



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:30 PM UTC

PDB ID : 7EI1 / pdb\_00007ei1  
Title : Structure of Pyrococcus furiosus Cas1Cas2 complex  
Authors : Yu, Y.; Chen, Q.  
Deposited on : 2021-03-30  
Resolution : 3.90 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:

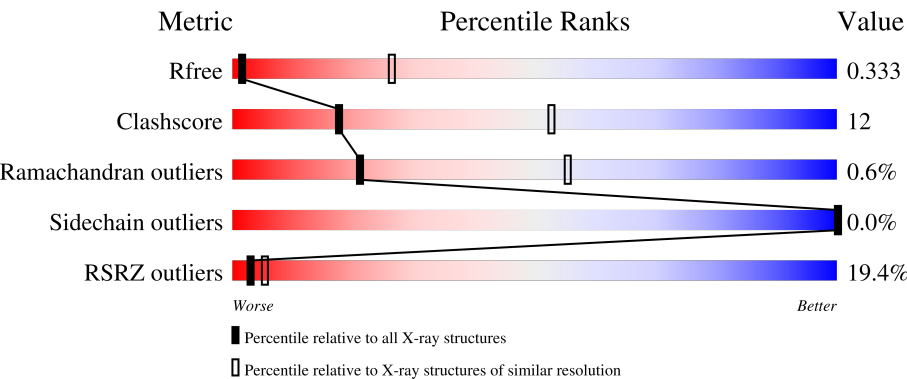
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

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 3.90 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1270 (4.10-3.70)                                      |
| Clashscore            | 190562                      | 1034 (4.08-3.72)                                      |
| Ramachandran outliers | 187476                      | 1251 (4.10-3.70)                                      |
| Sidechain outliers    | 187428                      | 1243 (4.10-3.70)                                      |
| RSRZ outliers         | 180081                      | 1269 (4.10-3.70)                                      |

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     | 322    | <div><div>26%</div><div><div></div><div>74%</div><div>21%</div><div>..</div></div></div> |
| 1   | B     | 322    | <div><div>13%</div><div><div></div><div>66%</div><div>29%</div><div>.</div></div></div>  |
| 1   | C     | 322    | <div><div>22%</div><div><div></div><div>66%</div><div>31%</div><div>.</div></div></div>  |
| 1   | D     | 322    | <div><div>9%</div><div><div></div><div>65%</div><div>28%</div><div>..</div></div></div>  |
| 1   | E     | 322    | <div><div>24%</div><div><div></div><div>70%</div><div>26%</div><div>.</div></div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 322    |                  |
| 1   | G     | 322    |                  |
| 1   | H     | 322    |                  |
| 1   | I     | 322    |                  |
| 1   | J     | 322    |                  |
| 1   | K     | 322    |                  |
| 1   | L     | 322    |                  |
| 1   | M     | 322    |                  |
| 1   | N     | 322    |                  |
| 1   | O     | 322    |                  |
| 1   | P     | 322    |                  |
| 2   | Q     | 85     |                  |
| 2   | R     | 85     |                  |
| 2   | S     | 85     |                  |
| 2   | T     | 85     |                  |
| 2   | U     | 85     |                  |
| 2   | V     | 85     |                  |
| 2   | W     | 85     |                  |
| 2   | X     | 85     |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 90949 atoms, of which 44675 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 CRISPR-associated endonuclease Cas1.

| Mol | Chain | Residues | Atoms         |           |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|----------|----------|--------|---------|---------|-------|
| 1   | A     | 311      | Total<br>5002 | C<br>1647 | H<br>2443 | N<br>449 | O<br>458 | S<br>5 | 0       | 0       | 0     |
| 1   | B     | 308      | Total<br>4941 | C<br>1633 | H<br>2409 | N<br>439 | O<br>455 | S<br>5 | 0       | 0       | 0     |
| 1   | C     | 312      | Total<br>5020 | C<br>1656 | H<br>2450 | N<br>450 | O<br>459 | S<br>5 | 0       | 0       | 0     |
| 1   | D     | 308      | Total<br>4937 | C<br>1633 | H<br>2405 | N<br>439 | O<br>455 | S<br>5 | 0       | 0       | 0     |
| 1   | E     | 312      | Total<br>5003 | C<br>1656 | H<br>2433 | N<br>450 | O<br>459 | S<br>5 | 0       | 0       | 0     |
| 1   | F     | 308      | Total<br>4950 | C<br>1633 | H<br>2418 | N<br>439 | O<br>455 | S<br>5 | 0       | 0       | 0     |
| 1   | G     | 312      | Total<br>5016 | C<br>1656 | H<br>2446 | N<br>450 | O<br>459 | S<br>5 | 0       | 0       | 0     |
| 1   | H     | 306      | Total<br>4926 | C<br>1624 | H<br>2408 | N<br>437 | O<br>452 | S<br>5 | 0       | 0       | 0     |
| 1   | K     | 310      | Total<br>5012 | C<br>1636 | H<br>2467 | N<br>447 | O<br>457 | S<br>5 | 0       | 0       | 0     |
| 1   | L     | 308      | Total<br>4958 | C<br>1633 | H<br>2426 | N<br>439 | O<br>455 | S<br>5 | 0       | 0       | 0     |
| 1   | M     | 314      | Total<br>5070 | C<br>1668 | H<br>2481 | N<br>455 | O<br>461 | S<br>5 | 0       | 0       | 0     |
| 1   | N     | 305      | Total<br>4905 | C<br>1619 | H<br>2396 | N<br>436 | O<br>449 | S<br>5 | 0       | 0       | 0     |
| 1   | I     | 312      | Total<br>5037 | C<br>1656 | H<br>2467 | N<br>450 | O<br>459 | S<br>5 | 0       | 0       | 0     |
| 1   | J     | 307      | Total<br>4924 | C<br>1629 | H<br>2399 | N<br>438 | O<br>453 | S<br>5 | 0       | 0       | 0     |
| 1   | O     | 311      | Total<br>5024 | C<br>1647 | H<br>2465 | N<br>449 | O<br>458 | S<br>5 | 0       | 0       | 0     |
| 1   | P     | 306      | Total<br>4937 | C<br>1624 | H<br>2419 | N<br>437 | O<br>452 | S<br>5 | 0       | 0       | 0     |

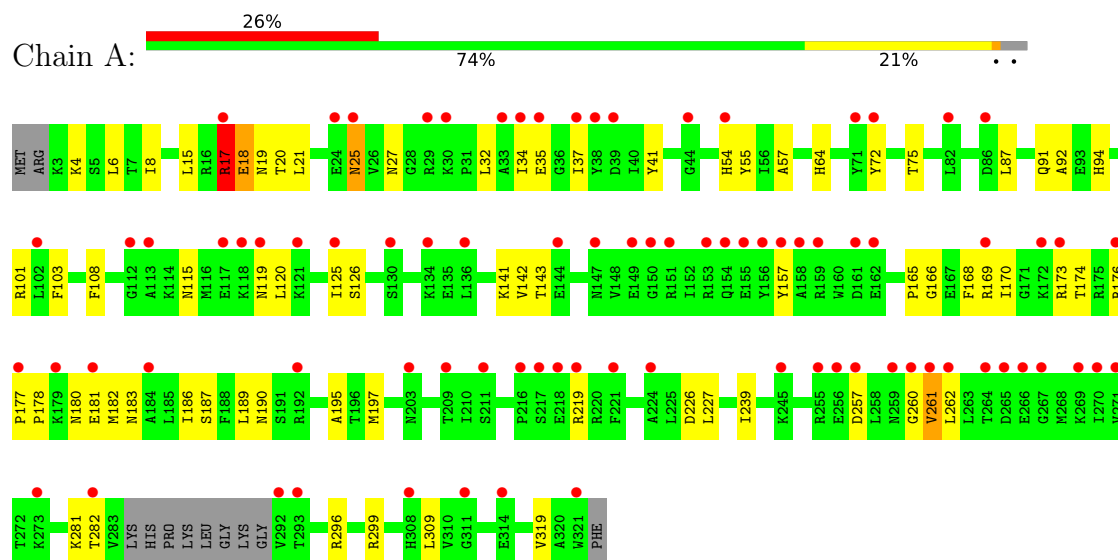
- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|---------|-------|
| 2   | Q     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1401  | 447 | 708 | 116 | 127 | 3 |         |         |       |
| 2   | R     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1413  | 447 | 720 | 116 | 127 | 3 |         |         |       |
| 2   | S     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1413  | 447 | 720 | 116 | 127 | 3 |         |         |       |
| 2   | T     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1413  | 447 | 720 | 116 | 127 | 3 |         |         |       |
| 2   | U     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1412  | 447 | 719 | 116 | 127 | 3 |         |         |       |
| 2   | V     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 447 | 718 | 116 | 127 | 3 |         |         |       |
| 2   | W     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1413  | 447 | 720 | 116 | 127 | 3 |         |         |       |
| 2   | X     | 84       | Total | C   | H   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 447 | 718 | 116 | 127 | 3 |         |         |       |

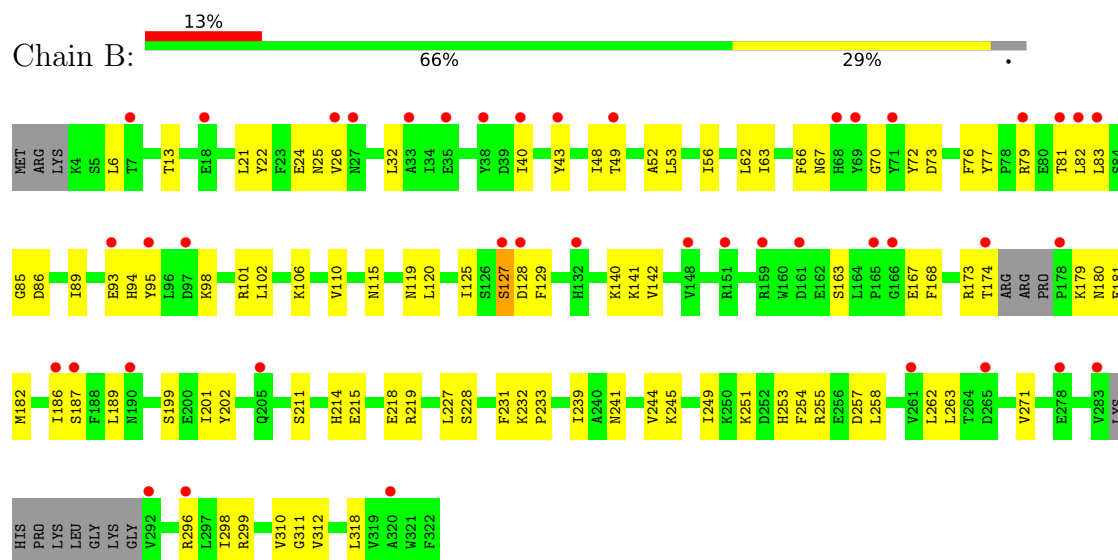
### 3 Residue-property plots [i](#)

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: CRISPR-associated endonuclease Cas1

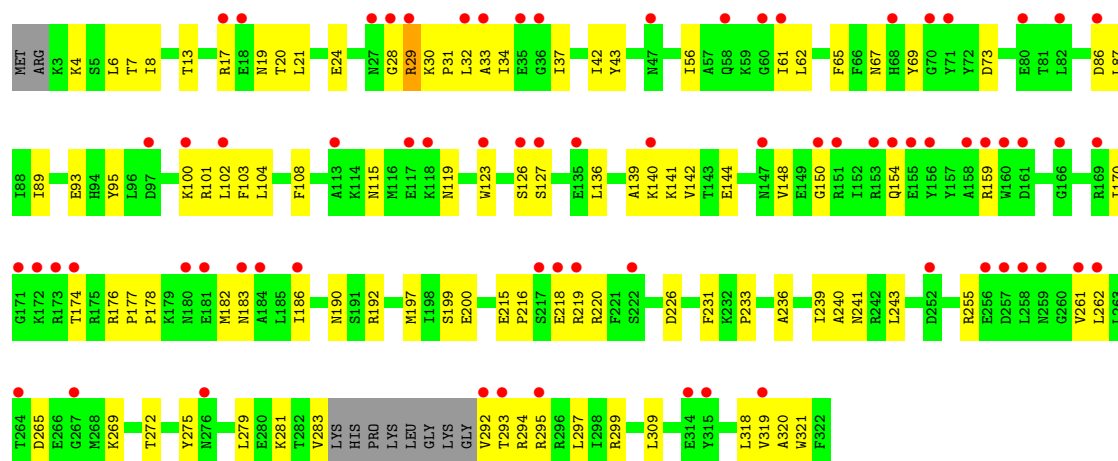


#### • Molecule 1: CRISPR-associated endonuclease Cas1

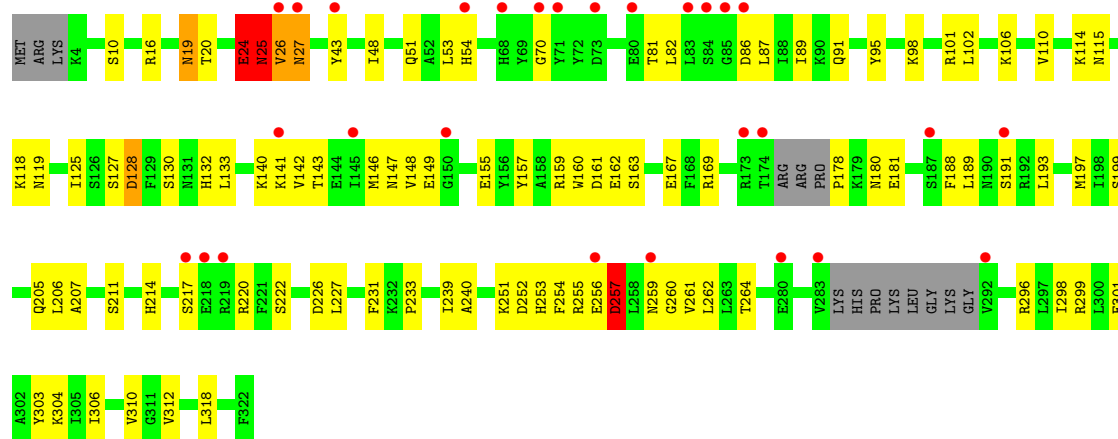


#### • Molecule 1: CRISPR-associated endonuclease Cas1

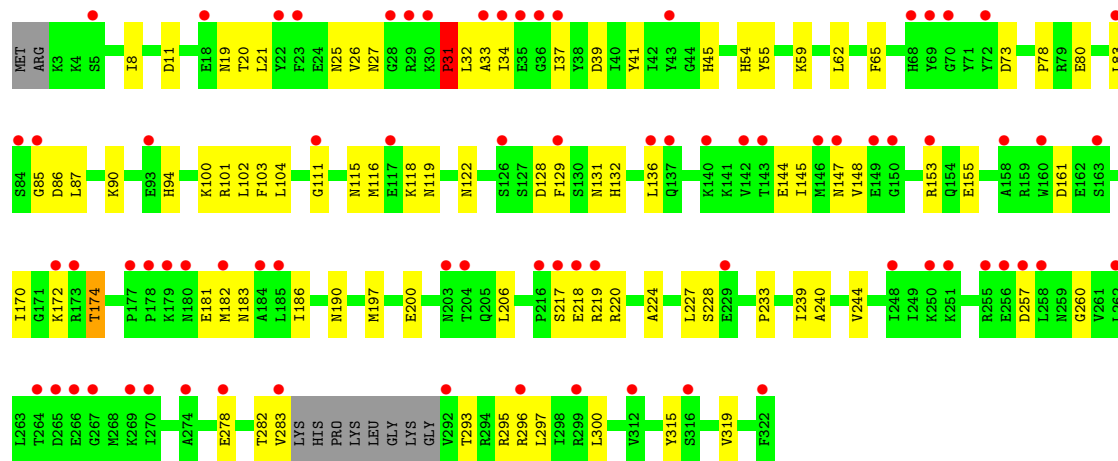




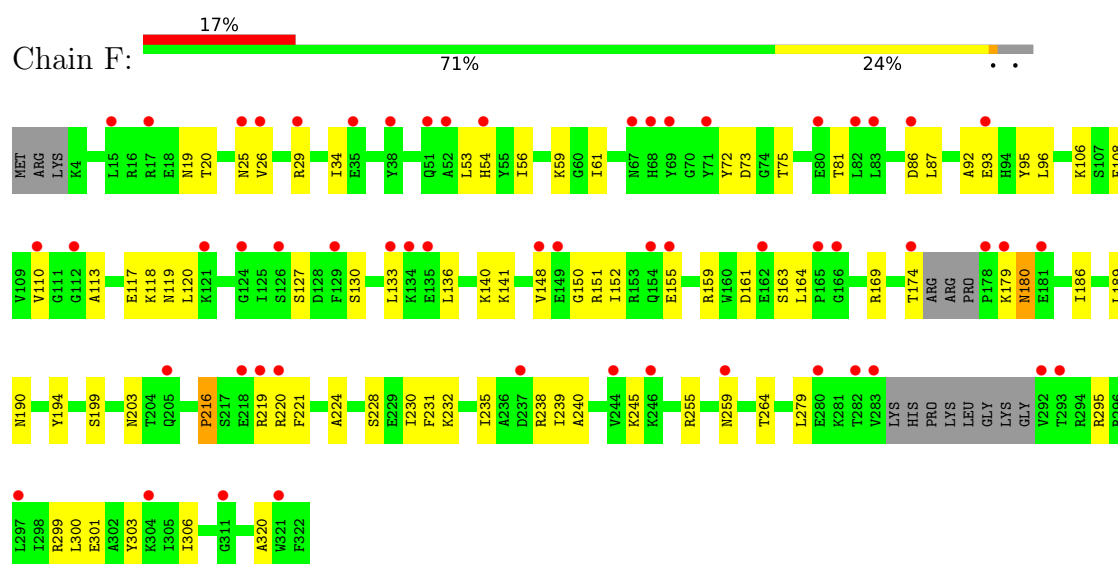
• Molecule 1: CRISPR-associated endonuclease Cas1



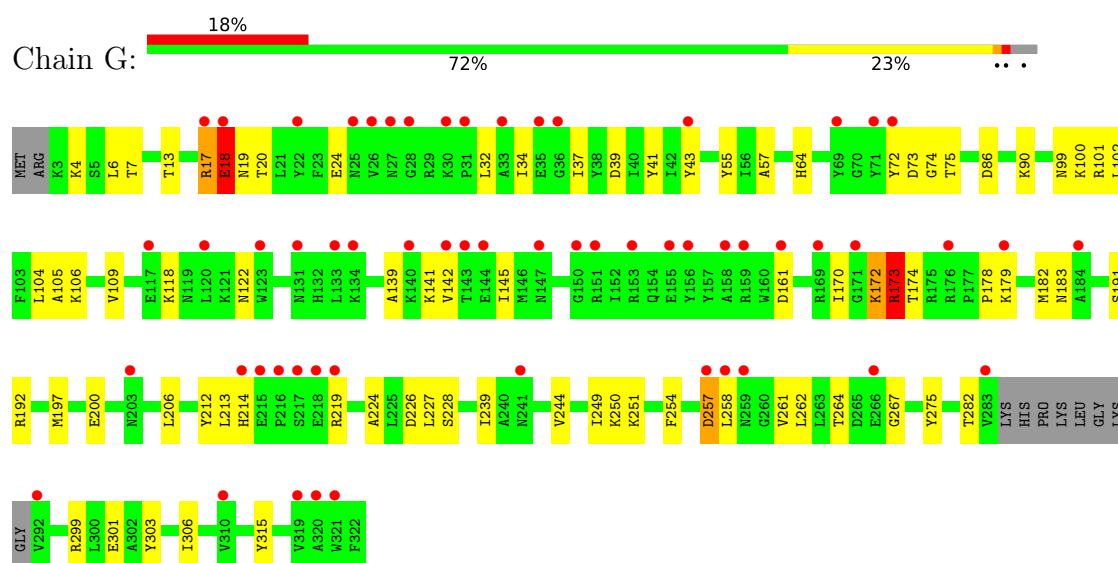
• Molecule 1: CRISPR-associated endonuclease Cas1



