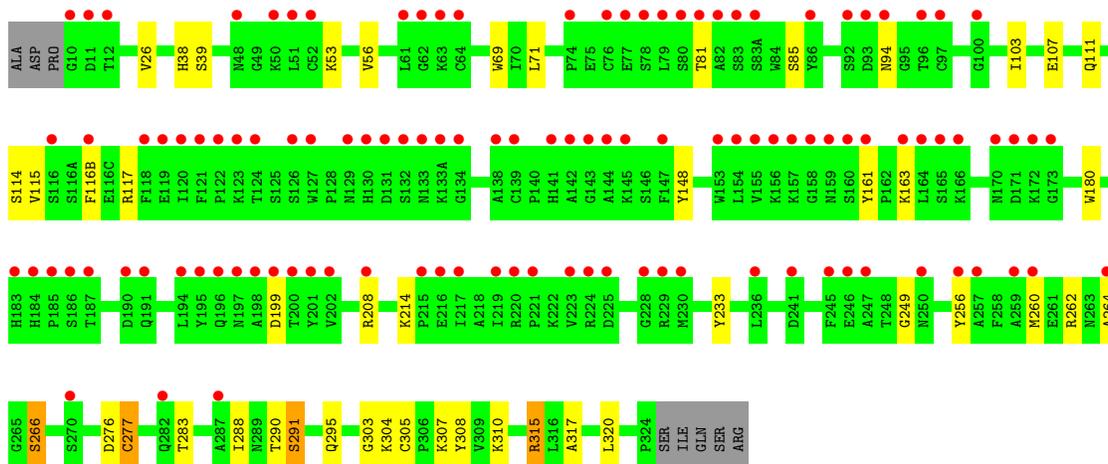
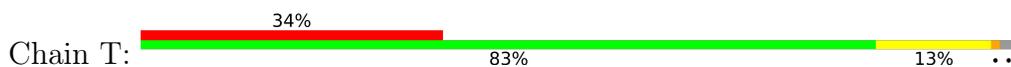




• Molecule 3: Hemagglutinin

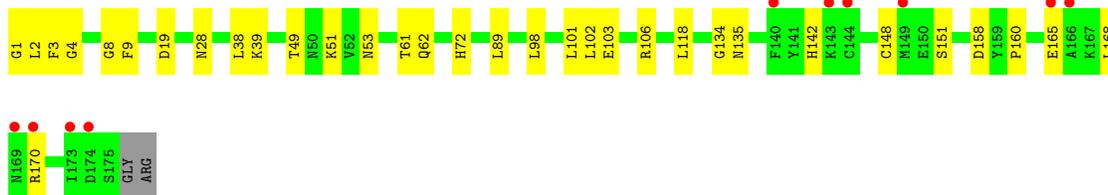


• Molecule 3: Hemagglutinin

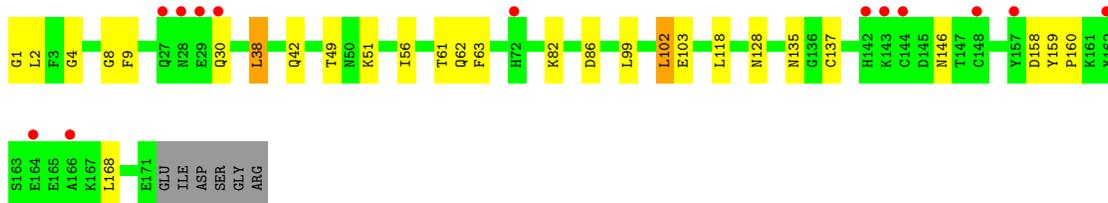
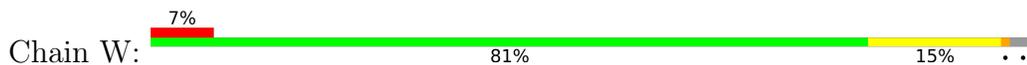




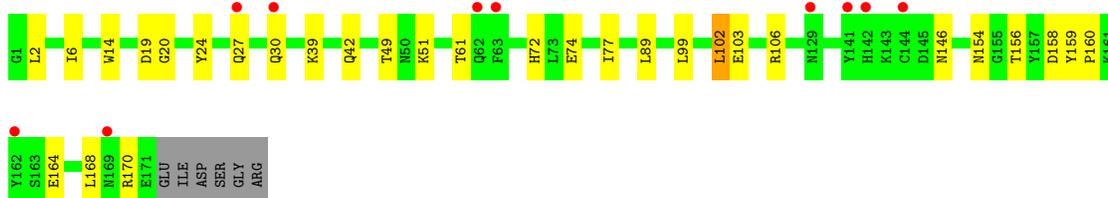
• Molecule 4: Hemagglutinin



• Molecule 4: Hemagglutinin



• Molecule 4: Hemagglutinin



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 190.58Å 191.49Å 391.05Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.45 – 3.49<br>49.45 – 3.49                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (49.45-3.49)<br>98.1 (49.45-3.49)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.13  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.58 (at 3.48Å)   | Xtrriage         |
| Refinement program  | PHENIX (1.12_2829: ???)                                     | Depositor        |
| R, $R_{free}$   | 0.246 , 0.268<br>0.246 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8910 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 90.1  | Xtrriage         |
| Anisotropy  | 0.148   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 52.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtrriage         |
| Estimated twinning fraction   | 0.008 for k,h,-l  | Xtrriage         |
| $F_o, F_c$ correlation  | 0.88  | EDS              |
| Total number of atoms   | 43322   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 101.0   | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 1   | A     | 1.09         | 3/1719 (0.2%)   | 0.83        | 2/2344 (0.1%)   |
| 1   | C     | 0.92         | 0/1719          | 0.82        | 1/2344 (0.0%)   |
| 1   | E     | 0.96         | 1/1719 (0.1%)   | 0.81        | 2/2344 (0.1%)   |
| 1   | G     | 0.92         | 1/1719 (0.1%)   | 0.81        | 2/2344 (0.1%)   |
| 1   | I     | 0.83         | 0/1719          | 0.75        | 1/2344 (0.0%)   |
| 1   | K     | 1.05         | 1/1719 (0.1%)   | 0.82        | 1/2344 (0.0%)   |
| 2   | B     | 1.19         | 0/1663          | 0.93        | 4/2260 (0.2%)   |
| 2   | D     | 0.98         | 1/1663 (0.1%)   | 0.85        | 2/2260 (0.1%)   |
| 2   | F     | 0.99         | 0/1663          | 0.83        | 0/2260          |
| 2   | H     | 1.00         | 0/1663          | 0.84        | 0/2260          |
| 2   | J     | 0.99         | 1/1663 (0.1%)   | 0.87        | 1/2260 (0.0%)   |
| 2   | L     | 1.14         | 1/1663 (0.1%)   | 0.88        | 2/2260 (0.1%)   |
| 3   | M     | 0.62         | 3/2593 (0.1%)   | 0.72        | 3/3524 (0.1%)   |
| 3   | N     | 0.62         | 0/2587          | 0.79        | 3/3516 (0.1%)   |
| 3   | O     | 0.57         | 1/2609 (0.0%)   | 0.74        | 2/3547 (0.1%)   |
| 3   | S     | 0.62         | 0/2593          | 0.73        | 4/3524 (0.1%)   |
| 3   | T     | 0.64         | 1/2587 (0.0%)   | 0.83        | 6/3516 (0.2%)   |
| 3   | U     | 0.60         | 0/2609          | 0.75        | 1/3547 (0.0%)   |
| 4   | P     | 1.01         | 1/1434 (0.1%)   | 0.87        | 0/1932          |
| 4   | Q     | 1.04         | 1/1403 (0.1%)   | 0.86        | 2/1890 (0.1%)   |
| 4   | R     | 0.94         | 2/1403 (0.1%)   | 0.86        | 1/1890 (0.1%)   |
| 4   | V     | 0.99         | 0/1434          | 0.90        | 3/1932 (0.2%)   |
| 4   | W     | 0.96         | 1/1403 (0.1%)   | 0.84        | 3/1890 (0.2%)   |
| 4   | X     | 0.90         | 1/1403 (0.1%)   | 0.89        | 3/1890 (0.2%)   |
| All | All   | 0.88         | 20/44350 (0.0%) | 0.82        | 49/60222 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | L     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (20) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | A     | 79     | TYR  | CE1-CZ  | -8.04 | 1.28        | 1.38     |
| 1   | E     | 211    | VAL  | C-N     | 7.65  | 1.51        | 1.34     |
| 2   | J     | 17     | GLU  | CB-CG   | -7.09 | 1.38        | 1.52     |
| 3   | M     | 14     | CYS  | CB-SG   | -6.31 | 1.71        | 1.82     |
| 4   | Q     | 21     | TRP  | CB-CG   | -6.09 | 1.39        | 1.50     |
| 2   | L     | 88     | CYS  | CB-SG   | -6.09 | 1.72        | 1.82     |
| 4   | W     | 137    | CYS  | CB-SG   | -6.07 | 1.72        | 1.82     |
| 2   | D     | 194    | CYS  | CB-SG   | -5.88 | 1.72        | 1.81     |
| 3   | O     | 14     | CYS  | CB-SG   | -5.87 | 1.72        | 1.81     |
| 4   | R     | 119    | TYR  | CD1-CE1 | -5.47 | 1.31        | 1.39     |
| 1   | A     | 100(A) | TYR  | CE1-CZ  | -5.34 | 1.31        | 1.38     |
| 1   | A     | 79     | TYR  | CE2-CZ  | -5.24 | 1.31        | 1.38     |
| 1   | K     | 96     | LEU  | C-N     | -5.17 | 1.22        | 1.34     |
| 4   | P     | 110    | TYR  | CE1-CZ  | -5.16 | 1.31        | 1.38     |
| 4   | R     | 137    | CYS  | CB-SG   | -5.13 | 1.73        | 1.81     |
| 3   | T     | 305    | CYS  | CB-SG   | -5.12 | 1.73        | 1.81     |
| 1   | G     | 96     | LEU  | C-N     | -5.10 | 1.22        | 1.34     |
| 3   | M     | 64     | CYS  | CB-SG   | -5.10 | 1.73        | 1.81     |
| 3   | M     | 52     | CYS  | CB-SG   | -5.09 | 1.73        | 1.81     |
| 4   | X     | 14     | TRP  | CB-CG   | -5.06 | 1.41        | 1.50     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|--------|-------------|----------|
| 3   | T     | 277   | CYS  | CA-CB-SG  | -15.68 | 85.77       | 114.00   |
| 3   | S     | 277   | CYS  | CA-CB-SG  | -8.97  | 97.85       | 114.00   |
| 3   | T     | 320   | LEU  | CB-CG-CD2 | -8.45  | 96.64       | 111.00   |
| 1   | I     | 82(B) | SER  | N-CA-C    | -8.29  | 88.63       | 111.00   |
| 3   | S     | 30    | LEU  | CB-CG-CD2 | -7.80  | 97.73       | 111.00   |
| 2   | B     | 30    | SER  | N-CA-CB   | 7.50   | 121.75      | 110.50   |
| 4   | V     | 106   | ARG  | NE-CZ-NH1 | -7.27  | 116.67      | 120.30   |
| 3   | N     | 277   | CYS  | CA-CB-SG  | -6.82  | 101.72      | 114.00   |
| 2   | B     | 32    | SER  | N-CA-C    | -6.72  | 92.85       | 111.00   |
| 2   | B     | 201   | LEU  | CA-CB-CG  | 6.65   | 130.60      | 115.30   |
| 3   | T     | 315   | ARG  | NE-CZ-NH1 | -6.57  | 117.01      | 120.30   |
| 3   | S     | 315   | ARG  | NE-CZ-NH1 | -6.48  | 117.06      | 120.30   |