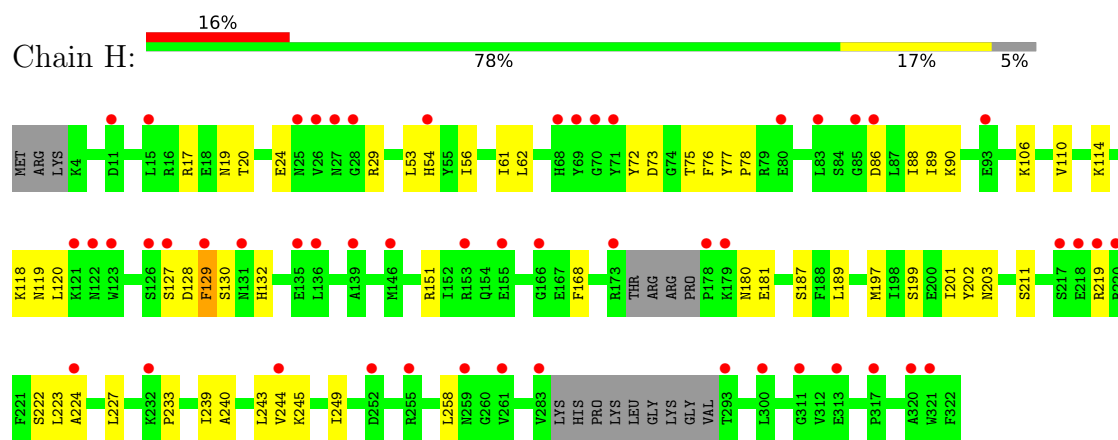
• Molecule 1: CRISPR-associated endonuclease Cas1



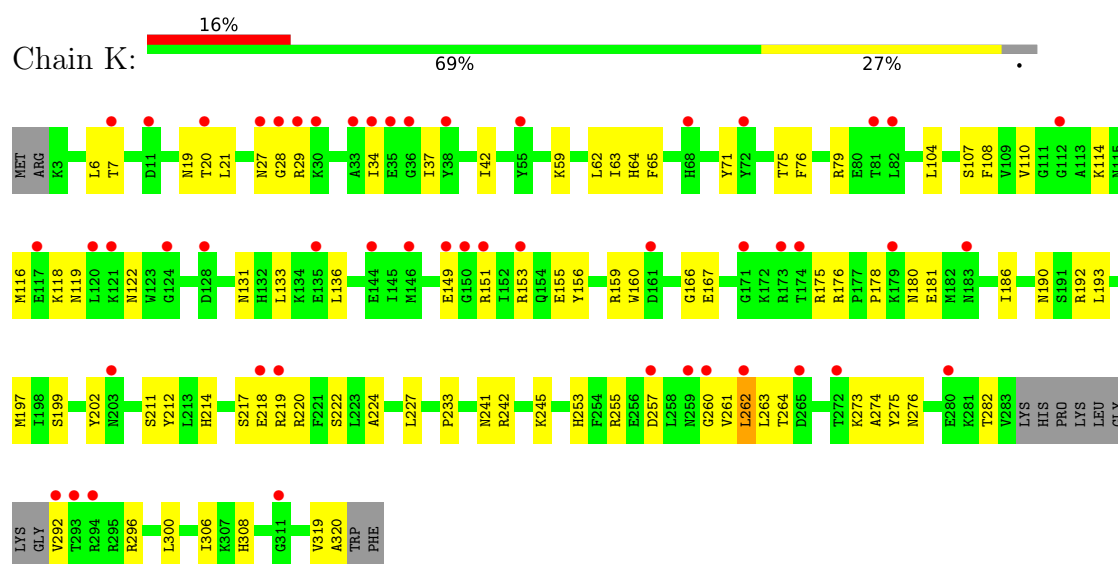
• Molecule 1: CRISPR-associated endonuclease Cas1



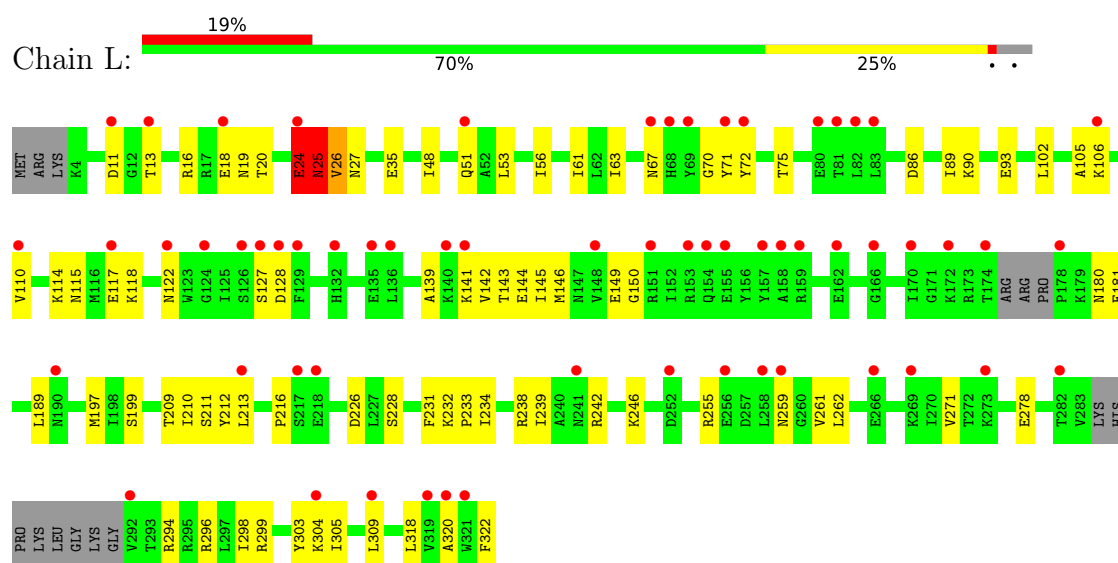
• Molecule 1: CRISPR-associated endonuclease Cas1



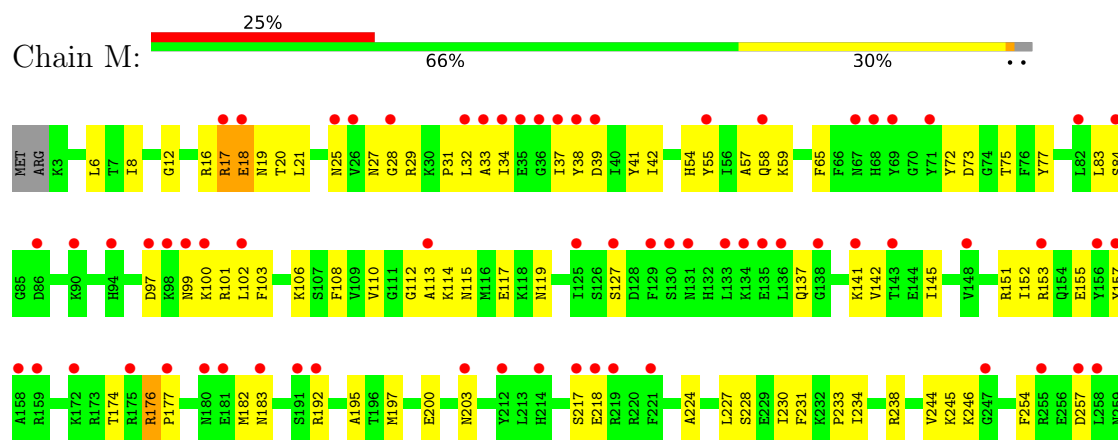
• Molecule 1: CRISPR-associated endonuclease Cas1

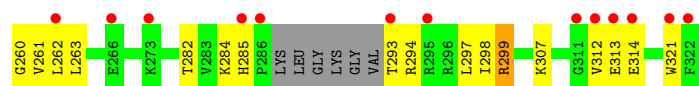


• Molecule 1: CRISPR-associated endonuclease Cas1

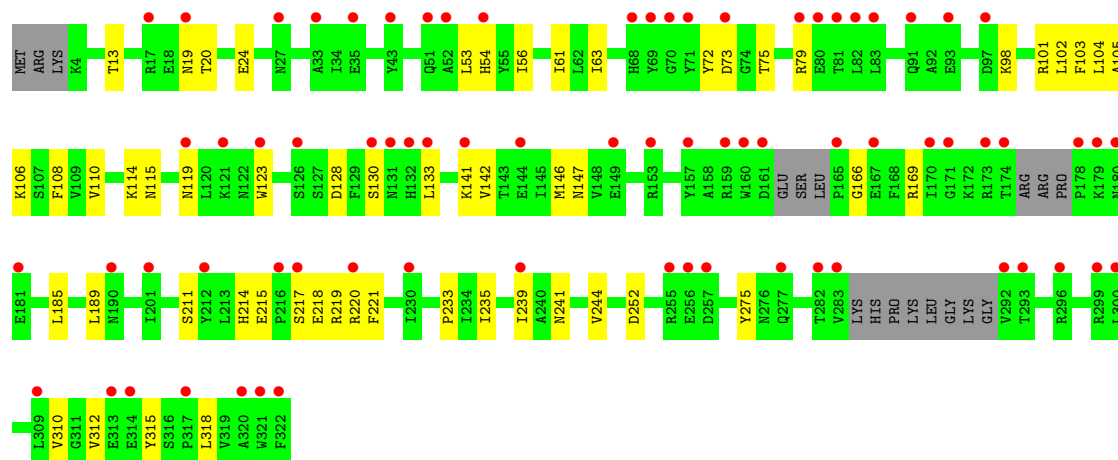
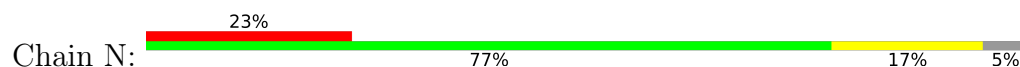


• Molecule 1: CRISPR-associated endonuclease Cas1

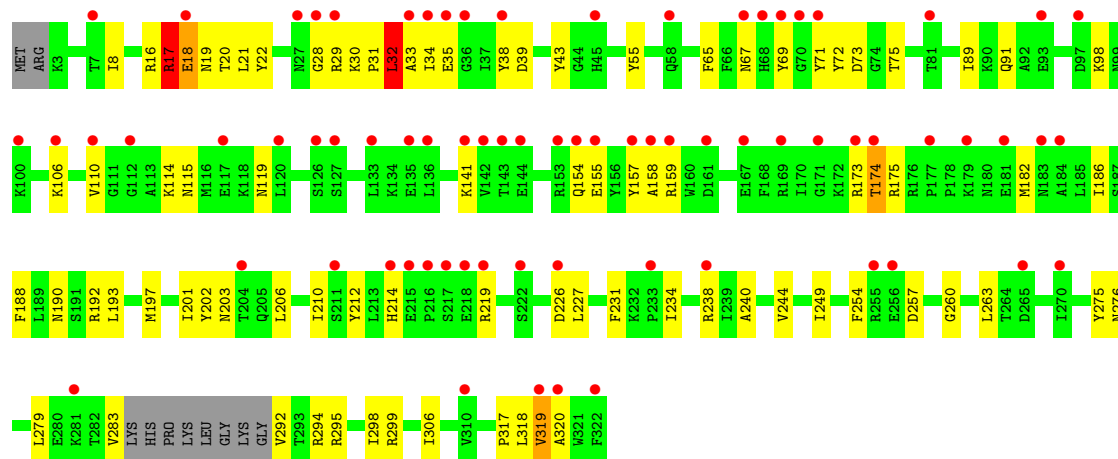




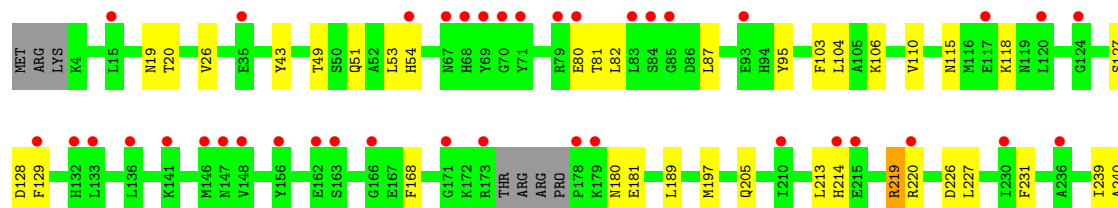
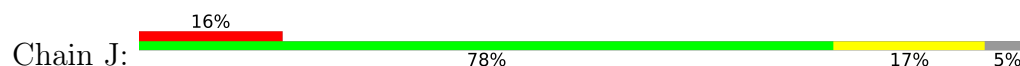
● Molecule 1: CRISPR-associated endonuclease Cas1

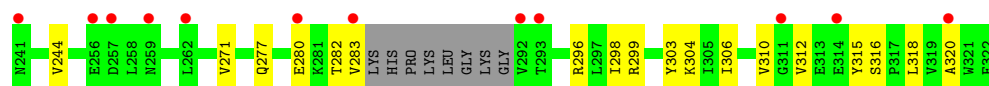


● Molecule 1: CRISPR-associated endonuclease Cas1

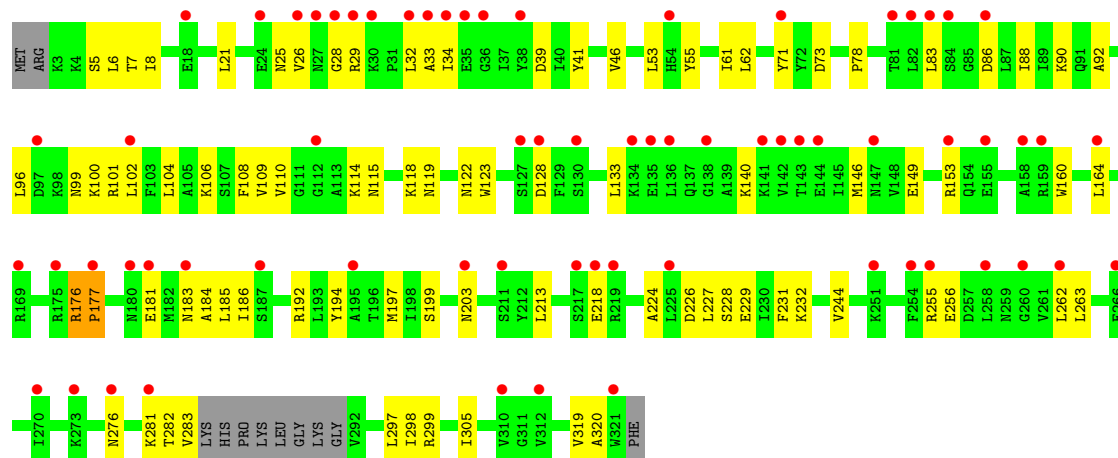


● Molecule 1: CRISPR-associated endonuclease Cas1

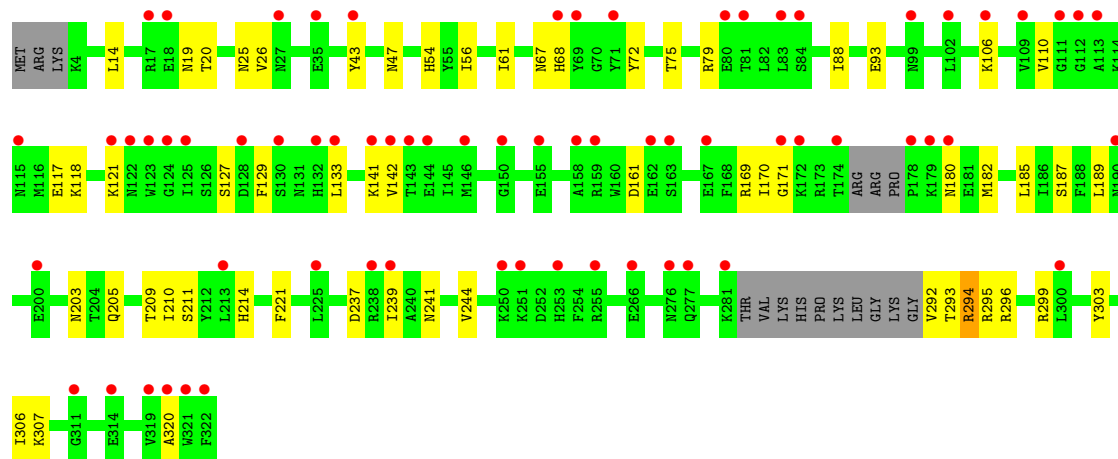
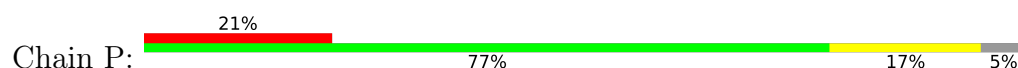




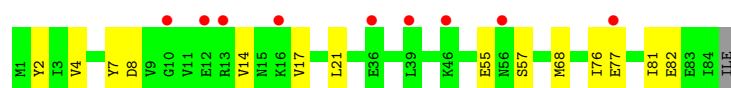
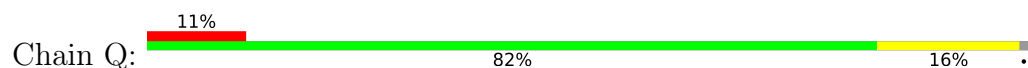
• Molecule 1: CRISPR-associated endonuclease Cas1



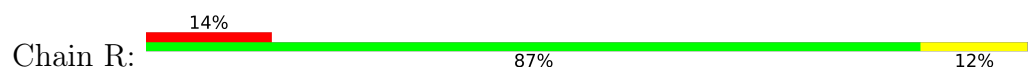
• Molecule 1: CRISPR-associated endonuclease Cas1



• Molecule 2: CRISPR-associated endonuclease Cas2

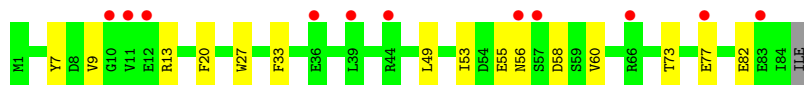
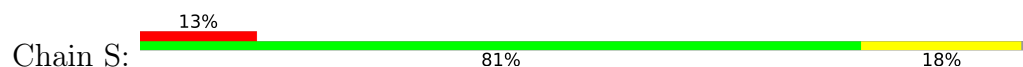


• Molecule 2: CRISPR-associated endonuclease Cas2

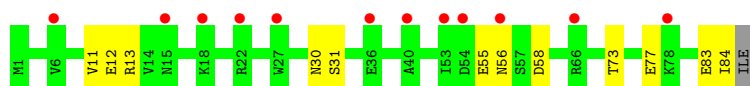
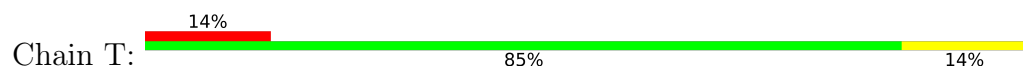




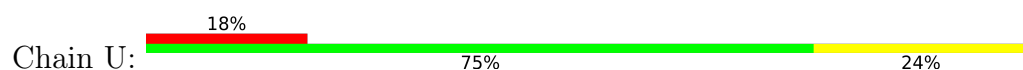
- Molecule 2: CRISPR-associated endoribonuclease Cas2