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| Mol | Chain | Res   | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 2   | L     | 200   | GLY  | N-CA-C    | -6.41 | 97.08       | 113.10   |
| 2   | L     | 201   | LEU  | N-CA-C    | -6.28 | 94.04       | 111.00   |
| 3   | O     | 316   | LEU  | CB-CG-CD2 | -6.27 | 100.34      | 111.00   |
| 1   | A     | 96    | LEU  | CA-CB-CG  | -6.21 | 101.02      | 115.30   |
| 1   | E     | 58    | LYS  | CD-CE-NZ  | 6.15  | 125.84      | 111.70   |
| 3   | M     | 30    | LEU  | CB-CG-CD2 | -6.01 | 100.78      | 111.00   |
| 3   | O     | 30    | LEU  | CB-CG-CD2 | -5.94 | 100.90      | 111.00   |
| 2   | J     | 17    | GLU  | N-CA-CB   | -5.84 | 100.08      | 110.60   |
| 2   | B     | 32(A) | TYR  | N-CA-C    | -5.83 | 95.27       | 111.00   |
| 2   | D     | 32    | SER  | N-CA-C    | -5.82 | 95.27       | 111.00   |
| 4   | V     | 39    | LYS  | CD-CE-NZ  | 5.76  | 124.95      | 111.70   |
| 3   | M     | 277   | CYS  | CA-CB-SG  | -5.67 | 103.80      | 114.00   |
| 4   | Q     | 118   | LEU  | CB-CG-CD1 | -5.67 | 101.37      | 111.00   |
| 4   | Q     | 106   | ARG  | NE-CZ-NH1 | -5.63 | 117.49      | 120.30   |
| 3   | T     | 310   | LYS  | CD-CE-NZ  | 5.60  | 124.57      | 111.70   |
| 3   | T     | 320   | LEU  | CB-CG-CD1 | -5.59 | 101.50      | 111.00   |
| 4   | W     | 1     | GLY  | N-CA-C    | -5.58 | 99.14       | 113.10   |
| 4   | X     | 102   | LEU  | CB-CG-CD2 | -5.57 | 101.54      | 111.00   |
| 4   | X     | 106   | ARG  | NE-CZ-NH1 | -5.48 | 117.56      | 120.30   |
| 4   | V     | 118   | LEU  | CB-CG-CD2 | -5.47 | 101.70      | 111.00   |
| 1   | K     | 58    | LYS  | CD-CE-NZ  | 5.46  | 124.25      | 111.70   |
| 1   | C     | 82(C) | LEU  | N-CA-C    | 5.45  | 125.71      | 111.00   |
| 3   | T     | 304   | LYS  | CG-CD-CE  | 5.37  | 128.00      | 111.90   |
| 4   | W     | 102   | LEU  | CB-CG-CD2 | -5.33 | 101.94      | 111.00   |
| 4   | X     | 24    | TYR  | CB-CG-CD2 | -5.25 | 117.85      | 121.00   |
| 1   | G     | 58    | LYS  | CD-CE-NZ  | 5.24  | 123.74      | 111.70   |
| 4   | R     | 38    | LEU  | CB-CG-CD2 | -5.22 | 102.12      | 111.00   |
| 4   | W     | 38    | LEU  | CB-CG-CD2 | -5.19 | 102.18      | 111.00   |
| 3   | M     | 12    | THR  | CA-CB-CG2 | -5.18 | 105.14      | 112.40   |
| 2   | D     | 70    | ASP  | CB-CG-OD1 | -5.17 | 113.64      | 118.30   |
| 1   | G     | 62    | LYS  | CD-CE-NZ  | 5.07  | 123.36      | 111.70   |
| 3   | N     | 320   | LEU  | CA-CB-CG  | 5.07  | 126.96      | 115.30   |
| 1   | E     | 94    | ARG  | NE-CZ-NH1 | -5.06 | 117.77      | 120.30   |
| 3   | N     | 315   | ARG  | NE-CZ-NH1 | -5.03 | 117.79      | 120.30   |
| 3   | S     | 316   | LEU  | CB-CG-CD2 | -5.02 | 102.46      | 111.00   |
| 3   | U     | 277   | CYS  | N-CA-CB   | -5.02 | 101.56      | 110.60   |
| 1   | A     | 82(A) | SER  | C-N-CA    | 5.01  | 134.23      | 121.70   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | G     | 148 | GLU  | Peptide   |
| 2   | L     | 198 | HIS  | Mainchain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1675  | 0        | 1642     | 62      | 0            |
| 1   | C     | 1675  | 0        | 1642     | 67      | 0            |
| 1   | E     | 1675  | 0        | 1643     | 43      | 0            |
| 1   | G     | 1675  | 0        | 1643     | 77      | 0            |
| 1   | I     | 1675  | 0        | 1643     | 69      | 0            |
| 1   | K     | 1675  | 0        | 1642     | 45      | 0            |
| 2   | B     | 1628  | 0        | 1592     | 63      | 0            |
| 2   | D     | 1628  | 0        | 1591     | 65      | 0            |
| 2   | F     | 1628  | 0        | 1592     | 30      | 0            |
| 2   | H     | 1628  | 0        | 1592     | 35      | 0            |
| 2   | J     | 1628  | 0        | 1590     | 63      | 0            |
| 2   | L     | 1628  | 0        | 1592     | 36      | 0            |
| 3   | M     | 2529  | 0        | 2479     | 46      | 0            |
| 3   | N     | 2523  | 0        | 2474     | 37      | 0            |
| 3   | O     | 2544  | 0        | 2490     | 54      | 0            |
| 3   | S     | 2529  | 0        | 2479     | 43      | 0            |
| 3   | T     | 2523  | 0        | 2474     | 30      | 0            |
| 3   | U     | 2544  | 0        | 2490     | 47      | 0            |
| 4   | P     | 1406  | 0        | 1326     | 32      | 0            |
| 4   | Q     | 1375  | 0        | 1300     | 28      | 0            |
| 4   | R     | 1375  | 0        | 1300     | 32      | 0            |
| 4   | V     | 1406  | 0        | 1326     | 33      | 0            |
| 4   | W     | 1375  | 0        | 1300     | 23      | 0            |
| 4   | X     | 1375  | 0        | 1300     | 26      | 0            |
| All | All   | 43322 | 0        | 42142    | 966     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (966) 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) |
|-----------------|--------------------|--------------------------|-------------------|
| 2:J:30:SER:OG   | 2:J:92:VAL:CG1     | 1.64                     | 1.44              |
| 2:B:94:THR:CB   | 2:B:95:PRO:HD3     | 1.33                     | 1.34              |
| 1:I:66:ARG:HB3  | 1:I:82(B):SER:CB   | 1.59                     | 1.33              |
| 2:B:94:THR:CB   | 2:B:95:PRO:CD      | 2.07                     | 1.32              |
| 1:I:17:SER:CB   | 1:I:82(A):SER:OG   | 1.76                     | 1.31              |
| 1:A:68:THR:O    | 1:A:81:ASP:CB      | 1.78                     | 1.29              |
| 1:I:17:SER:CA   | 1:I:82(A):SER:OG   | 1.83                     | 1.25              |
| 1:I:83:SER:O    | 1:I:111:VAL:HG11   | 1.33                     | 1.24              |
| 1:C:83:SER:O    | 1:C:111:VAL:HG11   | 1.27                     | 1.24              |
| 2:D:29:VAL:HG11 | 2:D:71:PHE:CZ      | 1.71                     | 1.24              |
| 1:A:83:SER:O    | 1:A:111:VAL:HG11   | 1.38                     | 1.23              |
| 1:A:68:THR:O    | 1:A:81:ASP:HB2     | 1.08                     | 1.23              |
| 2:D:112:ALA:HB2 | 2:D:200:GLY:O      | 1.36                     | 1.23              |
| 1:G:145:TYR:CE2 | 1:G:150:VAL:CG2    | 2.22                     | 1.21              |
| 2:J:30:SER:OG   | 2:J:92:VAL:HG11    | 1.17                     | 1.19              |
| 2:F:29:VAL:HG23 | 2:F:68:GLY:O       | 1.38                     | 1.19              |
| 1:G:145:TYR:CE1 | 1:G:176:TYR:HB2    | 1.78                     | 1.18              |
| 1:G:145:TYR:HE2 | 1:G:150:VAL:CG2    | 1.56                     | 1.16              |
| 1:G:145:TYR:HE1 | 1:G:176:TYR:CB     | 1.56                     | 1.16              |
| 1:G:83:SER:O    | 1:G:111:VAL:HG11   | 1.46                     | 1.15              |
| 1:I:66:ARG:HB3  | 1:I:82(B):SER:HB2  | 1.20                     | 1.14              |
| 1:I:66:ARG:CB   | 1:I:82(B):SER:HB3  | 1.76                     | 1.14              |
| 1:I:17:SER:HA   | 1:I:82(A):SER:OG   | 1.42                     | 1.14              |
| 1:G:145:TYR:CE2 | 1:G:150:VAL:HG23   | 1.80                     | 1.13              |
| 2:B:94:THR:HB   | 2:B:95:PRO:CD      | 1.71                     | 1.13              |
| 2:B:94:THR:OG1  | 2:B:95:PRO:CD      | 2.00                     | 1.10              |
| 1:A:67:VAL:HG23 | 1:A:81:ASP:O       | 1.51                     | 1.08              |
| 2:J:29:VAL:CG2  | 2:J:68:GLY:O       | 2.01                     | 1.08              |
| 1:I:66:ARG:CB   | 1:I:82(B):SER:CB   | 2.29                     | 1.07              |
| 2:D:29:VAL:HG11 | 2:D:71:PHE:CE2     | 1.89                     | 1.06              |
| 2:J:29:VAL:HG23 | 2:J:68:GLY:O       | 1.54                     | 1.05              |
| 1:G:145:TYR:CE1 | 1:G:176:TYR:CB     | 2.37                     | 1.05              |
| 1:A:68:THR:H    | 1:A:81:ASP:HB3     | 1.20                     | 1.04              |
| 2:B:31:SER:OG   | 2:B:32(A):TYR:HD2  | 1.41                     | 1.03              |
| 2:J:32:SER:O    | 2:J:50:GLY:O       | 1.76                     | 1.03              |
| 1:A:18:VAL:HG23 | 1:A:82(C):LEU:HD21 | 1.38                     | 1.02              |
| 1:K:66:ARG:O    | 1:K:82(A):SER:N    | 1.86                     | 1.02              |
| 1:G:145:TYR:CE2 | 1:G:150:VAL:HG21   | 1.90                     | 1.02              |
| 1:I:83:SER:O    | 1:I:111:VAL:CG1    | 2.09                     | 1.01              |
| 1:E:66:ARG:NH1  | 1:E:82(B):SER:OG   | 1.90                     | 1.01              |
| 2:B:94:THR:OG1  | 2:B:95:PRO:HD2     | 1.61                     | 1.01              |
| 1:G:145:TYR:HE1 | 1:G:176:TYR:HB3    | 1.22                     | 1.00              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:I:66:ARG:HB3   | 1:I:82(B):SER:HB3  | 1.37                     | 1.00              |
| 1:I:17:SER:HA    | 1:I:82(A):SER:HG   | 1.16                     | 0.99              |
| 1:G:28:THR:HG22  | 4:V:53:ASN:ND2     | 1.78                     | 0.98              |
| 1:C:83:SER:O     | 1:C:111:VAL:CG1    | 2.11                     | 0.98              |
| 1:A:68:THR:OG1   | 1:A:81:ASP:CG      | 2.03                     | 0.97              |
| 3:M:221:PRO:HG3  | 3:O:242:LYS:HB3    | 1.46                     | 0.97              |
| 1:A:74:SER:HB3   | 3:N:291:SER:HB3    | 1.43                     | 0.97              |
| 2:D:29:VAL:CG1   | 2:D:71:PHE:CZ      | 2.48                     | 0.97              |
| 1:I:66:ARG:HB2   | 1:I:82(B):SER:HB3  | 1.47                     | 0.97              |
| 1:C:27:GLY:O     | 1:C:28:THR:HG23    | 1.65                     | 0.96              |
| 1:A:68:THR:OG1   | 1:A:81:ASP:CB      | 2.14                     | 0.96              |
| 1:I:17:SER:HB3   | 1:I:82(A):SER:OG   | 1.64                     | 0.96              |
| 2:B:31:SER:OG    | 2:B:32(A):TYR:CD2  | 2.16                     | 0.95              |
| 2:D:33:LEU:HD12  | 2:D:89:GLN:O       | 1.67                     | 0.95              |
| 1:A:18:VAL:CG2   | 1:A:82(C):LEU:HD21 | 1.97                     | 0.94              |
| 2:B:29:VAL:HG11  | 2:B:71:PHE:CZ      | 2.02                     | 0.94              |
| 3:M:229:ARG:HH21 | 3:O:207:SER:HA     | 1.33                     | 0.94              |
| 1:G:83:SER:O     | 1:G:111:VAL:CG1    | 2.16                     | 0.93              |
| 2:D:29:VAL:CG1   | 2:D:71:PHE:HZ      | 1.80                     | 0.93              |
| 2:B:94:THR:OG1   | 2:B:95:PRO:HD3     | 1.64                     | 0.93              |
| 1:K:18:VAL:HG23  | 1:K:82(C):LEU:HD11 | 1.49                     | 0.93              |
| 1:C:66:ARG:HB2   | 1:C:82(B):SER:HB2  | 1.48                     | 0.93              |
| 1:I:17:SER:CA    | 1:I:82(A):SER:HG   | 1.73                     | 0.92              |
| 1:A:68:THR:C     | 1:A:81:ASP:HB2     | 1.90                     | 0.92              |
| 1:G:28:THR:HG22  | 4:V:53:ASN:HD21    | 1.35                     | 0.91              |
| 1:G:145:TYR:CD2  | 1:G:150:VAL:CG2    | 2.52                     | 0.91              |
| 1:A:68:THR:N     | 1:A:81:ASP:HB3     | 1.85                     | 0.91              |
| 1:G:28:THR:CG2   | 4:V:53:ASN:ND2     | 2.34                     | 0.90              |
| 1:C:27:GLY:C     | 1:C:28:THR:HG23    | 1.92                     | 0.90              |
| 1:A:83:SER:O     | 1:A:111:VAL:CG1    | 2.20                     | 0.90              |
| 1:G:145:TYR:CD2  | 1:G:150:VAL:HG21   | 2.06                     | 0.90              |
| 1:C:27:GLY:O     | 1:C:28:THR:CB      | 2.20                     | 0.89              |
| 2:D:29:VAL:HG11  | 2:D:71:PHE:HZ      | 1.34                     | 0.89              |
| 2:D:32:SER:CB    | 2:D:51:ALA:HB2     | 2.02                     | 0.88              |
| 2:J:30:SER:OG    | 2:J:92:VAL:CB      | 2.20                     | 0.88              |
| 1:A:67:VAL:CG2   | 1:A:81:ASP:O       | 2.22                     | 0.88              |
| 1:G:145:TYR:CD1  | 1:G:176:TYR:HB2    | 2.08                     | 0.88              |
| 1:C:27:GLY:O     | 1:C:28:THR:OG1     | 1.91                     | 0.88              |
| 2:J:30:SER:OG    | 2:J:92:VAL:HG12    | 1.74                     | 0.88              |
| 1:C:27:GLY:O     | 1:C:28:THR:CG2     | 2.22                     | 0.87              |
| 4:X:51:LYS:HE3   | 4:X:103:GLU:OE1    | 1.75                     | 0.87              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 1:A:28:THR:HG22 | 4:Q:53:ASN:HD22    | 1.41                     | 0.86              |
| 1:A:28:THR:HG22 | 4:Q:53:ASN:ND2     | 1.90                     | 0.86              |
| 1:A:18:VAL:HG23 | 1:A:82(C):LEU:CD2  | 2.06                     | 0.85              |
| 2:D:112:ALA:CB  | 2:D:200:GLY:O      | 2.24                     | 0.85              |
| 2:J:112:ALA:HB2 | 2:J:200:GLY:O      | 1.76                     | 0.85              |
| 2:B:94:THR:HB   | 2:B:95:PRO:HD3     | 0.85                     | 0.84              |
| 1:I:96:LEU:HD12 | 1:I:96:LEU:O       | 1.77                     | 0.84              |
| 1:I:17:SER:HB2  | 1:I:82(A):SER:OG   | 1.77                     | 0.82              |
| 2:D:29:VAL:HG12 | 2:D:68:GLY:O       | 1.80                     | 0.82              |
| 4:R:51:LYS:HE3  | 4:R:103:GLU:OE1    | 1.80                     | 0.82              |
| 3:N:114:SER:HB2 | 3:N:266:SER:HB2    | 1.62                     | 0.81              |
| 1:K:38:ARG:NH2  | 1:K:86:ASP:OD1     | 2.13                     | 0.81              |
| 1:G:28:THR:CG2  | 4:V:53:ASN:HD22    | 1.93                     | 0.81              |
| 1:A:47:TRP:CZ3  | 2:B:95:PRO:HA      | 2.14                     | 0.81              |
| 1:C:66:ARG:HB2  | 1:C:82(B):SER:CB   | 2.11                     | 0.80              |
| 2:B:29:VAL:HG11 | 2:B:71:PHE:HZ      | 1.46                     | 0.80              |
| 2:B:39:LYS:NZ   | 2:B:81:GLU:O       | 2.14                     | 0.80              |
| 3:M:242:LYS:HB3 | 3:N:221:PRO:HG3    | 1.63                     | 0.80              |
| 2:J:112:ALA:HB1 | 2:J:201:LEU:HD13   | 1.63                     | 0.80              |
| 2:F:31:SER:OG   | 2:F:32:SER:N       | 2.16                     | 0.79              |
| 1:I:66:ARG:CB   | 1:I:82(B):SER:HB2  | 2.02                     | 0.78              |
| 3:O:298:HIS:HE1 | 3:O:300:ILE:HD12   | 1.47                     | 0.78              |
| 2:J:29:VAL:HG22 | 2:J:68:GLY:O       | 1.84                     | 0.77              |
| 1:E:6:GLN:NE2   | 1:E:92:CYS:SG      | 2.58                     | 0.77              |
| 2:J:61:ARG:NH1  | 2:J:82:ASP:OD2     | 2.18                     | 0.77              |
| 2:L:112:ALA:HB2 | 2:L:200:GLY:O      | 1.85                     | 0.77              |
| 1:A:6:GLN:NE2   | 1:A:92:CYS:SG      | 2.58                     | 0.77              |
| 3:T:114:SER:HB2 | 3:T:266:SER:HB2    | 1.67                     | 0.76              |
| 4:P:51:LYS:HE3  | 4:P:103:GLU:OE1    | 1.84                     | 0.76              |
| 1:I:83:SER:OG   | 1:I:85:ASP:OD1     | 2.02                     | 0.76              |
| 2:B:198:HIS:CD2 | 2:B:200:GLY:H      | 2.04                     | 0.75              |
| 1:G:74:SER:HB3  | 3:S:291:SER:CB     | 2.16                     | 0.75              |
| 2:J:31:SER:OG   | 2:J:32:SER:N       | 2.18                     | 0.75              |
| 2:B:33:LEU:HD22 | 2:B:71:PHE:CD2     | 2.22                     | 0.74              |
| 1:G:18:VAL:HG23 | 1:G:82(C):LEU:CD2  | 2.17                     | 0.74              |
| 4:R:119:TYR:OH  | 4:R:132:GLU:OE2    | 2.04                     | 0.74              |
| 1:A:68:THR:O    | 1:A:81:ASP:N       | 2.20                     | 0.74              |
| 1:G:18:VAL:HG23 | 1:G:82(C):LEU:HD21 | 1.69                     | 0.74              |
| 2:J:29:VAL:HG21 | 2:J:71:PHE:HE2     | 1.52                     | 0.73              |
| 2:D:32:SER:OG   | 2:D:51:ALA:CB      | 2.36                     | 0.73              |
| 1:E:6:GLN:HG3   | 1:E:106:GLY:H      | 1.54                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:I:89:VAL:HG22    | 1:I:108:THR:HG22   | 1.70                     | 0.73              |
| 2:L:61:ARG:NH1     | 2:L:82:ASP:OD2     | 2.21                     | 0.73              |
| 3:U:116(B):PHE:HE1 | 3:U:260:MET:HE1    | 1.53                     | 0.73              |
| 1:G:74:SER:HB3     | 3:S:291:SER:OG     | 1.89                     | 0.73              |
| 1:C:74:SER:HB3     | 3:U:291:SER:HB2    | 1.69                     | 0.72              |
| 3:T:117:ARG:HD3    | 3:T:256:TYR:CD1    | 2.23                     | 0.72              |
| 1:G:83:SER:OG      | 1:G:85:ASP:OD1     | 2.06                     | 0.72              |
| 1:I:6:GLN:NE2      | 1:I:92:CYS:SG      | 2.62                     | 0.72              |
| 1:C:6:GLN:HG3      | 1:C:106:GLY:H      | 1.54                     | 0.72              |
| 1:G:6:GLN:NE2      | 1:G:92:CYS:SG      | 2.63                     | 0.72              |
| 1:A:66:ARG:HD2     | 1:A:82(B):SER:OG   | 1.90                     | 0.72              |
| 2:B:38:GLN:HE21    | 2:B:87:TYR:HE2     | 1.38                     | 0.72              |
| 2:L:32:SER:HB2     | 2:L:51:ALA:HB2     | 1.70                     | 0.71              |
| 2:B:198:HIS:HD2    | 2:B:200:GLY:H      | 1.36                     | 0.71              |
| 2:F:29:VAL:HG21    | 2:F:71:PHE:HE2     | 1.54                     | 0.70              |
| 1:G:145:TYR:CE1    | 1:G:176:TYR:HB3    | 2.15                     | 0.70              |
| 2:H:204:PRO:O      | 2:H:206:THR:HG22   | 1.91                     | 0.70              |
| 2:D:32:SER:HB2     | 2:D:51:ALA:HB2     | 1.71                     | 0.70              |
| 1:K:18:VAL:CG2     | 1:K:82(C):LEU:HD11 | 2.21                     | 0.70              |
| 3:M:114:SER:HB2    | 3:M:266:SER:HB2    | 1.73                     | 0.70              |
| 1:C:18:VAL:HG23    | 1:C:82(C):LEU:HD21 | 1.74                     | 0.70              |
| 2:D:32:SER:CB      | 2:D:51:ALA:CB      | 2.70                     | 0.70              |
| 2:B:29:VAL:HG11    | 2:B:71:PHE:CE2     | 2.26                     | 0.69              |
| 1:E:66:ARG:NH1     | 1:E:82(B):SER:HG   | 1.88                     | 0.69              |
| 1:G:74:SER:HB3     | 3:S:291:SER:HB2    | 1.73                     | 0.69              |
| 2:J:27:GLN:O       | 2:J:28:SER:O       | 2.09                     | 0.69              |
| 1:A:89:VAL:HG22    | 1:A:108:THR:HG22   | 1.75                     | 0.68              |
| 3:N:117:ARG:HD3    | 3:N:256:TYR:CD1    | 2.28                     | 0.68              |
| 2:B:27:GLN:O       | 2:B:28:SER:C       | 2.30                     | 0.68              |
| 1:I:74:SER:HB2     | 4:R:56:ILE:HG21    | 1.75                     | 0.68              |
| 3:U:298:HIS:HE1    | 3:U:300:ILE:HD12   | 1.58                     | 0.68              |
| 4:W:103:GLU:OE2    | 4:X:102:LEU:HD21   | 1.93                     | 0.68              |
| 2:D:32:SER:HB2     | 2:D:51:ALA:CB      | 2.24                     | 0.68              |
| 2:L:31:SER:OG      | 2:L:32:SER:N       | 2.24                     | 0.68              |
| 1:I:82(B):SER:O    | 1:I:86:ASP:OD2     | 2.11                     | 0.68              |
| 3:N:107:GLU:O      | 3:N:111:GLN:HG2    | 1.93                     | 0.68              |
| 1:E:82(B):SER:HB2  | 1:E:82(C):LEU:HA   | 1.75                     | 0.68              |
| 1:G:6:GLN:HG3      | 1:G:106:GLY:H      | 1.58                     | 0.68              |
| 1:A:119:PRO:HB3    | 1:A:145:TYR:HB3    | 1.76                     | 0.68              |
| 2:J:112:ALA:HB1    | 2:J:201:LEU:CD1    | 2.23                     | 0.68              |
| 1:A:68:THR:O       | 1:A:81:ASP:CA      | 2.42                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:J:30:SER:O       | 2:J:31:SER:CB      | 2.41                     | 0.67              |
| 1:I:163:VAL:HG22   | 1:I:182:VAL:HG22   | 1.76                     | 0.67              |
| 1:K:74:SER:HB3     | 3:T:291:SER:HB3    | 1.75                     | 0.67              |
| 1:C:66:ARG:CB      | 1:C:82(B):SER:HB2  | 2.23                     | 0.67              |
| 3:T:107:GLU:O      | 3:T:111:GLN:HG2    | 1.95                     | 0.67              |
| 2:B:38:GLN:NE2     | 2:B:87:TYR:HE2     | 1.91                     | 0.66              |
| 1:C:18:VAL:HG23    | 1:C:82(C):LEU:CD2  | 2.25                     | 0.66              |
| 2:D:32:SER:OG      | 2:D:51:ALA:HB2     | 1.93                     | 0.66              |
| 3:O:134:GLY:HA3    | 3:O:153:TRP:HB3    | 1.77                     | 0.66              |
| 1:K:119:PRO:HB3    | 1:K:145:TYR:HB3    | 1.77                     | 0.66              |
| 1:E:119:PRO:HB3    | 1:E:145:TYR:HB3    | 1.78                     | 0.66              |
| 1:A:68:THR:OG1     | 1:A:81:ASP:OD2     | 2.13                     | 0.66              |
| 2:J:29:VAL:HG21    | 2:J:71:PHE:CE2     | 2.30                     | 0.66              |
| 3:N:111:GLN:HE22   | 3:N:262:ARG:NH1    | 1.92                     | 0.66              |
| 4:W:51:LYS:HE3     | 4:W:103:GLU:OE1    | 1.95                     | 0.66              |
| 2:J:30:SER:OG      | 2:J:92:VAL:HB      | 1.96                     | 0.66              |
| 4:Q:51:LYS:HE3     | 4:Q:103:GLU:OE1    | 1.96                     | 0.66              |
| 1:C:16:SER:O       | 1:C:82(C):LEU:HB2  | 1.97                     | 0.65              |
| 2:J:201:LEU:HD21   | 2:J:205:VAL:HG12   | 1.79                     | 0.65              |
| 2:B:29:VAL:CG1     | 2:B:71:PHE:HZ      | 2.10                     | 0.65              |
| 1:A:67:VAL:HA      | 1:A:81:ASP:O       | 1.96                     | 0.65              |
| 1:C:53:ILE:HD13    | 4:X:49:THR:HA      | 1.79                     | 0.65              |
| 2:D:141:PRO:HG3    | 2:D:199:GLN:NE2    | 2.12                     | 0.65              |
| 2:B:29:VAL:CG1     | 2:B:71:PHE:CZ      | 2.78                     | 0.64              |
| 3:O:26:VAL:HG21    | 3:O:317:ALA:HB2    | 1.78                     | 0.64              |
| 1:G:119:PRO:HB3    | 1:G:145:TYR:HB3    | 1.78                     | 0.64              |
| 1:I:82(B):SER:O    | 1:I:82(B):SER:OG   | 2.09                     | 0.64              |
| 3:N:163:LYS:HB3    | 3:U:159:ASN:ND2    | 2.13                     | 0.64              |
| 2:L:166:GLN:HG3    | 2:L:173:TYR:CZ     | 2.33                     | 0.64              |
| 4:Q:69:GLU:O       | 4:R:76:ARG:NH1     | 2.28                     | 0.64              |
| 2:B:94:THR:HG1     | 2:B:95:PRO:CD      | 2.09                     | 0.64              |
| 1:C:36:TRP:CE2     | 1:C:80:MET:HB2     | 2.32                     | 0.64              |
| 1:I:66:ARG:O       | 1:I:82:LEU:HD12    | 1.98                     | 0.64              |
| 4:P:69:GLU:O       | 4:Q:76:ARG:NH1     | 2.31                     | 0.64              |
| 2:H:112:ALA:HB2    | 2:H:200:GLY:O      | 1.98                     | 0.64              |
| 2:F:170:ASP:OD1    | 2:F:172:THR:HG22   | 1.98                     | 0.63              |
| 2:H:61:ARG:NH1     | 2:H:82:ASP:OD2     | 2.32                     | 0.63              |
| 3:S:115:VAL:HG11   | 3:S:116(B):PHE:HB2 | 1.80                     | 0.63              |
| 2:F:29:VAL:HG21    | 2:F:71:PHE:CE2     | 2.34                     | 0.63              |
| 1:G:18:VAL:CG2     | 1:G:82(C):LEU:HD21 | 2.28                     | 0.63              |
| 3:U:116(B):PHE:CE1 | 3:U:260:MET:HE1    | 2.34                     | 0.63              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:X:154:ASN:OD1  | 4:X:156:THR:OG1    | 2.06                     | 0.63              |
| 2:L:158:ASN:OD1  | 2:L:158:ASN:N      | 2.28                     | 0.63              |
| 4:Q:30:GLN:OE1   | 4:Q:146:ASN:N      | 2.29                     | 0.63              |
| 3:S:307:LYS:HE2  | 4:V:61:THR:HG22    | 1.81                     | 0.63              |
| 1:I:52:SER:OG    | 1:I:54:PHE:HB3     | 1.99                     | 0.63              |
| 3:U:115:VAL:HG11 | 3:U:116(B):PHE:HB2 | 1.79                     | 0.63              |
| 2:B:170:ASP:OD1  | 2:B:172:THR:HG22   | 1.99                     | 0.63              |
| 1:G:145:TYR:CD2  | 1:G:150:VAL:HG23   | 2.26                     | 0.62              |
| 2:J:32:SER:HB2   | 2:J:51:ALA:HB2     | 1.80                     | 0.62              |
| 2:B:32:SER:HB2   | 2:B:51:ALA:HB2     | 1.81                     | 0.62              |
| 3:N:90:THR:OG1   | 3:N:92:SER:OG      | 2.10                     | 0.62              |
| 1:G:83:SER:O     | 1:G:111:VAL:CB     | 2.48                     | 0.62              |
| 3:M:115:VAL:HG11 | 3:M:116(B):PHE:HB2 | 1.80                     | 0.62              |
| 1:K:6:GLN:NE2    | 1:K:92:CYS:SG      | 2.73                     | 0.62              |
| 1:A:87:THR:OG1   | 1:A:110:THR:HA     | 1.99                     | 0.62              |
| 1:C:27:GLY:C     | 1:C:28:THR:CG2     | 2.61                     | 0.62              |
| 3:O:202:VAL:HG11 | 3:O:251:LEU:HD13   | 1.80                     | 0.62              |
| 2:L:141:PRO:HG3  | 2:L:199:GLN:NE2    | 2.15                     | 0.61              |
| 3:O:114:SER:HB2  | 3:O:266:SER:HB2    | 1.82                     | 0.61              |
| 4:R:30:GLN:OE1   | 4:R:146:ASN:N      | 2.31                     | 0.61              |
| 1:A:74:SER:HB2   | 4:Q:56:ILE:HG21    | 1.81                     | 0.61              |
| 3:O:38:HIS:CD2   | 3:O:39:SER:N       | 2.68                     | 0.61              |
| 1:K:6:GLN:HG3    | 1:K:106:GLY:H      | 1.63                     | 0.61              |
| 3:N:111:GLN:NE2  | 3:N:262:ARG:NH1    | 2.48                     | 0.61              |
| 1:C:119:PRO:HB3  | 1:C:145:TYR:HB3    | 1.82                     | 0.61              |
| 2:D:61:ARG:NH1   | 2:D:82:ASP:OD1     | 2.33                     | 0.61              |
| 2:F:166:GLN:HG3  | 2:F:173:TYR:CZ     | 2.35                     | 0.60              |
| 1:G:36:TRP:CE2   | 1:G:80:MET:HB2     | 2.36                     | 0.60              |
| 1:I:74:SER:HB3   | 3:O:291:SER:CB     | 2.31                     | 0.60              |
| 3:M:229:ARG:NH2  | 3:O:207:SER:HA     | 2.10                     | 0.60              |
| 3:O:42:LEU:HD11  | 3:O:316:LEU:HD22   | 1.82                     | 0.60              |
| 1:I:74:SER:HB3   | 3:O:291:SER:HB2    | 1.83                     | 0.60              |
| 4:V:158:ASP:OD1  | 4:V:160:PRO:HD2    | 2.01                     | 0.60              |
| 1:E:74:SER:HB3   | 3:M:291:SER:OG     | 2.01                     | 0.60              |
| 1:A:74:SER:HB3   | 3:N:291:SER:CB     | 2.25                     | 0.60              |
| 2:H:32:SER:HB2   | 2:H:51:ALA:HB2     | 1.84                     | 0.60              |
| 1:G:89:VAL:HG22  | 1:G:108:THR:HG22   | 1.83                     | 0.60              |
| 3:U:90:THR:OG1   | 3:U:92:SER:OG      | 2.08                     | 0.60              |
| 4:W:30:GLN:OE1   | 4:W:146:ASN:N      | 2.32                     | 0.60              |
| 1:A:68:THR:CA    | 1:A:81:ASP:HB3     | 2.30                     | 0.60              |
| 1:E:36:TRP:CZ3   | 1:E:92:CYS:HB3     | 2.37                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:201:TYR:OH    | 3:M:246:GLU:OE2   | 2.15                     | 0.60              |
| 1:K:42:GLY:O      | 1:K:43:GLN:NE2    | 2.30                     | 0.60              |
| 4:P:103:GLU:OE2   | 4:Q:102:LEU:HD21  | 2.01                     | 0.60              |
| 2:D:30:SER:OG     | 2:D:92:VAL:CG1    | 2.50                     | 0.60              |
| 1:A:61:GLN:N      | 1:A:61:GLN:OE1    | 2.35                     | 0.60              |
| 1:E:66:ARG:HH11   | 1:E:82(B):SER:HG  | 1.42                     | 0.60              |
| 2:D:27:GLN:O      | 2:D:28:SER:C      | 2.35                     | 0.60              |
| 1:E:36:TRP:CE2    | 1:E:80:MET:HB2    | 2.36                     | 0.59              |
| 2:J:205:VAL:HG13  | 2:J:205:VAL:O     | 2.02                     | 0.59              |
| 1:A:6:GLN:HG3     | 1:A:106:GLY:H     | 1.67                     | 0.59              |
| 2:B:158:ASN:N     | 2:B:158:ASN:OD1   | 2.33                     | 0.59              |
| 3:U:308:TYR:CD2   | 4:X:89:LEU:HD13   | 2.38                     | 0.59              |
| 2:D:29:VAL:HG22   | 2:D:29:VAL:O      | 2.03                     | 0.59              |
| 2:L:29:VAL:O      | 2:L:29:VAL:HG12   | 2.02                     | 0.59              |
| 4:V:51:LYS:HE3    | 4:V:103:GLU:OE1   | 2.03                     | 0.59              |
| 1:E:40:ALA:HB3    | 1:E:43:GLN:HG3    | 1.85                     | 0.58              |
| 1:G:36:TRP:CZ3    | 1:G:92:CYS:HB3    | 2.37                     | 0.58              |
| 2:H:27:GLN:O      | 2:H:28:SER:C      | 2.41                     | 0.58              |
| 2:J:30:SER:O      | 2:J:31:SER:OG     | 2.20                     | 0.58              |
| 4:V:9:PHE:O       | 4:V:135:ASN:HA    | 2.03                     | 0.58              |
| 1:G:87:THR:OG1    | 1:G:110:THR:HA    | 2.02                     | 0.58              |
| 2:J:32:SER:O      | 2:J:50:GLY:C      | 2.40                     | 0.58              |
| 1:I:5:VAL:HA      | 1:I:105:LYS:NZ    | 2.19                     | 0.58              |
| 2:J:61:ARG:NH1    | 2:J:82:ASP:CG     | 2.57                     | 0.58              |
| 1:K:36:TRP:CE2    | 1:K:80:MET:HB2    | 2.38                     | 0.58              |
| 2:F:158:ASN:OD1   | 2:F:158:ASN:N     | 2.35                     | 0.58              |
| 2:F:27:GLN:O      | 2:F:28:SER:C      | 2.41                     | 0.58              |
| 1:G:53:ILE:HD13   | 4:V:49:THR:HA     | 1.85                     | 0.58              |
| 2:H:158:ASN:OD1   | 2:H:158:ASN:N     | 2.36                     | 0.58              |
| 1:I:74:SER:HB3    | 3:O:291:SER:OG    | 2.03                     | 0.58              |
| 3:S:42:LEU:HD11   | 3:S:316:LEU:HD22  | 1.86                     | 0.58              |
| 1:C:63:PHE:HD2    | 1:C:66:ARG:HD2    | 1.68                     | 0.58              |
| 1:C:95:LYS:HE3    | 1:C:100(E):TYR:CZ | 2.39                     | 0.58              |
| 3:S:44:GLU:OE2    | 3:S:46:LYS:HG2    | 2.02                     | 0.58              |
| 1:A:28:THR:CG2    | 4:Q:53:ASN:HD22   | 2.13                     | 0.58              |
| 1:A:68:THR:OG1    | 1:A:81:ASP:HB2    | 2.02                     | 0.58              |
| 2:D:32(A):TYR:HD1 | 2:D:91:TYR:CE2    | 2.22                     | 0.58              |
| 2:D:158:ASN:OD1   | 2:D:158:ASN:N     | 2.37                     | 0.58              |
| 2:D:112:ALA:HB1   | 2:D:201:LEU:CD2   | 2.34                     | 0.58              |
| 1:I:119:PRO:HB3   | 1:I:145:TYR:HB3   | 1.86                     | 0.58              |
| 2:J:201:LEU:HD21  | 2:J:205:VAL:CG1   | 2.33                     | 0.58              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:Q:95:ASN:ND2   | 4:R:95:ASN:HD21    | 2.01                     | 0.58              |
| 4:P:134:GLY:O    | 4:P:135:ASN:OD1    | 2.23                     | 0.57              |
| 3:S:39:SER:OG    | 3:S:315:ARG:NE     | 2.32                     | 0.57              |
| 1:G:83:SER:OG    | 1:G:84:SER:N       | 2.35                     | 0.57              |
| 2:J:61:ARG:NH1   | 2:J:82:ASP:OD1     | 2.37                     | 0.57              |
| 3:U:199:ASP:OD1  | 3:U:214:LYS:NZ     | 2.37                     | 0.57              |
| 1:K:83:SER:O     | 1:K:83:SER:OG      | 2.17                     | 0.57              |
| 1:A:68:THR:C     | 1:A:81:ASP:CB      | 2.59                     | 0.57              |
| 3:U:114:SER:HB2  | 3:U:266:SER:HB2    | 1.86                     | 0.57              |
| 4:W:82:LYS:NZ    | 4:W:86:ASP:OD2     | 2.34                     | 0.57              |
| 1:C:96:LEU:CD1   | 1:C:102:VAL:HG21   | 2.35                     | 0.57              |
| 2:L:198:HIS:CG   | 2:L:199:GLN:H      | 2.23                     | 0.57              |
| 3:T:115:VAL:HG11 | 3:T:116(B):PHE:HB2 | 1.87                     | 0.57              |
| 2:D:166:GLN:HG3  | 2:D:173:TYR:CZ     | 2.39                     | 0.57              |
| 3:S:103:ILE:HG13 | 3:S:233:TYR:CE2    | 2.40                     | 0.57              |
| 3:O:163:LYS:NZ   | 3:O:201:TYR:OH     | 2.38                     | 0.57              |
| 3:S:114:SER:HB2  | 3:S:266:SER:HB2    | 1.86                     | 0.56              |
| 3:S:180:TRP:CE2  | 3:S:233:TYR:HB2    | 2.40                     | 0.56              |
| 1:G:5:VAL:HA     | 1:G:105:LYS:NZ     | 2.20                     | 0.56              |
| 3:N:42:LEU:HD11  | 3:N:316:LEU:HD22   | 1.87                     | 0.56              |
| 3:S:307:LYS:HE2  | 4:V:61:THR:CG2     | 2.36                     | 0.56              |
| 3:N:180:TRP:CE2  | 3:N:233:TYR:HB2    | 2.40                     | 0.56              |
| 1:I:159:LEU:HD21 | 1:I:182:VAL:HG11   | 1.88                     | 0.56              |
| 2:H:166:GLN:HG3  | 2:H:173:TYR:CZ     | 2.40                     | 0.56              |
| 1:I:36:TRP:CE2   | 1:I:80:MET:HB2     | 2.40                     | 0.56              |
| 3:N:26:VAL:HG21  | 3:N:317:ALA:HB2    | 1.88                     | 0.56              |
| 1:A:105:LYS:HE2  | 1:A:105:LYS:H      | 1.69                     | 0.56              |
| 1:E:87:THR:OG1   | 1:E:110:THR:HA     | 2.05                     | 0.56              |
| 3:M:207:SER:HA   | 3:N:229:ARG:HH21   | 1.71                     | 0.56              |
| 3:M:221:PRO:HG2  | 3:O:242:LYS:O      | 2.06                     | 0.56              |
| 1:C:66:ARG:HB3   | 1:C:82(B):SER:OG   | 2.06                     | 0.56              |
| 3:S:151:LEU:HB3  | 3:S:252:VAL:HG12   | 1.87                     | 0.56              |
| 3:T:180:TRP:CE2  | 3:T:233:TYR:HB2    | 2.41                     | 0.56              |
| 3:O:175:GLU:OE1  | 3:O:262:ARG:NH1    | 2.39                     | 0.55              |
| 4:P:76:ARG:NH1   | 4:R:69:GLU:O       | 2.39                     | 0.55              |
| 1:C:73:ILE:HD12  | 1:C:73:ILE:H       | 1.71                     | 0.55              |
| 1:G:5:VAL:HA     | 1:G:105:LYS:HZ3    | 1.71                     | 0.55              |
| 3:N:288:ILE:HG22 | 3:N:290:THR:HG22   | 1.88                     | 0.55              |
| 1:I:105:LYS:H    | 1:I:105:LYS:HE2    | 1.71                     | 0.55              |
| 3:U:42:LEU:HD11  | 3:U:316:LEU:HD22   | 1.87                     | 0.55              |
| 3:M:221:PRO:CG   | 3:O:242:LYS:HB3    | 2.28                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:136:LEU:N    | 2:B:136:LEU:HD23   | 2.22                     | 0.55              |
| 1:K:83:SER:O     | 1:K:85:ASP:N       | 2.36                     | 0.55              |
| 2:B:94:THR:HG1   | 2:B:95:PRO:HD3     | 1.68                     | 0.55              |
| 2:F:29:VAL:CG2   | 2:F:68:GLY:O       | 2.33                     | 0.55              |
| 2:L:170:ASP:OD1  | 2:L:172:THR:HG22   | 2.06                     | 0.55              |
| 2:D:206:THR:O    | 2:D:206:THR:OG1    | 2.22                     | 0.55              |
| 2:J:14:SER:N     | 2:J:17:GLU:OE2     | 2.39                     | 0.55              |
| 2:H:24:ARG:NH1   | 2:H:70:ASP:OD1     | 2.40                     | 0.55              |
| 3:S:26:VAL:HG21  | 3:S:317:ALA:HB2    | 1.89                     | 0.55              |
| 1:E:52:SER:O     | 1:E:53:ILE:N       | 2.40                     | 0.54              |
| 1:E:67:VAL:HA    | 1:E:81:ASP:O       | 2.08                     | 0.54              |
| 1:I:19:GLN:HG3   | 1:I:81:ASP:OD2     | 2.08                     | 0.54              |
| 2:B:37:GLN:HB2   | 2:B:47:LEU:HD11    | 1.88                     | 0.54              |
| 1:C:66:ARG:CB    | 1:C:82(B):SER:CB   | 2.82                     | 0.54              |
| 2:F:136:LEU:HD23 | 2:F:136:LEU:N      | 2.22                     | 0.54              |
| 1:E:19:GLN:HG3   | 1:E:81:ASP:OD2     | 2.06                     | 0.54              |
| 2:H:204:PRO:O    | 2:H:206:THR:CG2    | 2.56                     | 0.54              |
| 3:M:52:CYS:HB3   | 3:M:277:CYS:O      | 2.07                     | 0.54              |
| 3:O:18:HIS:O     | 3:O:320:LEU:HD11   | 2.07                     | 0.54              |
| 3:U:175:GLU:OE1  | 3:U:262:ARG:NH1    | 2.41                     | 0.54              |
| 2:B:38:GLN:NE2   | 2:B:87:TYR:CE2     | 2.75                     | 0.54              |
| 4:P:148:CYS:O    | 4:P:151:SER:OG     | 2.23                     | 0.54              |
| 3:T:277:CYS:O    | 3:T:277:CYS:SG     | 2.55                     | 0.54              |
| 1:I:38:ARG:HG3   | 1:I:90:TYR:CE1     | 2.43                     | 0.54              |
| 3:N:115:VAL:HG11 | 3:N:116(B):PHE:HB2 | 1.90                     | 0.54              |
| 1:K:163:VAL:HG22 | 1:K:182:VAL:HG22   | 1.90                     | 0.53              |
| 3:N:295:GLN:O    | 3:N:308:TYR:HA     | 2.08                     | 0.53              |
| 3:O:77:GLU:HG3   | 3:O:149:LYS:HE3    | 1.90                     | 0.53              |
| 4:Q:82:LYS:NZ    | 4:Q:86:ASP:OD2     | 2.36                     | 0.53              |
| 1:C:66:ARG:HD3   | 1:C:82(B):SER:HB2  | 1.89                     | 0.53              |
| 1:K:59:TYR:HE1   | 1:K:69:ILE:HG13    | 1.74                     | 0.53              |
| 3:U:202:VAL:HG11 | 3:U:251:LEU:HD13   | 1.90                     | 0.53              |
| 1:E:84:SER:HA    | 1:E:111:VAL:HB     | 1.90                     | 0.53              |
| 3:N:103:ILE:HG13 | 3:N:233:TYR:CE2    | 2.44                     | 0.53              |
| 2:J:201:LEU:CD2  | 2:J:205:VAL:HG12   | 2.38                     | 0.53              |
| 3:O:111:GLN:OE1  | 3:O:262:ARG:NE     | 2.42                     | 0.53              |
| 4:X:27:GLN:O     | 4:X:27:GLN:HG3     | 2.08                     | 0.53              |
| 1:C:74:SER:CB    | 3:U:291:SER:HB2    | 2.37                     | 0.53              |
| 2:D:29:VAL:CG1   | 2:D:71:PHE:CE2     | 2.76                     | 0.53              |
| 2:H:136:LEU:N    | 2:H:136:LEU:HD23   | 2.24                     | 0.53              |
| 1:I:105:LYS:H    | 1:I:105:LYS:CE     | 2.21                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:F:27:GLN:O      | 2:F:28:SER:O       | 2.27                     | 0.53              |
| 1:G:114:ALA:HB3   | 1:G:146:PHE:CE2    | 2.43                     | 0.53              |
| 1:I:96:LEU:HD12   | 1:I:96:LEU:C       | 2.22                     | 0.53              |
| 3:N:58:PRO:HB3    | 3:N:86:TYR:CZ      | 2.44                     | 0.53              |
| 2:D:30:SER:OG     | 2:D:92:VAL:HG12    | 2.09                     | 0.53              |
| 2:L:32(A):TYR:HB2 | 2:L:92:VAL:HG12    | 1.91                     | 0.53              |
| 4:V:103:GLU:OE2   | 4:W:102:LEU:HD21   | 2.09                     | 0.53              |
| 2:B:32:SER:HB2    | 2:B:51:ALA:CB      | 2.39                     | 0.52              |
| 1:I:6:GLN:HG3     | 1:I:106:GLY:H      | 1.74                     | 0.52              |
| 2:J:158:ASN:OD1   | 2:J:158:ASN:N      | 2.40                     | 0.52              |
| 3:U:180:TRP:CE2   | 3:U:233:TYR:HB2    | 2.44                     | 0.52              |
| 4:V:62:GLN:H      | 4:V:62:GLN:CD      | 2.13                     | 0.52              |
| 3:O:115:VAL:HG11  | 3:O:116(B):PHE:HB2 | 1.91                     | 0.52              |
| 2:L:136:LEU:HD21  | 2:L:196:VAL:HG21   | 1.90                     | 0.52              |
| 3:T:307:LYS:HE2   | 4:W:61:THR:HG22    | 1.90                     | 0.52              |
| 2:D:30:SER:OG     | 2:D:92:VAL:HG11    | 2.10                     | 0.52              |
| 2:F:119:PRO:HB3   | 2:F:209:PHE:CE2    | 2.44                     | 0.52              |
| 3:T:307:LYS:HE2   | 4:W:61:THR:CG2     | 2.40                     | 0.52              |
| 3:M:26:VAL:HG21   | 3:M:317:ALA:HB2    | 1.92                     | 0.52              |
| 4:P:62:GLN:NE2    | 4:Q:86:ASP:HB3     | 2.24                     | 0.52              |
| 4:V:134:GLY:O     | 4:V:135:ASN:OD1    | 2.27                     | 0.52              |
| 1:K:84:SER:H      | 1:K:111:VAL:HG11   | 1.75                     | 0.52              |
| 3:O:38:HIS:CD2    | 3:O:39:SER:H       | 2.26                     | 0.52              |
| 1:I:5:VAL:HA      | 1:I:105:LYS:HZ1    | 1.75                     | 0.52              |
| 1:A:68:THR:H      | 1:A:81:ASP:CB      | 2.08                     | 0.52              |
| 1:A:210:ARG:HH12  | 1:A:212:GLU:HB3    | 1.75                     | 0.52              |
| 2:J:37:GLN:HG3    | 2:J:86:TYR:CE2     | 2.45                     | 0.52              |
| 3:N:134:GLY:HA3   | 3:N:153:TRP:HB3    | 1.92                     | 0.52              |
| 1:C:96:LEU:HD13   | 1:C:102:VAL:CG2    | 2.40                     | 0.51              |
| 2:H:170:ASP:OD1   | 2:H:172:THR:HG22   | 2.09                     | 0.51              |
| 1:G:52:SER:O      | 1:G:53:ILE:N       | 2.43                     | 0.51              |
| 3:M:284:PRO:HD3   | 3:M:300:ILE:O      | 2.09                     | 0.51              |
| 2:J:27:GLN:O      | 2:J:28:SER:C       | 2.44                     | 0.51              |
| 3:N:163:LYS:HB3   | 3:U:159:ASN:HD21   | 1.74                     | 0.51              |
| 1:I:154:TRP:CH2   | 1:I:196:CYS:HB3    | 2.45                     | 0.51              |
| 1:A:52:SER:O      | 1:A:53:ILE:N       | 2.44                     | 0.51              |
| 1:C:52:SER:O      | 1:C:53:ILE:N       | 2.43                     | 0.51              |
| 1:E:5:VAL:HA      | 1:E:105:LYS:NZ     | 2.24                     | 0.51              |
| 1:C:163:VAL:HG22  | 1:C:182:VAL:HG22   | 1.93                     | 0.51              |
| 1:I:87:THR:OG1    | 1:I:110:THR:HA     | 2.11                     | 0.51              |
| 3:M:288:ILE:HG21  | 3:M:297:ILE:HG13   | 1.93                     | 0.51              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:B:166:GLN:HG3    | 2:B:173:TYR:CZ   | 2.46                     | 0.51              |
| 2:D:141:PRO:O      | 2:D:198:HIS:HE1  | 1.93                     | 0.51              |
| 1:E:148:GLU:OE1    | 1:E:149:PRO:HA   | 2.11                     | 0.51              |
| 3:N:100:GLY:HA3    | 3:N:230:MET:O    | 2.10                     | 0.51              |
| 2:B:32:SER:O       | 2:B:32:SER:OG    | 2.21                     | 0.51              |
| 2:D:112:ALA:HB1    | 2:D:201:LEU:HD23 | 1.93                     | 0.51              |
| 1:G:38:ARG:HG3     | 1:G:90:TYR:CE1   | 2.46                     | 0.50              |
| 1:C:38:ARG:HG3     | 1:C:90:TYR:CE1   | 2.46                     | 0.50              |
| 1:K:100(A):TYR:HD2 | 4:W:42:GLN:OE1   | 1.93                     | 0.50              |
| 1:A:59:TYR:HE1     | 1:A:69:ILE:HG13  | 1.77                     | 0.50              |
| 1:C:74:SER:HB3     | 3:U:291:SER:CB   | 2.38                     | 0.50              |
| 2:H:175:LEU:HD12   | 2:H:176:SER:H    | 1.77                     | 0.50              |
| 3:M:103:ILE:HG13   | 3:M:233:TYR:CE2  | 2.47                     | 0.50              |
| 1:E:32:TYR:HB3     | 1:E:100:TYR:CD1  | 2.46                     | 0.50              |
| 1:G:28:THR:HG21    | 4:V:53:ASN:HD22  | 1.71                     | 0.50              |
| 3:T:69:TRP:HE1     | 3:T:81:THR:HG21  | 1.77                     | 0.50              |
| 1:A:68:THR:CA      | 1:A:81:ASP:CB    | 2.89                     | 0.50              |
| 2:D:29:VAL:HG11    | 2:D:71:PHE:HE2   | 1.69                     | 0.50              |
| 2:F:47:LEU:HD23    | 2:F:58:ILE:HD12  | 1.94                     | 0.50              |
| 2:J:32:SER:HB2     | 2:J:51:ALA:CB    | 2.42                     | 0.50              |
| 2:L:115:VAL:HG22   | 2:L:136:LEU:HD22 | 1.93                     | 0.50              |
| 3:O:100:GLY:HA3    | 3:O:230:MET:O    | 2.11                     | 0.50              |
| 4:Q:95:ASN:HD21    | 4:R:95:ASN:HD21  | 1.58                     | 0.50              |
| 4:V:98:LEU:O       | 4:V:102:LEU:HG   | 2.11                     | 0.50              |
| 1:A:105:LYS:H      | 1:A:105:LYS:CE   | 2.25                     | 0.50              |
| 2:B:119:PRO:HB3    | 2:B:209:PHE:CE2  | 2.46                     | 0.50              |
| 3:M:151:LEU:HB3    | 3:M:252:VAL:HG12 | 1.94                     | 0.50              |
| 3:U:77:GLU:HG3     | 3:U:149:LYS:HE3  | 1.94                     | 0.50              |
| 1:E:59:TYR:HE1     | 1:E:69:ILE:HG13  | 1.76                     | 0.49              |
| 4:P:158:ASP:OD1    | 4:P:160:PRO:HD2  | 2.12                     | 0.49              |
| 1:K:74:SER:HB2     | 4:W:56:ILE:HG21  | 1.93                     | 0.49              |
| 2:L:119:PRO:HB3    | 2:L:209:PHE:CE2  | 2.47                     | 0.49              |
| 3:N:11:ASP:OD1     | 4:Q:28:ASN:HA    | 2.11                     | 0.49              |
| 4:P:70:PHE:CE2     | 4:P:78:GLU:HA    | 2.47                     | 0.49              |
| 3:S:134:GLY:HA3    | 3:S:153:TRP:HB3  | 1.93                     | 0.49              |
| 4:W:62:GLN:CD      | 4:W:62:GLN:H     | 2.14                     | 0.49              |
| 3:O:189:ALA:HA     | 3:U:189:ALA:CB   | 2.42                     | 0.49              |
| 3:M:111:GLN:OE1    | 3:M:262:ARG:NH1  | 2.41                     | 0.49              |
| 2:B:32(A):TYR:HD1  | 2:B:91:TYR:CE2   | 2.30                     | 0.49              |
| 2:J:170:ASP:OD1    | 2:J:172:THR:HG22 | 2.12                     | 0.49              |
| 2:D:24:ARG:NH1     | 2:D:70:ASP:OD1   | 2.45                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:74:SER:HB3   | 3:T:291:SER:CB    | 2.40                     | 0.49              |
| 4:P:9:PHE:O      | 4:P:135:ASN:HA    | 2.12                     | 0.49              |
| 1:E:36:TRP:CH2   | 1:E:92:CYS:HB3    | 2.47                     | 0.49              |
| 1:G:145:TYR:HD2  | 1:G:150:VAL:CG2   | 2.19                     | 0.49              |
| 3:S:50:LYS:HD2   | 3:S:275:HIS:HB2   | 1.94                     | 0.49              |
| 1:G:145:TYR:CD1  | 1:G:145:TYR:C     | 2.85                     | 0.49              |
| 1:I:83:SER:O     | 1:I:111:VAL:CB    | 2.59                     | 0.49              |
| 3:U:284:PRO:HD3  | 3:U:300:ILE:O     | 2.13                     | 0.49              |
| 1:C:66:ARG:CB    | 1:C:82(B):SER:OG  | 2.61                     | 0.49              |
| 1:I:52:SER:O     | 1:I:53:ILE:N      | 2.46                     | 0.49              |
| 3:T:103:ILE:HG13 | 3:T:233:TYR:CE2   | 2.47                     | 0.49              |
| 2:B:30:SER:OG    | 2:B:92:VAL:HG11   | 2.12                     | 0.48              |
| 2:D:67:SER:HA    | 2:D:71:PHE:CE1    | 2.47                     | 0.48              |
| 2:B:29:VAL:CG1   | 2:B:71:PHE:CE2    | 2.95                     | 0.48              |
| 1:C:47:TRP:CG    | 2:D:96:LEU:HB2    | 2.48                     | 0.48              |
| 2:F:32:SER:HB2   | 2:F:51:ALA:HB2    | 1.95                     | 0.48              |
| 1:K:84:SER:O     | 1:K:87:THR:HG22   | 2.13                     | 0.48              |
| 1:E:95:LYS:HE3   | 1:E:100(E):TYR:CZ | 2.48                     | 0.48              |
| 1:G:42:GLY:O     | 1:G:43:GLN:NE2    | 2.43                     | 0.48              |
| 1:G:145:TYR:HD1  | 1:G:145:TYR:O     | 1.97                     | 0.48              |
| 3:O:284:PRO:HD3  | 3:O:300:ILE:O     | 2.14                     | 0.48              |
| 2:B:105:GLU:OE1  | 2:B:173:TYR:OH    | 2.26                     | 0.48              |
| 1:C:87:THR:OG1   | 1:C:110:THR:HA    | 2.13                     | 0.48              |
| 1:G:25:SER:O     | 1:G:25:SER:OG     | 2.19                     | 0.48              |
| 2:J:4:LEU:HD11   | 2:J:90:GLN:HB3    | 1.96                     | 0.48              |
| 2:L:141:PRO:O    | 2:L:198:HIS:HE1   | 1.97                     | 0.48              |
| 3:S:123:LYS:NZ   | 3:S:133:ASN:HD21  | 2.10                     | 0.48              |
| 1:E:74:SER:HB3   | 3:M:291:SER:CB    | 2.43                     | 0.48              |
| 1:K:52:SER:O     | 1:K:53:ILE:N      | 2.46                     | 0.48              |
| 3:O:186:SER:HA   | 3:O:218:ALA:O     | 2.12                     | 0.48              |
| 2:F:83:PHE:HA    | 2:F:104:VAL:HG23  | 1.96                     | 0.48              |
| 1:G:73:ILE:H     | 1:G:73:ILE:HD12   | 1.79                     | 0.48              |
| 1:I:123:PRO:HD2  | 2:J:121:SER:HB3   | 1.94                     | 0.48              |
| 3:T:199:ASP:OD1  | 3:T:214:LYS:NZ    | 2.42                     | 0.48              |
| 4:X:158:ASP:OD1  | 4:X:160:PRO:HD2   | 2.13                     | 0.48              |
| 4:X:159:TYR:HB3  | 4:X:160:PRO:HD3   | 1.95                     | 0.48              |
| 2:D:61:ARG:NH1   | 2:D:82:ASP:OD2    | 2.47                     | 0.48              |
| 1:E:38:ARG:HG3   | 1:E:90:TYR:CE1    | 2.48                     | 0.48              |
| 2:L:198:HIS:CG   | 2:L:199:GLN:N     | 2.81                     | 0.48              |
| 3:O:66:ILE:HD12  | 3:O:109:ARG:CZ    | 2.44                     | 0.48              |
| 2:D:30:SER:OG    | 2:D:31:SER:N      | 2.46                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:E:36:TRP:CG      | 1:E:80:MET:HG3    | 2.48                     | 0.48              |
| 1:E:53:ILE:HD13    | 4:P:49:THR:HA     | 1.96                     | 0.48              |
| 3:O:307:LYS:NZ     | 4:P:90:ASP:OD2    | 2.41                     | 0.48              |
| 1:C:40:ALA:HB3     | 1:C:43:GLN:HB2    | 1.95                     | 0.48              |
| 2:D:163:VAL:HG22   | 2:D:175:LEU:HD13  | 1.96                     | 0.48              |
| 1:I:47:TRP:CG      | 2:J:96:LEU:HB2    | 2.49                     | 0.48              |
| 1:I:82(C):LEU:HD12 | 1:I:82(C):LEU:HA  | 1.53                     | 0.48              |
| 1:I:95:LYS:HE3     | 1:I:100(E):TYR:CZ | 2.49                     | 0.48              |
| 4:R:164:GLU:O      | 4:R:168:LEU:HD13  | 2.13                     | 0.48              |
| 1:A:7:SER:HB3      | 1:A:21:SER:OG     | 2.14                     | 0.47              |
| 1:C:6:GLN:NE2      | 1:C:92:CYS:SG     | 2.87                     | 0.47              |
| 2:D:32:SER:C       | 2:D:50:GLY:O      | 2.52                     | 0.47              |
| 1:I:47:TRP:CD2     | 2:J:96:LEU:HB2    | 2.49                     | 0.47              |
| 3:U:100:GLY:HA3    | 3:U:230:MET:O     | 2.14                     | 0.47              |
| 1:C:100(B):PHE:CE1 | 4:X:19:ASP:HA     | 2.49                     | 0.47              |
| 1:K:51:ILE:HD11    | 1:K:71:ALA:HB2    | 1.96                     | 0.47              |
| 3:O:159:ASN:ND2    | 3:T:163:LYS:NZ    | 2.62                     | 0.47              |
| 3:T:288:ILE:HG22   | 3:T:290:THR:HG22  | 1.96                     | 0.47              |
| 1:C:47:TRP:NE1     | 2:D:96:LEU:HD12   | 2.29                     | 0.47              |
| 1:E:143:LYS:HE3    | 1:E:144:ASP:OD1   | 2.14                     | 0.47              |
| 1:K:105:LYS:HE2    | 1:K:105:LYS:H     | 1.80                     | 0.47              |
| 2:L:141:PRO:CG     | 2:L:199:GLN:NE2   | 2.77                     | 0.47              |
| 3:S:44:GLU:HG2     | 3:S:290:THR:HG21  | 1.97                     | 0.47              |
| 4:V:102:LEU:CD2    | 4:X:103:GLU:OE2   | 2.62                     | 0.47              |
| 1:I:100(B):PHE:CE1 | 4:R:19:ASP:HA     | 2.49                     | 0.47              |
| 3:M:307:LYS:HE2    | 4:P:61:THR:HG22   | 1.97                     | 0.47              |
| 3:T:111:GLN:HE22   | 3:T:262:ARG:NH1   | 2.11                     | 0.47              |
| 3:U:48:ASN:O       | 3:U:50:LYS:HG2    | 2.14                     | 0.47              |
| 2:D:8:PRO:HG2      | 2:D:10:THR:O      | 2.14                     | 0.47              |
| 1:G:129:LYS:HE2    | 1:G:129:LYS:HA    | 1.96                     | 0.47              |
| 2:L:136:LEU:N      | 2:L:136:LEU:HD23  | 2.28                     | 0.47              |
| 1:C:59:TYR:HE1     | 1:C:69:ILE:HG13   | 1.80                     | 0.47              |
| 2:D:47:LEU:O       | 2:D:48:ILE:HD13   | 2.15                     | 0.47              |
| 3:S:123:LYS:HZ1    | 3:S:133:ASN:ND2   | 2.12                     | 0.47              |
| 1:A:32:TYR:HB3     | 1:A:100:TYR:CD1   | 2.50                     | 0.47              |
| 1:A:38:ARG:HG3     | 1:A:90:TYR:CE1    | 2.50                     | 0.47              |
| 1:G:159:LEU:HD21   | 1:G:182:VAL:HG11  | 1.96                     | 0.47              |
| 3:M:100:GLY:HA3    | 3:M:230:MET:O     | 2.15                     | 0.47              |
| 3:S:185:PRO:O      | 3:S:217:ILE:HA    | 2.15                     | 0.47              |
| 3:U:262:ARG:HG3    | 3:U:262:ARG:HH11  | 1.78                     | 0.47              |
| 3:U:307:LYS:HE2    | 4:X:61:THR:HG22   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:47:TRP:NE1   | 2:J:96:LEU:HD12  | 2.30                     | 0.47              |
| 3:N:307:LYS:HE2  | 4:Q:61:THR:CG2   | 2.45                     | 0.47              |
| 3:O:195:TYR:CZ   | 3:O:250:ASN:HA   | 2.49                     | 0.47              |
| 3:T:38:HIS:CD2   | 3:T:39:SER:N     | 2.83                     | 0.47              |
| 2:B:175:LEU:HD12 | 2:B:176:SER:H    | 1.79                     | 0.47              |
| 1:C:38:ARG:NH2   | 1:C:86:ASP:OD1   | 2.48                     | 0.47              |
| 3:S:202:VAL:HG11 | 3:S:251:LEU:HD13 | 1.97                     | 0.47              |
| 1:I:144:ASP:OD1  | 1:I:171:GLN:NE2  | 2.43                     | 0.46              |
| 3:O:56:VAL:HB    | 3:O:85:SER:HB3   | 1.98                     | 0.46              |
| 2:L:113:PRO:HB3  | 2:L:139:PHE:HB3  | 1.97                     | 0.46              |
| 3:S:100:GLY:HA3  | 3:S:230:MET:O    | 2.15                     | 0.46              |
| 1:A:61:GLN:HA    | 1:A:64:GLN:HB2   | 1.98                     | 0.46              |
| 3:M:50:LYS:HD2   | 3:M:275:HIS:HB2  | 1.97                     | 0.46              |
| 3:M:58:PRO:HB3   | 3:M:86:TYR:CZ    | 2.51                     | 0.46              |
| 1:C:105:LYS:HE2  | 1:C:105:LYS:H    | 1.80                     | 0.46              |
| 1:G:105:LYS:H    | 1:G:105:LYS:HE2  | 1.80                     | 0.46              |
| 1:K:94:ARG:NE    | 1:K:95:LYS:O     | 2.41                     | 0.46              |
| 4:X:30:GLN:OE1   | 4:X:146:ASN:N    | 2.42                     | 0.46              |
| 2:B:21:LEU:N     | 2:B:21:LEU:HD12  | 2.31                     | 0.46              |
| 1:K:129:LYS:HE2  | 1:K:129:LYS:HA   | 1.96                     | 0.46              |
| 3:M:114:SER:HB2  | 3:M:266:SER:CB   | 2.44                     | 0.46              |
| 3:N:110:GLU:HG3  | 4:R:75:LYS:HE3   | 1.96                     | 0.46              |
| 3:U:58:PRO:HB3   | 3:U:86:TYR:CZ    | 2.50                     | 0.46              |
| 4:V:142:HIS:HB2  | 4:V:165:GLU:CD   | 2.36                     | 0.46              |
| 2:F:30:SER:HB2   | 2:F:92:VAL:CG1   | 2.46                     | 0.46              |
| 2:H:67:SER:HA    | 2:H:71:PHE:CE1   | 2.51                     | 0.46              |
| 3:N:163:LYS:CB   | 3:U:159:ASN:ND2  | 2.78                     | 0.46              |
| 4:P:102:LEU:HD23 | 4:P:102:LEU:HA   | 1.77                     | 0.46              |
| 3:S:107:GLU:O    | 3:S:111:GLN:HG2  | 2.15                     | 0.46              |
| 3:S:123:LYS:NZ   | 3:S:133:ASN:ND2  | 2.64                     | 0.46              |
| 3:T:111:GLN:NE2  | 3:T:262:ARG:NH1  | 2.63                     | 0.46              |
| 1:A:67:VAL:CA    | 1:A:81:ASP:O     | 2.63                     | 0.46              |
| 2:B:89:GLN:HG2   | 2:B:90:GLN:N     | 2.31                     | 0.46              |
| 1:C:154:TRP:CH2  | 1:C:196:CYS:HB3  | 2.50                     | 0.46              |
| 2:J:47:LEU:HD11  | 2:J:86:TYR:HE2   | 1.81                     | 0.46              |
| 2:J:89:GLN:HG2   | 2:J:90:GLN:N     | 2.31                     | 0.46              |
| 2:J:192:TYR:HB2  | 2:J:209:PHE:CE1  | 2.51                     | 0.46              |
| 1:K:84:SER:H     | 1:K:111:VAL:CG1  | 2.29                     | 0.46              |
| 3:U:208:ARG:NH1  | 4:V:72:HIS:CD2   | 2.83                     | 0.46              |
| 2:B:206:THR:O    | 2:B:206:THR:OG1  | 2.26                     | 0.46              |
| 1:G:52:SER:OG    | 1:G:54:PHE:HB3   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:202:VAL:HG11  | 3:M:251:LEU:HD13  | 1.96                     | 0.46              |
| 4:R:158:ASP:OD1   | 4:R:160:PRO:HD2   | 2.16                     | 0.46              |
| 1:C:53:ILE:CD1    | 4:X:49:THR:HA     | 2.46                     | 0.46              |
| 2:F:119:PRO:HB3   | 2:F:209:PHE:CZ    | 2.51                     | 0.46              |
| 1:I:59:TYR:HE1    | 1:I:69:ILE:HG13   | 1.81                     | 0.46              |
| 2:L:21:LEU:HD12   | 2:L:21:LEU:N      | 2.30                     | 0.46              |
| 3:O:107:GLU:O     | 3:O:111:GLN:HG2   | 2.16                     | 0.46              |
| 3:O:303:GLY:HA2   | 4:R:63:PHE:CE2    | 2.50                     | 0.46              |
| 4:W:4:GLY:O       | 4:W:8:GLY:HA3     | 2.15                     | 0.46              |
| 2:D:141:PRO:CG    | 2:D:199:GLN:NE2   | 2.77                     | 0.46              |
| 1:E:47:TRP:CG     | 2:F:96:LEU:HB2    | 2.51                     | 0.46              |
| 2:H:198:HIS:CD2   | 2:H:199:GLN:O     | 2.68                     | 0.46              |
| 3:O:167:SER:OG    | 3:O:244:THR:HG22  | 2.16                     | 0.46              |
| 3:S:284:PRO:HD3   | 3:S:300:ILE:O     | 2.15                     | 0.46              |
| 2:D:136:LEU:N     | 2:D:136:LEU:HD23  | 2.31                     | 0.45              |
| 2:D:150:VAL:HG13  | 2:D:155:GLN:HG2   | 1.98                     | 0.45              |
| 2:H:200:GLY:O     | 2:H:201:LEU:HD23  | 2.16                     | 0.45              |
| 3:S:38:HIS:CD2    | 3:S:39:SER:N      | 2.84                     | 0.45              |
| 1:A:36:TRP:CD2    | 1:A:80:MET:HG3    | 2.52                     | 0.45              |
| 3:N:38:HIS:CD2    | 3:N:39:SER:N      | 2.84                     | 0.45              |
| 1:A:47:TRP:HZ3    | 2:B:95:PRO:HA     | 1.75                     | 0.45              |
| 1:E:96:LEU:HD12   | 1:E:96:LEU:HA     | 1.75                     | 0.45              |
| 1:G:4:LEU:HD11    | 1:G:94:ARG:HG2    | 1.99                     | 0.45              |
| 1:G:87:THR:HG1    | 1:G:110:THR:HA    | 1.81                     | 0.45              |
| 1:G:145:TYR:CD1   | 1:G:145:TYR:O     | 2.70                     | 0.45              |
| 3:U:107:GLU:O     | 3:U:111:GLN:HG2   | 2.17                     | 0.45              |
| 4:V:102:LEU:HD21  | 4:X:103:GLU:OE2   | 2.16                     | 0.45              |
| 2:D:175:LEU:HD12  | 2:D:176:SER:H     | 1.81                     | 0.45              |
| 2:J:136:LEU:N     | 2:J:136:LEU:HD23  | 2.31                     | 0.45              |
| 4:W:9:PHE:O       | 4:W:135:ASN:HA    | 2.16                     | 0.45              |
| 1:G:95:LYS:HE3    | 1:G:100(E):TYR:CZ | 2.51                     | 0.45              |
| 1:I:72:ASP:OD1    | 3:O:291:SER:OG    | 2.30                     | 0.45              |
| 2:J:33:LEU:HD22   | 2:J:71:PHE:CG     | 2.52                     | 0.45              |
| 2:J:203:SER:OG    | 2:J:203:SER:O     | 2.34                     | 0.45              |
| 3:N:69:TRP:HE1    | 3:N:81:THR:HG21   | 1.81                     | 0.45              |
| 4:R:74:GLU:HB3    | 4:R:77:ILE:HD11   | 1.98                     | 0.45              |
| 3:U:134:GLY:HA3   | 3:U:153:TRP:HB3   | 1.98                     | 0.45              |
| 2:F:141:PRO:HG3   | 2:F:199:GLN:NE2   | 2.31                     | 0.45              |
| 2:H:32(A):TYR:HB2 | 2:H:92:VAL:HG12   | 1.99                     | 0.45              |
| 2:J:38:GLN:NE2    | 2:J:87:TYR:HE2    | 2.14                     | 0.45              |
| 2:L:112:ALA:CB    | 2:L:200:GLY:O     | 2.60                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:X:39:LYS:HB2    | 4:X:39:LYS:HE3    | 1.69                     | 0.45              |
| 1:A:5:VAL:HA      | 1:A:105:LYS:NZ    | 2.32                     | 0.45              |
| 1:C:83:SER:O      | 1:C:111:VAL:CB    | 2.64                     | 0.45              |
| 2:J:21:LEU:HD12   | 2:J:21:LEU:N      | 2.32                     | 0.45              |
| 1:C:131:THR:HA    | 1:C:136:ALA:HA    | 1.97                     | 0.45              |
| 2:F:139:PHE:HD2   | 2:F:198:HIS:CE1   | 2.34                     | 0.45              |
| 1:G:83:SER:O      | 1:G:111:VAL:HB    | 2.17                     | 0.45              |
| 2:J:105:GLU:OE1   | 2:J:173:TYR:OH    | 2.27                     | 0.45              |
| 3:O:321:ARG:HD2   | 3:O:323:ILE:HD11  | 1.98                     | 0.45              |
| 2:L:148:TRP:O     | 2:L:154:LEU:HD12  | 2.17                     | 0.45              |