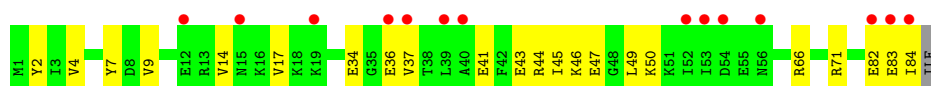
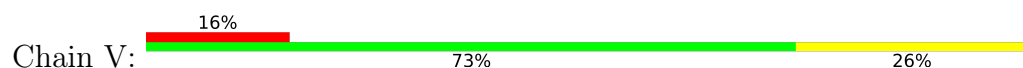
- Molecule 2: CRISPR-associated endoribonuclease Cas2



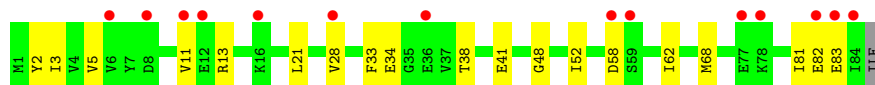
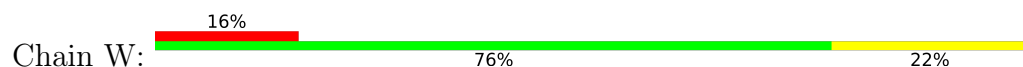
- Molecule 2: CRISPR-associated endoribonuclease Cas2



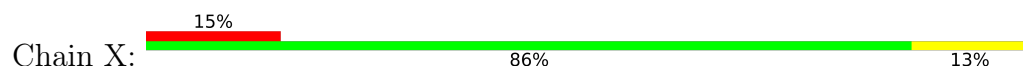
- Molecule 2: CRISPR-associated endoribonuclease Cas2



- Molecule 2: CRISPR-associated endoribonuclease Cas2



- Molecule 2: CRISPR-associated endoribonuclease Cas2



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 98.76Å 180.47Å 338.85Å<br>90.00° 94.43° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 36.53 – 3.90<br>36.53 – 3.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.4 (36.53-3.90)<br>93.6 (36.53-3.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.71 (at 3.87Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.15.2_3472                                          | Depositor        |
| R, $R_{free}$                                                           | 0.281 , 0.328<br>0.280 , 0.333                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 978 reflections (0.91%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.363                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 39.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.81                                                        | EDS              |
| Total number of atoms                                                   | 90949                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.18         | 0/2612         | 0.48        | 2/3517 (0.1%)   |
| 1   | B     | 0.16         | 0/2584         | 0.47        | 1/3478 (0.0%)   |
| 1   | C     | 0.19         | 0/2624         | 0.44        | 0/3533          |
| 1   | D     | 0.17         | 0/2584         | 0.47        | 2/3478 (0.1%)   |
| 1   | E     | 0.19         | 0/2624         | 0.46        | 1/3533 (0.0%)   |
| 1   | F     | 0.16         | 0/2584         | 0.44        | 0/3478          |
| 1   | G     | 0.16         | 0/2624         | 0.46        | 1/3533 (0.0%)   |
| 1   | H     | 0.16         | 0/2570         | 0.39        | 0/3458          |
| 1   | I     | 0.21         | 0/2624         | 0.53        | 2/3533 (0.1%)   |
| 1   | J     | 0.14         | 0/2577         | 0.36        | 0/3468          |
| 1   | K     | 0.19         | 0/2596         | 0.48        | 0/3494          |
| 1   | L     | 0.17         | 0/2584         | 0.45        | 1/3478 (0.0%)   |
| 1   | M     | 0.24         | 1/2645 (0.0%)  | 0.49        | 1/3561 (0.0%)   |
| 1   | N     | 0.14         | 0/2560         | 0.38        | 0/3443          |
| 1   | O     | 0.16         | 0/2612         | 0.43        | 0/3517          |
| 1   | P     | 0.13         | 0/2570         | 0.34        | 0/3458          |
| 2   | Q     | 0.15         | 0/704          | 0.36        | 0/947           |
| 2   | R     | 0.12         | 0/704          | 0.32        | 0/947           |
| 2   | S     | 0.14         | 0/704          | 0.33        | 0/947           |
| 2   | T     | 0.17         | 0/704          | 0.36        | 0/947           |
| 2   | U     | 0.13         | 0/704          | 0.39        | 0/947           |
| 2   | V     | 0.15         | 0/704          | 0.41        | 0/947           |
| 2   | W     | 0.13         | 0/704          | 0.38        | 0/947           |
| 2   | X     | 0.12         | 0/704          | 0.30        | 0/947           |
| All | All   | 0.17         | 1/47206 (0.0%) | 0.44        | 11/63536 (0.0%) |

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

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

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 3                   |
| 1   | E     | 0                   | 3                   |
| 1   | F     | 0                   | 1                   |
| 1   | G     | 0                   | 4                   |
| 1   | I     | 0                   | 2                   |
| 1   | J     | 0                   | 1                   |
| 1   | K     | 0                   | 1                   |
| 1   | L     | 0                   | 1                   |
| 1   | M     | 0                   | 2                   |
| 1   | O     | 0                   | 1                   |
| All | All   | 0                   | 21                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 299 | ARG  | CZ-NH2 | -5.23 | 1.26        | 1.33     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 18  | GLU  | N-CA-C     | 6.41  | 124.45      | 110.80   |
| 1   | E     | 31  | PRO  | N-CA-C     | 6.15  | 125.14      | 112.47   |
| 1   | D     | 261 | VAL  | CG1-CB-CG2 | 5.94  | 123.88      | 110.80   |
| 1   | L     | 25  | ASN  | N-CA-C     | 5.92  | 123.41      | 110.80   |
| 1   | B     | 127 | SER  | N-CA-C     | 5.62  | 122.77      | 110.80   |
| 1   | I     | 32  | LEU  | N-CA-C     | 5.54  | 122.60      | 110.80   |
| 1   | A     | 261 | VAL  | CG1-CB-CG2 | 5.44  | 122.78      | 110.80   |
| 1   | M     | 17  | ARG  | N-CA-C     | -5.34 | 99.42       | 110.80   |
| 1   | A     | 17  | ARG  | N-CA-C     | -5.31 | 101.47      | 109.60   |
| 1   | G     | 173 | ARG  | N-CA-C     | -5.28 | 99.56       | 110.80   |
| 1   | D     | 257 | ASP  | N-CA-C     | -5.21 | 99.70       | 110.80   |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 17  | ARG  | Peptide |
| 1   | C     | 17  | ARG  | Peptide |
| 1   | D     | 149 | GLU  | Peptide |
| 1   | D     | 24  | GLU  | Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 25  | ASN  | Peptide   |
| 1   | E     | 111 | GLY  | Peptide   |
| 1   | E     | 174 | THR  | Peptide   |
| 1   | E     | 31  | PRO  | Peptide   |
| 1   | F     | 216 | PRO  | Peptide   |
| 1   | G     | 17  | ARG  | Peptide   |
| 1   | G     | 172 | LYS  | Peptide   |
| 1   | G     | 18  | GLU  | Mainchain |
| 1   | G     | 257 | ASP  | Peptide   |
| 1   | I     | 17  | ARG  | Peptide   |
| 1   | I     | 174 | THR  | Peptide   |
| 1   | J     | 219 | ARG  | Peptide   |
| 1   | K     | 176 | ARG  | Peptide   |
| 1   | L     | 24  | GLU  | Peptide   |
| 1   | M     | 16  | ARG  | Peptide   |
| 1   | M     | 176 | ARG  | Peptide   |
| 1   | O     | 176 | ARG  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2559  | 2443     | 2609     | 75      | 0            |
| 1   | B     | 2532  | 2409     | 2572     | 76      | 1            |
| 1   | C     | 2570  | 2450     | 2618     | 103     | 0            |
| 1   | D     | 2532  | 2405     | 2572     | 74      | 1            |
| 1   | E     | 2570  | 2433     | 2618     | 90      | 0            |
| 1   | F     | 2532  | 2418     | 2572     | 66      | 1            |
| 1   | G     | 2570  | 2446     | 2618     | 69      | 0            |
| 1   | H     | 2518  | 2408     | 2556     | 46      | 1            |
| 1   | I     | 2570  | 2467     | 2618     | 81      | 0            |
| 1   | J     | 2525  | 2399     | 2565     | 40      | 1            |
| 1   | K     | 2545  | 2467     | 2599     | 75      | 0            |
| 1   | L     | 2532  | 2426     | 2572     | 69      | 1            |
| 1   | M     | 2589  | 2481     | 2636     | 104     | 0            |
| 1   | N     | 2509  | 2396     | 2550     | 44      | 1            |
| 1   | O     | 2559  | 2465     | 2609     | 85      | 0            |
| 1   | P     | 2518  | 2419     | 2556     | 49      | 1            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | Q     | 693   | 708      | 721      | 11      | 0            |
| 2   | R     | 693   | 720      | 721      | 9       | 0            |
| 2   | S     | 693   | 720      | 721      | 11      | 0            |
| 2   | T     | 693   | 720      | 721      | 9       | 0            |
| 2   | U     | 693   | 719      | 721      | 18      | 0            |
| 2   | V     | 693   | 718      | 721      | 17      | 0            |
| 2   | W     | 693   | 720      | 721      | 15      | 0            |
| 2   | X     | 693   | 718      | 721      | 9       | 0            |
| All | All   | 46274 | 44675    | 47208    | 1155    | 4            |

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 12.