| 3:M:282:GLN:OE1   | 3:M:287:ALA:HB2   | 2.17                     | 0.45              |
| 3:O:45:ASP:C      | 3:O:297:ILE:HD11  | 2.36                     | 0.45              |
| 4:W:158:ASP:OD1   | 4:W:160:PRO:HD2   | 2.17                     | 0.45              |
| 4:X:6:ILE:HD13    | 4:X:6:ILE:HG21    | 1.73                     | 0.45              |
| 2:D:33:LEU:HD12   | 2:D:89:GLN:C      | 2.33                     | 0.45              |
| 2:J:113:PRO:HB3   | 2:J:139:PHE:HB3   | 1.99                     | 0.45              |
| 2:L:32(A):TYR:HB2 | 2:L:92:VAL:CG1    | 2.47                     | 0.45              |
| 3:M:221:PRO:HG3   | 3:O:242:LYS:CB    | 2.32                     | 0.45              |
| 4:V:4:GLY:O       | 4:V:8:GLY:HA3     | 2.17                     | 0.45              |
| 4:V:38:LEU:HA     | 4:V:38:LEU:HD23   | 1.77                     | 0.45              |
| 1:C:96:LEU:CD1    | 1:C:102:VAL:CG2   | 2.95                     | 0.44              |
| 4:V:2:LEU:HD12    | 4:V:2:LEU:HA      | 1.69                     | 0.44              |
| 1:G:66:ARG:HB3    | 1:G:82(A):SER:O   | 2.18                     | 0.44              |
| 2:J:166:GLN:HG3   | 2:J:173:TYR:CZ    | 2.52                     | 0.44              |
| 1:K:66:ARG:HB3    | 1:K:82(A):SER:HB2 | 1.03                     | 0.44              |
| 3:N:137:ALA:HA    | 3:N:145:LYS:HG2   | 1.99                     | 0.44              |
| 4:Q:9:PHE:O       | 4:Q:135:ASN:HA    | 2.18                     | 0.44              |
| 3:U:90(A):PRO:HD2 | 3:U:271:ASP:OD1   | 2.17                     | 0.44              |
| 4:V:3:PHE:CZ      | 4:W:2:LEU:HG      | 2.52                     | 0.44              |
| 1:C:209:LYS:HD2   | 1:C:209:LYS:HA    | 1.86                     | 0.44              |
| 2:D:37:GLN:HB2    | 2:D:47:LEU:HD11   | 1.98                     | 0.44              |
| 1:G:53:ILE:CD1    | 4:V:49:THR:HA     | 2.47                     | 0.44              |
| 1:G:197:ASN:ND2   | 1:G:208:ASP:OD2   | 2.45                     | 0.44              |
| 3:M:314:LEU:HD23  | 3:M:314:LEU:HA    | 1.85                     | 0.44              |
| 3:T:69:TRP:HE1    | 3:T:81:THR:CG2    | 2.31                     | 0.44              |
| 3:T:295:GLN:O     | 3:T:308:TYR:HA    | 2.17                     | 0.44              |
| 4:V:1:GLY:O       | 4:V:2:LEU:C       | 2.56                     | 0.44              |
| 2:B:145:LYS:HE2   | 2:B:147:GLN:NE2   | 2.32                     | 0.44              |
| 1:C:66:ARG:CD     | 1:C:82(B):SER:HB2 | 2.47                     | 0.44              |
| 2:D:47:LEU:HD23   | 2:D:58:ILE:HD12   | 1.98                     | 0.44              |
| 2:D:161:GLU:HA    | 2:D:177:SER:HA    | 1.99                     | 0.44              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:J:33:LEU:HD22    | 2:J:71:PHE:CD2   | 2.52                     | 0.44              |
| 3:U:111:GLN:OE1    | 3:U:262:ARG:NE   | 2.50                     | 0.44              |
| 1:A:53:ILE:HD13    | 4:Q:49:THR:HA    | 1.98                     | 0.44              |
| 1:A:66:ARG:HB3     | 1:A:82(B):SER:OG | 2.18                     | 0.44              |
| 2:D:33:LEU:HD12    | 2:D:33:LEU:HA    | 1.70                     | 0.44              |
| 2:J:163:VAL:HG22   | 2:J:175:LEU:HD13 | 1.99                     | 0.44              |
| 2:J:175:LEU:HD12   | 2:J:176:SER:H    | 1.82                     | 0.44              |
| 1:K:73:ILE:HD12    | 1:K:73:ILE:H     | 1.81                     | 0.44              |
| 3:M:90(A):PRO:HD2  | 3:M:271:ASP:OD1  | 2.18                     | 0.44              |
| 3:O:180:TRP:CE2    | 3:O:233:TYR:HB2  | 2.52                     | 0.44              |
| 3:S:30:LEU:HD23    | 3:S:30:LEU:HA    | 1.61                     | 0.44              |
| 3:T:56:VAL:HB      | 3:T:85:SER:HB3   | 1.99                     | 0.44              |
| 4:X:2:LEU:HD12     | 4:X:2:LEU:HA     | 1.75                     | 0.44              |
| 1:C:32:TYR:HB3     | 1:C:100:TYR:CD1  | 2.53                     | 0.44              |
| 1:C:63:PHE:CD2     | 1:C:66:ARG:HD2   | 2.51                     | 0.44              |
| 1:C:154:TRP:CZ3    | 1:C:196:CYS:HB3  | 2.52                     | 0.44              |
| 2:F:78:LEU:HD23    | 2:F:78:LEU:HA    | 1.73                     | 0.44              |
| 2:F:175:LEU:HD12   | 2:F:176:SER:H    | 1.83                     | 0.44              |
| 2:H:118:PHE:HB2    | 2:H:133:VAL:HB   | 2.00                     | 0.44              |
| 2:L:18:ARG:HG2     | 2:L:76:THR:HA    | 1.99                     | 0.44              |
| 3:O:52:CYS:HB3     | 3:O:277:CYS:O    | 2.16                     | 0.44              |
| 2:B:11:LEU:O       | 2:B:104:VAL:HA   | 2.18                     | 0.44              |
| 2:B:39:LYS:HG2     | 2:B:84:ALA:HB2   | 1.98                     | 0.44              |
| 2:F:21:LEU:N       | 2:F:21:LEU:HD12  | 2.33                     | 0.44              |
| 1:G:36:TRP:CH2     | 1:G:92:CYS:HB3   | 2.52                     | 0.44              |
| 1:G:178:LEU:C      | 1:G:178:LEU:HD12 | 2.38                     | 0.44              |
| 3:M:71:LEU:O       | 3:M:148:TYR:HB3  | 2.18                     | 0.44              |
| 3:S:314:LEU:HD23   | 3:S:314:LEU:HA   | 1.71                     | 0.44              |
| 3:U:45:ASP:O       | 3:U:46:LYS:HD2   | 2.18                     | 0.44              |
| 1:A:51:ILE:HD11    | 1:A:71:ALA:HB2   | 2.00                     | 0.44              |
| 1:A:73:ILE:HD12    | 1:A:73:ILE:H     | 1.82                     | 0.44              |
| 2:B:31:SER:HB2     | 2:B:32:SER:H     | 1.63                     | 0.44              |
| 2:B:33:LEU:HD12    | 2:B:89:GLN:O     | 2.18                     | 0.44              |
| 4:R:102:LEU:HD23   | 4:R:102:LEU:HA   | 1.73                     | 0.44              |
| 3:T:53:LYS:HE3     | 3:T:276:ASP:OD1  | 2.18                     | 0.44              |
| 2:H:175:LEU:HD12   | 2:H:176:SER:N    | 2.32                     | 0.44              |
| 1:I:53:ILE:HD13    | 4:R:49:THR:HA    | 2.00                     | 0.44              |
| 1:I:100(A):TYR:HD2 | 4:R:42:GLN:OE1   | 2.01                     | 0.44              |
| 2:L:202:SER:O      | 2:L:202:SER:OG   | 2.30                     | 0.44              |
| 3:M:107:GLU:O      | 3:M:111:GLN:HG2  | 2.17                     | 0.44              |
| 3:M:138:ALA:HB2    | 3:M:226:GLN:HE21 | 1.82                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:I:16:SER:O     | 1:I:82(C):LEU:HB2  | 2.17                     | 0.43              |
| 1:I:73:ILE:HD12  | 1:I:73:ILE:H       | 1.83                     | 0.43              |
| 2:J:14:SER:O     | 2:J:17:GLU:OE2     | 2.36                     | 0.43              |
| 3:O:15:ILE:HD11  | 4:R:122:VAL:HG21   | 2.00                     | 0.43              |
| 3:O:151:LEU:HB3  | 3:O:252:VAL:HG12   | 1.99                     | 0.43              |
| 1:A:51:ILE:CD1   | 1:A:71:ALA:HB2     | 2.48                     | 0.43              |
| 2:D:191:VAL:O    | 2:D:191:VAL:HG13   | 2.18                     | 0.43              |
| 3:M:163:LYS:HE3  | 3:M:246:GLU:OE2    | 2.18                     | 0.43              |
| 3:N:45:ASP:C     | 3:N:297:ILE:HD11   | 2.39                     | 0.43              |
| 3:O:197:ASN:HB2  | 3:O:200:THR:HG22   | 2.00                     | 0.43              |
| 4:Q:17:MET:SD    | 4:Q:23:GLY:HA3     | 2.58                     | 0.43              |
| 1:A:169:VAL:O    | 1:A:176:TYR:HA     | 2.18                     | 0.43              |
| 2:B:33:LEU:CD2   | 2:B:71:PHE:CD2     | 2.97                     | 0.43              |
| 1:G:41:PRO:O     | 1:G:43:GLN:HG2     | 2.18                     | 0.43              |
| 2:J:37:GLN:HG3   | 2:J:86:TYR:CZ      | 2.54                     | 0.43              |
| 3:M:218:ALA:HB3  | 3:O:203:PHE:CE2    | 2.53                     | 0.43              |
| 3:N:64:CYS:O     | 3:N:92:SER:HB3     | 2.18                     | 0.43              |
| 4:Q:6:ILE:HD13   | 4:Q:6:ILE:HG21     | 1.79                     | 0.43              |
| 4:R:2:LEU:HA     | 4:R:2:LEU:HD12     | 1.58                     | 0.43              |
| 3:S:195:TYR:CZ   | 3:S:250:ASN:HA     | 2.53                     | 0.43              |
| 4:W:128:ASN:ND2  | 4:W:159:TYR:OH     | 2.47                     | 0.43              |
| 4:X:164:GLU:O    | 4:X:168:LEU:HD13   | 2.18                     | 0.43              |
| 4:P:126:LEU:HA   | 4:P:126:LEU:HD23   | 1.70                     | 0.43              |
| 4:X:74:GLU:HB3   | 4:X:77:ILE:HD11    | 2.00                     | 0.43              |
| 1:G:51:ILE:HD11  | 1:G:71:ALA:HB2     | 1.99                     | 0.43              |
| 1:G:130:SER:HA   | 2:H:116:PHE:HD1    | 1.83                     | 0.43              |
| 4:W:2:LEU:HD12   | 4:W:2:LEU:HA       | 1.54                     | 0.43              |
| 2:D:32:SER:O     | 2:D:50:GLY:O       | 2.36                     | 0.43              |
| 2:D:61:ARG:NH1   | 2:D:82:ASP:CG      | 2.72                     | 0.43              |
| 1:K:105:LYS:H    | 1:K:105:LYS:CE     | 2.32                     | 0.43              |
| 1:K:192:GLN:OE1  | 1:K:193:THR:N      | 2.51                     | 0.43              |
| 3:M:176:VAL:HA   | 3:M:258:PHE:O      | 2.18                     | 0.43              |
| 3:O:189:ALA:HA   | 3:U:189:ALA:HB1    | 2.00                     | 0.43              |
| 3:T:208:ARG:HH11 | 4:X:72:HIS:CE1     | 2.37                     | 0.43              |
| 2:B:31:SER:OG    | 2:B:32(A):TYR:CE2  | 2.69                     | 0.43              |
| 1:C:18:VAL:CG2   | 1:C:82(C):LEU:HD21 | 2.44                     | 0.43              |
| 1:E:82(B):SER:CB | 1:E:82(C):LEU:HA   | 2.46                     | 0.43              |
| 1:G:145:TYR:CD1  | 1:G:176:TYR:O      | 2.72                     | 0.43              |
| 4:P:62:GLN:CD    | 4:P:62:GLN:H       | 2.22                     | 0.43              |
| 4:P:102:LEU:HD21 | 4:R:103:GLU:OE2    | 2.18                     | 0.43              |
| 4:P:105:GLU:CG   | 4:R:106:ARG:HH12   | 2.31                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:S:315:ARG:HH11   | 3:S:315:ARG:HD2  | 1.62                     | 0.43              |
| 1:C:84:SER:HA      | 1:C:111:VAL:HB   | 2.00                     | 0.43              |
| 1:E:32:TYR:HB3     | 1:E:100:TYR:CE1  | 2.53                     | 0.43              |
| 1:K:53:ILE:HD13    | 4:W:49:THR:HA    | 2.01                     | 0.43              |
| 3:T:161:TYR:CZ     | 3:T:249:GLY:HA2  | 2.54                     | 0.43              |
| 3:T:315:ARG:HH11   | 3:T:315:ARG:HD2  | 1.60                     | 0.43              |
| 2:J:88:CYS:O       | 2:J:99:GLY:N     | 2.51                     | 0.43              |
| 3:M:53:LYS:HG2     | 3:M:57:ALA:HA    | 2.00                     | 0.43              |
| 3:O:314:LEU:HD23   | 3:O:314:LEU:HA   | 1.76                     | 0.43              |
| 4:P:95:ASN:ND2     | 4:Q:95:ASN:HD21  | 2.17                     | 0.43              |
| 3:U:308:TYR:HD2    | 4:X:89:LEU:HD13  | 1.81                     | 0.43              |
| 4:W:99:LEU:HD12    | 4:W:99:LEU:HA    | 1.78                     | 0.43              |
| 2:B:175:LEU:HD12   | 2:B:176:SER:N    | 2.33                     | 0.43              |
| 1:E:159:LEU:HD21   | 1:E:182:VAL:HG11 | 2.01                     | 0.43              |
| 2:H:201:LEU:HD23   | 2:H:201:LEU:HA   | 1.73                     | 0.43              |
| 3:O:177:LEU:HA     | 3:O:236:LEU:HD23 | 2.01                     | 0.43              |
| 4:Q:68:LYS:HE3     | 4:R:79:ASN:HB2   | 2.00                     | 0.43              |
| 4:R:27:GLN:O       | 4:R:27:GLN:HG3   | 2.18                     | 0.43              |
| 3:U:167:SER:OG     | 3:U:244:THR:HG22 | 2.18                     | 0.43              |
| 1:C:82(C):LEU:HD12 | 1:C:82(C):LEU:HA | 1.55                     | 0.42              |
| 1:G:146:PHE:O      | 1:G:200:HIS:HE1  | 2.02                     | 0.42              |
| 1:G:154:TRP:CZ3    | 1:G:196:CYS:HB3  | 2.53                     | 0.42              |
| 1:I:83:SER:OG      | 1:I:84:SER:N     | 2.51                     | 0.42              |
| 2:B:58:ILE:HD13    | 2:B:58:ILE:HA    | 1.83                     | 0.42              |
| 1:C:89:VAL:HG22    | 1:C:108:THR:HG22 | 2.02                     | 0.42              |
| 2:L:136:LEU:CD2    | 2:L:196:VAL:HG21 | 2.48                     | 0.42              |
| 3:M:123:LYS:HZ2    | 3:M:133:ASN:HD21 | 1.66                     | 0.42              |
| 4:Q:158:ASP:OD1    | 4:Q:160:PRO:HD2  | 2.19                     | 0.42              |
| 2:B:122:ASP:O      | 2:B:125:LEU:N    | 2.51                     | 0.42              |
| 2:B:203:SER:HA     | 2:B:204:PRO:HD3  | 1.53                     | 0.42              |
| 1:E:178:LEU:C      | 1:E:178:LEU:HD12 | 2.39                     | 0.42              |
| 2:F:61:ARG:NH1     | 2:F:82:ASP:OD1   | 2.52                     | 0.42              |
| 2:H:204:PRO:O      | 2:H:205:VAL:C    | 2.55                     | 0.42              |
| 4:Q:103:GLU:OE2    | 4:R:102:LEU:HD21 | 2.19                     | 0.42              |
| 3:U:26:VAL:HG21    | 3:U:317:ALA:HB2  | 2.00                     | 0.42              |
| 4:W:102:LEU:HD23   | 4:W:102:LEU:HA   | 1.60                     | 0.42              |
| 2:D:29:VAL:O       | 2:D:29:VAL:HG13  | 2.18                     | 0.42              |
| 2:F:198:HIS:CD2    | 2:F:200:GLY:H    | 2.37                     | 0.42              |
| 2:H:205:VAL:O      | 2:H:205:VAL:HG12 | 2.18                     | 0.42              |
| 1:I:123:PRO:HD2    | 2:J:121:SER:CB   | 2.49                     | 0.42              |
| 1:I:154:TRP:CZ3    | 1:I:196:CYS:HB3  | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K:52:SER:OG      | 1:K:54:PHE:HB3     | 2.20                     | 0.42              |
| 3:O:30:LEU:HA      | 3:O:30:LEU:HD23    | 1.82                     | 0.42              |
| 4:P:70:PHE:CD2     | 4:P:78:GLU:HA      | 2.53                     | 0.42              |
| 3:S:116(A):SER:O   | 3:S:260:MET:HA     | 2.20                     | 0.42              |
| 3:T:116(B):PHE:HE1 | 3:T:260:MET:HE1    | 1.84                     | 0.42              |
| 3:U:103:ILE:N      | 3:U:103:ILE:HD12   | 2.34                     | 0.42              |
| 1:A:25:SER:O       | 1:A:25:SER:OG      | 2.24                     | 0.42              |
| 1:A:40:ALA:HB3     | 1:A:43:GLN:HB2     | 2.01                     | 0.42              |
| 2:B:29:VAL:HG12    | 2:B:68:GLY:O       | 2.20                     | 0.42              |
| 1:C:143:LYS:HE3    | 1:C:144:ASP:OD1    | 2.20                     | 0.42              |
| 1:E:100(A):TYR:HD2 | 4:P:42:GLN:OE1     | 2.03                     | 0.42              |
| 2:F:54:ARG:HG2     | 2:F:58:ILE:HB      | 2.02                     | 0.42              |
| 2:J:191:VAL:HG13   | 2:J:191:VAL:O      | 2.19                     | 0.42              |
| 1:K:181:VAL:HG11   | 2:L:135:LEU:CD2    | 2.50                     | 0.42              |
| 3:M:177:LEU:HD11   | 3:M:234:TRP:HB2    | 2.01                     | 0.42              |
| 3:O:298:HIS:CE1    | 3:O:300:ILE:HD12   | 2.38                     | 0.42              |
| 4:W:118:LEU:HA     | 4:W:118:LEU:HD12   | 1.75                     | 0.42              |
| 2:B:2:ILE:HG12     | 2:B:27:GLN:HB2     | 2.02                     | 0.42              |
| 1:E:5:VAL:HA       | 1:E:105:LYS:HZ1    | 1.83                     | 0.42              |
| 1:K:127:SER:H      | 1:K:130:SER:HB2    | 1.83                     | 0.42              |
| 2:L:32:SER:HB2     | 2:L:51:ALA:CB      | 2.46                     | 0.42              |
| 2:L:198:HIS:CD2    | 2:L:199:GLN:O      | 2.72                     | 0.42              |
| 3:N:137:ALA:HB2    | 3:N:145:LYS:HE3    | 2.01                     | 0.42              |
| 3:O:103:ILE:N      | 3:O:103:ILE:HD12   | 2.34                     | 0.42              |
| 4:P:168:LEU:HD23   | 4:P:168:LEU:HA     | 1.78                     | 0.42              |
| 3:T:26:VAL:HG21    | 3:T:317:ALA:HB2    | 2.00                     | 0.42              |
| 3:U:8:ASP:N        | 3:U:9:PRO:HD2      | 2.33                     | 0.42              |
| 2:H:32(A):TYR:HB2  | 2:H:92:VAL:CG1     | 2.49                     | 0.42              |
| 1:I:51:ILE:CD1     | 1:I:71:ALA:HB2     | 2.50                     | 0.42              |
| 2:J:206:THR:O      | 2:J:206:THR:OG1    | 2.32                     | 0.42              |
| 3:M:106:GLU:CD     | 4:P:71:ASN:HB3     | 2.39                     | 0.42              |
| 3:U:66:ILE:HD12    | 3:U:109:ARG:HG2    | 2.00                     | 0.42              |
| 1:E:163:VAL:HG22   | 1:E:182:VAL:HG22   | 2.01                     | 0.42              |
| 2:F:203:SER:HA     | 2:F:204:PRO:HD3    | 1.78                     | 0.42              |
| 1:K:51:ILE:HD13    | 1:K:51:ILE:HG21    | 1.68                     | 0.42              |
| 3:M:123:LYS:NZ     | 3:M:133:ASN:HD21   | 2.17                     | 0.42              |
| 4:V:168:LEU:HA     | 4:V:168:LEU:HD23   | 1.80                     | 0.42              |
| 1:A:210:ARG:NH1    | 1:A:212:GLU:HB3    | 2.35                     | 0.42              |
| 2:F:141:PRO:O      | 2:F:198:HIS:HE1    | 2.02                     | 0.42              |
| 2:F:198:HIS:HD2    | 2:F:200:GLY:H      | 1.68                     | 0.42              |
| 1:G:18:VAL:HG23    | 1:G:82(C):LEU:HD22 | 1.99                     | 0.42              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:181:VAL:HG11   | 2:H:135:LEU:HD22 | 2.02                     | 0.42              |
| 2:H:120:PRO:HD3    | 2:H:132:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:82(C):LEU:HD12 | 1:A:82(C):LEU:HA | 1.75                     | 0.42              |
| 1:C:146:PHE:HA     | 1:C:147:PRO:HA   | 1.79                     | 0.42              |
| 1:K:181:VAL:HG11   | 2:L:135:LEU:HD22 | 2.02                     | 0.42              |
| 2:L:163:VAL:HG22   | 2:L:175:LEU:HD13 | 2.02                     | 0.42              |
| 2:L:198:HIS:CD2    | 2:L:199:GLN:H    | 2.37                     | 0.42              |
| 3:U:119:GLU:CD     | 3:U:122:PRO:HA   | 2.39                     | 0.42              |
| 2:B:24:ARG:NH1     | 2:B:70:ASP:OD1   | 2.53                     | 0.41              |
| 1:C:17:SER:HA      | 1:C:82(A):SER:HA | 1.96                     | 0.41              |
| 1:C:51:ILE:HG21    | 1:C:51:ILE:HD13  | 1.71                     | 0.41              |
| 2:H:29:VAL:O       | 2:H:29:VAL:CG1   | 2.68                     | 0.41              |
| 1:K:61:GLN:N       | 1:K:61:GLN:OE1   | 2.52                     | 0.41              |
| 1:K:95:LYS:HE2     | 1:K:97:GLU:O     | 2.19                     | 0.41              |
| 3:O:116(B):PHE:CE1 | 3:O:260:MET:HE2  | 2.54                     | 0.41              |
| 3:S:45:ASP:C       | 3:S:297:ILE:HD11 | 2.40                     | 0.41              |
| 2:B:32(A):TYR:CD1  | 2:B:91:TYR:CE2   | 3.08                     | 0.41              |
| 2:D:29:VAL:CG1     | 2:D:68:GLY:O     | 2.61                     | 0.41              |
| 1:E:61:GLN:OE1     | 1:E:61:GLN:N     | 2.54                     | 0.41              |
| 2:H:32:SER:HB2     | 2:H:51:ALA:CB    | 2.49                     | 0.41              |
| 2:H:123:GLU:HA     | 2:H:126:LYS:HE2  | 2.03                     | 0.41              |
| 2:J:205:VAL:HG12   | 2:J:205:VAL:H    | 1.59                     | 0.41              |
| 4:P:95:ASN:HD21    | 4:R:95:ASN:ND2   | 2.17                     | 0.41              |
| 4:P:99:LEU:HA      | 4:P:99:LEU:HD12  | 1.86                     | 0.41              |
| 3:S:58:PRO:HB3     | 3:S:86:TYR:CZ    | 2.55                     | 0.41              |
| 3:S:152:ILE:HD11   | 3:S:255:ARG:HD2  | 2.02                     | 0.41              |
| 1:E:51:ILE:HG21    | 1:E:51:ILE:HD13  | 1.72                     | 0.41              |
| 1:E:209:LYS:HD2    | 1:E:209:LYS:HA   | 1.77                     | 0.41              |
| 2:F:112:ALA:HB2    | 2:F:200:GLY:HA3  | 2.02                     | 0.41              |
| 1:G:72:ASP:OD1     | 3:S:291:SER:OG   | 2.28                     | 0.41              |
| 2:H:33:LEU:HD22    | 2:H:71:PHE:CG    | 2.55                     | 0.41              |
| 2:H:35:TRP:CZ3     | 2:H:88:CYS:HB3   | 2.55                     | 0.41              |
| 2:H:78:LEU:HD23    | 2:H:78:LEU:HA    | 1.83                     | 0.41              |
| 1:I:129:LYS:HE2    | 1:I:129:LYS:HA   | 2.03                     | 0.41              |
| 1:K:18:VAL:HG12    | 1:K:19:GLN:N     | 2.35                     | 0.41              |
| 3:N:151:LEU:HB3    | 3:N:252:VAL:HG12 | 2.02                     | 0.41              |
| 4:R:170:ARG:HH11   | 4:R:170:ARG:HD2  | 1.72                     | 0.41              |
| 3:S:11:ASP:OD1     | 4:V:28:ASN:HA    | 2.20                     | 0.41              |
| 3:U:8:ASP:N        | 3:U:9:PRO:CD     | 2.84                     | 0.41              |
| 3:U:174:LYS:CA     | 3:U:239:PRO:HG3  | 2.50                     | 0.41              |
| 2:D:119:PRO:HB3    | 2:D:209:PHE:CE2  | 2.55                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:105:LYS:HE2    | 1:E:105:LYS:H    | 1.84                     | 0.41              |
| 3:M:207:SER:OG     | 3:M:241:ASP:OD1  | 2.27                     | 0.41              |
| 3:S:90(A):PRO:HD2  | 3:S:271:ASP:OD1  | 2.19                     | 0.41              |
| 3:U:186:SER:HA     | 3:U:218:ALA:O    | 2.20                     | 0.41              |
| 4:X:102:LEU:HD23   | 4:X:102:LEU:HA   | 1.87                     | 0.41              |
| 2:B:119:PRO:HB3    | 2:B:209:PHE:CZ   | 2.56                     | 0.41              |
| 1:C:148:GLU:HG2    | 1:C:176:TYR:CD2  | 2.55                     | 0.41              |
| 1:K:6:GLN:HG3      | 1:K:106:GLY:N    | 2.33                     | 0.41              |
| 4:P:3:PHE:CZ       | 4:Q:2:LEU:HG     | 2.55                     | 0.41              |
| 4:R:159:TYR:HB3    | 4:R:160:PRO:HD3  | 2.01                     | 0.41              |
| 2:B:79:GLU:HB3     | 2:B:80:PRO:HD2   | 2.02                     | 0.41              |
| 2:B:95:PRO:O       | 2:B:95:PRO:CG    | 2.69                     | 0.41              |
| 2:D:120:PRO:HD3    | 2:D:132:VAL:HG22 | 2.01                     | 0.41              |
| 2:D:201:LEU:HD23   | 2:D:201:LEU:HA   | 1.85                     | 0.41              |
| 1:G:74:SER:CB      | 3:S:291:SER:HB2  | 2.45                     | 0.41              |
| 1:G:144:ASP:OD1    | 1:G:171:GLN:NE2  | 2.52                     | 0.41              |
| 3:O:195:TYR:O      | 3:O:197:ASN:N    | 2.49                     | 0.41              |
| 4:R:38:LEU:HA      | 4:R:38:LEU:HD23  | 1.61                     | 0.41              |
| 3:S:308:TYR:CD2    | 4:V:89:LEU:HD13  | 2.56                     | 0.41              |
| 4:V:1:GLY:O        | 4:V:4:GLY:N      | 2.51                     | 0.41              |
| 1:G:100(A):TYR:OH  | 4:V:19:ASP:O     | 2.32                     | 0.41              |
| 1:K:100(A):TYR:HB3 | 4:W:42:GLN:OE1   | 2.20                     | 0.41              |
| 3:M:15:ILE:N       | 3:M:15:ILE:HD12  | 2.35                     | 0.41              |
| 3:M:180:TRP:CE2    | 3:M:233:TYR:HB2  | 2.56                     | 0.41              |
| 3:N:94:ASN:HD22    | 3:N:94:ASN:HA    | 1.69                     | 0.41              |
| 1:A:53:ILE:CD1     | 4:Q:49:THR:HA    | 2.50                     | 0.41              |
| 2:B:32(A):TYR:CB   | 2:B:92:VAL:HG12  | 2.51                     | 0.41              |
| 2:B:61:ARG:NH1     | 2:B:82:ASP:OD1   | 2.54                     | 0.41              |
| 1:C:38:ARG:NH1     | 1:C:46:GLU:OE2   | 2.48                     | 0.41              |
| 1:C:51:ILE:HD11    | 1:C:71:ALA:HB2   | 2.03                     | 0.41              |
| 1:G:96:LEU:HA      | 1:G:96:LEU:HD12  | 1.84                     | 0.41              |
| 1:K:129:LYS:HZ3    | 2:L:207:LYS:HD3  | 1.85                     | 0.41              |
| 1:K:146:PHE:CE1    | 1:K:147:PRO:HB3  | 2.56                     | 0.41              |
| 3:S:41:ASN:ND2     | 3:S:43:LEU:O     | 2.54                     | 0.41              |
| 3:S:184:HIS:HB3    | 3:S:216:GLU:O    | 2.21                     | 0.41              |
| 3:U:262:ARG:NH1    | 3:U:262:ARG:HG3  | 2.36                     | 0.41              |
| 1:C:36:TRP:CZ2     | 1:C:80:MET:HB2   | 2.55                     | 0.41              |
| 2:D:35:TRP:CZ3     | 2:D:88:CYS:HB3   | 2.55                     | 0.41              |
| 2:D:83:PHE:HA      | 2:D:104:VAL:HG23 | 2.03                     | 0.41              |
| 2:D:131:SER:HA     | 2:D:179:LEU:O    | 2.21                     | 0.41              |
| 1:E:89:VAL:HG22    | 1:E:108:THR:HG22 | 2.03                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:H:11:LEU:O       | 2:H:104:VAL:HA   | 2.20                     | 0.41              |
| 1:I:47:TRP:HB3     | 2:J:96:LEU:O     | 2.21                     | 0.41              |
| 1:K:61:GLN:HA      | 1:K:64:GLN:HB2   | 2.02                     | 0.41              |
| 1:K:96:LEU:HA      | 1:K:96:LEU:HD12  | 1.82                     | 0.41              |
| 2:L:122:ASP:O      | 2:L:125:LEU:N    | 2.54                     | 0.41              |
| 3:M:308:TYR:CD2    | 4:P:89:LEU:HD13  | 2.56                     | 0.41              |
| 3:N:54:LEU:HA      | 3:N:54:LEU:HD12  | 1.82                     | 0.41              |
| 3:O:176:VAL:HA     | 3:O:258:PHE:O    | 2.20                     | 0.41              |
| 4:P:1:GLY:O        | 4:P:2:LEU:C      | 2.57                     | 0.41              |
| 4:P:2:LEU:HD12     | 4:P:2:LEU:HA     | 1.62                     | 0.41              |
| 4:P:74:GLU:HB3     | 4:P:77:ILE:HD11  | 2.03                     | 0.41              |
| 4:R:39:LYS:HE3     | 4:R:39:LYS:HB2   | 1.79                     | 0.41              |
| 3:U:18:HIS:HB2     | 4:X:20:GLY:O     | 2.21                     | 0.41              |
| 4:V:170:ARG:HH11   | 4:V:170:ARG:HD2  | 1.74                     | 0.41              |
| 4:X:170:ARG:HH11   | 4:X:170:ARG:HD2  | 1.72                     | 0.41              |
| 3:N:310:LYS:HD3    | 3:N:310:LYS:HA   | 1.90                     | 0.41              |
| 3:O:262:ARG:HH11   | 3:O:262:ARG:HG3  | 1.85                     | 0.41              |
| 4:P:142:HIS:CE1    | 4:P:162:TYR:CG   | 3.09                     | 0.41              |
| 4:Q:62:GLN:NE2     | 4:R:86:ASP:HB3   | 2.35                     | 0.41              |
| 3:T:303:GLY:HA2    | 4:W:63:PHE:CE2   | 2.56                     | 0.41              |
| 4:V:101:LEU:HD23   | 4:V:101:LEU:HA   | 1.75                     | 0.41              |
| 4:X:99:LEU:HA      | 4:X:99:LEU:HD12  | 1.87                     | 0.41              |
| 1:C:100(A):TYR:HD2 | 4:X:42:GLN:OE1   | 2.04                     | 0.40              |
| 2:D:89:GLN:HG2     | 2:D:90:GLN:N     | 2.35                     | 0.40              |
| 2:H:19:ALA:HB2     | 2:H:78:LEU:HD11  | 2.03                     | 0.40              |
| 1:I:61:GLN:N       | 1:I:61:GLN:OE1   | 2.54                     | 0.40              |
| 1:I:146:PHE:HA     | 1:I:147:PRO:HA   | 1.90                     | 0.40              |
| 3:M:42:LEU:HD11    | 3:M:316:LEU:HD22 | 2.03                     | 0.40              |
| 3:M:321:ARG:HH11   | 3:M:321:ARG:HD2  | 1.75                     | 0.40              |
| 4:P:23:GLY:HA3     | 4:P:36:ALA:HA    | 2.02                     | 0.40              |
| 4:Q:62:GLN:H       | 4:Q:62:GLN:CD    | 2.24                     | 0.40              |
| 3:U:52:CYS:HB3     | 3:U:277:CYS:O    | 2.20                     | 0.40              |
| 4:V:148:CYS:O      | 4:V:151:SER:OG   | 2.29                     | 0.40              |
| 1:C:47:TRP:CD1     | 2:D:96:LEU:HD12  | 2.57                     | 0.40              |
| 1:E:146:PHE:HA     | 1:E:147:PRO:HA   | 1.91                     | 0.40              |
| 1:G:89:VAL:HA      | 1:G:108:THR:HA   | 2.03                     | 0.40              |
| 1:I:38:ARG:NH2     | 1:I:86:ASP:OD1   | 2.55                     | 0.40              |
| 1:I:145:TYR:CE1    | 1:I:150:VAL:HG23 | 2.57                     | 0.40              |
| 2:L:13:LEU:HD23    | 2:L:13:LEU:HA    | 1.75                     | 0.40              |
| 2:L:141:PRO:HG3    | 2:L:199:GLN:HE22 | 1.82                     | 0.40              |
| 3:T:71:LEU:O       | 3:T:148:TYR:HB3  | 2.21                     | 0.40              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:D:21:LEU:HD12    | 2:D:21:LEU:N     | 2.36                     | 0.40              |
| 1:I:12:LYS:HD2     | 1:I:12:LYS:HA    | 1.94                     | 0.40              |
| 2:J:203:SER:HA     | 2:J:204:PRO:HD3  | 1.63                     | 0.40              |
| 1:K:41:PRO:O       | 1:K:43:GLN:HG2   | 2.21                     | 0.40              |
| 4:Q:73:LEU:HD23    | 4:Q:73:LEU:HA    | 1.84                     | 0.40              |
| 4:R:141:TYR:O      | 4:R:166:ALA:HA   | 2.21                     | 0.40              |
| 4:R:157:TYR:CE2    | 4:R:159:TYR:HA   | 2.56                     | 0.40              |
| 4:W:38:LEU:HA      | 4:W:38:LEU:HD23  | 1.82                     | 0.40              |
| 1:E:51:ILE:HD11    | 1:E:71:ALA:HB2   | 2.03                     | 0.40              |
| 2:H:83:PHE:HA      | 2:H:104:VAL:HG23 | 2.04                     | 0.40              |
| 3:N:41:ASN:ND2     | 3:N:43:LEU:O     | 2.53                     | 0.40              |
| 3:S:20:ASN:C       | 3:S:20:ASN:OD1   | 2.60                     | 0.40              |
| 3:T:94:ASN:HD22    | 3:T:94:ASN:HA    | 1.75                     | 0.40              |
| 1:A:42:GLY:O       | 1:A:43:GLN:NE2   | 2.44                     | 0.40              |
| 1:C:105:LYS:H      | 1:C:105:LYS:CE   | 2.35                     | 0.40              |
| 2:D:203:SER:HB3    | 2:D:204:PRO:HD2  | 2.02                     | 0.40              |
| 1:G:82(C):LEU:HD12 | 1:G:82(C):LEU:HA | 1.81                     | 0.40              |
| 2:H:167:ASP:O      | 2:H:171:SER:HA   | 2.22                     | 0.40              |
| 2:J:47:LEU:HD11    | 2:J:86:TYR:CE2   | 2.57                     | 0.40              |
| 2:J:58:ILE:HA      | 2:J:59:PRO:HD2   | 1.89                     | 0.40              |
| 3:S:42:LEU:HA      | 3:S:42:LEU:HD23  | 1.67                     | 0.40              |
| 3:U:54:LEU:HD12    | 3:U:54:LEU:HA    | 1.92                     | 0.40              |