All (1155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:4:LYS:NZ     | 2:Q:77:GLU:OE2   | 1.74                     | 1.21              |
| 1:K:133:LEU:O    | 1:K:136:LEU:CD2  | 1.99                     | 1.10              |
| 1:L:278:GLU:OE2  | 1:L:294:ARG:NH1  | 1.85                     | 1.09              |
| 1:K:133:LEU:O    | 1:K:136:LEU:HD22 | 1.55                     | 1.06              |
| 1:M:38:TYR:OH    | 1:M:299:ARG:NH1  | 1.88                     | 1.06              |
| 1:K:6:LEU:HD12   | 1:K:37:ILE:HD13  | 1.40                     | 1.01              |
| 1:C:28:GLY:C     | 1:C:29:ARG:HD3   | 1.87                     | 1.00              |
| 1:K:6:LEU:CD1    | 1:K:37:ILE:HD13  | 1.92                     | 0.99              |
| 1:M:38:TYR:OH    | 1:M:299:ARG:CZ   | 2.16                     | 0.94              |
| 1:B:163:SER:O    | 1:B:245:LYS:NZ   | 2.01                     | 0.93              |
| 1:O:71:TYR:HE2   | 1:P:79:ARG:NH1   | 1.66                     | 0.93              |
| 1:M:203:ASN:CG   | 1:M:299:ARG:NH1  | 2.25                     | 0.92              |
| 1:L:189:LEU:HD22 | 1:L:239:ILE:HD11 | 1.51                     | 0.92              |
| 1:M:72:TYR:OH    | 1:M:75:THR:OG1   | 1.87                     | 0.91              |
| 1:C:115:ASN:ND2  | 1:C:319:VAL:O    | 2.03                     | 0.90              |
| 2:X:83:GLU:OE2   | 1:O:276:ASN:ND2  | 2.04                     | 0.90              |
| 1:L:16:ARG:NH1   | 1:L:18:GLU:O     | 2.04                     | 0.89              |
| 1:L:25:ASN:O     | 1:L:27:ASN:N     | 2.04                     | 0.89              |
| 1:K:133:LEU:O    | 1:K:136:LEU:HD23 | 1.73                     | 0.88              |
| 1:A:17:ARG:O     | 1:A:18:GLU:O     | 1.92                     | 0.87              |
| 1:H:189:LEU:HD22 | 1:H:239:ILE:HD11 | 1.57                     | 0.87              |
| 1:M:284:LYS:O    | 1:M:285:HIS:ND1  | 2.08                     | 0.86              |
| 1:O:153:ARG:NH2  | 1:O:229:GLU:OE1  | 2.08                     | 0.86              |
| 1:H:189:LEU:CD2  | 1:H:239:ILE:HD11 | 2.05                     | 0.86              |
| 1:A:115:ASN:ND2  | 1:A:319:VAL:O    | 2.09                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:54:HIS:ND1   | 1:N:73:ASP:OD1   | 2.08                     | 0.84              |
| 1:H:219:ARG:HG3  | 1:H:219:ARG:HH11 | 1.39                     | 0.84              |
| 1:M:17:ARG:O     | 1:M:18:GLU:O     | 1.96                     | 0.83              |
| 1:O:115:ASN:ND2  | 1:O:319:VAL:O    | 2.10                     | 0.83              |
| 1:H:239:ILE:HD12 | 1:H:240:ALA:N    | 1.93                     | 0.83              |
| 1:F:190:ASN:OD1  | 1:F:232:LYS:NZ   | 2.10                     | 0.83              |
| 1:A:87:LEU:HD21  | 1:A:309:LEU:HD23 | 1.59                     | 0.83              |
| 1:B:163:SER:OG   | 1:B:245:LYS:NZ   | 2.11                     | 0.83              |
| 1:E:39:ASP:OD2   | 1:E:41:TYR:OH    | 1.96                     | 0.83              |
| 1:K:28:GLY:O     | 1:K:29:ARG:HG3   | 1.77                     | 0.83              |
| 1:O:73:ASP:OD2   | 1:P:54:HIS:ND1   | 2.11                     | 0.83              |
| 2:X:34:GLU:OE2   | 2:X:71:ARG:NH2   | 2.11                     | 0.83              |
| 1:M:102:LEU:HD12 | 1:M:103:PHE:N    | 1.94                     | 0.82              |
| 1:H:128:ASP:O    | 1:H:130:SER:N    | 2.13                     | 0.81              |
| 1:N:72:TYR:OH    | 1:N:75:THR:OG1   | 1.98                     | 0.81              |
| 1:O:28:GLY:C     | 1:O:29:ARG:HD3   | 2.05                     | 0.81              |
| 1:A:120:LEU:CD2  | 1:A:125:ILE:HB   | 2.11                     | 0.81              |
| 1:E:219:ARG:HB3  | 1:F:81:THR:HG21  | 1.60                     | 0.81              |
| 1:G:17:ARG:O     | 1:G:18:GLU:O     | 1.97                     | 0.81              |
| 1:C:176:ARG:HB2  | 1:G:258:LEU:HD21 | 1.61                     | 0.81              |
| 1:M:102:LEU:HD12 | 1:M:103:PHE:H    | 1.45                     | 0.81              |
| 1:A:72:TYR:HH    | 1:A:75:THR:HG1   | 1.04                     | 0.81              |
| 1:B:119:ASN:ND2  | 1:B:233:PRO:O    | 2.15                     | 0.80              |
| 1:G:257:ASP:O    | 1:G:258:LEU:HD12 | 1.82                     | 0.80              |
| 1:C:219:ARG:HB3  | 1:D:81:THR:HG21  | 1.65                     | 0.79              |
| 1:M:203:ASN:CG   | 1:M:299:ARG:HH12 | 1.91                     | 0.79              |
| 1:D:189:LEU:HD13 | 1:D:239:ILE:HD11 | 1.64                     | 0.79              |
| 2:W:13:ARG:NH2   | 2:W:58:ASP:OD2   | 2.16                     | 0.79              |
| 1:L:72:TYR:OH    | 1:L:75:THR:OG1   | 2.00                     | 0.79              |
| 1:P:118:LYS:HE3  | 1:P:320:ALA:O    | 1.83                     | 0.79              |
| 1:O:6:LEU:HD23   | 1:O:7:THR:N      | 1.97                     | 0.78              |
| 1:O:71:TYR:CE2   | 1:P:79:ARG:NH1   | 2.52                     | 0.78              |
| 1:O:118:LYS:O    | 1:O:122:ASN:ND2  | 2.17                     | 0.78              |
| 1:I:234:ILE:O    | 1:I:238:ARG:NE   | 2.16                     | 0.77              |
| 1:E:34:ILE:HD11  | 1:E:55:TYR:CE2   | 2.20                     | 0.77              |
| 1:F:161:ASP:O    | 1:F:169:ARG:NH1  | 2.17                     | 0.77              |
| 1:N:106:LYS:O    | 1:N:110:VAL:HG23 | 1.84                     | 0.77              |
| 1:L:19:ASN:O     | 1:L:20:THR:OG1   | 2.02                     | 0.77              |
| 1:A:178:PRO:O    | 1:A:261:VAL:HG22 | 1.86                     | 0.75              |
| 1:B:189:LEU:HD13 | 1:B:239:ILE:HD11 | 1.68                     | 0.75              |
| 1:B:219:ARG:HG3  | 1:B:219:ARG:HH11 | 1.51                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:38:TYR:CE2   | 1:M:299:ARG:NH2  | 2.54                     | 0.75              |
| 1:M:174:THR:O    | 1:M:183:ASN:ND2  | 2.18                     | 0.75              |
| 1:A:186:ILE:O    | 1:A:190:ASN:ND2  | 2.20                     | 0.75              |
| 2:T:83:GLU:OE1   | 1:K:276:ASN:ND2  | 2.19                     | 0.75              |
| 1:I:73:ASP:OD2   | 1:J:54:HIS:ND1   | 2.20                     | 0.75              |
| 1:H:86:ASP:O     | 1:H:90:LYS:HG2   | 1.87                     | 0.75              |
| 1:F:161:ASP:HA   | 1:F:164:LEU:HD21 | 1.68                     | 0.74              |
| 1:K:257:ASP:OD1  | 1:K:260:GLY:N    | 2.20                     | 0.74              |
| 1:N:19:ASN:O     | 1:N:20:THR:OG1   | 2.06                     | 0.74              |
| 1:A:219:ARG:HB2  | 1:B:81:THR:OG1   | 1.89                     | 0.73              |
| 1:C:126:SER:O    | 1:C:159:ARG:NE   | 2.22                     | 0.73              |
| 1:C:67:ASN:OD1   | 1:C:176:ARG:NH2  | 2.20                     | 0.73              |
| 1:C:119:ASN:ND2  | 1:C:233:PRO:O    | 2.22                     | 0.73              |
| 1:E:115:ASN:ND2  | 1:E:319:VAL:O    | 2.21                     | 0.73              |
| 1:M:21:LEU:HB3   | 1:M:32:LEU:HD22  | 1.71                     | 0.73              |
| 1:D:119:ASN:ND2  | 1:D:233:PRO:O    | 2.21                     | 0.73              |
| 1:I:28:GLY:O     | 1:I:29:ARG:HG3   | 1.88                     | 0.73              |
| 1:I:19:ASN:O     | 1:I:20:THR:HG23  | 1.89                     | 0.72              |
| 1:A:170:ILE:O    | 1:A:170:ILE:HD12 | 1.89                     | 0.72              |
| 1:G:224:ALA:O    | 1:G:228:SER:OG   | 2.05                     | 0.72              |
| 1:A:25:ASN:OD1   | 1:A:25:ASN:N     | 2.22                     | 0.72              |
| 1:M:200:GLU:HB3  | 1:M:299:ARG:HG2  | 1.71                     | 0.72              |
| 1:H:114:LYS:O    | 1:H:118:LYS:HG2  | 1.90                     | 0.72              |
| 1:E:32:LEU:HD21  | 1:E:37:ILE:HD11  | 1.70                     | 0.71              |
| 1:F:174:THR:OG1  | 1:F:179:LYS:O    | 2.08                     | 0.71              |
| 1:C:19:ASN:O     | 1:C:20:THR:OG1   | 2.06                     | 0.71              |
| 1:N:110:VAL:HG12 | 1:N:114:LYS:HD2  | 1.70                     | 0.71              |
| 1:J:213:LEU:N    | 1:J:226:ASP:OD2  | 2.23                     | 0.71              |
| 1:F:72:TYR:HH    | 1:F:75:THR:HG1   | 1.33                     | 0.71              |
| 1:B:70:GLY:O     | 1:B:199:SER:OG   | 2.07                     | 0.71              |
| 1:F:163:SER:OG   | 1:F:245:LYS:NZ   | 2.24                     | 0.71              |
| 1:J:189:LEU:HD22 | 1:J:239:ILE:HD11 | 1.72                     | 0.71              |
| 1:P:43:TYR:OH    | 1:P:299:ARG:NH2  | 2.24                     | 0.71              |
| 1:P:141:LYS:NZ   | 1:P:142:VAL:HG12 | 2.06                     | 0.70              |
| 1:C:28:GLY:O     | 1:C:29:ARG:HD3   | 1.92                     | 0.70              |
| 1:J:115:ASN:ND2  | 1:J:318:LEU:O    | 2.24                     | 0.70              |
| 1:C:6:LEU:CD1    | 1:C:37:ILE:HG12  | 2.22                     | 0.70              |
| 1:C:6:LEU:HD12   | 1:C:37:ILE:HG12  | 1.72                     | 0.70              |
| 1:L:141:LYS:HG2  | 1:L:142:VAL:H    | 1.57                     | 0.69              |
| 1:P:293:THR:O    | 1:P:296:ARG:N    | 2.21                     | 0.69              |
| 2:Q:82:GLU:OE1   | 2:Q:82:GLU:N     | 2.25                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:197:MET:HE3  | 1:K:227:LEU:HB3  | 1.74                     | 0.69              |
| 1:K:211:SER:OG   | 1:K:214:HIS:O    | 2.09                     | 0.69              |
| 1:L:35:GLU:N     | 1:L:35:GLU:OE1   | 2.24                     | 0.69              |
| 1:D:211:SER:OG   | 1:D:214:HIS:O    | 2.07                     | 0.69              |
| 1:G:174:THR:N    | 1:G:183:ASN:OD1  | 2.26                     | 0.69              |
| 1:C:6:LEU:HD12   | 1:C:37:ILE:CG1   | 2.22                     | 0.68              |
| 1:D:180:ASN:OD1  | 1:D:181:GLU:N    | 2.26                     | 0.68              |
| 1:J:189:LEU:HD21 | 1:J:271:VAL:CG1  | 2.22                     | 0.68              |
| 1:A:197:MET:HE3  | 1:A:227:LEU:HB3  | 1.76                     | 0.68              |
| 2:S:13:ARG:NH2   | 2:S:58:ASP:OD2   | 2.26                     | 0.68              |
| 1:K:21:LEU:CD1   | 1:K:34:ILE:HD12  | 2.24                     | 0.68              |
| 1:D:162:GLU:N    | 1:D:162:GLU:OE2  | 2.27                     | 0.67              |
| 1:D:301:GLU:OE1  | 1:D:304:LYS:NZ   | 2.27                     | 0.67              |
| 1:H:239:ILE:HD12 | 1:H:239:ILE:C    | 2.19                     | 0.67              |
| 1:I:318:LEU:O    | 1:I:320:ALA:N    | 2.26                     | 0.67              |
| 2:R:66:ARG:O     | 1:I:29:ARG:NH1   | 2.27                     | 0.67              |
| 1:E:161:ASP:OD2  | 1:E:170:ILE:N    | 2.28                     | 0.67              |
| 1:D:19:ASN:O     | 1:D:20:THR:OG1   | 2.12                     | 0.66              |
| 1:D:189:LEU:CD1  | 1:D:239:ILE:HD11 | 2.24                     | 0.66              |
| 1:P:19:ASN:O     | 1:P:20:THR:OG1   | 2.12                     | 0.66              |
| 1:I:91:GLN:NE2   | 1:I:210:ILE:O    | 2.29                     | 0.66              |
| 1:E:119:ASN:ND2  | 1:E:233:PRO:O    | 2.27                     | 0.66              |
| 1:J:127:SER:OG   | 1:J:128:ASP:N    | 2.29                     | 0.66              |
| 1:J:106:LYS:O    | 1:J:110:VAL:HG22 | 1.95                     | 0.66              |
| 1:L:238:ARG:HH11 | 1:L:278:GLU:HG3  | 1.60                     | 0.66              |
| 1:B:115:ASN:ND2  | 1:B:318:LEU:O    | 2.29                     | 0.65              |
| 1:D:132:HIS:NE2  | 1:D:155:GLU:OE2  | 2.29                     | 0.65              |
| 1:H:219:ARG:HH11 | 1:H:219:ARG:CG   | 2.08                     | 0.65              |
| 2:T:83:GLU:OE1   | 1:K:276:ASN:CG   | 2.39                     | 0.65              |
| 1:L:239:ILE:HA   | 1:L:242:ARG:HD2  | 1.77                     | 0.65              |
| 1:M:203:ASN:ND2  | 1:M:299:ARG:HH12 | 1.94                     | 0.65              |
| 1:M:72:TYR:HH    | 1:M:75:THR:HG1   | 1.38                     | 0.65              |
| 1:B:311:GLY:O    | 1:E:147:ASN:ND2  | 2.28                     | 0.65              |
| 1:F:92:ALA:O     | 1:F:95:TYR:N     | 2.28                     | 0.65              |
| 1:M:203:ASN:CB   | 1:M:299:ARG:HH11 | 2.10                     | 0.65              |
| 1:F:194:TYR:OH   | 1:F:220:ARG:O    | 2.14                     | 0.65              |
| 1:I:214:HIS:ND1  | 1:I:226:ASP:OD1  | 2.30                     | 0.65              |
| 1:H:199:SER:O    | 1:H:203:ASN:N    | 2.30                     | 0.65              |
| 1:A:18:GLU:HG2   | 1:A:19:ASN:N     | 2.12                     | 0.64              |
| 1:C:215:GLU:O    | 1:C:220:ARG:NH1  | 2.29                     | 0.64              |
| 1:D:114:LYS:O    | 1:D:118:LYS:HG2  | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:170:ILE:O    | 1:A:170:ILE:CD1  | 2.45                     | 0.64              |
| 1:F:118:LYS:HG2  | 1:F:320:ALA:O    | 1.97                     | 0.64              |
| 1:P:292:VAL:HG11 | 1:P:296:ARG:NH2  | 2.12                     | 0.64              |
| 1:F:299:ARG:O    | 1:F:303:TYR:N    | 2.29                     | 0.64              |
| 1:A:18:GLU:O     | 1:A:20:THR:N     | 2.29                     | 0.64              |
| 2:U:34:GLU:OE2   | 2:U:71:ARG:NH1   | 2.30                     | 0.64              |
| 1:P:106:LYS:O    | 1:P:110:VAL:HG23 | 1.96                     | 0.64              |
| 1:C:176:ARG:CB   | 1:G:258:LEU:HD21 | 2.26                     | 0.64              |
| 1:O:110:VAL:HG22 | 1:O:133:LEU:HD11 | 1.80                     | 0.64              |
| 1:D:98:LYS:HZ3   | 1:D:141:LYS:HZ2  | 1.44                     | 0.63              |
| 1:E:83:LEU:HD21  | 1:F:221:PHE:CE1  | 2.33                     | 0.63              |
| 1:L:26:VAL:O     | 1:L:27:ASN:OD1   | 2.17                     | 0.63              |
| 2:V:43:GLU:O     | 2:V:47:GLU:N     | 2.28                     | 0.63              |
| 1:M:115:ASN:HB3  | 1:M:233:PRO:HB2  | 1.79                     | 0.63              |
| 1:B:102:LEU:HD21 | 1:B:140:LYS:O    | 1.99                     | 0.63              |
| 1:M:83:LEU:HD21  | 1:N:221:PHE:CE1  | 2.33                     | 0.63              |
| 1:M:200:GLU:OE1  | 1:M:299:ARG:NE   | 2.31                     | 0.63              |
| 1:B:173:ARG:O    | 1:B:174:THR:OG1  | 2.15                     | 0.63              |
| 1:F:186:ILE:O    | 1:F:190:ASN:ND2  | 2.31                     | 0.63              |
| 1:N:13:THR:N     | 1:N:24:GLU:O     | 2.31                     | 0.63              |
| 1:A:178:PRO:HD2  | 1:A:261:VAL:HG21 | 1.81                     | 0.62              |
| 1:K:217:SER:OG   | 1:K:220:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:19:ASN:O     | 1:A:20:THR:HG23  | 1.99                     | 0.62              |
| 1:B:98:LYS:O     | 1:B:102:LEU:HD13 | 2.00                     | 0.62              |
| 1:M:38:TYR:HE2   | 1:M:299:ARG:NH2  | 1.97                     | 0.62              |
| 1:L:189:LEU:HD21 | 1:L:271:VAL:CG1  | 2.30                     | 0.62              |
| 1:H:189:LEU:HD21 | 1:H:239:ILE:HD11 | 1.82                     | 0.62              |
| 1:C:218:GLU:OE2  | 1:D:205:GLN:HG2  | 1.99                     | 0.62              |
| 1:P:72:TYR:HH    | 1:P:75:THR:HG1   | 1.35                     | 0.62              |
| 1:G:257:ASP:O    | 1:G:258:LEU:CD1  | 2.48                     | 0.61              |
| 1:F:120:LEU:HD13 | 1:F:127:SER:HB3  | 1.82                     | 0.61              |
| 1:A:87:LEU:CD2   | 1:A:309:LEU:HD23 | 2.29                     | 0.61              |
| 1:K:6:LEU:HD13   | 1:K:37:ILE:HD13  | 1.80                     | 0.61              |
| 1:C:139:ALA:HB1  | 1:C:144:GLU:HB3  | 1.81                     | 0.61              |
| 1:C:219:ARG:HB2  | 1:D:81:THR:OG1   | 1.99                     | 0.61              |
| 1:H:219:ARG:HG3  | 1:H:219:ARG:NH1  | 2.14                     | 0.61              |
| 1:L:118:LYS:HG2  | 1:L:320:ALA:O    | 2.01                     | 0.61              |
| 1:N:130:SER:O    | 1:N:133:LEU:N    | 2.29                     | 0.61              |
| 1:P:141:LYS:HZ3  | 1:P:142:VAL:HG12 | 1.66                     | 0.61              |
| 1:E:131:ASN:OD1  | 1:E:132:HIS:N    | 2.34                     | 0.60              |
| 1:M:203:ASN:CB   | 1:M:299:ARG:NH1  | 2.63                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:169:ARG:O    | 1:D:180:ASN:ND2  | 2.35                     | 0.60              |
| 1:B:219:ARG:HG3  | 1:B:219:ARG:NH1  | 2.14                     | 0.60              |
| 1:B:249:ILE:HG12 | 1:B:253:HIS:HD2  | 1.65                     | 0.60              |
| 1:G:301:GLU:OE2  | 1:G:315:TYR:OH   | 2.09                     | 0.60              |
| 1:P:67:ASN:OD1   | 1:P:68:HIS:N     | 2.33                     | 0.60              |
| 1:B:43:TYR:HB3   | 1:B:66:PHE:HB2   | 1.83                     | 0.60              |
| 1:O:197:MET:HE1  | 1:O:231:PHE:CD1  | 2.36                     | 0.60              |
| 1:P:117:GLU:HG2  | 1:P:127:SER:HB2  | 1.83                     | 0.60              |
| 1:B:189:LEU:CD1  | 1:B:239:ILE:HD11 | 2.31                     | 0.60              |
| 1:M:115:ASN:O    | 1:M:119:ASN:N    | 2.34                     | 0.60              |