There are no symmetry-related clashes.

## 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     | 223/225 (99%) | 204 (92%) | 16 (7%) | 3 (1%)   | <b>12</b> 48        |
| 1   | C     | 223/225 (99%) | 200 (90%) | 20 (9%) | 3 (1%)   | <b>12</b> 48        |
| 1   | E     | 223/225 (99%) | 207 (93%) | 15 (7%) | 1 (0%)   | <b>34</b> <b>72</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | G     | 223/225 (99%)   | 203 (91%)  | 18 (8%)  | 2 (1%)   | 17          | 56  |
| 1   | I     | 223/225 (99%)   | 205 (92%)  | 17 (8%)  | 1 (0%)   | 34          | 72  |
| 1   | K     | 223/225 (99%)   | 203 (91%)  | 17 (8%)  | 3 (1%)   | 12          | 48  |
| 2   | B     | 211/213 (99%)   | 189 (90%)  | 16 (8%)  | 6 (3%)   | 5           | 32  |
| 2   | D     | 211/213 (99%)   | 191 (90%)  | 17 (8%)  | 3 (1%)   | 11          | 46  |
| 2   | F     | 211/213 (99%)   | 192 (91%)  | 16 (8%)  | 3 (1%)   | 11          | 46  |
| 2   | H     | 211/213 (99%)   | 192 (91%)  | 17 (8%)  | 2 (1%)   | 17          | 56  |
| 2   | J     | 211/213 (99%)   | 190 (90%)  | 15 (7%)  | 6 (3%)   | 5           | 32  |
| 2   | L     | 211/213 (99%)   | 193 (92%)  | 15 (7%)  | 3 (1%)   | 11          | 46  |
| 3   | M     | 322/331 (97%)   | 312 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 3   | N     | 321/331 (97%)   | 312 (97%)  | 8 (2%)   | 1 (0%)   | 41          | 75  |
| 3   | O     | 324/331 (98%)   | 312 (96%)  | 10 (3%)  | 2 (1%)   | 25          | 64  |
| 3   | S     | 322/331 (97%)   | 312 (97%)  | 9 (3%)   | 1 (0%)   | 41          | 75  |
| 3   | T     | 321/331 (97%)   | 312 (97%)  | 8 (2%)   | 1 (0%)   | 41          | 75  |
| 3   | U     | 324/331 (98%)   | 312 (96%)  | 10 (3%)  | 2 (1%)   | 25          | 64  |
| 4   | P     | 173/177 (98%)   | 169 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 4   | Q     | 169/177 (96%)   | 167 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 4   | R     | 169/177 (96%)   | 167 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 4   | V     | 173/177 (98%)   | 169 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 4   | W     | 169/177 (96%)   | 166 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 4   | X     | 169/177 (96%)   | 167 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| All | All   | 5560/5676 (98%) | 5246 (94%) | 271 (5%) | 43 (1%)  | 19          | 58  |