| 1:E:118:LYS:HG3  | 1:E:122:ASN:ND2  | 2.17                     | 0.60              |
| 1:J:180:ASN:OD1  | 1:J:181:GLU:N    | 2.30                     | 0.59              |
| 1:H:132:HIS:CE1  | 1:H:151:ARG:HG2  | 2.37                     | 0.59              |
| 1:M:19:ASN:O     | 1:M:20:THR:OG1   | 2.19                     | 0.59              |
| 1:G:174:THR:HG21 | 1:G:179:LYS:H    | 1.66                     | 0.59              |
| 1:H:219:ARG:CG   | 1:H:219:ARG:NH1  | 2.62                     | 0.59              |
| 1:F:19:ASN:O     | 1:F:20:THR:OG1   | 2.16                     | 0.59              |
| 1:H:180:ASN:OD1  | 1:H:181:GLU:N    | 2.33                     | 0.59              |
| 1:K:180:ASN:OD1  | 1:K:181:GLU:N    | 2.34                     | 0.59              |
| 1:I:283:VAL:CG1  | 1:I:292:VAL:HG12 | 2.33                     | 0.59              |
| 1:I:158:ALA:C    | 1:I:159:ARG:HE   | 2.10                     | 0.59              |
| 2:V:34:GLU:OE1   | 2:V:71:ARG:NH2   | 2.36                     | 0.59              |
| 1:M:285:HIS:HB2  | 1:M:321:TRP:CZ2  | 2.38                     | 0.59              |
| 1:O:86:ASP:O     | 1:O:90:LYS:HG2   | 2.03                     | 0.59              |
| 1:E:296:ARG:C    | 1:E:296:ARG:HD3  | 2.28                     | 0.58              |
| 1:B:201:ILE:HD11 | 1:B:227:LEU:CD1  | 2.33                     | 0.58              |
| 1:N:103:PHE:O    | 1:N:104:LEU:HB2  | 2.03                     | 0.58              |
| 1:K:156:TYR:O    | 1:K:160:TRP:N    | 2.37                     | 0.58              |
| 1:H:17:ARG:NH1   | 1:H:29:ARG:HH12  | 2.01                     | 0.58              |
| 1:I:283:VAL:HG11 | 1:I:292:VAL:HG12 | 1.85                     | 0.58              |
| 1:C:6:LEU:CD1    | 1:C:37:ILE:CD1   | 2.82                     | 0.58              |
| 1:H:106:LYS:O    | 1:H:110:VAL:HG23 | 2.02                     | 0.58              |
| 1:M:39:ASP:OD2   | 1:M:41:TYR:OH    | 2.10                     | 0.58              |
| 1:K:197:MET:HB3  | 1:K:224:ALA:HB1  | 1.84                     | 0.58              |
| 1:O:92:ALA:O     | 1:O:96:LEU:HD12  | 2.04                     | 0.58              |
| 1:M:28:GLY:O     | 1:M:29:ARG:HG3   | 2.04                     | 0.58              |
| 1:N:211:SER:OG   | 1:N:214:HIS:O    | 2.19                     | 0.58              |
| 1:M:203:ASN:HB3  | 1:M:299:ARG:HH11 | 1.69                     | 0.58              |
| 1:E:33:ALA:HB2   | 2:U:70:PRO:HB3   | 1.86                     | 0.58              |
| 1:K:34:ILE:HD11  | 1:K:59:LYS:HG3   | 1.86                     | 0.58              |
| 1:B:6:LEU:HD21   | 1:B:40:ILE:HG12  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:55:TYR:O     | 1:M:58:GLN:N     | 2.37                     | 0.57              |
| 1:M:257:ASP:OD1  | 1:M:260:GLY:N    | 2.37                     | 0.57              |
| 1:P:72:TYR:OH    | 1:P:75:THR:OG1   | 2.13                     | 0.57              |
| 1:C:6:LEU:CD1    | 1:C:37:ILE:HD11  | 2.35                     | 0.57              |
| 2:R:39:LEU:O     | 2:R:39:LEU:HD23  | 2.04                     | 0.57              |
| 1:A:72:TYR:OH    | 1:A:75:THR:OG1   | 1.98                     | 0.57              |
| 2:S:13:ARG:NH1   | 2:S:58:ASP:OD2   | 2.37                     | 0.57              |
| 1:K:19:ASN:O     | 1:K:20:THR:HG23  | 2.05                     | 0.57              |
| 1:L:26:VAL:O     | 1:L:27:ASN:CG    | 2.47                     | 0.57              |
| 1:O:283:VAL:HG21 | 1:O:297:LEU:HD11 | 1.87                     | 0.57              |
| 1:A:101:ARG:NH2  | 1:A:142:VAL:HG21 | 2.18                     | 0.57              |
| 1:H:72:TYR:OH    | 1:H:75:THR:OG1   | 2.16                     | 0.57              |
| 1:L:122:ASN:ND2  | 1:L:322:PHE:O    | 2.38                     | 0.57              |
| 1:O:71:TYR:HE2   | 1:P:79:ARG:HH12  | 1.52                     | 0.57              |
| 1:C:87:LEU:HD23  | 1:C:87:LEU:O     | 2.04                     | 0.57              |
| 1:J:103:PHE:O    | 1:J:104:LEU:HB2  | 2.04                     | 0.57              |
| 1:C:29:ARG:HH11  | 1:C:29:ARG:HG2   | 1.69                     | 0.57              |
| 1:L:232:LYS:HG2  | 1:L:233:PRO:HD3  | 1.87                     | 0.57              |
| 1:N:141:LYS:HG2  | 1:N:142:VAL:H    | 1.68                     | 0.57              |
| 1:C:7:THR:HG21   | 1:C:192:ARG:NH2  | 2.20                     | 0.57              |
| 1:G:19:ASN:O     | 1:G:20:THR:HG23  | 2.05                     | 0.57              |
| 1:K:118:LYS:O    | 1:K:122:ASN:ND2  | 2.35                     | 0.57              |
| 1:N:185:LEU:O    | 1:N:189:LEU:HD12 | 2.04                     | 0.57              |
| 1:F:72:TYR:OH    | 1:F:75:THR:OG1   | 2.06                     | 0.56              |
| 1:A:157:TYR:HB3  | 1:A:170:ILE:HD13 | 1.86                     | 0.56              |
| 1:M:203:ASN:CG   | 1:M:299:ARG:HH11 | 2.09                     | 0.56              |
| 1:C:28:GLY:O     | 1:C:29:ARG:NH1   | 2.37                     | 0.56              |
| 1:E:54:HIS:HD1   | 1:F:73:ASP:CG    | 2.13                     | 0.56              |
| 1:C:182:MET:HE1  | 1:C:240:ALA:HB1  | 1.87                     | 0.56              |
| 1:E:54:HIS:ND1   | 1:F:73:ASP:OD2   | 2.37                     | 0.56              |
| 1:K:218:GLU:HB2  | 1:L:86:ASP:HA    | 1.87                     | 0.56              |
| 1:F:140:LYS:HD2  | 1:F:141:LYS:CE   | 2.36                     | 0.56              |
| 1:O:115:ASN:O    | 1:O:119:ASN:N    | 2.37                     | 0.56              |
| 1:D:10:SER:HB3   | 1:D:26:VAL:HG21  | 1.86                     | 0.56              |
| 1:K:104:LEU:HD13 | 1:K:212:TYR:CE1  | 2.41                     | 0.56              |
| 1:G:7:THR:HG21   | 1:G:192:ARG:NH2  | 2.21                     | 0.56              |
| 1:G:74:GLY:HA3   | 1:H:78:PRO:HA    | 1.87                     | 0.56              |
| 2:R:67:SER:HB3   | 1:I:29:ARG:HD3   | 1.87                     | 0.56              |
| 2:V:37:VAL:HB    | 2:V:41:GLU:OE1   | 2.06                     | 0.56              |
| 2:V:66:ARG:O     | 1:M:29:ARG:NH1   | 2.39                     | 0.56              |
| 1:L:189:LEU:HD21 | 1:L:271:VAL:HG13 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:296:ARG:O    | 1:B:299:ARG:N    | 2.39                     | 0.56              |
| 1:A:34:ILE:HG13  | 1:A:35:GLU:H     | 1.69                     | 0.56              |
| 1:M:38:TYR:CZ    | 1:M:299:ARG:NH2  | 2.73                     | 0.56              |
| 1:M:203:ASN:OD1  | 1:M:299:ARG:NH1  | 2.38                     | 0.56              |
| 1:E:83:LEU:HD21  | 1:F:221:PHE:HE1  | 1.70                     | 0.55              |
| 1:I:155:GLU:O    | 1:I:159:ARG:HG2  | 2.06                     | 0.55              |
| 1:O:6:LEU:HD22   | 1:O:8:ILE:HG23   | 1.88                     | 0.55              |
| 1:L:117:GLU:HG3  | 1:L:127:SER:HB2  | 1.87                     | 0.55              |
| 1:L:146:MET:O    | 1:L:149:GLU:N    | 2.39                     | 0.55              |
| 1:J:197:MET:HE1  | 1:J:227:LEU:HD22 | 1.89                     | 0.55              |
| 1:E:186:ILE:O    | 1:E:190:ASN:ND2  | 2.40                     | 0.55              |
| 1:H:120:LEU:HD13 | 1:H:127:SER:HB3  | 1.88                     | 0.55              |
| 1:M:38:TYR:OH    | 1:M:299:ARG:NH2  | 2.39                     | 0.55              |
| 1:M:293:THR:HG22 | 1:M:294:ARG:H    | 1.71                     | 0.55              |
| 1:E:39:ASP:OD1   | 1:E:39:ASP:N     | 2.39                     | 0.55              |
| 1:C:100:LYS:O    | 1:C:104:LEU:HD12 | 2.06                     | 0.55              |
| 1:I:279:LEU:O    | 1:I:279:LEU:HD23 | 2.07                     | 0.55              |
| 1:O:34:ILE:HD11  | 1:O:61:ILE:HD12  | 1.89                     | 0.55              |
| 1:C:281:LYS:O    | 1:C:294:ARG:HB2  | 2.06                     | 0.55              |
| 1:E:55:TYR:CE2   | 1:E:59:LYS:HG3   | 2.41                     | 0.55              |
| 1:J:19:ASN:O     | 1:J:20:THR:OG1   | 2.20                     | 0.55              |
| 1:C:159:ARG:HG2  | 1:C:159:ARG:O    | 2.07                     | 0.55              |
| 1:G:39:ASP:N     | 1:G:39:ASP:OD1   | 2.40                     | 0.55              |
| 1:G:86:ASP:O     | 1:G:90:LYS:HG2   | 2.07                     | 0.55              |
| 1:K:133:LEU:C    | 1:K:136:LEU:HD22 | 2.31                     | 0.55              |
| 1:H:128:ASP:OD1  | 1:H:129:PHE:N    | 2.40                     | 0.55              |
| 1:K:79:ARG:O     | 1:K:202:TYR:OH   | 2.22                     | 0.55              |
| 1:M:113:ALA:HB2  | 1:M:152:ILE:HG21 | 1.89                     | 0.55              |
| 1:D:239:ILE:C    | 1:D:239:ILE:HD12 | 2.31                     | 0.54              |
| 1:E:239:ILE:HD11 | 1:E:278:GLU:HB2  | 1.89                     | 0.54              |
| 1:C:127:SER:OG   | 1:C:159:ARG:HD3  | 2.07                     | 0.54              |
| 1:C:186:ILE:O    | 1:C:190:ASN:ND2  | 2.41                     | 0.54              |
| 1:K:42:ILE:HD11  | 1:K:63:ILE:HD11  | 1.89                     | 0.54              |
| 1:F:140:LYS:HG2  | 1:F:141:LYS:HD3  | 1.90                     | 0.54              |
| 2:R:83:GLU:OE1   | 1:I:276:ASN:ND2  | 2.39                     | 0.54              |
| 2:X:30:ASN:O     | 2:X:31:SER:OG    | 2.21                     | 0.54              |
| 1:I:158:ALA:O    | 1:I:159:ARG:NE   | 2.40                     | 0.54              |
| 1:E:11:ASP:O     | 1:E:26:VAL:CG1   | 2.56                     | 0.54              |
| 1:F:279:LEU:HB3  | 1:F:295:ARG:HB2  | 1.89                     | 0.54              |
| 1:A:91:GLN:CG    | 1:A:309:LEU:HD21 | 2.38                     | 0.54              |
| 1:C:292:VAL:N    | 2:T:56:ASN:OD1   | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:261:VAL:O    | 1:K:262:LEU:O    | 2.25                     | 0.54              |
| 1:K:292:VAL:HG13 | 1:K:292:VAL:O    | 2.08                     | 0.54              |
| 1:I:115:ASN:CG   | 1:I:319:VAL:HG13 | 2.32                     | 0.54              |
| 1:K:63:ILE:HG22  | 1:K:76:PHE:HB3   | 1.89                     | 0.54              |
| 1:P:110:VAL:HG22 | 1:P:133:LEU:HD11 | 1.89                     | 0.54              |
| 1:D:161:ASP:OD2  | 1:D:169:ARG:HG3  | 2.07                     | 0.54              |
| 1:L:180:ASN:OD1  | 1:L:181:GLU:N    | 2.41                     | 0.54              |
| 1:L:213:LEU:N    | 1:L:226:ASP:OD2  | 2.38                     | 0.54              |
| 1:O:176:ARG:HG2  | 1:O:177:PRO:HD3  | 1.90                     | 0.54              |
| 1:E:32:LEU:CD2   | 1:E:37:ILE:HD11  | 2.38                     | 0.53              |
| 1:E:80:GLU:O     | 1:E:83:LEU:HD23  | 2.08                     | 0.53              |
| 1:K:211:SER:HB3  | 1:K:222:SER:O    | 2.08                     | 0.53              |
| 1:M:97:ASP:O     | 1:M:99:ASN:N     | 2.41                     | 0.53              |
| 1:N:115:ASN:ND2  | 1:N:318:LEU:O    | 2.39                     | 0.53              |
| 1:I:158:ALA:O    | 1:I:159:ARG:NH2  | 2.41                     | 0.53              |
| 1:C:19:ASN:C     | 1:C:20:THR:HG1   | 2.14                     | 0.53              |
| 1:G:17:ARG:C     | 1:G:18:GLU:O     | 2.50                     | 0.53              |
| 1:P:189:LEU:HD11 | 1:P:239:ILE:CG1  | 2.38                     | 0.53              |
| 1:D:220:ARG:NH1  | 1:D:222:SER:OG   | 2.36                     | 0.53              |
| 1:L:11:ASP:N     | 1:L:11:ASP:OD1   | 2.41                     | 0.53              |
| 1:J:118:LYS:HG2  | 1:J:320:ALA:O    | 2.08                     | 0.53              |
| 1:F:56:ILE:HG23  | 1:F:61:ILE:HB    | 1.88                     | 0.53              |
| 1:B:211:SER:OG   | 1:B:214:HIS:O    | 2.27                     | 0.53              |
| 2:W:81:ILE:O     | 2:W:81:ILE:HG22  | 2.08                     | 0.53              |
| 1:I:318:LEU:C    | 1:I:318:LEU:HD12 | 2.34                     | 0.53              |
| 1:C:6:LEU:HD12   | 1:C:37:ILE:CD1   | 2.39                     | 0.53              |
| 1:E:296:ARG:NE   | 1:E:300:LEU:HD21 | 2.24                     | 0.53              |
| 1:P:169:ARG:O    | 1:P:180:ASN:ND2  | 2.41                     | 0.53              |
| 1:D:102:LEU:HD11 | 1:D:140:LYS:O    | 2.09                     | 0.53              |
| 1:E:296:ARG:HE   | 1:E:300:LEU:HD21 | 1.72                     | 0.53              |
| 1:O:96:LEU:HD21  | 1:P:93:GLU:HB2   | 1.91                     | 0.53              |
| 1:A:115:ASN:O    | 1:A:119:ASN:N    | 2.40                     | 0.52              |
| 1:D:98:LYS:NZ    | 1:D:141:LYS:HZ2  | 2.07                     | 0.52              |
| 1:K:131:ASN:C    | 1:K:131:ASN:HD22 | 2.10                     | 0.52              |
| 1:I:32:LEU:HD23  | 1:I:33:ALA:O     | 2.08                     | 0.52              |
| 1:B:95:TYR:CD2   | 1:B:95:TYR:O     | 2.62                     | 0.52              |
| 2:W:28:VAL:HG22  | 2:W:81:ILE:HG13  | 1.91                     | 0.52              |
| 1:L:70:GLY:O     | 1:L:199:SER:OG   | 2.21                     | 0.52              |
| 1:M:21:LEU:CB    | 1:M:32:LEU:HD22  | 2.39                     | 0.52              |
| 1:P:170:ILE:HG22 | 1:P:171:GLY:H    | 1.73                     | 0.52              |
| 1:C:218:GLU:HG3  | 1:C:219:ARG:HD2  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:279:LEU:CD2  | 1:C:295:ARG:HB2  | 2.40                     | 0.52              |
| 1:F:106:LYS:O    | 1:F:110:VAL:HG23 | 2.10                     | 0.52              |
| 1:M:27:ASN:OD1   | 1:M:27:ASN:N     | 2.42                     | 0.52              |
| 1:I:72:TYR:OH    | 1:I:75:THR:OG1   | 1.96                     | 0.52              |
| 1:O:6:LEU:CD1    | 1:O:32:LEU:HD11  | 2.40                     | 0.52              |
| 1:C:174:THR:N    | 1:C:183:ASN:OD1  | 2.39                     | 0.52              |
| 1:I:38:TYR:OH    | 1:I:295:ARG:NH1  | 2.42                     | 0.52              |
| 1:J:303:TYR:O    | 1:J:306:ILE:N    | 2.42                     | 0.52              |
| 1:C:87:LEU:HD21  | 1:C:309:LEU:HD13 | 1.91                     | 0.52              |
| 2:V:66:ARG:CD    | 2:V:66:ARG:H     | 2.22                     | 0.52              |
| 1:L:139:ALA:HB1  | 1:L:144:GLU:HB3  | 1.91                     | 0.52              |
| 1:M:176:ARG:HG3  | 1:M:177:PRO:HD3  | 1.90                     | 0.52              |
| 1:O:213:LEU:HB3  | 1:O:226:ASP:OD2  | 2.08                     | 0.52              |
| 1:L:238:ARG:NH1  | 1:L:239:ILE:HG22 | 2.24                     | 0.52              |
| 1:B:189:LEU:HD21 | 1:B:271:VAL:CG1  | 2.40                     | 0.52              |
| 1:B:257:ASP:OD1  | 1:B:258:LEU:N    | 2.40                     | 0.52              |
| 1:C:21:LEU:HD13  | 1:C:34:ILE:HD12  | 1.92                     | 0.52              |
| 1:B:101:ARG:NH2  | 1:B:215:GLU:OE2  | 2.40                     | 0.52              |
| 1:H:132:HIS:CE1  | 1:H:151:ARG:HD3  | 2.45                     | 0.52              |
| 1:O:109:VAL:HG22 | 1:O:213:LEU:HD11 | 1.91                     | 0.52              |
| 1:P:211:SER:OG   | 1:P:214:HIS:O    | 2.12                     | 0.52              |
| 1:L:141:LYS:NZ   | 1:L:142:VAL:HG12 | 2.25                     | 0.51              |
| 1:J:168:PHE:CD1  | 1:J:244:VAL:HG13 | 2.45                     | 0.51              |
| 1:P:127:SER:O    | 1:P:129:PHE:HD2  | 1.92                     | 0.51              |
| 1:A:91:GLN:HG2   | 1:A:309:LEU:HD21 | 1.92                     | 0.51              |
| 1:D:48:ILE:HG21  | 1:D:53:LEU:HD11  | 1.92                     | 0.51              |
| 2:V:66:ARG:H     | 2:V:66:ARG:HD3   | 1.74                     | 0.51              |
| 1:K:160:TRP:HZ2  | 1:K:241:ASN:HB2  | 1.74                     | 0.51              |
| 1:D:26:VAL:O     | 1:D:27:ASN:HB2   | 2.11                     | 0.51              |
| 1:L:238:ARG:NH1  | 1:L:278:GLU:HG3  | 2.24                     | 0.51              |
| 1:M:39:ASP:OD1   | 1:M:39:ASP:N     | 2.43                     | 0.51              |
| 1:B:127:SER:O    | 1:B:129:PHE:CD1  | 2.63                     | 0.51              |
| 1:E:11:ASP:O     | 1:E:26:VAL:HG13  | 2.10                     | 0.51              |
| 2:V:41:GLU:HA    | 2:V:44:ARG:CD    | 2.39                     | 0.51              |
| 1:K:262:LEU:C    | 1:K:262:LEU:HD12 | 2.35                     | 0.51              |
| 1:O:39:ASP:OD1   | 1:O:39:ASP:N     | 2.43                     | 0.51              |
| 1:P:293:THR:O    | 1:P:295:ARG:N    | 2.42                     | 0.51              |
| 1:E:240:ALA:O    | 1:E:244:VAL:HG23 | 2.10                     | 0.51              |
| 1:G:105:ALA:O    | 1:G:109:VAL:HG23 | 2.11                     | 0.51              |
| 2:T:13:ARG:NH1   | 2:T:58:ASP:OD2   | 2.44                     | 0.51              |
| 1:C:176:ARG:HB2  | 1:G:258:LEU:CD2  | 2.38                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:53:LEU:HD23  | 1:O:53:LEU:C     | 2.36                     | 0.51              |
| 1:D:51:GLN:HA    | 1:D:54:HIS:HD2   | 1.75                     | 0.51              |
| 1:E:296:ARG:HE   | 1:E:300:LEU:CD2  | 2.23                     | 0.51              |
| 1:F:136:LEU:HB3  | 1:F:148:VAL:HG11 | 1.92                     | 0.51              |
| 1:N:101:ARG:O    | 1:N:102:LEU:HB2  | 2.11                     | 0.51              |