All (43) Ramachandran outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 82(B) | SER  |
| 2   | B     | 30    | SER  |
| 2   | B     | 94    | THR  |
| 1   | C     | 28    | THR  |
| 1   | G     | 149   | PRO  |
| 2   | J     | 30    | SER  |
| 1   | K     | 82(A) | SER  |
| 1   | A     | 27    | GLY  |
| 2   | D     | 31    | SER  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 2   | F     | 204   | PRO  |
| 2   | H     | 204   | PRO  |
| 2   | J     | 28    | SER  |
| 2   | B     | 204   | PRO  |
| 1   | C     | 82(C) | LEU  |
| 2   | J     | 31    | SER  |
| 1   | K     | 84    | SER  |
| 2   | B     | 201   | LEU  |
| 2   | B     | 203   | SER  |
| 2   | J     | 203   | SER  |
| 2   | L     | 203   | SER  |
| 2   | F     | 28    | SER  |
| 2   | L     | 201   | LEU  |
| 3   | O     | 264   | ALA  |
| 3   | U     | 264   | ALA  |
| 3   | N     | 264   | ALA  |
| 3   | O     | 9     | PRO  |
| 3   | S     | 264   | ALA  |
| 3   | T     | 264   | ALA  |
| 3   | U     | 9     | PRO  |
| 2   | D     | 204   | PRO  |
| 1   | E     | 52(A) | PRO  |
| 1   | G     | 52(A) | PRO  |
| 2   | J     | 204   | PRO  |
| 1   | A     | 52(A) | PRO  |
| 2   | B     | 2     | ILE  |
| 1   | C     | 52(A) | PRO  |
| 2   | D     | 2     | ILE  |
| 2   | F     | 2     | ILE  |
| 2   | H     | 2     | ILE  |
| 2   | J     | 2     | ILE  |
| 1   | K     | 52(A) | PRO  |
| 2   | L     | 2     | ILE  |
| 1   | I     | 52(A) | PRO  |