| 1:O:262:LEU:HD12 | 1:O:263:LEU:O    | 2.11                     | 0.51              |
| 1:M:73:ASP:O     | 1:N:79:ARG:N     | 2.43                     | 0.51              |
| 1:M:73:ASP:OD2   | 1:N:54:HIS:ND1   | 2.44                     | 0.51              |
| 1:A:261:VAL:O    | 1:A:262:LEU:HB2  | 2.11                     | 0.51              |
| 1:D:253:HIS:O    | 1:D:264:THR:HG22 | 2.11                     | 0.51              |
| 1:L:56:ILE:HG21  | 1:L:63:ILE:HD11  | 1.92                     | 0.51              |
| 1:P:121:LYS:HG3  | 1:P:127:SER:HB3  | 1.91                     | 0.50              |
| 1:C:150:GLY:O    | 1:C:154:GLN:NE2  | 2.43                     | 0.50              |
| 1:K:62:LEU:HD12  | 1:K:62:LEU:O     | 2.10                     | 0.50              |
| 1:M:197:MET:HE1  | 1:M:231:PHE:CD1  | 2.46                     | 0.50              |
| 1:O:184:ALA:C    | 1:O:186:ILE:H    | 2.19                     | 0.50              |
| 1:A:21:LEU:HB2   | 1:A:34:ILE:CG2   | 2.41                     | 0.50              |
| 1:C:192:ARG:HH22 | 1:C:272:THR:HG23 | 1.76                     | 0.50              |
| 1:E:80:GLU:HG3   | 1:E:83:LEU:HD23  | 1.93                     | 0.50              |
| 1:K:253:HIS:O    | 1:K:264:THR:HG22 | 2.11                     | 0.50              |
| 1:L:56:ILE:HG23  | 1:L:61:ILE:HB    | 1.93                     | 0.50              |
| 1:L:141:LYS:HG2  | 1:L:142:VAL:N    | 2.27                     | 0.50              |
| 1:O:255:ARG:HG2  | 1:O:256:GLU:H    | 1.76                     | 0.50              |
| 1:B:106:LYS:O    | 1:B:110:VAL:HG23 | 2.10                     | 0.50              |
| 1:C:6:LEU:HD12   | 1:C:37:ILE:HD11  | 1.92                     | 0.50              |
| 1:C:13:THR:N     | 1:C:24:GLU:O     | 2.36                     | 0.50              |
| 2:U:56:ASN:CG    | 1:M:282:THR:HG1  | 2.19                     | 0.50              |
| 1:I:257:ASP:OD1  | 1:I:260:GLY:N    | 2.43                     | 0.50              |
| 1:A:87:LEU:O     | 1:A:87:LEU:HD23  | 2.12                     | 0.50              |
| 1:D:16:ARG:HB3   | 1:D:51:GLN:OE1   | 2.11                     | 0.50              |
| 1:O:62:LEU:HD23  | 1:O:78:PRO:HD2   | 1.93                     | 0.50              |
| 1:K:7:THR:CG2    | 1:K:192:ARG:HH12 | 2.23                     | 0.50              |
| 1:O:99:ASN:C     | 1:O:101:ARG:H    | 2.20                     | 0.50              |
| 1:A:125:ILE:HG22 | 1:A:126:SER:N    | 2.26                     | 0.50              |
| 1:K:167:GLU:O    | 1:K:167:GLU:HG2  | 2.12                     | 0.50              |
| 1:K:263:LEU:H    | 1:K:263:LEU:HD23 | 1.76                     | 0.50              |
| 1:M:245:LYS:O    | 1:M:246:LYS:HB2  | 2.12                     | 0.50              |
| 1:D:141:LYS:HG3  | 1:D:143:THR:H    | 1.75                     | 0.50              |
| 1:G:192:ARG:HH11 | 1:G:192:ARG:HB3  | 1.77                     | 0.50              |
| 1:O:228:SER:HB2  | 1:O:232:LYS:HE3  | 1.94                     | 0.50              |
| 1:C:87:LEU:HD21  | 1:C:309:LEU:CD1  | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:219:ARG:HH22 | 1:D:82:LEU:HD11  | 1.77                     | 0.49              |
| 1:L:303:TYR:O    | 1:L:304:LYS:HB2  | 2.12                     | 0.49              |
| 1:D:98:LYS:NZ    | 1:D:141:LYS:NZ   | 2.60                     | 0.49              |
| 1:F:92:ALA:O     | 1:F:96:LEU:HD12  | 2.12                     | 0.49              |
| 1:F:179:LYS:O    | 1:F:180:ASN:HB2  | 2.11                     | 0.49              |
| 1:K:218:GLU:OE1  | 1:K:219:ARG:NH1  | 2.45                     | 0.49              |
| 1:L:105:ALA:O    | 1:L:106:LYS:HB2  | 2.12                     | 0.49              |
| 1:A:15:LEU:CD1   | 1:A:17:ARG:H     | 2.25                     | 0.49              |
| 1:C:102:LEU:HD11 | 1:C:140:LYS:HA   | 1.94                     | 0.49              |
| 1:C:176:ARG:HA   | 1:C:178:PRO:HD3  | 1.94                     | 0.49              |
| 1:D:24:GLU:O     | 1:D:25:ASN:O     | 2.30                     | 0.49              |
| 1:B:6:LEU:CD2    | 1:B:40:ILE:HG12  | 2.42                     | 0.49              |
| 2:T:73:THR:OG1   | 2:T:77:GLU:OE2   | 2.30                     | 0.49              |
| 1:O:21:LEU:HD13  | 1:O:55:TYR:CE2   | 2.48                     | 0.49              |
| 1:C:6:LEU:HD11   | 1:C:37:ILE:CD1   | 2.42                     | 0.49              |
| 1:E:73:ASP:OD2   | 1:F:54:HIS:HB2   | 2.12                     | 0.49              |
| 2:V:83:GLU:O     | 2:V:84:ILE:HG13  | 2.13                     | 0.49              |
| 1:M:106:LYS:HD3  | 1:M:137:GLN:HG2  | 1.95                     | 0.49              |
| 1:M:113:ALA:CB   | 1:M:152:ILE:HG21 | 2.41                     | 0.49              |
| 1:P:303:TYR:HA   | 1:P:306:ILE:HG12 | 1.93                     | 0.49              |
| 1:A:197:MET:CE   | 1:A:227:LEU:HB3  | 2.40                     | 0.49              |
| 1:C:6:LEU:CD1    | 1:C:37:ILE:CG1   | 2.85                     | 0.49              |
| 1:C:176:ARG:O    | 1:G:258:LEU:HD11 | 2.11                     | 0.49              |
| 1:C:218:GLU:HG3  | 1:C:219:ARG:CD   | 2.43                     | 0.49              |
| 1:C:318:LEU:HD13 | 1:C:319:VAL:N    | 2.27                     | 0.49              |
| 1:M:57:ALA:HB1   | 1:N:73:ASP:O     | 2.12                     | 0.49              |
| 1:E:118:LYS:HE3  | 1:E:122:ASN:HD21 | 1.78                     | 0.49              |
| 1:G:299:ARG:O    | 1:G:303:TYR:N    | 2.44                     | 0.49              |
| 1:K:71:TYR:OH    | 1:K:178:PRO:HG3  | 2.12                     | 0.49              |
| 1:J:127:SER:O    | 1:J:129:PHE:CD2  | 2.66                     | 0.49              |
| 1:A:183:ASN:HA   | 1:A:186:ILE:HG22 | 1.95                     | 0.49              |
| 1:D:157:TYR:O    | 1:D:160:TRP:N    | 2.29                     | 0.49              |
| 1:F:303:TYR:O    | 1:F:306:ILE:HG22 | 2.13                     | 0.49              |
| 1:I:106:LYS:O    | 1:I:110:VAL:HG12 | 2.12                     | 0.49              |
| 1:J:189:LEU:HD21 | 1:J:271:VAL:HG13 | 1.93                     | 0.49              |
| 1:C:95:TYR:CE1   | 1:C:101:ARG:NH1  | 2.81                     | 0.49              |
| 1:C:239:ILE:O    | 1:C:240:ALA:HB3  | 2.11                     | 0.49              |
| 1:C:197:MET:HE1  | 1:C:231:PHE:CD1  | 2.47                     | 0.48              |
| 1:D:101:ARG:NH2  | 1:D:142:VAL:HG21 | 2.28                     | 0.48              |
| 1:F:194:TYR:OH   | 1:F:220:ARG:HG3  | 2.12                     | 0.48              |
| 1:B:52:ALA:O     | 1:B:56:ILE:HD13  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:29:ARG:HG2   | 1:C:29:ARG:NH1   | 2.28                     | 0.48              |
| 1:C:32:LEU:HD23  | 1:C:33:ALA:N     | 2.28                     | 0.48              |
| 1:H:24:GLU:HG3   | 1:H:29:ARG:CG    | 2.43                     | 0.48              |
| 1:L:231:PHE:CE2  | 1:L:298:ILE:HA   | 2.48                     | 0.48              |
| 1:I:91:GLN:NE2   | 1:I:210:ILE:HG23 | 2.28                     | 0.48              |
| 1:B:49:THR:HG23  | 1:B:52:ALA:H     | 1.78                     | 0.48              |
| 1:B:167:GLU:OE2  | 1:B:251:LYS:HG3  | 2.13                     | 0.48              |
| 1:E:161:ASP:OD2  | 1:E:170:ILE:O    | 2.31                     | 0.48              |
| 1:G:13:THR:N     | 1:G:24:GLU:O     | 2.46                     | 0.48              |
| 2:S:73:THR:HG23  | 2:S:77:GLU:OE2   | 2.13                     | 0.48              |
| 2:U:14:VAL:O     | 2:U:17:VAL:HG22  | 2.13                     | 0.48              |
| 2:U:62:ILE:HG23  | 2:U:62:ILE:O     | 2.13                     | 0.48              |
| 1:M:31:PRO:O     | 1:M:32:LEU:HB2   | 2.14                     | 0.48              |
| 1:O:110:VAL:HG22 | 1:O:133:LEU:CD1  | 2.43                     | 0.48              |
| 1:P:182:MET:HE1  | 1:P:244:VAL:HG21 | 1.95                     | 0.48              |
| 1:C:255:ARG:HA   | 1:C:255:ARG:NE   | 2.28                     | 0.48              |
| 1:D:26:VAL:O     | 1:D:26:VAL:HG12  | 2.13                     | 0.48              |
| 1:D:82:LEU:HB3   | 1:G:172:LYS:NZ   | 2.28                     | 0.48              |
| 1:D:252:ASP:OD1  | 1:D:253:HIS:ND1  | 2.46                     | 0.48              |
| 1:E:174:THR:HG22 | 1:E:183:ASN:HB3  | 1.95                     | 0.48              |
| 1:E:197:MET:CG   | 1:E:227:LEU:HD11 | 2.43                     | 0.48              |
| 1:E:296:ARG:HD3  | 1:E:297:LEU:N    | 2.28                     | 0.48              |
| 1:O:6:LEU:CD2    | 1:O:8:ILE:HG23   | 2.43                     | 0.48              |
| 1:G:174:THR:OG1  | 1:G:178:PRO:HA   | 2.13                     | 0.48              |
| 2:Q:81:ILE:HG22  | 2:Q:81:ILE:O     | 2.13                     | 0.48              |
| 1:F:279:LEU:O    | 1:F:295:ARG:HB2  | 2.13                     | 0.48              |
| 1:A:189:LEU:HD21 | 1:A:239:ILE:HB   | 1.94                     | 0.48              |
| 1:G:34:ILE:HG12  | 1:G:55:TYR:CE1   | 2.48                     | 0.48              |
| 1:G:212:TYR:O    | 1:G:226:ASP:OD2  | 2.31                     | 0.48              |
| 1:J:49:THR:HB    | 1:J:51:GLN:OE1   | 2.14                     | 0.48              |
| 1:D:231:PHE:CE2  | 1:D:298:ILE:HA   | 2.49                     | 0.48              |
| 1:E:136:LEU:CD1  | 1:E:148:VAL:HG21 | 2.44                     | 0.48              |
| 1:N:101:ARG:C    | 1:N:103:PHE:H    | 2.20                     | 0.48              |
| 1:I:159:ARG:NE   | 1:I:159:ARG:HA   | 2.29                     | 0.48              |
| 1:O:118:LYS:O    | 1:O:118:LYS:HD2  | 2.14                     | 0.48              |
| 1:P:25:ASN:O     | 1:P:26:VAL:C     | 2.56                     | 0.48              |
| 1:E:87:LEU:HD21  | 1:E:206:LEU:HD23 | 1.95                     | 0.48              |
| 1:L:110:VAL:HG12 | 1:L:114:LYS:HD3  | 1.95                     | 0.48              |
| 1:M:119:ASN:OD1  | 1:M:238:ARG:NH2  | 2.47                     | 0.48              |
| 1:M:200:GLU:OE1  | 1:M:299:ARG:CD   | 2.62                     | 0.48              |
| 1:C:200:GLU:HG3  | 1:C:299:ARG:HG3  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:142:VAL:HG13 | 1:L:143:THR:N    | 2.29                     | 0.47              |
| 1:M:192:ARG:O    | 1:M:195:ALA:O    | 2.31                     | 0.47              |
| 1:I:39:ASP:N     | 1:I:39:ASP:OD1   | 2.46                     | 0.47              |
| 1:I:279:LEU:CD2  | 1:I:295:ARG:HB3  | 2.43                     | 0.47              |
| 1:A:219:ARG:HE   | 1:B:62:LEU:HB2   | 1.79                     | 0.47              |
| 2:X:70:PRO:HB3   | 1:O:33:ALA:CB    | 2.44                     | 0.47              |
| 1:I:28:GLY:O     | 1:I:29:ARG:CG    | 2.62                     | 0.47              |
| 1:A:296:ARG:O    | 1:A:299:ARG:N    | 2.47                     | 0.47              |
| 1:B:180:ASN:OD1  | 1:B:181:GLU:N    | 2.47                     | 0.47              |
| 1:G:257:ASP:CG   | 1:G:258:LEU:H    | 2.22                     | 0.47              |
| 1:N:104:LEU:O    | 1:N:108:PHE:CD2  | 2.66                     | 0.47              |
| 1:J:80:GLU:O     | 1:J:81:THR:OG1   | 2.31                     | 0.47              |
| 1:B:89:ILE:O     | 1:B:93:GLU:N     | 2.42                     | 0.47              |
| 1:C:8:ILE:HD11   | 1:C:42:ILE:HG12  | 1.97                     | 0.47              |
| 1:I:279:LEU:O    | 1:I:294:ARG:HB2  | 2.14                     | 0.47              |
| 1:D:91:GLN:NE2   | 1:D:207:ALA:O    | 2.46                     | 0.47              |
| 2:Q:7:TYR:HE2    | 2:Q:21:LEU:HD12  | 1.79                     | 0.47              |
| 1:M:197:MET:HE1  | 1:M:231:PHE:HD1  | 1.79                     | 0.47              |
| 1:I:98:LYS:NZ    | 1:I:141:LYS:HG3  | 2.29                     | 0.47              |
| 1:C:28:GLY:O     | 1:C:29:ARG:CD    | 2.61                     | 0.47              |
| 1:E:11:ASP:CG    | 1:E:45:HIS:H     | 2.22                     | 0.47              |
| 1:F:117:GLU:OE2  | 1:F:130:SER:N    | 2.48                     | 0.47              |
| 1:H:88:ILE:HG23  | 1:H:89:ILE:HD12  | 1.97                     | 0.47              |
| 1:I:173:ARG:O    | 1:I:174:THR:OG1  | 2.21                     | 0.47              |
| 1:O:231:PHE:HE1  | 1:O:298:ILE:HA   | 1.78                     | 0.47              |
| 1:A:34:ILE:HG13  | 1:A:35:GLU:N     | 2.29                     | 0.47              |
| 1:B:72:TYR:CD1   | 1:B:202:TYR:HB3  | 2.50                     | 0.47              |
| 1:C:170:ILE:O    | 1:C:170:ILE:HG13 | 2.15                     | 0.47              |
| 1:F:194:TYR:HE1  | 1:F:224:ALA:HB3  | 1.80                     | 0.47              |
| 1:G:161:ASP:CG   | 1:G:170:ILE:O    | 2.58                     | 0.47              |
| 1:G:174:THR:HG21 | 1:G:179:LYS:N    | 2.27                     | 0.47              |
| 1:K:119:ASN:ND2  | 1:K:233:PRO:O    | 2.44                     | 0.47              |
| 1:L:211:SER:H    | 1:L:216:PRO:HB3  | 1.80                     | 0.47              |
| 1:L:255:ARG:CZ   | 1:L:262:LEU:HD11 | 2.44                     | 0.47              |
| 1:M:102:LEU:CD1  | 1:M:103:PHE:N    | 2.73                     | 0.47              |
| 1:I:157:TYR:O    | 1:I:158:ALA:HB3  | 2.15                     | 0.47              |
| 1:O:55:TYR:CD2   | 1:O:55:TYR:C     | 2.93                     | 0.47              |
| 1:D:127:SER:O    | 1:D:128:ASP:HB3  | 2.15                     | 0.47              |
| 1:D:255:ARG:HE   | 1:D:262:LEU:HD11 | 1.80                     | 0.47              |
| 2:S:53:ILE:HD13  | 2:S:60:VAL:HG21  | 1.97                     | 0.47              |
| 1:K:116:MET:HG2  | 1:K:233:PRO:HB3  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:90:LYS:O     | 1:L:93:GLU:N     | 2.48                     | 0.47              |
| 1:O:28:GLY:O     | 1:O:29:ARG:HD3   | 2.12                     | 0.47              |
| 1:O:88:ILE:HG21  | 1:P:88:ILE:HD11  | 1.96                     | 0.47              |
| 1:D:197:MET:HE1  | 1:D:227:LEU:HD23 | 1.96                     | 0.47              |
| 1:D:239:ILE:HD12 | 1:D:240:ALA:N    | 2.30                     | 0.47              |
| 1:G:178:PRO:HG2  | 1:G:261:VAL:O    | 2.15                     | 0.47              |
| 1:G:182:MET:HE3  | 1:G:244:VAL:HG21 | 1.96                     | 0.47              |
| 1:D:25:ASN:C     | 1:D:27:ASN:H     | 2.23                     | 0.46              |
| 1:E:136:LEU:HD12 | 1:E:148:VAL:HG21 | 1.96                     | 0.46              |
| 1:H:201:ILE:HD11 | 1:H:227:LEU:HD22 | 1.96                     | 0.46              |
| 1:L:106:LYS:O    | 1:L:110:VAL:HG23 | 2.15                     | 0.46              |
| 1:L:242:ARG:HD3  | 1:L:242:ARG:C    | 2.39                     | 0.46              |
| 1:L:305:ILE:O    | 1:L:309:LEU:HG   | 2.16                     | 0.46              |
| 1:I:21:LEU:HD11  | 1:I:55:TYR:CD1   | 2.50                     | 0.46              |
| 1:I:174:THR:O    | 1:I:175:ARG:C    | 2.57                     | 0.46              |
| 1:E:21:LEU:HB3   | 1:E:32:LEU:HD22  | 1.96                     | 0.46              |
| 1:J:81:THR:O     | 1:J:82:LEU:C     | 2.58                     | 0.46              |
| 1:P:14:LEU:N     | 1:P:47:ASN:O     | 2.48                     | 0.46              |
| 1:A:8:ILE:HG13   | 1:A:8:ILE:O      | 2.15                     | 0.46              |
| 1:C:29:ARG:O     | 1:C:31:PRO:CD    | 2.63                     | 0.46              |
| 1:E:87:LEU:O     | 1:E:90:LYS:N     | 2.49                     | 0.46              |
| 1:E:172:LYS:HD2  | 1:E:172:LYS:O    | 2.16                     | 0.46              |
| 1:G:118:LYS:HG2  | 1:G:122:ASN:OD1  | 2.16                     | 0.46              |
| 1:G:219:ARG:HD3  | 1:H:62:LEU:HD11  | 1.98                     | 0.46              |
| 2:V:41:GLU:HA    | 2:V:44:ARG:HD2   | 1.98                     | 0.46              |
| 1:L:86:ASP:HB3   | 1:L:89:ILE:HD12  | 1.96                     | 0.46              |
| 1:L:197:MET:HE1  | 1:L:231:PHE:HD2  | 1.80                     | 0.46              |
| 1:A:25:ASN:HB2   | 1:A:27:ASN:OD1   | 2.16                     | 0.46              |
| 1:B:168:PHE:CD1  | 1:B:244:VAL:HG22 | 2.50                     | 0.46              |
| 1:E:94:HIS:O     | 1:E:101:ARG:HB2  | 2.15                     | 0.46              |
| 1:P:189:LEU:HD11 | 1:P:239:ILE:HG12 | 1.97                     | 0.46              |
| 1:A:72:TYR:CD2   | 1:B:79:ARG:HB2   | 2.50                     | 0.46              |
| 1:B:63:ILE:HG12  | 1:B:76:PHE:HB3   | 1.97                     | 0.46              |
| 1:G:57:ALA:HB1   | 1:H:73:ASP:O     | 2.16                     | 0.46              |
| 1:N:310:VAL:HG23 | 1:N:312:VAL:HG23 | 1.98                     | 0.46              |
| 1:A:157:TYR:CE2  | 1:A:173:ARG:HD3  | 2.51                     | 0.46              |
| 1:B:21:LEU:HD22  | 1:B:32:LEU:HB2   | 1.98                     | 0.46              |
| 1:C:174:THR:HG23 | 1:C:174:THR:O    | 2.15                     | 0.46              |
| 1:E:172:LYS:HD2  | 1:E:172:LYS:C    | 2.41                     | 0.46              |
| 1:F:231:PHE:HE2  | 1:F:301:GLU:HG2  | 1.81                     | 0.46              |
| 1:G:182:MET:CE   | 1:G:244:VAL:HG21 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:56:ASN:OD1   | 1:K:282:THR:OG1  | 2.33                     | 0.46              |
| 1:K:155:GLU:O    | 1:K:159:ARG:N    | 2.47                     | 0.46              |
| 1:I:158:ALA:O    | 1:I:159:ARG:CZ   | 2.63                     | 0.46              |
| 1:B:6:LEU:HD21   | 1:B:40:ILE:HG23  | 1.97                     | 0.46              |
| 1:C:43:TYR:OH    | 1:C:192:ARG:NH1  | 2.48                     | 0.46              |
| 1:C:141:LYS:HG2  | 1:C:142:VAL:H    | 1.80                     | 0.46              |
| 1:D:106:LYS:O    | 1:D:110:VAL:HG23 | 2.16                     | 0.46              |
| 1:K:242:ARG:HH22 | 1:K:274:ALA:HB1  | 1.81                     | 0.46              |
| 1:O:176:ARG:HG2  | 1:O:177:PRO:CD   | 2.45                     | 0.46              |
| 1:O:228:SER:CB   | 1:O:232:LYS:HE3  | 2.46                     | 0.46              |
| 1:C:28:GLY:C     | 1:C:29:ARG:CD    | 2.76                     | 0.46              |
| 1:C:275:TYR:CZ   | 1:C:279:LEU:HD12 | 2.51                     | 0.46              |
| 1:E:25:ASN:ND2   | 1:E:27:ASN:OD1   | 2.45                     | 0.46              |
| 1:F:29:ARG:HG2   | 1:F:29:ARG:O     | 2.14                     | 0.46              |
| 1:G:206:LEU:HG   | 1:G:306:ILE:HD11 | 1.98                     | 0.46              |
| 1:K:319:VAL:HG12 | 1:K:320:ALA:N    | 2.30                     | 0.46              |
| 1:M:102:LEU:O    | 1:M:106:LYS:HB2  | 2.16                     | 0.46              |
| 1:J:231:PHE:CE2  | 1:J:298:ILE:HA   | 2.51                     | 0.46              |
| 1:O:184:ALA:O    | 1:O:185:LEU:HB3  | 2.15                     | 0.46              |
| 1:C:192:ARG:HG3  | 1:C:275:TYR:CZ   | 2.51                     | 0.46              |
| 1:F:189:LEU:HD11 | 1:F:240:ALA:HB2  | 1.98                     | 0.46              |
| 2:S:55:GLU:OE1   | 2:S:55:GLU:N     | 2.46                     | 0.46              |
| 1:L:238:ARG:HH11 | 1:L:239:ILE:HG22 | 1.80                     | 0.46              |
| 1:M:261:VAL:HG12 | 1:M:262:LEU:N    | 2.31                     | 0.46              |
| 1:I:21:LEU:CD1   | 1:I:55:TYR:CD1   | 2.99                     | 0.46              |
| 1:P:67:ASN:CG    | 1:P:68:HIS:N     | 2.73                     | 0.46              |
| 1:A:120:LEU:HD22 | 1:A:125:ILE:HB   | 1.96                     | 0.46              |
| 1:B:254:PHE:CE2  | 1:B:263:LEU:HD22 | 2.50                     | 0.46              |
| 1:L:211:SER:N    | 1:L:216:PRO:HB3  | 2.31                     | 0.46              |
| 1:M:99:ASN:C     | 1:M:100:LYS:HG3  | 2.41                     | 0.46              |
| 1:N:241:ASN:HA   | 1:N:244:VAL:HG22 | 1.98                     | 0.46              |
| 1:O:197:MET:HE3  | 1:O:227:LEU:HB3  | 1.98                     | 0.46              |
| 1:E:136:LEU:HD22 | 1:E:144:GLU:CD   | 2.42                     | 0.45              |
| 1:H:72:TYR:CD2   | 1:H:202:TYR:HB3  | 2.50                     | 0.45              |
| 2:W:28:VAL:HG21  | 2:W:34:GLU:HG2   | 1.97                     | 0.45              |
| 2:X:70:PRO:HB3   | 1:O:33:ALA:HB2   | 1.98                     | 0.45              |
| 1:L:303:TYR:C    | 1:L:305:ILE:H    | 2.23                     | 0.45              |
| 1:M:34:ILE:HD13  | 1:M:55:TYR:CZ    | 2.51                     | 0.45              |
| 1:M:254:PHE:CE1  | 1:M:263:LEU:HD22 | 2.51                     | 0.45              |
| 1:O:231:PHE:CE1  | 1:O:298:ILE:HA   | 2.51                     | 0.45              |
| 1:B:81:THR:HG22  | 1:B:82:LEU:O     | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:101:ARG:CZ   | 1:B:142:VAL:HG11 | 2.46                     | 0.45              |
| 1:D:43:TYR:OH    | 1:D:299:ARG:NH2  | 2.50                     | 0.45              |
| 1:D:181:GLU:HB3  | 1:D:254:PHE:CD1  | 2.52                     | 0.45              |
| 1:H:132:HIS:CE1  | 1:H:151:ARG:CD   | 3.00                     | 0.45              |
| 1:M:37:ILE:HG22  | 1:M:38:TYR:N     | 2.32                     | 0.45              |
| 1:M:99:ASN:C     | 1:M:101:ARG:H    | 2.23                     | 0.45              |
| 1:N:119:ASN:ND2  | 1:N:233:PRO:O    | 2.42                     | 0.45              |
| 1:I:206:LEU:HG   | 1:I:306:ILE:HD11 | 1.97                     | 0.45              |
| 1:J:296:ARG:O    | 1:J:299:ARG:N    | 2.49                     | 0.45              |
| 1:O:146:MET:O    | 1:O:149:GLU:N    | 2.50                     | 0.45              |
| 1:A:34:ILE:HD13  | 1:A:55:TYR:CE2   | 2.50                     | 0.45              |
| 1:C:89:ILE:HG12  | 1:D:95:TYR:CD1   | 2.51                     | 0.45              |
| 1:D:296:ARG:O    | 1:D:299:ARG:N    | 2.49                     | 0.45              |
| 1:F:87:LEU:HD21  | 1:F:306:ILE:HG13 | 1.99                     | 0.45              |
| 1:G:99:ASN:C     | 1:G:101:ARG:H    | 2.24                     | 0.45              |
| 2:T:84:ILE:HB    | 1:K:7:THR:O      | 2.16                     | 0.45              |
| 1:O:197:MET:HB3  | 1:O:224:ALA:HB1  | 1.98                     | 0.45              |
| 1:O:319:VAL:O    | 1:O:320:ALA:HB2  | 2.16                     | 0.45              |
| 1:A:54:HIS:NE2   | 1:B:67:ASN:OD1   | 2.50                     | 0.45              |
| 1:B:241:ASN:OD1  | 1:B:245:LYS:HD2  | 2.16                     | 0.45              |
| 1:D:146:MET:O    | 1:D:147:ASN:HB3  | 2.17                     | 0.45              |
| 1:F:150:GLY:O    | 1:F:151:ARG:HB3  | 2.16                     | 0.45              |
| 1:G:34:ILE:HG12  | 1:G:55:TYR:HE1   | 1.81                     | 0.45              |
| 2:S:13:ARG:CZ    | 2:S:58:ASP:OD2   | 2.64                     | 0.45              |
| 1:M:141:LYS:HG2  | 1:M:142:VAL:N    | 2.32                     | 0.45              |
| 1:I:188:PHE:CD1  | 1:I:188:PHE:C    | 2.93                     | 0.45              |
| 1:O:102:LEU:HD11 | 1:O:140:LYS:HA   | 1.97                     | 0.45              |
| 1:O:123:TRP:CZ3  | 1:O:160:TRP:NE1  | 2.85                     | 0.45              |
| 1:D:146:MET:C    | 1:D:148:VAL:H    | 2.24                     | 0.45              |
| 2:U:62:ILE:O     | 2:U:62:ILE:CG2   | 2.65                     | 0.45              |
| 2:V:82:GLU:OE2   | 2:V:82:GLU:N     | 2.41                     | 0.45              |
| 1:M:106:LYS:O    | 1:M:110:VAL:HG12 | 2.16                     | 0.45              |
| 1:A:64:HIS:ND1   | 1:A:195:ALA:HB1  | 2.31                     | 0.45              |
| 1:E:197:MET:HE3  | 1:E:228:SER:HA   | 1.99                     | 0.45              |
| 1:G:264:THR:O    | 1:G:267:GLY:N    | 2.49                     | 0.45              |
| 2:T:55:GLU:OE1   | 2:T:55:GLU:N     | 2.49                     | 0.45              |
| 1:L:115:ASN:OD1  | 1:L:320:ALA:HB2  | 2.17                     | 0.45              |
| 1:O:227:LEU:HD21 | 1:O:305:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:255:ARG:CZ   | 1:B:262:LEU:HD11 | 2.47                     | 0.45              |
| 1:E:219:ARG:HB3  | 1:F:81:THR:CG2   | 2.40                     | 0.45              |
| 2:V:14:VAL:O     | 2:V:17:VAL:HG22  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:21:LEU:HD11  | 1:K:34:ILE:HD12  | 1.99                     | 0.45              |
| 1:M:12:GLY:HA3   | 1:M:25:ASN:HA    | 1.97                     | 0.45              |
| 1:O:118:LYS:HG2  | 1:O:320:ALA:HB3  | 1.99                     | 0.45              |
| 1:P:292:VAL:HG11 | 1:P:296:ARG:HH22 | 1.81                     | 0.45              |
| 1:B:43:TYR:HB3   | 1:B:66:PHE:CB    | 2.46                     | 0.45              |
| 1:D:256:GLU:O    | 1:D:257:ASP:HB2  | 2.16                     | 0.45              |
| 1:E:34:ILE:HD11  | 1:E:55:TYR:CZ    | 2.51                     | 0.45              |
| 1:H:19:ASN:O     | 1:H:20:THR:HG23  | 2.17                     | 0.45              |
| 1:H:132:HIS:HE1  | 1:H:151:ARG:HD3  | 1.81                     | 0.45              |
| 1:K:273:LYS:O    | 1:K:274:ALA:HB3  | 2.17                     | 0.45              |
| 1:L:25:ASN:C     | 1:L:27:ASN:H     | 2.12                     | 0.45              |
| 1:M:108:PHE:O    | 1:M:112:GLY:N    | 2.46                     | 0.45              |
| 1:J:189:LEU:HD21 | 1:J:271:VAL:HG12 | 1.99                     | 0.45              |
| 1:J:310:VAL:HG23 | 1:J:312:VAL:HG23 | 1.98                     | 0.45              |
| 1:B:94:HIS:O     | 1:B:95:TYR:HB3   | 2.16                     | 0.45              |
| 1:C:37:ILE:HD12  | 1:C:37:ILE:HA    | 1.82                     | 0.45              |
| 1:C:279:LEU:HD23 | 1:C:279:LEU:O    | 2.17                     | 0.45              |
| 1:D:125:ILE:HG21 | 1:D:159:ARG:O    | 2.16                     | 0.45              |
| 2:Q:55:GLU:OE1   | 2:Q:55:GLU:N     | 2.48                     | 0.45              |
| 2:W:5:VAL:HG12   | 2:W:62:ILE:HG12  | 1.99                     | 0.45              |
| 1:K:149:GLU:O    | 1:K:153:ARG:HG2  | 2.17                     | 0.45              |
| 1:I:34:ILE:CD1   | 1:I:35:GLU:OE2   | 2.65                     | 0.45              |
| 1:O:203:ASN:OD1  | 1:O:299:ARG:NH1  | 2.44                     | 0.45              |
| 1:P:56:ILE:HG23  | 1:P:61:ILE:HB    | 1.98                     | 0.45              |
| 1:F:113:ALA:HB3  | 1:F:133:LEU:HD21 | 1.98                     | 0.45              |
| 1:G:17:ARG:O     | 1:G:18:GLU:C     | 2.60                     | 0.45              |
| 1:L:67:ASN:HB2   | 1:L:71:TYR:HB3   | 1.99                     | 0.45              |
| 1:M:73:ASP:HA    | 1:N:79:ARG:HD3   | 1.99                     | 0.45              |
| 1:O:102:LEU:O    | 1:O:106:LYS:HG3  | 2.17                     | 0.45              |
| 1:B:25:ASN:O     | 1:B:26:VAL:C     | 2.59                     | 0.44              |
| 1:D:178:PRO:O    | 1:D:260:GLY:HA3  | 2.17                     | 0.44              |
| 1:E:282:THR:O    | 1:E:283:VAL:HG23 | 2.18                     | 0.44              |
| 2:W:82:GLU:O     | 2:W:83:GLU:HB3   | 2.16                     | 0.44              |
| 2:X:29:GLN:HG2   | 2:X:30:ASN:N     | 2.32                     | 0.44              |
| 1:K:255:ARG:O    | 1:K:261:VAL:O    | 2.35                     | 0.44              |
| 1:M:73:ASP:O     | 1:N:79:ARG:HB3   | 2.17                     | 0.44              |
| 1:M:84:SER:HA    | 1:N:218:GLU:O    | 2.16                     | 0.44              |
| 1:M:153:ARG:NH2  | 1:M:157:TYR:OH   | 2.51                     | 0.44              |
| 1:I:231:PHE:CE2  | 1:I:298:ILE:HA   | 2.52                     | 0.44              |
| 1:P:43:TYR:OH    | 1:P:203:ASN:OD1  | 2.33                     | 0.44              |
| 1:C:141:LYS:HG2  | 1:C:142:VAL:N    | 2.31                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:72:TYR:HH    | 1:G:75:THR:HG1   | 1.56                     | 0.44              |
| 1:B:127:SER:O    | 1:B:129:PHE:N    | 2.50                     | 0.44              |
| 1:E:197:MET:HB3  | 1:E:224:ALA:HB1  | 2.00                     | 0.44              |
| 1:H:245:LYS:HE2  | 1:H:245:LYS:HA   | 1.99                     | 0.44              |
| 1:M:6:LEU:HD21   | 1:M:37:ILE:HD13  | 1.98                     | 0.44              |
| 1:N:146:MET:O    | 1:N:147:ASN:HB2  | 2.18                     | 0.44              |
| 1:J:104:LEU:HD23 | 1:J:315:TYR:CD2  | 2.51                     | 0.44              |
| 1:J:168:PHE:HD1  | 1:J:244:VAL:HG13 | 1.80                     | 0.44              |
| 1:B:86:ASP:HB2   | 1:B:89:ILE:HG22  | 1.99                     | 0.44              |
| 1:C:62:LEU:CD1   | 1:C:199:SER:HA   | 2.47                     | 0.44              |
| 1:C:65:PHE:CE1   | 1:D:53:LEU:HD12  | 2.53                     | 0.44              |
| 1:E:197:MET:SD   | 1:E:227:LEU:HD11 | 2.57                     | 0.44              |
| 1:G:250:LYS:HG3  | 1:G:251:LYS:H    | 1.83                     | 0.44              |
| 1:M:197:MET:HE2  | 1:M:228:SER:HA   | 1.99                     | 0.44              |
| 1:J:87:LEU:HD12  | 1:J:205:GLN:HB3  | 2.00                     | 0.44              |
| 1:O:34:ILE:HD13  | 1:O:55:TYR:HE2   | 1.82                     | 0.44              |
| 1:D:87:LEU:HD22  | 1:D:206:LEU:HD23 | 1.99                     | 0.44              |
| 1:E:118:LYS:HG3  | 1:E:122:ASN:HD21 | 1.82                     | 0.44              |
| 1:E:218:GLU:N    | 1:F:86:ASP:OD1   | 2.51                     | 0.44              |
| 1:M:231:PHE:CE1  | 1:M:298:ILE:HA   | 2.53                     | 0.44              |
| 1:N:123:TRP:CH2  | 1:N:241:ASN:CG   | 2.96                     | 0.44              |
| 1:I:219:ARG:HB3  | 1:J:81:THR:HB    | 1.99                     | 0.44              |
| 1:B:254:PHE:CD2  | 1:B:263:LEU:HD22 | 2.52                     | 0.44              |
| 1:C:86:ASP:HB2   | 1:D:217:SER:CB   | 2.48                     | 0.44              |
| 1:D:167:GLU:OE2  | 1:D:251:LYS:HG3  | 2.18                     | 0.44              |
| 1:E:174:THR:HG22 | 1:E:183:ASN:CG   | 2.42                     | 0.44              |
| 1:G:141:LYS:HG2  | 1:G:142:VAL:N    | 2.33                     | 0.44              |
| 1:K:193:LEU:O    | 1:K:197:MET:HB2  | 2.18                     | 0.44              |
| 1:N:104:LEU:HD23 | 1:N:315:TYR:CD2  | 2.51                     | 0.44              |
| 1:I:275:TYR:CE1  | 1:I:279:LEU:HD12 | 2.52                     | 0.44              |
| 1:J:168:PHE:HD2  | 1:J:181:GLU:HG2  | 1.83                     | 0.44              |
| 1:J:219:ARG:O    | 1:J:220:ARG:HG2  | 2.18                     | 0.44              |
| 1:O:34:ILE:HD13  | 1:O:55:TYR:CE2   | 2.53                     | 0.44              |
| 1:P:203:ASN:OD1  | 1:P:299:ARG:NH2  | 2.50                     | 0.44              |
| 1:C:56:ILE:HG23  | 1:C:61:ILE:HB    | 1.99                     | 0.44              |
| 1:G:6:LEU:HD22   | 1:G:32:LEU:HD22  | 1.98                     | 0.44              |
| 1:G:32:LEU:HB3   | 1:G:37:ILE:HD11  | 1.99                     | 0.44              |
| 1:H:243:LEU:HB3  | 1:H:249:ILE:CD1  | 2.48                     | 0.44              |
| 2:V:46:LYS:O     | 2:V:50:LYS:HG3   | 2.17                     | 0.44              |
| 1:K:7:THR:HG22   | 1:K:192:ARG:HH12 | 1.83                     | 0.44              |
| 1:M:112:GLY:HA2  | 1:M:230:ILE:HA   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:176:ARG:O    | 1:M:177:PRO:C    | 2.61                     | 0.44              |
| 1:N:239:ILE:CD1  | 1:N:275:TYR:HA   | 2.47                     | 0.44              |
| 1:A:18:GLU:CG    | 1:A:19:ASN:N     | 2.79                     | 0.44              |
| 1:A:32:LEU:C     | 1:A:32:LEU:HD23  | 2.43                     | 0.44              |
| 1:A:103:PHE:CD1  | 1:A:103:PHE:C    | 2.96                     | 0.44              |
| 1:D:188:PHE:O    | 1:D:191:SER:OG   | 2.32                     | 0.44              |
| 1:F:224:ALA:O    | 1:F:228:SER:OG   | 2.20                     | 0.44              |
| 1:E:128:ASP:O    | 1:E:131:ASN:ND2  | 2.51                     | 0.44              |
| 2:V:45:ILE:O     | 2:V:49:LEU:HB2   | 2.18                     | 0.44              |
| 1:L:16:ARG:HE    | 1:L:51:GLN:HB3   | 1.82                     | 0.44              |
| 1:M:18:GLU:O     | 1:M:20:THR:N     | 2.49                     | 0.44              |
| 1:M:195:ALA:C    | 1:M:197:MET:H    | 2.26                     | 0.44              |
| 1:J:26:VAL:HG23  | 1:J:26:VAL:O     | 2.17                     | 0.44              |
| 1:A:141:LYS:HD2  | 1:A:142:VAL:H    | 1.83                     | 0.43              |
| 2:Q:14:VAL:O     | 2:Q:17:VAL:HG22  | 2.17                     | 0.43              |
| 1:K:241:ASN:O    | 1:K:245:LYS:HG2  | 2.18                     | 0.43              |
| 1:L:212:TYR:CD1  | 1:L:212:TYR:N    | 2.85                     | 0.43              |
| 1:I:30:LYS:N     | 1:I:30:LYS:CD    | 2.81                     | 0.43              |
| 1:C:89:ILE:O     | 1:C:93:GLU:N     | 2.42                     | 0.43              |
| 1:G:172:LYS:O    | 1:G:173:ARG:NE   | 2.51                     | 0.43              |
| 1:K:166:GLY:O    | 1:K:167:GLU:HB3  | 2.18                     | 0.43              |
| 1:J:127:SER:O    | 1:J:129:PHE:HD2  | 2.01                     | 0.43              |
| 1:P:303:TYR:O    | 1:P:307:LYS:HG2  | 2.17                     | 0.43              |
| 2:Q:76:ILE:CG2   | 2:R:56:ASN:HA    | 2.48                     | 0.43              |
| 1:K:21:LEU:HD12  | 1:K:34:ILE:HD12  | 1.98                     | 0.43              |
| 1:L:232:LYS:CG   | 1:L:233:PRO:HD3  | 2.47                     | 0.43              |
| 1:M:32:LEU:HD21  | 1:M:37:ILE:CD1   | 2.48                     | 0.43              |
| 1:N:219:ARG:O    | 1:N:220:ARG:HG2  | 2.18                     | 0.43              |
| 1:I:89:ILE:HD12  | 1:J:95:TYR:CD2   | 2.53                     | 0.43              |
| 1:I:182:MET:SD   | 1:I:244:VAL:HG21 | 2.58                     | 0.43              |
| 1:B:13:THR:O     | 1:B:24:GLU:HB2   | 2.19                     | 0.43              |
| 1:E:83:LEU:CD2   | 1:F:221:PHE:HE1  | 2.31                     | 0.43              |
| 1:E:296:ARG:C    | 1:E:296:ARG:CD   | 2.90                     | 0.43              |
| 2:X:38:THR:HG23  | 2:X:41:GLU:H     | 1.84                     | 0.43              |
| 1:M:200:GLU:OE1  | 1:M:299:ARG:CZ   | 2.66                     | 0.43              |
| 1:I:91:GLN:HG2   | 1:I:212:TYR:OH   | 2.19                     | 0.43              |
| 1:D:197:MET:HE1  | 1:D:227:LEU:CD2  | 2.49                     | 0.43              |