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

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 189/189 (100%)  | 175 (93%)  | 14 (7%)  | 13          | 44  |
| 1   | C     | 189/189 (100%)  | 177 (94%)  | 12 (6%)  | 18          | 51  |
| 1   | E     | 189/189 (100%)  | 180 (95%)  | 9 (5%)   | 25          | 60  |
| 1   | G     | 189/189 (100%)  | 176 (93%)  | 13 (7%)  | 15          | 47  |
| 1   | I     | 189/189 (100%)  | 179 (95%)  | 10 (5%)  | 22          | 55  |
| 1   | K     | 189/189 (100%)  | 178 (94%)  | 11 (6%)  | 20          | 53  |
| 2   | B     | 184/184 (100%)  | 176 (96%)  | 8 (4%)   | 29          | 62  |
| 2   | D     | 184/184 (100%)  | 175 (95%)  | 9 (5%)   | 25          | 59  |
| 2   | F     | 184/184 (100%)  | 174 (95%)  | 10 (5%)  | 22          | 55  |
| 2   | H     | 184/184 (100%)  | 173 (94%)  | 11 (6%)  | 19          | 52  |
| 2   | J     | 184/184 (100%)  | 175 (95%)  | 9 (5%)   | 25          | 59  |
| 2   | L     | 184/184 (100%)  | 171 (93%)  | 13 (7%)  | 14          | 46  |
| 3   | M     | 284/290 (98%)   | 278 (98%)  | 6 (2%)   | 53          | 79  |
| 3   | N     | 283/290 (98%)   | 279 (99%)  | 4 (1%)   | 67          | 85  |
| 3   | O     | 286/290 (99%)   | 283 (99%)  | 3 (1%)   | 76          | 88  |
| 3   | S     | 284/290 (98%)   | 279 (98%)  | 5 (2%)   | 59          | 81  |
| 3   | T     | 283/290 (98%)   | 280 (99%)  | 3 (1%)   | 73          | 88  |
| 3   | U     | 286/290 (99%)   | 283 (99%)  | 3 (1%)   | 76          | 88  |
| 4   | P     | 150/151 (99%)   | 150 (100%) | 0        | 100         | 100 |
| 4   | Q     | 146/151 (97%)   | 145 (99%)  | 1 (1%)   | 84          | 93  |
| 4   | R     | 146/151 (97%)   | 146 (100%) | 0        | 100         | 100 |
| 4   | V     | 150/151 (99%)   | 150 (100%) | 0        | 100         | 100 |
| 4   | W     | 146/151 (97%)   | 145 (99%)  | 1 (1%)   | 84          | 93  |
| 4   | X     | 146/151 (97%)   | 146 (100%) | 0        | 100         | 100 |
| All | All   | 4828/4884 (99%) | 4673 (97%) | 155 (3%) | 39          | 69  |

All (155) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | VAL  |
| 1   | A     | 25  | SER  |
| 1   | A     | 28  | THR  |
| 1   | A     | 38  | ARG  |
| 1   | A     | 66  | ARG  |
| 1   | A     | 81  | ASP  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 82         | LEU         |
| 1          | A            | 82(A)      | SER         |
| 1          | A            | 82(C)      | LEU         |
| 1          | A            | 83         | SER         |
| 1          | A            | 100        | TYR         |
| 1          | A            | 100(F)     | MET         |
| 1          | A            | 105        | LYS         |
| 1          | A            | 208        | ASP         |
| 2          | B            | 22         | SER         |
| 2          | B            | 28         | SER         |
| 2          | B            | 122        | ASP         |
| 2          | B            | 143        | GLU         |
| 2          | B            | 150        | VAL         |
| 2          | B            | 199        | GLN         |
| 2          | B            | 203        | SER         |
| 2          | B            | 204        | PRO         |
| 1          | C            | 11         | VAL         |
| 1          | C            | 38         | ARG         |
| 1          | C            | 82         | LEU         |
| 1          | C            | 82(A)      | SER         |
| 1          | C            | 82(B)      | SER         |
| 1          | C            | 82(C)      | LEU         |
| 1          | C            | 96         | LEU         |
| 1          | C            | 97         | GLU         |
| 1          | C            | 100        | TYR         |
| 1          | C            | 100(F)     | MET         |
| 1          | C            | 105        | LYS         |
| 1          | C            | 208        | ASP         |
| 2          | D            | 22         | SER         |
| 2          | D            | 32         | SER         |
| 2          | D            | 61         | ARG         |
| 2          | D            | 122        | ASP         |
| 2          | D            | 125        | LEU         |
| 2          | D            | 143        | GLU         |
| 2          | D            | 150        | VAL         |
| 2          | D            | 202        | SER         |
| 2          | D            | 205        | VAL         |
| 1          | E            | 11         | VAL         |
| 1          | E            | 38         | ARG         |
| 1          | E            | 66         | ARG         |
| 1          | E            | 81         | ASP         |
| 1          | E            | 82(B)      | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | E            | 100        | TYR         |
| 1          | E            | 100(F)     | MET         |
| 1          | E            | 105        | LYS         |
| 1          | E            | 208        | ASP         |
| 2          | F            | 22         | SER         |
| 2          | F            | 28         | SER         |
| 2          | F            | 29         | VAL         |
| 2          | F            | 122        | ASP         |
| 2          | F            | 125        | LEU         |
| 2          | F            | 143        | GLU         |
| 2          | F            | 150        | VAL         |
| 2          | F            | 202        | SER         |
| 2          | F            | 205        | VAL         |
| 2          | F            | 206        | THR         |
| 1          | G            | 11         | VAL         |
| 1          | G            | 38         | ARG         |
| 1          | G            | 66         | ARG         |
| 1          | G            | 82(A)      | SER         |
| 1          | G            | 82(C)      | LEU         |
| 1          | G            | 83         | SER         |
| 1          | G            | 84         | SER         |
| 1          | G            | 100        | TYR         |
| 1          | G            | 100(F)     | MET         |
| 1          | G            | 105        | LYS         |
| 1          | G            | 145        | TYR         |
| 1          | G            | 148        | GLU         |
| 1          | G            | 208        | ASP         |
| 2          | H            | 22         | SER         |
| 2          | H            | 28         | SER         |
| 2          | H            | 29         | VAL         |
| 2          | H            | 30         | SER         |
| 2          | H            | 122        | ASP         |
| 2          | H            | 125        | LEU         |
| 2          | H            | 143        | GLU         |
| 2          | H            | 150        | VAL         |
| 2          | H            | 199        | GLN         |
| 2          | H            | 205        | VAL         |
| 2          | H            | 206        | THR         |
| 1          | I            | 38         | ARG         |
| 1          | I            | 66         | ARG         |
| 1          | I            | 81         | ASP         |
| 1          | I            | 82(A)      | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | I            | 82(B)      | SER         |
| 1          | I            | 83         | SER         |
| 1          | I            | 100        | TYR         |
| 1          | I            | 100(F)     | MET         |
| 1          | I            | 105        | LYS         |
| 1          | I            | 208        | ASP         |
| 2          | J            | 22         | SER         |
| 2          | J            | 28         | SER         |
| 2          | J            | 29         | VAL         |
| 2          | J            | 30         | SER         |
| 2          | J            | 122        | ASP         |
| 2          | J            | 125        | LEU         |
| 2          | J            | 143        | GLU         |
| 2          | J            | 150        | VAL         |
| 2          | J            | 199        | GLN         |
| 1          | K            | 11         | VAL         |
| 1          | K            | 28         | THR         |
| 1          | K            | 38         | ARG         |
| 1          | K            | 66         | ARG         |
| 1          | K            | 82         | LEU         |
| 1          | K            | 82(B)      | SER         |
| 1          | K            | 84         | SER         |
| 1          | K            | 100        | TYR         |
| 1          | K            | 100(F)     | MET         |
| 1          | K            | 105        | LYS         |
| 1          | K            | 208        | ASP         |
| 2          | L            | 22         | SER         |
| 2          | L            | 26         | SER         |
| 2          | L            | 27         | GLN         |
| 2          | L            | 28         | SER         |
| 2          | L            | 29         | VAL         |
| 2          | L            | 30         | SER         |
| 2          | L            | 61         | ARG         |
| 2          | L            | 122        | ASP         |
| 2          | L            | 143        | GLU         |
| 2          | L            | 150        | VAL         |
| 2          | L            | 199        | GLN         |
| 2          | L            | 205        | VAL         |
| 2          | L            | 206        | THR         |
| 3          | M            | 63         | LYS         |
| 3          | M            | 208        | ARG         |
| 3          | M            | 266        | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 3          | M            | 277        | CYS         |
| 3          | M            | 283        | THR         |
| 3          | M            | 320        | LEU         |
| 3          | N            | 266        | SER         |
| 3          | N            | 283        | THR         |
| 3          | N            | 291        | SER         |
| 3          | N            | 310        | LYS         |
| 3          | O            | 63         | LYS         |
| 3          | O            | 266        | SER         |
| 3          | O            | 283        | THR         |
| 4          | Q            | 168        | LEU         |
| 3          | S            | 63         | LYS         |
| 3          | S            | 208        | ARG         |
| 3          | S            | 266        | SER         |
| 3          | S            | 283        | THR         |
| 3          | S            | 320        | LEU         |
| 3          | T            | 266        | SER         |
| 3          | T            | 283        | THR         |
| 3          | T            | 291        | SER         |
| 3          | U            | 63         | LYS         |
| 3          | U            | 266        | SER         |
| 3          | U            | 283        | THR         |
| 4          | W            | 168        | LEU         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 6          | GLN         |
| 2          | B            | 38         | GLN         |
| 2          | B            | 198        | HIS         |
| 2          | B            | 199        | GLN         |
| 2          | D            | 38         | GLN         |
| 2          | D            | 198        | HIS         |
| 2          | D            | 199        | GLN         |
| 1          | E            | 39         | GLN         |
| 1          | E            | 199        | ASN         |
| 2          | F            | 38         | GLN         |
| 2          | F            | 198        | HIS         |
| 2          | H            | 198        | HIS         |
| 1          | I            | 39         | GLN         |
| 2          | J            | 38         | GLN         |
| 2          | J            | 199        | GLN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 6   | GLN  |
| 2   | L     | 198 | HIS  |
| 2   | L     | 199 | GLN  |
| 3   | M     | 94  | ASN  |
| 3   | M     | 133 | ASN  |
| 3   | M     | 226 | GLN  |
| 3   | N     | 94  | ASN  |
| 3   | N     | 111 | GLN  |
| 3   | O     | 38  | HIS  |
| 3   | O     | 94  | ASN  |
| 3   | O     | 159 | ASN  |
| 3   | O     | 226 | GLN  |
| 4   | P     | 43  | ASN  |
| 4   | P     | 95  | ASN  |
| 4   | Q     | 53  | ASN  |
| 4   | Q     | 95  | ASN  |
| 4   | Q     | 154 | ASN  |
| 4   | R     | 25  | HIS  |
| 4   | R     | 79  | ASN  |
| 3   | S     | 94  | ASN  |
| 3   | S     | 133 | ASN  |
| 3   | T     | 111 | GLN  |
| 3   | T     | 226 | GLN  |
| 3   | U     | 94  | ASN  |
| 3   | U     | 159 | ASN  |
| 3   | U     | 226 | GLN  |
| 3   | U     | 275 | HIS  |
| 4   | V     | 43  | ASN  |
| 4   | V     | 53  | ASN  |
| 4   | V     | 95  | ASN  |
| 4   | W     | 25  | HIS  |
| 4   | W     | 95  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 225/225 (100%) | 0.56   | 14 (6%) 20 18 | 51, 74, 96, 116       | 0     |
| 1   | C     | 225/225 (100%) | 0.53   | 11 (4%) 29 26 | 59, 78, 95, 114       | 0     |
| 1   | E     | 225/225 (100%) | 0.54   | 10 (4%) 34 30 | 55, 79, 99, 111       | 0     |
| 1   | G     | 225/225 (100%) | 0.64   | 12 (5%) 26 24 | 54, 81, 105, 124      | 0     |
| 1   | I     | 225/225 (100%) | 0.92   | 34 (15%) 2 3  | 59, 91, 116, 128      | 0     |
| 1   | K     | 225/225 (100%) | 0.55   | 13 (5%) 23 20 | 51, 72, 98, 114       | 0     |
| 2   | B     | 213/213 (100%) | 0.23   | 1 (0%) 91 88  | 53, 61, 76, 85        | 0     |
| 2   | D     | 213/213 (100%) | 0.38   | 1 (0%) 91 88  | 62, 71, 83, 94        | 0     |
| 2   | F     | 213/213 (100%) | 0.30   | 0 100 100     | 58, 68, 83, 92        | 0     |
| 2   | H     | 213/213 (100%) | 0.29   | 3 (1%) 75 69  | 54, 68, 86, 98        | 0     |
| 2   | J     | 213/213 (100%) | 0.33   | 4 (1%) 66 61  | 55, 71, 89, 106       | 0     |
| 2   | L     | 213/213 (100%) | 0.17   | 1 (0%) 91 88  | 51, 61, 76, 88        | 0     |
| 3   | M     | 324/331 (97%)  | 2.28   | 146 (45%) 0 0 | 55, 175, 212, 218     | 0     |
| 3   | N     | 323/331 (97%)  | 2.01   | 137 (42%) 0 0 | 50, 168, 205, 211     | 0     |
| 3   | O     | 326/331 (98%)  | 2.48   | 165 (50%) 0 0 | 54, 196, 228, 232     | 0     |
| 3   | S     | 324/331 (97%)  | 1.69   | 114 (35%) 0 0 | 55, 153, 182, 186     | 0     |
| 3   | T     | 323/331 (97%)  | 1.72   | 114 (35%) 0 0 | 52, 157, 192, 196     | 0     |
| 3   | U     | 326/331 (98%)  | 1.73   | 116 (35%) 0 0 | 55, 159, 190, 197     | 0     |
| 4   | P     | 175/177 (98%)  | 0.62   | 11 (6%) 20 18 | 51, 73, 141, 170      | 0     |
| 4   | Q     | 171/177 (96%)  | 0.53   | 10 (5%) 23 20 | 50, 72, 133, 157      | 0     |
| 4   | R     | 171/177 (96%)  | 0.51   | 8 (4%) 31 28  | 51, 74, 134, 156      | 0     |
| 4   | V     | 175/177 (98%)  | 0.57   | 10 (5%) 23 21 | 52, 77, 128, 147      | 0     |
| 4   | W     | 171/177 (96%)  | 0.57   | 13 (7%) 13 14 | 51, 72, 113, 141      | 0     |
| 4   | X     | 171/177 (96%)  | 0.52   | 10 (5%) 23 20 | 53, 77, 116, 142      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------|-----------------------|-------|
| All | All   | 5608/5676 (98%) | 1.01   | 958 (17%) <b>1</b> <b>1</b> | 50, 80, 199, 232      | 0     |

All (958) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | O     | 165 | SER  | 13.2 |
| 3   | O     | 164 | LEU  | 11.8 |
| 3   | N     | 198 | ALA  | 11.7 |
| 3   | O     | 250 | ASN  | 10.9 |
| 3   | M     | 127 | TRP  | 9.4  |
| 3   | O     | 138 | ALA  | 9.4  |
| 3   | O     | 154 | LEU  | 9.2  |
| 3   | M     | 187 | THR  | 9.1  |
| 3   | M     | 250 | ASN  | 8.9  |
| 1   | A     | 215 | SER  | 8.7  |
| 3   | M     | 76  | CYS  | 8.6  |
| 3   | M     | 224 | ARG  | 8.6  |
| 3   | N     | 186 | SER  | 8.5  |
| 3   | N     | 138 | ALA  | 8.5  |
| 3   | N     | 127 | TRP  | 8.4  |
| 3   | M     | 225 | ASP  | 8.2  |
| 3   | M     | 195 | TYR  | 8.1  |
| 3   | M     | 74  | PRO  | 8.1  |
| 3   | S     | 183 | HIS  | 8.0  |
| 3   | M     | 154 | LEU  | 7.8  |
| 3   | O     | 123 | LYS  | 7.8  |
| 3   | O     | 8   | ASP  | 7.7  |
| 3   | S     | 154 | LEU  | 7.7  |
| 3   | O     | 246 | GLU  | 7.6  |
| 3   | M     | 260 | MET  | 7.6  |
| 3   | M     | 142 | ALA  | 7.6  |
| 3   | O     | 247 | ALA  | 7.6  |
| 3   | N     | 167 | SER  | 7.4  |
| 3   | O     | 243 | ILE  | 7.3  |
| 1   | G     | 215 | SER  | 7.3  |
| 3   | N     | 199 | ASP  | 7.3  |
| 3   | O     | 205 | GLY  | 7.2  |
| 3   | T     | 173 | GLY  | 7.2  |
| 3   | M     | 55  | ARG  | 7.0  |
| 3   | T     | 154 | LEU  | 6.9  |
| 3   | O     | 155 | VAL  | 6.9  |
| 3   | M     | 172 | LYS  | 6.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | O            | 163        | LYS         | 6.8         |
| 3          | M            | 155        | VAL         | 6.8         |
| 3          | U            | 81         | THR         | 6.8         |
| 3          | M            | 123        | LYS         | 6.7         |
| 1          | I            | 131        | THR         | 6.7         |
| 1          | I            | 215        | SER         | 6.7         |
| 3          | M            | 217        | ILE         | 6.7         |
| 3          | O            | 127        | TRP         | 6.7         |
| 3          | O            | 133(A)     | LYS         | 6.7         |
| 3          | N            | 77         | GLU         | 6.6         |
| 3          | T            | 132        | SER         | 6.6         |
| 3          | S            | 134        | GLY         | 6.6         |
| 3          | T            | 224        | ARG         | 6.5         |
| 3          | O            | 141        | HIS         | 6.5         |
| 3          | O            | 199        | ASP         | 6.5         |
| 3          | O            | 101        | ASP         | 6.4         |
| 3          | N            | 224        | ARG         | 6.4         |
| 3          | T            | 250        | ASN         | 6.4         |
| 3          | O            | 76         | CYS         | 6.3         |
| 3          | O            | 159        | ASN         | 6.3         |
| 3          | S            | 138        | ALA         | 6.3         |
| 3          | O            | 213        | PHE         | 6.2         |
| 3          | O            | 132        | SER         | 6.2         |
| 3          | M            | 143        | GLY         | 6.2         |
| 3          | U            | 154        | LEU         | 6.2         |
| 3          | M            | 229        | ARG         | 6.2         |
| 3          | U            | 138        | ALA         | 6.2         |
| 3          | O            | 74         | PRO         | 6.1         |
| 3          | O            | 79         | LEU         | 6.1         |
| 3          | N            | 216        | GLU         | 6.1         |
| 3          | O            | 148        | TYR         | 6.1         |
| 3          | U            | 163        | LYS         | 6.1         |
| 3          | U            | 76         | CYS         | 6.1         |
| 3          | N            | 154        | LEU         | 6.0         |
| 3          | S            | 155        | VAL         | 6.0         |
| 4          | P            | 175        | SER         | 6.0         |
| 3          | U            | 134        | GLY         | 6.0         |
| 3          | N            | 116(C)     | GLU         | 6.0         |
| 3          | S            | 153        | TRP         | 5.9         |
| 3          | U            | 153        | TRP         | 5.9         |
| 3          | N            | 76         | CYS         | 5.9         |
| 3          | T            | 198        | ALA         | 5.9         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | N            | 155        | VAL         | 5.8         |
| 3          | O            | 173        | GLY         | 5.8         |
| 3          | M            | 134        | GLY         | 5.8         |
| 3          | O            | 77         | GLU         | 5.8         |
| 3          | O            | 216        | GLU         | 5.8         |
| 3          | T            | 155        | VAL         | 5.8         |
| 3          | O            | 187        | THR         | 5.8         |
| 3          | T            | 160        | SER         | 5.8         |
| 4          | P            | 174        | ASP         | 5.8         |
| 3          | N            | 187        | THR         | 5.7         |
| 3          | M            | 213        | PHE         | 5.7         |
| 3          | T            | 123        | LYS         | 5.7         |
| 3          | T            | 142        | ALA         | 5.7         |
| 3          | M            | 186        | SER         | 5.7         |
| 3          | M            | 230        | MET         | 5.7         |
| 3          | M            | 197        | ASN         | 5.7         |
| 3          | O            | 116(C)     | GLU         | 5.7         |
| 3          | N            | 250        | ASN         | 5.7         |
| 3          | U            | 139        | CYS         | 5.6         |
| 3          | M            | 80         | SER         | 5.6         |
| 3          | N            | 223        | VAL         | 5.6         |
| 3          | O            | 153        | TRP         | 5.6         |
| 3          | O            | 139        | CYS         | 5.6         |
| 3          | S            | 172        | LYS         | 5.6         |
| 3          | M            | 147        | PHE         | 5.5         |
| 3          | M            | 93         | ASP         | 5.5         |
| 3          | U            | 142        | ALA         | 5.5         |
| 3          | O            | 195        | TYR         | 5.5         |
| 3          | U            | 250        | ASN         | 5.5         |
| 3          | M            | 138        | ALA         | 5.5         |
| 3          | M            | 135        | VAL         | 5.4         |
| 3          | M            | 161        | TYR         | 5.4         |
| 3          | T            | 153        | TRP         | 5.4         |
| 1          | K            | 215        | SER         | 5.4         |
| 3          | T            | 195        | TYR         | 5.4         |
| 3          | O            | 245        | PHE         | 5.4         |
| 3          | S            | 64         | CYS         | 5.3         |
| 3          | M            | 150        | ASN         | 5.3         |
| 3          | N            | 96         | THR         | 5.3         |
| 3          | S            | 116(C)     | GLU         | 5.3         |
| 3          | O            | 241        | ASP         | 5.3         |
| 3          | M            | 144        | ALA         | 5.2         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | O            | 93         | ASP         | 5.1         |
| 3          | M            | 75         | GLU         | 5.1         |
| 3          | M            | 97         | CYS         | 5.1         |
| 3          | N            | 159        | ASN         | 5.1         |
| 3          | U            | 61         | LEU         | 5.0         |
| 3          | U            | 63         | LYS         | 5.0         |
| 3          | M            | 215        | PRO         | 5.0         |
| 3          | O            | 203        | PHE         | 5.0         |
| 3          | M            | 82         | ALA         | 5.0         |
| 3          | M            | 153        | TRP         | 4.9         |
| 3          | M            | 163        | LYS         | 4.9         |
| 3          | N            | 132        | SER         | 4.9         |
| 3          | M            | 139        | CYS         | 4.9         |
| 3          | M            | 200        | THR         | 4.9         |
| 3          | O            | 88         | VAL         | 4.9         |
| 3          | N            | 141        | HIS         | 4.9         |
| 3          | O            | 251        | LEU         | 4.9         |
| 3          | N            | 126        | SER         | 4.9         |
| 3          | T            | 161        | TYR         | 4.9         |
| 3          | U            | 116(C)     | GLU         | 4.9         |
| 3          | T            | 196        | GLN         | 4.8         |
| 3          | M            | 133(A)     | LYS         | 4.8         |
| 1          | K            | 130        | SER         | 4.8         |
| 3          | U            | 8          | ASP         | 4.8         |
| 3          | U            | 160        | SER         | 4.8         |
| 3          | O            | 194        | LEU         | 4.8         |
| 3          | N            | 251        | LEU         | 4.8         |
| 3          | O            | 181        | GLY         | 4.8         |
| 3          | T            | 127        | TRP         | 4.8         |
| 3          | S            | 127        | TRP         | 4.7         |
| 3          | M            | 51         | LEU         | 4.7         |
| 3          | M            | 116(B)     | PHE         | 4.7         |
| 3          | S            | 152        | ILE         | 4.7         |
| 3          | O            | 9          | PRO         | 4.7         |
| 3          | T            | 97         | CYS         | 4.7         |
| 3          | T            | 228        | GLY         | 4.7         |
| 3          | U            | 223        | VAL         | 4.7         |
| 3          | M            | 183        | HIS         | 4.7         |
| 3          | N            | 246        | GLU         | 4.7         |
| 3          | T            | 78         | SER         | 4.7         |
| 3          | M            | 121        | PHE         | 4.7         |
| 3          | U            | 216        | GLU         | 4.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | M            | 228        | GLY         | 4.7         |
| 3          | N            | 158        | GLY         | 4.7         |
| 3          | O            | 62         | GLY         | 4.7         |
| 3          | O            | 73         | ASN         | 4.7         |
| 3          | M            | 132        | SER         | 4.6         |
| 3          | S            | 230        | MET         | 4.6         |
| 3          | O            | 229        | ARG         | 4.6         |
| 3          | O            | 116(B)     | PHE         | 4.6         |
| 3          | M            | 220        | ARG         | 4.6         |
| 4          | P            | 173        | ILE         | 4.6         |
| 3          | O            | 214        | LYS         | 4.6         |
| 3          | N            | 173        | GLY         | 4.6         |
| 3          | T            | 129        | ASN         | 4.6         |
| 3          | T            | 122        | PRO         | 4.6         |
| 3          | T            | 141        | HIS         | 4.6         |
| 3          | N            | 153        | TRP         | 4.6         |
| 3          | S            | 197        | ASN         | 4.6         |
| 3          | U            | 217        | ILE         | 4.6         |
| 3          | O            | 172        | LYS         | 4.5         |
| 3          | O            | 201        | TYR         | 4.5         |
| 3          | U            | 260        | MET         | 4.5         |
| 3          | N            | 194        | LEU         | 4.5         |
| 3          | N            | 260        | MET         | 4.5         |
| 3          | U            | 127        | TRP         | 4.5         |
| 3          | O            | 61         | LEU         | 4.5         |
| 3          | T            | 229        | ARG         | 4.4         |
| 3          | O            | 80         | SER         | 4.4         |
| 3          | O            | 249        | GLY         | 4.4         |
| 3          | O            | 204        | VAL         | 4.4         |
| 3          | N            | 197        | ASN         | 4.4         |
| 3          | M            | 141        | HIS         | 4.4         |
| 3          | O            | 166        | LYS         | 4.4         |
| 3          | M            | 287        | ALA         | 4.4         |
| 3          | O            | 90(A)      | PRO         | 4.4         |
| 1          | G            | 130        | SER         | 4.4         |
| 3          | O            | 152        | ILE         | 4.4         |
| 1          | G            | 131        | THR         | 4.4         |
| 3          | T            | 172        | LYS         | 4.3         |
| 3          | M            | 140        | PRO         | 4.3         |
| 3          | T            | 126        | SER         | 4.3         |
| 3          | U            | 55(A)      | GLY         | 4.3         |
| 3          | S            | 79         | LEU         | 4.3         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | T            | 121        | PHE         | 4.3         |
| 3          | O            | 131        | ASP         | 4.3         |
| 3          | N            | 160        | SER         | 4.3         |
| 3          | O            | 134        | GLY         | 4.3         |
| 3          | T            | 138        | ALA         | 4.3         |
| 3          | N            | 163        | LYS         | 4.3         |
| 3          | T            | 185        | PRO         | 4.3         |
| 3          | U            | 230        | MET         | 4.3         |
| 3          | S            | 156        | LYS         | 4.3         |
| 3          | U            | 161        | TYR         | 4.3         |
| 3          | N            | 245        | PHE         | 4.2         |
| 4          | V            | 174        | ASP         | 4.2         |
| 3          | T            | 77         | GLU         | 4.2         |
| 3          | O            | 51         | LEU         | 4.2         |
| 3          | O            | 81         | THR         | 4.2         |
| 3          | O            | 215        | PRO         | 4.2         |
| 3          | M            | 162        | PRO         | 4.2         |
| 3          | T            | 80         | SER         | 4.2         |
| 3          | M            | 219        | ILE         | 4.2         |
| 3          | O            | 252        | VAL         | 4.2         |
| 3          | S            | 198        | ALA         | 4.2         |
| 3          | S            | 248        | THR         | 4.2         |
| 3          | N            | 229        | ARG         | 4.1         |
| 3          | N            | 161        | TYR         | 4.1         |
| 1          | A            | 131        | THR         | 4.1         |
| 3          | M            | 73         | ASN         | 4.1         |
| 3          | N            | 79         | LEU         | 4.1         |
| 3          | N            | 201        | TYR         | 4.1         |
| 3          | N            | 241        | ASP         | 4.1         |
| 3          | T            | 216        | GLU         | 4.1         |
| 3          | N            | 157        | LYS         | 4.1         |
| 3          | N            | 185        | PRO         | 4.1         |
| 3          | O            | 162        | PRO         | 4.1         |
| 3          | O            | 207        | SER         | 4.1         |
| 3          | M            | 173        | GLY         | 4.1         |
| 3          | M            | 126        | SER         | 4.1         |
| 3          | T            | 79         | LEU         | 4.1         |
| 3          | M            | 122        | PRO         | 4.1         |
| 3          | M            | 77         | GLU         | 4.1         |
| 3          | M            | 196        | GLN         | 4.1         |
| 3          | T            | 100        | GLY         | 4.1         |
| 3          | N            | 97         | CYS         | 4.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | N            | 152        | ILE         | 4.1         |
| 4          | X            | 144        | CYS         | 4.1         |
| 3          | M            | 288        | ILE         | 4.0         |
| 3          | M            | 72         | GLY         | 4.0         |
| 3          | M            | 96         | THR         | 4.0         |
| 3          | O            | 104        | ASP         | 4.0         |
| 3          | N            | 191        | GLN         | 4.0         |
| 3          | M            | 245        | PHE         | 4.0         |
| 3          | S            | 247        | ALA         | 4.0         |
| 3          | M            | 94         | ASN         | 4.0         |
| 3          | O            | 191        | GLN         | 4.0         |
| 3          | T            | 120        | ILE         | 4.0         |
| 3          | S            | 166        | LYS         | 4.0         |
| 3          | N            | 129        | ASN         | 4.0         |
| 3          | U            | 215        | PRO         | 4.0         |
| 3          | M            | 223        | VAL         | 4.0         |
| 3          | M            | 81         | THR         | 4.0         |
| 3          | T            | 260        | MET         | 4.0         |
| 3          | T            | 223        | VAL         | 3.9         |
| 1          | I            | 214        | LYS         | 3.9         |
| 3          | M            | 118        | PHE         | 3.9         |
| 3          | O            | 171        | ASP         | 3.9         |
| 1          | I            | 132        | SER         | 3.9         |
| 3          | N            | 156        | LYS         | 3.9         |
| 3          | S            | 63         | LYS         | 3.9         |
| 3          | T            | 134        | GLY         | 3.9         |
| 3          | U            | 116(B)     | PHE         | 3.9         |
| 4          | V            | 143        | LYS         | 3.9         |
| 3          | O            | 122        | PRO         | 3.9         |
| 3          | U            | 123        | LYS         | 3.9         |
| 3          | N            | 83(A)      | SER         | 3.9         |
| 3          | O            | 185        | PRO         | 3.9         |
| 3          | S            | 168        | TYR         | 3.9         |
| 3          | O            | 224        | ARG         | 3.9         |
| 1          | I            | 130        | SER         | 3.9         |
| 3          | O            | 223        | VAL         | 3.9         |
| 1          | K            | 214        | LYS         | 3.9         |
| 3          | S            | 157        | LYS         | 3.9         |
| 3          | M            | 92         | SER         | 3.9         |
| 3          | T            | 220        | ARG         | 3.9         |
| 3          | N            | 221        | PRO         | 3.8         |
| 3          | U            | 214        | LYS         | 3.8         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | N            | 270        | SER         | 3.8         |
| 3          | S            | 123        | LYS         | 3.8         |
| 3          | T            | 156        | LYS         | 3.8         |
| 1          | I            | 196        | CYS         | 3.8         |
| 3          | M            | 64         | CYS         | 3.8         |
| 3          | T            | 11         | ASP         | 3.8         |
| 3          | N            | 166        | LYS         | 3.8         |
| 3          | T            | 157        | LYS         | 3.8         |
| 3          | M            | 190        | ASP         | 3.8         |
| 3          | S            | 76         | CYS         | 3.8         |
| 1          | C            | 215        | SER         | 3.8         |
| 3          | O            | 266        | SER         | 3.8         |
| 3          | S            | 160        | SER         | 3.8         |
| 3          | U            | 157        | LYS         | 3.8         |
| 3          | O            | 156        | LYS         | 3.8         |
| 3          | U            | 77         | GLU         | 3.8         |
| 1          | I            | 198        | VAL         | 3.8         |
| 3          | M            | 152        | ILE         | 3.8         |
| 3          | S            | 139        | CYS         | 3.8         |
| 3          | S            | 161        | TYR         | 3.8         |
| 3          | M            | 198        | ALA         | 3.7         |
| 3          | T            | 63         | LYS         | 3.7         |
| 3          | T            | 159        | ASN         | 3.7         |
| 3          | M            | 120        | ILE         | 3.7         |
| 3          | U            | 148        | TYR         | 3.7         |
| 3          | M            | 124        | THR         | 3.7         |
| 3          | M            | 191        | GLN         | 3.7         |
| 3          | N            | 134        | GLY         | 3.7         |
| 3          | N            | 184        | HIS         | 3.7         |
| 3          | S            | 118        | PHE         | 3.7         |
| 1          | E            | 215        | SER         | 3.7         |
| 3          | O            | 279        | THR         | 3.7         |
| 3          | U            | 224        | ARG         | 3.7         |
| 4          | Q            | 142        | HIS         | 3.7         |
| 3          | U            | 164        | LEU         | 3.6         |
| 3          | M            | 116(A)     | SER         | 3.6         |
| 3          | M            | 87         | ILE         | 3.6         |
| 3          | O            | 116(A)     | SER         | 3.6         |
| 3          | O            | 228        | GLY         | 3.6         |
| 3          | N            | 78         | SER         | 3.6         |
| 3          | O            | 83(A)      | SER         | 3.6         |
| 3          | O            | 98         | TYR         | 3.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | O            | 58         | PRO         | 3.6         |
| 3          | O            | 124        | THR         | 3.6         |
| 3          | N            | 183        | HIS         | 3.6         |
| 3          | S            | 77         | GLU         | 3.6         |
| 3          | S            | 174        | LYS         | 3.6         |
| 3          | U            | 11         | ASP         | 3.6         |
| 3          | U            | 80         | SER         | 3.6         |
| 3          | O            | 150        | ASN         | 3.6         |
| 3          | T            | 147        | PHE         | 3.6         |
| 4          | V            | 173        | ILE         | 3.6         |
| 3          | T            | 200        | THR         | 3.6         |
| 3          | N            | 195        | TYR         | 3.6         |
| 3          | T            | 116        | SER         | 3.6         |
| 3          | M            | 62         | GLY         | 3.5         |
| 3          | N            | 55         | ARG         | 3.5         |
| 3          | N            | 172        | LYS         | 3.5         |
| 3          | M            | 60         | HIS         | 3.5         |
| 3          | O            | 59         | LEU         | 3.5         |
| 3          | M            | 83         | SER         | 3.5         |
| 3          | N            | 165        | SER         | 3.5         |
| 3          | N            | 259        | ALA         | 3.5         |
| 3          | N            | 140        | PRO         | 3.5         |
| 3          | T            | 62         | GLY         | 3.5         |
| 3          | M            | 276        | ASP         | 3.5         |
| 3          | O            | 244        | THR         | 3.5         |
| 3          | S            | 261        | GLU         | 3.5         |
| 3          | T            | 197        | ASN         | 3.5         |
| 3          | O            | 97         | CYS         | 3.5         |
| 3          | U            | 196        | GLN         | 3.5         |
| 3          | M            | 100        | GLY         | 3.5         |
| 3          | N            | 170        | ASN         | 3.5         |
| 3          | U            | 62         | GLY         | 3.5         |
| 1          | I            | 112        | SER         | 3.5         |
| 3          | N            | 121        | PHE         | 3.5         |
| 3          | U            | 229        | ARG         | 3.4         |
| 3          | N            | 74         | PRO         | 3.4         |
| 3          | S            | 74         | PRO         | 3.4         |
| 3          | U            | 79         | LEU         | 3.4         |
| 3          | S            | 62         | GLY         | 3.4         |
| 4          | V            | 140        | PHE         | 3.4         |
| 3          | M            | 137        | ALA         | 3.4         |
| 3          | S            | 117        | ARG         | 3.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | M            | 151        | LEU         | 3.4         |
| 3          | O            | 146        | SER         | 3.4         |
| 3          | S            | 187        | THR         | 3.4         |
| 1          | A            | 214        | LYS         | 3.4         |
| 3          | U            | 173        | GLY         | 3.4         |
| 3          | N            | 175        | GLU         | 3.4         |
| 1          | E            | 189        | LEU         | 3.4         |
| 3          | N            | 202        | VAL         | 3.4         |
| 4          | X            | 129        | ASN         | 3.4         |
| 1          | K            | 131        | THR         | 3.4         |
| 3          | O            | 183        | HIS         | 3.4         |
| 3          | O            | 157        | LYS         | 3.4         |
| 3          | U            | 133(A)     | LYS         | 3.4         |
| 3          | M            | 216        | GLU         | 3.4         |
| 3          | T            | 230        | MET         | 3.4         |
| 1          | I            | 82(B)      | SER         | 3.4         |
| 3          | U            | 247        | ALA         | 3.4         |
| 3          | M            | 218        | ALA         | 3.4         |
| 3          | O            | 125        | SER         | 3.4         |
| 4          | P            | 144        | CYS         | 3.4         |
| 3          | S            | 171        | ASP         | 3.4         |
| 3          | O            | 220        | ARG         | 3.4         |
| 3          | S            | 10         | GLY         | 3.4         |
| 3          | S            | 55         | ARG         | 3.4         |
| 3          | S            | 224        | ARG         | 3.4         |
| 3          | S            | 195        | TYR         | 3.3         |
| 3          | O            | 126        | SER         | 3.3         |
| 3          | M            | 54         | LEU         | 3.3         |
| 3          | N            | 122        | PRO         | 3.3         |
| 3          | U            | 97         | CYS         | 3.3         |
| 3          | U            | 147        | PHE         | 3.3         |
| 3          | S            | 173        | GLY         | 3.3         |
| 3          | U            | 199        | ASP         | 3.3         |
| 3          | M            | 251        | LEU         | 3.3         |
| 3          | N            | 88         | VAL         | 3.3         |
| 3          | O            | 259        | ALA         | 3.3         |
| 3          | S            | 245        | PHE         | 3.3         |
| 3          | N            | 139        | CYS         | 3.3         |
| 1          | E            | 198        | VAL         | 3.3         |
| 3          | M            | 257        | ALA         | 3.3         |
| 3          | N            | 11         | ASP         | 3.3         |
| 3          | T            | 139        | CYS         | 3.3         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | S            | 147        | PHE         | 3.3         |
| 3          | O            | 260        | MET         | 3.3         |
| 3          | O            | 161        | TYR         | 3.3         |
| 1          | K            | 129        | LYS         | 3.3         |
| 3          | M            | 270        | SER         | 3.3         |
| 3          | O            | 174        | LYS         | 3.3         |
| 1          | K            | 189        | LEU         | 3.3         |
| 3          | M            | 79         | LEU         | 3.3         |
| 3          | S            | 251        | LEU         | 3.3         |
| 3          | T            | 245        | PHE         | 3.3         |
| 4          | W            | 144        | CYS         | 3.3         |
| 3          | U            | 171        | ASP         | 3.3         |
| 3          | N            | 123        | LYS         | 3.2         |
| 3          | S            | 199        | ASP         | 3.2         |
| 3          | T            | 76         | CYS         | 3.2         |
| 3          | U            | 197        | ASN         | 3.2         |
| 3          | T            | 219        | ILE         | 3.2         |
| 1          | E            | 131        | THR         | 3.2         |
| 3          | O            | 202        | VAL         | 3.2         |
| 3          | T            | 96         | THR         | 3.2         |
| 3          | O            | 218        | ALA         | 3.2         |
| 4          | P            | 143        | LYS         | 3.2         |
| 3          | M            | 70         | ILE         | 3.2         |
| 3          | U            | 90(A)      | PRO         | 3.2         |
| 3          | O            | 116        | SER         | 3.2         |
| 3          | O            | 167        | SER         | 3.2         |
| 3          | S            | 246        | GLU         | 3.2         |
| 3          | O            | 282        | GLN         | 3.2         |
| 1          | I            | 159        | LEU         | 3.2         |
| 4          | R            | 144        | CYS         | 3.2         |
| 3          | M            | 50         | LYS         | 3.2         |
| 3          | O            | 94         | ASN         | 3.2         |
| 3          | N            | 118        | PHE         | 3.2         |
| 3          | O            | 192        | GLN         | 3.2         |
| 3          | S            | 96         | THR         | 3.2         |
| 3          | M            | 98         | TYR         | 3.2         |
| 4          | X            | 141        | TYR         | 3.2         |
| 3          | O            | 182        | ILE         | 3.2         |
| 3          | T            | 124        | THR         | 3.2         |
| 3          | O            | 273        | PRO         | 3.1         |
| 3          | N            | 289        | ASN         | 3.1         |
| 3          | S            | 194        | LEU         | 3.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 4          | V            | 144        | CYS         | 3.1         |
| 3          | S            | 260        | MET         | 3.1         |
| 1          | I            | 207        | VAL         | 3.1         |
| 3          | S            | 95         | GLY         | 3.1         |
| 3          | T            | 247        | ALA         | 3.1         |
| 3          | T            | 187        | THR         | 3.1         |
| 3          | O            | 158        | GLY         | 3.1         |
| 3          | O            | 240        | GLY         | 3.1         |
| 3          | N            | 61         | LEU         | 3.1         |
| 3          | S            | 94         | ASN         | 3.1         |
| 3          | M            | 104        | ASP         | 3.1         |
| 3          | N            | 263        | ASN         | 3.1         |
| 1          | I            | 212        | GLU         | 3.1         |
| 3          | O            | 206        | SER         | 3.1         |
| 3          | O            | 254        | PRO         | 3.1         |
| 3          | O            | 90         | THR         | 3.1         |
| 3          | M            | 240        | GLY         | 3.1         |
| 3          | U            | 73         | ASN         | 3.1         |
| 3          | O            | 147        | PHE         | 3.1         |
| 3          | M            | 221        | PRO         | 3.0         |
| 3          | M            | 160        | SER         | 3.0         |
| 3          | N            | 219        | ILE         | 3.0         |
| 3          | O            | 186        | SER         | 3.0         |
| 3          | U            | 155        | VAL         | 3.0         |
| 3          | U            | 279        | THR         | 3.0         |
| 4          | Q            | 162        | TYR         | 3.0         |
| 3          | S            | 93         | ASP         | 3.0         |
| 3          | T            | 131        | ASP         | 3.0         |
| 3          | O            | 257        | ALA         | 3.0         |
| 3          | T            | 130        | HIS         | 3.0         |
| 3          | T            | 201        | TYR         | 3.0         |
| 1          | I            | 144        | ASP         | 3.0         |
| 3          | S            | 121        | PHE         | 3.0         |
| 1          | C            | 210        | ARG         | 3.0         |
| 3          | S            | 51         | LEU         | 3.0         |
| 3          | O            | 102        | PHE         | 3.0         |
| 3          | M            | 259        | ALA         | 3.0         |
| 3          | O            | 188        | SER         | 3.0         |
| 3          | T            | 165        | SER         | 3.0         |
| 3          | M            | 116(C)     | GLU         | 3.0         |
| 3          | T            | 143        | GLY         | 3.0         |
| 3          | O            | 60         | HIS         | 3.0         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | T            | 221        | PRO         | 3.0         |
| 1          | G            | 191        | THR         | 3.0         |
| 3          | S            | 290        | THR         | 3.0         |
| 3          | N            | 94         | ASN         | 3.0         |
| 3          | S            | 250        | ASN         | 3.0         |
| 3          | U            | 219        | ILE         | 3.0         |
| 3          | S            | 61         | LEU         | 3.0         |
| 3          | O            | 149        | LYS         | 3.0         |
| 3          | O            | 48         | ASN         | 3.0         |
| 3          | S            | 167        | SER         | 3.0         |
| 3          | U            | 231        | ASN         | 3.0         |
| 4          | R            | 143        | LYS         | 3.0         |
| 3          | N            | 64         | CYS         | 3.0         |
| 3          | S            | 277        | CYS         | 3.0         |
| 1          | I            | 154        | TRP         | 2.9         |
| 3          | S            | 133(A)     | LYS         | 2.9         |
| 3          | M            | 68         | GLY         | 2.9         |
| 3          | M            | 136        | THR         | 2.9         |
| 1          | A            | 189        | LEU         | 2.9         |
| 4          | W            | 27         | GLN         | 2.9         |
| 3          | U            | 288        | ILE         | 2.9         |
| 3          | N            | 142        | ALA         | 2.9         |
| 3          | N            | 100        | GLY         | 2.9         |
| 3          | O            | 226        | GLN         | 2.9         |
| 3          | U            | 207        | SER         | 2.9         |
| 3          | O            | 96         | THR         | 2.9         |
| 3          | O            | 290        | THR         | 2.9         |
| 3          | U            | 246        | GLU         | 2.9         |
| 3          | U            | 182        | ILE         | 2.9         |
| 3          | S            | 263        | ASN         | 2.9         |
| 3          | T            | 74         | PRO         | 2.9         |
| 3          | U            | 150        | ASN         | 2.9         |
| 3          | S            | 88         | VAL         | 2.9         |
| 1          | A            | 130        | SER         | 2.9         |
| 3          | S            | 122        | PRO         | 2.9         |
| 3          | S            | 215        | PRO         | 2.9         |
| 3          | U            | 195        | TYR         | 2.9         |
| 3          | N            | 119        | GLU         | 2.9         |
| 3          | O            | 118        | PHE         | 2.9         |
| 3          | M            | 159        | ASN         | 2.9         |
| 3          | N            | 208        | ARG         | 2.9         |
| 3          | S            | 124        | THR         | 2.9         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | S            | 229        | ARG         | 2.9         |
| 3          | S            | 184        | HIS         | 2.9         |
| 3          | N            | 249        | GLY         | 2.9         |
| 3          | T            | 144        | ALA         | 2.9         |
| 3          | M            | 95         | GLY         | 2.9         |
| 3          | S            | 55(A)      | GLY         | 2.9         |
| 3          | M            | 236        | LEU         | 2.9         |
| 3          | U            | 186        | SER         | 2.9         |
| 3          | M            | 71         | LEU         | 2.9         |
| 3          | T            | 61         | LEU         | 2.9         |
| 3          | O            | 92         | SER         | 2.8         |
| 3          | U            | 159        | ASN         | 2.8         |
| 3          | O            | 190        | ASP         | 2.8         |
| 3          | T            | 158        | GLY         | 2.8         |
| 3          | U            | 141        | HIS         | 2.8         |
| 3          | M            | 212        | LYS         | 2.8         |
| 3          | N            | 257        | ALA         | 2.8         |
| 3          | S            | 73         | ASN         | 2.8         |
| 3          | T            | 81         | THR         | 2.8         |
| 4          | R            | 63         | PHE         | 2.8         |
| 3          | S            | 186        | SER         | 2.8         |
| 3          | S            | 231        | ASN         | 2.8         |
| 3          | O            | 69         | TRP         | 2.8         |
| 3          | N            | 144        | ALA         | 2.8         |
| 3          | T            | 82         | ALA         | 2.8         |
| 3          | O            | 100        | GLY         | 2.8         |
| 3          | M            | 263        | ASN         | 2.8         |
| 3          | N            | 190        | ASP         | 2.8         |
| 3          | O            | 140        | PRO         | 2.8         |
| 4          | Q            | 141        | TYR         | 2.8         |
| 1          | E            | 16         | SER         | 2.8         |
| 3          | S            | 83(A)      | SER         | 2.8         |
| 3          | U            | 245        | PHE         | 2.8         |
| 3          | T            | 170        | ASN         | 2.8         |
| 3          | M            | 194        | LEU         | 2.8         |
| 3          | O            | 168        | TYR         | 2.8         |
| 4          | W            | 142        | HIS         | 2.8         |
| 3          | M            | 91         | SER         | 2.8         |
| 3          | O            | 277        | CYS         | 2.8         |
| 3          | S            | 282        | GLN         | 2.8         |
| 1          | K            | 194        | TYR         | 2.8         |
| 3          | T            | 118        | PHE         | 2.8         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | T            | 171        | ASP         | 2.8         |
| 3          | S            | 78         | SER         | 2.8         |
| 3          | T            | 64         | CYS         | 2.8         |
| 3          | T            | 191        | GLN         | 2.7         |
| 3          | S            | 146        | SER         | 2.7         |
| 3          | O            | 121        | PHE         | 2.7         |
| 3          | U            | 60         | HIS         | 2.7         |
| 3          | T            | 92         | SER         | 2.7         |
| 3          | M            | 90(A)      | PRO         | 2.7         |
| 3          | N            | 254        | PRO         | 2.7         |
| 3          | T            | 241        | ASP         | 2.7         |
| 3          | U            | 200        | THR         | 2.7         |
| 3          | U            | 248        | THR         | 2.7         |
| 3          | U            | 168        | TYR         | 2.7         |
| 3          | U            | 201        | TYR         | 2.7         |
| 3          | U            | 51         | LEU         | 2.7         |
| 3          | N            | 268        | ILE         | 2.7         |
| 3          | N            | 90(A)      | PRO         | 2.7         |
| 1          | I            | 145        | TYR         | 2.7         |
| 3          | S            | 287        | ALA         | 2.7         |
| 1          | I            | 66         | ARG         | 2.7         |
| 3          | U            | 166        | LYS         | 2.7         |
| 3          | N            | 51         | LEU         | 2.7         |
| 3          | S            | 83         | SER         | 2.7         |
| 3          | T            | 215        | PRO         | 2.7         |
| 3          | M            | 214        | LYS         | 2.7         |
| 4          | Q            | 144        | CYS         | 2.7         |
| 1          | E            | 130        | SER         | 2.7         |
| 3          | M            | 63         | LYS         | 2.7         |
| 3          | N            | 124        | THR         | 2.7         |
| 3          | N            | 200        | THR         | 2.7         |
| 3          | S            | 202        | VAL         | 2.7         |
| 3          | S            | 272        | THR         | 2.7         |
| 3          | T            | 202        | VAL         | 2.7         |
| 3          | N            | 164        | LEU         | 2.7         |
| 3          | M            | 78         | SER         | 2.7         |
| 3          | U            | 99         | PRO         | 2.7         |
| 4          | W            | 148        | CYS         | 2.7         |
| 3          | S            | 223        | VAL         | 2.7         |
| 3          | N            | 218        | ALA         | 2.7         |
| 3          | N            | 174        | LYS         | 2.7         |
| 3          | N            | 282        | GLN         | 2.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | U            | 10         | GLY         | 2.7         |
| 4          | V            | 149        | MET         | 2.7         |
| 3          | O            | 75         | GLU         | 2.7         |
| 3          | M            | 53         | LYS         | 2.7         |
| 3          | M            | 157        | LYS         | 2.7         |
| 1          | K            | 128        | SER         | 2.7         |
| 3          | S            | 200        | THR         | 2.7         |
| 3          | N            | 147        | PHE         | 2.7         |
| 3          | M            | 261        | GLU         | 2.7         |
| 4          | P            | 142        | HIS         | 2.7         |
| 2          | L            | 30         | SER         | 2.6         |
| 3          | M            | 222        | LYS         | 2.6         |
| 1          | I            | 206        | LYS         | 2.6         |
| 3          | O            | 212        | LYS         | 2.6         |
| 3          | U            | 74         | PRO         | 2.6         |
| 3          | T            | 184        | HIS         | 2.6         |
| 3          | U            | 146        | SER         | 2.6         |
| 1          | I            | 1          | GLN         | 2.6         |
| 3          | O            | 10         | GLY         | 2.6         |
| 3          | O            | 242        | LYS         | 2.6         |
| 3          | N            | 162        | PRO         | 2.6         |
| 3          | N            | 212        | LYS         | 2.6         |
| 3          | S            | 129        | ASN         | 2.6         |
| 3          | T            | 50         | LYS         | 2.6         |
| 4          | W            | 143        | LYS         | 2.6         |
| 3          | M            | 59         | LEU         | 2.6         |
| 3          | T            | 52         | CYS         | 2.6         |
| 3          | S            | 185        | PRO         | 2.6         |
| 3          | N            | 145        | LYS         | 2.6         |
| 2          | J            | 77         | ARG         | 2.6         |
| 3          | O            | 63         | LYS         | 2.6         |
| 3          | S            | 270        | SER         | 2.6         |
| 3          | N            | 217        | ILE         | 2.6         |
| 3          | N            | 278        | ASN         | 2.6         |
| 3          | N            | 148        | TYR         | 2.6         |
| 3          | N            | 102        | PHE         | 2.6         |
| 3          | M            | 184        | HIS         | 2.6         |
| 3          | S            | 75         | GLU         | 2.6         |
| 3          | T            | 270        | SER         | 2.6         |
| 3          | O            | 120        | ILE         | 2.6         |
| 3          | N            | 73         | ASN         | 2.6         |
| 3          | S            | 289        | ASN         | 2.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | C            | 194        | TYR         | 2.6         |
| 1          | E            | 144        | ASP         | 2.6         |
| 3          | U            | 218        | ALA         | 2.6         |
| 1          | I            | 199        | ASN         | 2.6         |
| 3          | M            | 275        | HIS         | 2.6         |
| 3          | S            | 11         | ASP         | 2.6         |
| 3          | S            | 214        | LYS         | 2.6         |
| 3          | O            | 219        | ILE         | 2.6         |
| 1          | I            | 64         | GLN         | 2.6         |
| 3          | N            | 99         | PRO         | 2.6         |
| 3          | U            | 118        | PHE         | 2.6         |
| 3          | S            | 149        | LYS         | 2.6         |
| 1          | I            | 119        | PRO         | 2.6         |
| 3          | U            | 9          | PRO         | 2.6         |
| 3          | N            | 196        | GLN         | 2.5         |
| 3          | N            | 264        | ALA         | 2.5         |
| 1          | I            | 23         | ARG         | 2.5         |
| 3          | S            | 48         | ASN         | 2.5         |
| 3          | M            | 256        | TYR         | 2.5         |
| 3          | S            | 192        | GLN         | 2.5         |
| 3          | O            | 49         | GLY         | 2.5         |
| 3          | M            | 131        | ASP         | 2.5         |
| 3          | N            | 116(B)     | PHE         | 2.5         |
| 3          | U            | 172        | LYS         | 2.5         |
| 2          | J            | 129        | THR         | 2.5         |
| 3          | O            | 119        | GLU         | 2.5         |
| 3          | S            | 82         | ALA         | 2.5         |
| 3          | T            | 133(A)     | LYS         | 2.5         |
| 2          | B            | 62         | PHE         | 2.5         |
| 3          | U            | 184        | HIS         | 2.5         |
| 3          | N            | 236        | LEU         | 2.5         |
| 3          | U            | 270        | SER         | 2.5         |
| 4          | P            | 165        | GLU         | 2.5         |
| 3          | U            | 190        | ASP         | 2.5         |
| 3          | M            | 192        | GLN         | 2.5         |
| 3          | M            | 170        | ASN         | 2.5         |
| 1          | I            | 191        | THR         | 2.5         |
| 3          | N            | 54         | LEU         | 2.5         |
| 3          | S            | 140        | PRO         | 2.5         |
| 3          | M            | 182        | ILE         | 2.5         |
| 3          | U            | 12         | THR         | 2.5         |
| 3          | U            | 89         | GLU         | 2.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | M            | 208        | ARG         | 2.5         |
| 1          | C            | 189        | LEU         | 2.5         |
| 3          | S            | 158        | GLY         | 2.5         |
| 3          | U            | 262        | ARG         | 2.5         |
| 3          | M            | 290        | THR         | 2.5         |
| 3          | U            | 187        | THR         | 2.5         |
| 3          | U            | 198        | ALA         | 2.5         |
| 4          | W            | 164        | GLU         | 2.5         |
| 3          | M            | 274        | VAL         | 2.5         |
| 3          | T            | 12         | THR         | 2.5         |
| 3          | N            | 131        | ASP         | 2.5         |
| 3          | T            | 246        | GLU         | 2.5         |
| 3          | N            | 230        | MET         | 2.4         |
| 3          | N            | 143        | GLY         | 2.4         |
| 3          | T            | 259        | ALA         | 2.4         |
| 1          | I            | 126        | PRO         | 2.4         |
| 3          | S            | 191        | GLN         | 2.4         |
| 3          | S            | 221        | PRO         | 2.4         |
| 3          | O            | 175        | GLU         | 2.4         |
| 1          | G            | 112        | SER         | 2.4         |
| 3          | U            | 167        | SER         | 2.4         |
| 3          | U            | 54         | LEU         | 2.4         |
| 3          | M            | 148        | TYR         | 2.4         |
| 1          | I            | 129        | LYS         | 2.4         |
| 3          | S            | 225        | ASP         | 2.4         |
| 3          | U            | 116        | SER         | 2.4         |
| 3          | U            | 220        | ARG         | 2.4         |
| 1          | I            | 204        | ASN         | 2.4         |
| 3          | U            | 88         | VAL         | 2.4         |
| 3          | N            | 80         | SER         | 2.4         |
| 3          | O            | 55         | ARG         | 2.4         |
| 3          | U            | 129        | ASN         | 2.4         |
| 4          | W            | 162        | TYR         | 2.4         |
| 3          | N            | 98         | TYR         | 2.4         |
| 3          | S            | 143        | GLY         | 2.4         |
| 3          | U            | 290        | THR         | 2.4         |
| 1          | G            | 194        | TYR         | 2.4         |
| 3          | M            | 11         | ASP         | 2.4         |
| 3          | O            | 71         | LEU         | 2.4         |
| 3          | U            | 183        | HIS         | 2.4         |
| 1          | G            | 132        | SER         | 2.4         |
| 3          | O            | 52         | CYS         | 2.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | N            | 130        | HIS         | 2.4         |
| 3          | U            | 131        | ASP         | 2.4         |
| 3          | T            | 194        | LEU         | 2.4         |
| 1          | G            | 192        | GLN         | 2.4         |
| 1          | I            | 211        | VAL         | 2.4         |
| 2          | D            | 62         | PHE         | 2.4         |
| 3          | T            | 186        | SER         | 2.4         |
| 3          | M            | 185        | PRO         | 2.4         |
| 3          | N            | 215        | PRO         | 2.4         |
| 3          | N            | 12         | THR         | 2.4         |
| 3          | N            | 120        | ILE         | 2.4         |
| 3          | T            | 163        | LYS         | 2.4         |
| 3          | T            | 257        | ALA         | 2.4         |
| 4          | P            | 141        | TYR         | 2.4         |
| 3          | T            | 93         | ASP         | 2.4         |
| 3          | M            | 88         | VAL         | 2.4         |
| 1          | E            | 112        | SER         | 2.4         |
| 1          | G            | 1          | GLN         | 2.4         |
| 4          | Q            | 157        | TYR         | 2.4         |
| 1          | I            | 205        | THR         | 2.4         |
| 3          | U            | 66         | ILE         | 2.4         |
| 3          | N            | 135        | VAL         | 2.3         |
| 3          | T            | 217        | ILE         | 2.3         |
| 3          | U            | 100        | GLY         | 2.3         |
| 3          | M            | 175        | GLU         | 2.3         |
| 4          | W            | 166        | ALA         | 2.3         |
| 3          | O            | 84         | TRP         | 2.3         |
| 3          | U            | 64         | CYS         | 2.3         |
| 3          | O            | 268        | ILE         | 2.3         |
| 1          | A            | 207        | VAL         | 2.3         |
| 1          | K            | 1          | GLN         | 2.3         |
| 3          | M            | 168        | TYR         | 2.3         |
| 3          | T            | 133        | ASN         | 2.3         |
| 3          | T            | 183        | HIS         | 2.3         |
| 3          | O            | 217        | ILE         | 2.3         |
| 3          | O            | 258        | PHE         | 2.3         |
| 1          | G            | 209        | LYS         | 2.3         |
| 3          | O            | 135        | VAL         | 2.3         |
| 3          | S            | 204        | VAL         | 2.3         |
| 4          | V            | 165        | GLU         | 2.3         |
| 4          | X            | 30         | GLN         | 2.3         |
| 4          | X            | 62         | GLN         | 2.3         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 4          | Q            | 60         | ASN         | 2.3         |
| 1          | C            | 214        | LYS         | 2.3         |
| 3          | N            | 128        | PRO         | 2.3         |
| 3          | N            | 222        | LYS         | 2.3         |
| 1          | A            | 1          | GLN         | 2.3         |
| 3          | U            | 130        | HIS         | 2.3         |
| 3          | T            | 86         | TYR         | 2.3         |
| 3          | T            | 287        | ALA         | 2.3         |
| 3          | N            | 243        | ILE         | 2.3         |
| 3          | O            | 304        | LYS         | 2.3         |
| 3          | T            | 225        | ASP         | 2.3         |
| 1          | K            | 4          | LEU         | 2.3         |
| 3          | U            | 191        | GLN         | 2.3         |
| 3          | O            | 55(A)      | GLY         | 2.3         |
| 3          | S            | 288        | ILE         | 2.3         |
| 3          | N            | 91         | SER         | 2.3         |
| 3          | N            | 95         | GLY         | 2.2         |
| 1          | C            | 23         | ARG         | 2.2         |
| 3          | O            | 302        | ILE         | 2.2         |
| 1          | K            | 211        | VAL         | 2.2         |
| 1          | C            | 199        | ASN         | 2.2         |
| 4          | X            | 63         | PHE         | 2.2         |
| 3          | T            | 264        | ALA         | 2.2         |
| 3          | U            | 282        | GLN         | 2.2         |
| 4          | R            | 29         | GLU         | 2.2         |
| 4          | X            | 162        | TYR         | 2.2         |
| 3          | M            | 234        | TRP         | 2.2         |
| 3          | T            | 51         | LEU         | 2.2         |
| 3          | O            | 230        | MET         | 2.2         |
| 1          | A            | 81         | ASP         | 2.2         |
| 4          | Q            | 140        | PHE         | 2.2         |
| 3          | N            | 252        | VAL         | 2.2         |
| 3          | T            | 145        | LYS         | 2.2         |
| 3          | U            | 174        | LYS         | 2.2         |
| 1          | I            | 17         | SER         | 2.2         |
| 3          | S            | 276        | ASP         | 2.2         |
| 3          | O            | 301        | THR         | 2.2         |
| 4          | R            | 142        | HIS         | 2.2         |
| 1          | A            | 186        | SER         | 2.2         |
| 3          | T            | 83(A)      | SER         | 2.2         |
| 3          | O            | 255        | ARG         | 2.2         |
| 3          | M            | 249        | GLY         | 2.2         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | I            | 140        | CYS         | 2.2         |
| 4          | W            | 72         | HIS         | 2.2         |
| 3          | O            | 262        | ARG         | 2.2         |
| 1          | C            | 119        | PRO         | 2.2         |
| 1          | I            | 197        | ASN         | 2.2         |
| 3          | T            | 116(B)     | PHE         | 2.2         |
| 3          | T            | 208        | ARG         | 2.2         |
| 3          | M            | 267        | ILE         | 2.2         |
| 1          | I            | 189        | LEU         | 2.2         |
| 2          | H            | 70         | ASP         | 2.2         |
| 3          | T            | 190        | ASP         | 2.2         |
| 3          | S            | 227        | GLU         | 2.2         |
| 3          | T            | 10         | GLY         | 2.2         |
| 3          | U            | 132        | SER         | 2.2         |
| 1          | A            | 198        | VAL         | 2.2         |
| 3          | N            | 10         | GLY         | 2.2         |
| 3          | S            | 126        | SER         | 2.2         |
| 1          | C            | 1          | GLN         | 2.2         |
| 3          | T            | 282        | GLN         | 2.2         |
| 3          | O            | 170        | ASN         | 2.2         |
| 3          | S            | 235        | THR         | 2.2         |
| 3          | M            | 262        | ARG         | 2.2         |
| 3          | U            | 117        | ARG         | 2.2         |
| 1          | E            | 159        | LEU         | 2.2         |
| 3          | U            | 212        | LYS         | 2.2         |
| 4          | Q            | 165        | GLU         | 2.2         |
| 3          | N            | 290        | THR         | 2.2         |
| 3          | U            | 121        | PHE         | 2.1         |
| 1          | I            | 213        | PRO         | 2.1         |
| 3          | M            | 199        | ASP         | 2.1         |
| 3          | S            | 104        | ASP         | 2.1         |
| 3          | U            | 202        | VAL         | 2.1         |
| 4          | P            | 140        | PHE         | 2.1         |
| 3          | N            | 146        | SER         | 2.1         |
| 3          | O            | 276        | ASP         | 2.1         |
| 3          | T            | 236        | LEU         | 2.1         |
| 1          | C            | 205        | THR         | 2.1         |
| 3          | M            | 211        | LYS         | 2.1         |
| 4          | W            | 28         | ASN         | 2.1         |
| 3          | T            | 199        | ASP         | 2.1         |
| 3          | T            | 256        | TYR         | 2.1         |
| 3          | U            | 69         | TRP         | 2.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 4          | V            | 169        | ASN         | 2.1         |
| 4          | V            | 170        | ARG         | 2.1         |
| 4          | X            | 142        | HIS         | 2.1         |
| 3          | O            | 297        | ILE         | 2.1         |
| 3          | S            | 217        | ILE         | 2.1         |
| 3          | T            | 48         | ASN         | 2.1         |
| 3          | U            | 265        | GLY         | 2.1         |
| 4          | R            | 170        | ARG         | 2.1         |
| 3          | N            | 168        | TYR         | 2.1         |
| 3          | O            | 89         | GLU         | 2.1         |
| 3          | U            | 227        | GLU         | 2.1         |
| 3          | M            | 279        | THR         | 2.1         |
| 3          | N            | 240        | GLY         | 2.1         |
| 3          | S            | 159        | ASN         | 2.1         |
| 3          | S            | 279        | THR         | 2.1         |
| 3          | T            | 166        | LYS         | 2.1         |
| 1          | A            | 194        | TYR         | 2.1         |
| 1          | G            | 128        | SER         | 2.1         |
| 3          | U            | 257        | ALA         | 2.1         |
| 3          | O            | 184        | HIS         | 2.1         |
| 3          | O            | 234        | TRP         | 2.1         |
| 4          | Q            | 72         | HIS         | 2.1         |
| 3          | U            | 143        | GLY         | 2.1         |
| 1          | A            | 199        | ASN         | 2.1         |
| 4          | P            | 149        | MET         | 2.1         |
| 4          | Q            | 28         | ASN         | 2.1         |
| 1          | E            | 145        | TYR         | 2.1         |
| 1          | C            | 207        | VAL         | 2.1         |
| 2          | H            | 77         | ARG         | 2.1         |
| 3          | N            | 225        | ASP         | 2.1         |
| 2          | H            | 62         | PHE         | 2.1         |
| 3          | U            | 203        | PHE         | 2.1         |
| 3          | N            | 248        | THR         | 2.1         |
| 3          | M            | 201        | TYR         | 2.1         |
| 3          | M            | 273        | PRO         | 2.1         |
| 4          | R            | 69         | GLU         | 2.1         |
| 3          | O            | 253        | VAL         | 2.1         |
| 3          | S            | 142        | ALA         | 2.1         |
| 4          | V            | 166        | ALA         | 2.1         |
| 3          | N            | 59         | LEU         | 2.1         |
| 3          | N            | 116(A)     | SER         | 2.1         |
| 4          | W            | 30         | GLN         | 2.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | O            | 256        | TYR         | 2.1         |
| 3          | S            | 144        | ALA         | 2.1         |
| 3          | U            | 96         | THR         | 2.1         |
| 4          | P            | 171        | GLU         | 2.1         |
| 3          | N            | 53         | LYS         | 2.0         |
| 3          | S            | 116(B)     | PHE         | 2.0         |
| 1          | A            | 119        | PRO         | 2.0         |
| 3          | T            | 94         | ASN         | 2.0         |
| 4          | R            | 169        | ASN         | 2.0         |
| 3          | M            | 268        | ILE         | 2.0         |
| 3          | N            | 112        | LEU         | 2.0         |
| 2          | J            | 32         | SER         | 2.0         |
| 4          | X            | 27         | GLN         | 2.0         |
| 3          | U            | 277        | CYS         | 2.0         |
| 2          | J            | 125        | LEU         | 2.0         |
| 3          | O            | 278        | ASN         | 2.0         |
| 3          | T            | 164        | LEU         | 2.0         |
| 3          | N            | 214        | LYS         | 2.0         |
| 4          | W            | 29         | GLU         | 2.0         |
| 4          | W            | 157        | TYR         | 2.0         |
| 1          | G            | 189        | LEU         | 2.0         |
| 3          | O            | 133        | ASN         | 2.0         |
| 3          | U            | 119        | GLU         | 2.0         |
| 3          | N            | 232        | TYR         | 2.0         |
| 3          | O            | 54         | LEU         | 2.0         |
| 3          | O            | 66         | ILE         | 2.0         |
| 3          | S            | 259        | ALA         | 2.0         |
| 4          | X            | 169        | ASN         | 2.0         |
| 1          | A            | 144        | ASP         | 2.0         |
| 1          | I            | 156        | SER         | 2.0         |
| 1          | K            | 127        | SER         | 2.0         |
| 3          | M            | 125        | SER         | 2.0         |
| 3          | S            | 53         | LYS         | 2.0         |
| 3          | T            | 83         | SER         | 2.0         |
| 3          | S            | 182        | ILE         | 2.0         |
| 3          | U            | 240        | GLY         | 2.0         |
| 3          | T            | 119        | GLU         | 2.0         |
| 1          | K            | 23         | ARG         | 2.0         |
| 3          | M            | 61         | LEU         | 2.0         |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.