| 1:H:197:MET:HG3  | 1:H:224:ALA:HB1  | 1.99                     | 0.43              |
| 1:I:22:TYR:HB3   | 1:I:30:LYS:HB2   | 2.00                     | 0.43              |
| 1:A:197:MET:HE2  | 1:A:227:LEU:C    | 2.43                     | 0.43              |
| 1:B:310:VAL:HG23 | 1:B:312:VAL:HG23 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:155:GLU:HG2  | 1:F:159:ARG:NH1  | 2.34                     | 0.43              |
| 1:G:261:VAL:HG12 | 1:G:262:LEU:H    | 1.84                     | 0.43              |
| 2:W:21:LEU:HD12  | 2:W:33:PHE:CD1   | 2.54                     | 0.43              |
| 1:K:64:HIS:HD1   | 1:K:75:THR:HG23  | 1.84                     | 0.43              |
| 1:K:242:ARG:NH2  | 1:K:274:ALA:HB1  | 2.33                     | 0.43              |
| 1:M:217:SER:O    | 1:M:218:GLU:CG   | 2.66                     | 0.43              |
| 1:I:159:ARG:NE   | 1:I:159:ARG:CA   | 2.82                     | 0.43              |
| 1:O:5:SER:HG     | 1:O:41:TYR:HE1   | 1.67                     | 0.43              |
| 1:C:216:PRO:HB2  | 1:D:86:ASP:OD1   | 2.19                     | 0.43              |
| 1:E:19:ASN:O     | 1:E:20:THR:HG23  | 2.18                     | 0.43              |
| 1:E:116:MET:HE2  | 1:E:153:ARG:NH1  | 2.34                     | 0.43              |
| 1:E:217:SER:HB3  | 1:E:220:ARG:HB3  | 2.01                     | 0.43              |
| 1:F:300:LEU:HA   | 1:F:303:TYR:HB2  | 2.00                     | 0.43              |
| 2:R:11:VAL:O     | 2:R:12:GLU:HB2   | 2.18                     | 0.43              |
| 2:V:2:TYR:HD1    | 2:V:36:GLU:HG2   | 1.84                     | 0.43              |
| 1:N:166:GLY:O    | 1:N:169:ARG:HG3  | 2.18                     | 0.43              |
| 1:G:172:LYS:O    | 1:G:173:ARG:HB3  | 2.18                     | 0.43              |
| 2:R:55:GLU:O     | 2:R:56:ASN:CG    | 2.62                     | 0.43              |
| 1:K:110:VAL:O    | 1:K:114:LYS:HB2  | 2.19                     | 0.43              |
| 1:L:242:ARG:O    | 1:L:246:LYS:HB2  | 2.19                     | 0.43              |
| 1:I:193:LEU:O    | 1:I:197:MET:HG2  | 2.19                     | 0.43              |
| 1:I:203:ASN:CG   | 1:I:299:ARG:NH1  | 2.77                     | 0.43              |
| 1:B:56:ILE:HD12  | 1:B:56:ILE:H     | 1.83                     | 0.43              |
| 1:C:42:ILE:HD12  | 1:C:65:PHE:CE1   | 2.54                     | 0.43              |
| 1:F:120:LEU:HD13 | 1:F:127:SER:CB   | 2.47                     | 0.43              |
| 1:G:43:TYR:OH    | 1:G:192:ARG:NE   | 2.52                     | 0.43              |
| 1:G:100:LYS:O    | 1:G:104:LEU:HD12 | 2.19                     | 0.43              |
| 1:K:63:ILE:HG23  | 1:K:63:ILE:O     | 2.19                     | 0.43              |
| 1:L:106:LYS:HG3  | 1:L:145:ILE:HD12 | 2.00                     | 0.43              |
| 1:M:313:GLU:O    | 1:M:314:GLU:C    | 2.61                     | 0.43              |
| 1:N:103:PHE:C    | 1:N:105:ALA:H    | 2.25                     | 0.43              |
| 1:I:115:ASN:OD1  | 1:I:234:ILE:HD11 | 2.19                     | 0.43              |
| 1:I:283:VAL:HG12 | 1:I:292:VAL:O    | 2.18                     | 0.43              |
| 1:A:186:ILE:HG23 | 1:A:187:SER:N    | 2.34                     | 0.43              |
| 1:C:126:SER:HB3  | 1:C:159:ARG:HH21 | 1.83                     | 0.43              |
| 1:E:293:THR:O    | 1:E:296:ARG:HG3  | 2.19                     | 0.43              |
| 1:I:110:VAL:O    | 1:I:114:LYS:HB2  | 2.19                     | 0.43              |
| 1:J:304:LYS:NZ   | 1:J:316:SER:O    | 2.45                     | 0.43              |
| 1:O:7:THR:HG22   | 1:O:41:TYR:HB2   | 2.01                     | 0.43              |
| 1:O:8:ILE:CD1    | 1:O:46:VAL:HG21  | 2.49                     | 0.43              |
| 1:O:25:ASN:O     | 1:O:26:VAL:C     | 2.61                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:108:PHE:CE2  | 1:C:226:ASP:HB3  | 2.54                     | 0.42              |
| 1:E:32:LEU:HD21  | 1:E:37:ILE:CD1   | 2.43                     | 0.42              |
| 2:U:39:LEU:O     | 2:U:40:ALA:C     | 2.62                     | 0.42              |
| 2:W:2:TYR:HD1    | 2:W:3:ILE:N      | 2.17                     | 0.42              |
| 1:K:186:ILE:O    | 1:K:190:ASN:ND2  | 2.49                     | 0.42              |
| 1:J:239:ILE:HG13 | 1:J:240:ALA:N    | 2.34                     | 0.42              |
| 1:A:92:ALA:HB1   | 1:B:89:ILE:HD12  | 2.00                     | 0.42              |
| 1:B:174:THR:HG21 | 1:B:179:LYS:H    | 1.84                     | 0.42              |
| 1:E:257:ASP:N    | 1:E:260:GLY:O    | 2.51                     | 0.42              |
| 1:G:197:MET:HE3  | 1:G:227:LEU:HB3  | 2.00                     | 0.42              |
| 1:H:128:ASP:C    | 1:H:130:SER:H    | 2.25                     | 0.42              |
| 1:K:107:SER:O    | 1:K:108:PHE:HB2  | 2.20                     | 0.42              |
| 1:L:13:THR:OG1   | 1:L:24:GLU:HB3   | 2.19                     | 0.42              |
| 1:M:231:PHE:HE1  | 1:M:298:ILE:HA   | 1.84                     | 0.42              |
| 1:O:128:ASP:OD1  | 1:O:128:ASP:O    | 2.37                     | 0.42              |
| 1:A:17:ARG:C     | 1:A:18:GLU:O     | 2.60                     | 0.42              |
| 1:C:136:LEU:HD23 | 1:C:148:VAL:HG11 | 2.00                     | 0.42              |
| 1:D:86:ASP:HB2   | 1:D:89:ILE:HD12  | 2.02                     | 0.42              |
| 1:G:64:HIS:CD2   | 1:G:75:THR:HG23  | 2.54                     | 0.42              |
| 1:G:212:TYR:O    | 1:G:213:LEU:HB3  | 2.19                     | 0.42              |
| 1:L:261:VAL:HG12 | 1:L:262:LEU:N    | 2.33                     | 0.42              |
| 1:M:8:ILE:HD11   | 1:M:42:ILE:CD1   | 2.49                     | 0.42              |
| 1:M:141:LYS:HG2  | 1:M:142:VAL:H    | 1.84                     | 0.42              |
| 1:I:16:ARG:O     | 1:I:17:ARG:O     | 2.37                     | 0.42              |
| 1:O:228:SER:OG   | 1:O:232:LYS:HE3  | 2.19                     | 0.42              |
| 1:A:257:ASP:OD1  | 1:A:260:GLY:N    | 2.51                     | 0.42              |
| 1:C:87:LEU:CD2   | 1:C:309:LEU:HD13 | 2.49                     | 0.42              |
| 1:D:130:SER:O    | 1:D:133:LEU:N    | 2.52                     | 0.42              |
| 1:H:258:LEU:HD23 | 1:H:258:LEU:O    | 2.19                     | 0.42              |
| 1:I:43:TYR:OH    | 1:I:192:ARG:HD2  | 2.19                     | 0.42              |
| 1:I:115:ASN:O    | 1:I:119:ASN:N    | 2.45                     | 0.42              |
| 1:I:197:MET:HE1  | 1:I:227:LEU:HB3  | 2.01                     | 0.42              |
| 1:O:160:TRP:O    | 1:O:160:TRP:CD1  | 2.72                     | 0.42              |
| 1:O:164:LEU:HD23 | 1:O:244:VAL:HG11 | 2.02                     | 0.42              |
| 1:P:161:ASP:OD2  | 1:P:170:ILE:O    | 2.36                     | 0.42              |
| 1:B:189:LEU:HD22 | 1:B:239:ILE:HD11 | 2.01                     | 0.42              |
| 1:C:101:ARG:HH21 | 1:C:142:VAL:HG11 | 1.84                     | 0.42              |
| 1:E:282:THR:CG2  | 2:U:76:ILE:HG21  | 2.50                     | 0.42              |
| 1:E:315:TYR:CD1  | 1:E:315:TYR:C    | 2.97                     | 0.42              |
| 1:F:239:ILE:HG13 | 1:F:240:ALA:N    | 2.35                     | 0.42              |
| 1:H:127:SER:O    | 1:H:128:ASP:CG   | 2.62                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:U:30:ASN:O     | 2:U:31:SER:OG    | 2.30                     | 0.42              |
| 1:L:189:LEU:CD2  | 1:L:239:ILE:HD11 | 2.35                     | 0.42              |
| 1:M:32:LEU:HD23  | 1:M:33:ALA:N     | 2.33                     | 0.42              |
| 1:M:77:TYR:N     | 1:N:75:THR:O     | 2.43                     | 0.42              |
| 1:M:294:ARG:O    | 1:M:297:LEU:HB3  | 2.19                     | 0.42              |
| 1:I:8:ILE:O      | 1:I:8:ILE:HG13   | 2.18                     | 0.42              |
| 1:O:6:LEU:HD12   | 1:O:32:LEU:HD11  | 2.01                     | 0.42              |
| 1:O:8:ILE:O      | 1:O:8:ILE:HG13   | 2.20                     | 0.42              |
| 1:B:48:ILE:HG22  | 1:B:49:THR:N     | 2.35                     | 0.42              |
| 1:C:219:ARG:CD   | 1:C:219:ARG:N    | 2.83                     | 0.42              |
| 1:C:219:ARG:NH2  | 1:D:82:LEU:HD11  | 2.35                     | 0.42              |
| 1:E:200:GLU:OE2  | 1:E:295:ARG:NH1  | 2.52                     | 0.42              |
| 1:F:140:LYS:HD3  | 1:F:141:LYS:NZ   | 2.35                     | 0.42              |
| 1:G:102:LEU:O    | 1:G:106:LYS:HB2  | 2.20                     | 0.42              |
| 1:H:239:ILE:CD1  | 1:H:240:ALA:N    | 2.75                     | 0.42              |
| 2:U:68:MET:HE1   | 2:U:84:ILE:HD12  | 2.01                     | 0.42              |
| 1:K:65:PHE:CZ    | 1:L:53:LEU:HD23  | 2.54                     | 0.42              |
| 1:M:197:MET:HB3  | 1:M:224:ALA:HB1  | 2.01                     | 0.42              |
| 1:N:141:LYS:HG2  | 1:N:142:VAL:N    | 2.32                     | 0.42              |
| 1:I:188:PHE:CD2  | 1:I:263:LEU:HD12 | 2.54                     | 0.42              |
| 1:I:249:ILE:HG21 | 1:I:254:PHE:CE2  | 2.55                     | 0.42              |
| 1:O:99:ASN:C     | 1:O:100:LYS:HG3  | 2.45                     | 0.42              |
| 1:P:293:THR:C    | 1:P:295:ARG:N    | 2.77                     | 0.42              |
| 1:A:176:ARG:HA   | 1:A:177:PRO:HA   | 1.92                     | 0.42              |
| 1:A:178:PRO:HD2  | 1:A:261:VAL:CG2  | 2.47                     | 0.42              |
| 1:A:181:GLU:O    | 1:A:182:MET:HB3  | 2.18                     | 0.42              |
| 1:B:95:TYR:HD2   | 1:B:101:ARG:HD2  | 1.85                     | 0.42              |
| 1:B:186:ILE:HG13 | 1:B:187:SER:N    | 2.35                     | 0.42              |
| 1:C:69:TYR:CD2   | 1:C:262:LEU:CD2  | 3.02                     | 0.42              |
| 1:C:103:PHE:CD1  | 1:C:103:PHE:C    | 2.97                     | 0.42              |
| 1:C:240:ALA:HA   | 1:C:243:LEU:HB3  | 2.00                     | 0.42              |
| 1:D:70:GLY:O     | 1:D:199:SER:OG   | 2.29                     | 0.42              |
| 1:D:214:HIS:N    | 1:D:226:ASP:OD1  | 2.49                     | 0.42              |
| 1:E:86:ASP:O     | 1:E:90:LYS:HG2   | 2.19                     | 0.42              |
| 1:G:200:GLU:OE1  | 1:G:299:ARG:NE   | 2.50                     | 0.42              |
| 1:K:27:ASN:OD1   | 1:K:27:ASN:N     | 2.52                     | 0.42              |
| 1:L:231:PHE:HE1  | 1:L:318:LEU:HD22 | 1.83                     | 0.42              |
| 1:N:215:GLU:O    | 1:N:217:SER:N    | 2.52                     | 0.42              |
| 1:I:21:LEU:HD11  | 1:I:55:TYR:HD1   | 1.84                     | 0.42              |
| 1:I:159:ARG:HE   | 1:I:159:ARG:N    | 2.17                     | 0.42              |
| 1:O:6:LEU:HD11   | 1:O:32:LEU:HD11  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:283:VAL:HG22 | 1:C:293:THR:OG1  | 2.19                     | 0.42              |
| 1:E:296:ARG:NH2  | 1:E:300:LEU:HD21 | 2.35                     | 0.42              |
| 1:F:140:LYS:HB3  | 1:F:140:LYS:HE3  | 1.86                     | 0.42              |
| 1:G:282:THR:OG1  | 2:X:56:ASN:OD1   | 2.33                     | 0.42              |
| 2:U:29:GLN:HG2   | 2:U:30:ASN:N     | 2.35                     | 0.42              |
| 1:K:104:LEU:HD11 | 1:K:308:HIS:CD2  | 2.54                     | 0.42              |
| 1:M:73:ASP:OD2   | 1:N:54:HIS:CE1   | 2.72                     | 0.42              |
| 1:M:142:VAL:O    | 1:M:145:ILE:HG22 | 2.20                     | 0.42              |
| 1:N:235:ILE:O    | 1:N:239:ILE:HG22 | 2.19                     | 0.42              |
| 1:I:32:LEU:HD23  | 1:I:32:LEU:C     | 2.45                     | 0.42              |
| 1:I:186:ILE:O    | 1:I:190:ASN:ND2  | 2.47                     | 0.42              |
| 1:I:254:PHE:CE2  | 1:I:263:LEU:CD2  | 3.03                     | 0.42              |
| 1:O:6:LEU:CD2    | 1:O:7:THR:N      | 2.76                     | 0.42              |
| 1:P:293:THR:O    | 1:P:294:ARG:C    | 2.62                     | 0.42              |
| 1:A:15:LEU:C     | 1:A:15:LEU:HD12  | 2.45                     | 0.42              |
| 1:A:15:LEU:HD12  | 1:A:17:ARG:H     | 1.85                     | 0.42              |
| 1:A:281:LYS:O    | 1:A:282:THR:HB   | 2.19                     | 0.42              |
| 1:G:72:TYR:HB2   | 1:G:191:SER:HB3  | 2.02                     | 0.42              |
| 1:H:211:SER:OG   | 1:H:222:SER:C    | 2.63                     | 0.42              |
| 2:S:20:PHE:HE2   | 2:S:49:LEU:N     | 2.18                     | 0.42              |
| 1:N:56:ILE:HG23  | 1:N:61:ILE:HB    | 2.00                     | 0.42              |
| 1:N:56:ILE:HG21  | 1:N:63:ILE:HD11  | 2.01                     | 0.42              |
| 1:I:67:ASN:N     | 1:I:71:TYR:O     | 2.51                     | 0.42              |
| 1:J:277:GLN:O    | 1:J:280:GLU:HG3  | 2.19                     | 0.42              |
| 1:O:7:THR:HG21   | 1:O:192:ARG:NH1  | 2.35                     | 0.42              |
| 1:O:228:SER:O    | 1:O:232:LYS:HD3  | 2.19                     | 0.42              |
| 1:P:292:VAL:CG1  | 1:P:296:ARG:NH2  | 2.82                     | 0.42              |
| 1:A:6:LEU:HD13   | 1:A:37:ILE:HG21  | 2.02                     | 0.42              |
| 1:E:8:ILE:O      | 1:E:8:ILE:HG13   | 2.20                     | 0.42              |
| 1:G:4:LYS:H      | 1:G:4:LYS:HG2    | 1.71                     | 0.42              |
| 1:G:41:TYR:HD2   | 1:G:192:ARG:HH22 | 1.68                     | 0.42              |
| 1:G:41:TYR:HE1   | 1:G:64:HIS:HD1   | 1.67                     | 0.42              |
| 2:V:7:TYR:CD1    | 2:V:9:VAL:HG23   | 2.55                     | 0.42              |
| 2:W:48:GLY:O     | 2:W:52:ILE:HG13  | 2.19                     | 0.42              |
| 1:K:306:ILE:N    | 1:K:306:ILE:HD12 | 2.35                     | 0.42              |
| 1:L:141:LYS:HZ2  | 1:L:142:VAL:HG12 | 1.85                     | 0.42              |
| 1:M:65:PHE:CZ    | 1:N:53:LEU:HD23  | 2.55                     | 0.42              |
| 1:I:318:LEU:O    | 1:I:318:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:18:GLU:HG2   | 1:A:19:ASN:H     | 1.84                     | 0.41              |
| 1:A:108:PHE:CE2  | 1:A:226:ASP:HB3  | 2.54                     | 0.41              |
| 1:C:29:ARG:O     | 1:C:31:PRO:HD2   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:8:ILE:HG22   | 2:U:84:ILE:HG23  | 2.02                     | 0.41              |
| 1:E:182:MET:CE   | 1:E:240:ALA:HB1  | 2.50                     | 0.41              |
| 1:E:227:LEU:C    | 1:E:227:LEU:HD12 | 2.45                     | 0.41              |
| 1:F:174:THR:HG21 | 1:F:179:LYS:HB2  | 2.00                     | 0.41              |
| 1:G:73:ASP:OD2   | 1:H:54:HIS:HB2   | 2.20                     | 0.41              |
| 2:U:39:LEU:O     | 2:U:42:PHE:N     | 2.52                     | 0.41              |
| 1:K:64:HIS:CE1   | 1:K:75:THR:HG23  | 2.55                     | 0.41              |
| 1:O:6:LEU:CD2    | 1:O:6:LEU:C      | 2.92                     | 0.41              |
| 1:F:150:GLY:C    | 1:F:152:ILE:H    | 2.27                     | 0.41              |
| 1:F:235:ILE:HG21 | 1:F:279:LEU:HD21 | 2.02                     | 0.41              |
| 2:W:2:TYR:CD2    | 2:W:68:MET:HA    | 2.54                     | 0.41              |
| 1:M:55:TYR:HE2   | 1:M:59:LYS:CG    | 2.32                     | 0.41              |
| 1:M:231:PHE:HD2  | 1:M:234:ILE:HD12 | 1.85                     | 0.41              |
| 1:A:94:HIS:O     | 1:A:101:ARG:HB2  | 2.20                     | 0.41              |
| 1:B:53:LEU:HD11  | 1:B:76:PHE:CD2   | 2.55                     | 0.41              |
| 1:B:141:LYS:HG2  | 1:B:142:VAL:N    | 2.36                     | 0.41              |
| 1:B:232:LYS:HB2  | 1:B:233:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:293:THR:O    | 1:C:297:LEU:HG   | 2.21                     | 0.41              |
| 1:E:37:ILE:H     | 1:E:37:ILE:HD12  | 1.85                     | 0.41              |
| 1:G:75:THR:O     | 1:H:77:TYR:N     | 2.48                     | 0.41              |
| 1:H:168:PHE:CD1  | 1:H:244:VAL:HG23 | 2.56                     | 0.41              |
| 2:V:4:VAL:O      | 2:V:4:VAL:HG23   | 2.20                     | 0.41              |
| 2:W:2:TYR:HE1    | 2:W:34:GLU:HB2   | 1.85                     | 0.41              |
| 1:K:151:ARG:O    | 1:K:155:GLU:HB2  | 2.19                     | 0.41              |
| 1:L:48:ILE:HG21  | 1:L:53:LEU:HD22  | 2.02                     | 0.41              |
| 1:J:282:THR:O    | 1:J:283:VAL:C    | 2.63                     | 0.41              |
| 1:P:209:THR:HG23 | 1:P:210:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:75:THR:O     | 1:B:77:TYR:N     | 2.53                     | 0.41              |
| 1:E:104:LEU:HD23 | 1:E:315:TYR:HD2  | 1.84                     | 0.41              |
| 1:E:174:THR:HG22 | 1:E:183:ASN:CB   | 2.50                     | 0.41              |
| 1:H:56:ILE:HG23  | 1:H:61:ILE:HB    | 2.03                     | 0.41              |
| 2:S:27:TRP:HD1   | 2:S:33:PHE:CZ    | 2.39                     | 0.41              |
| 1:K:62:LEU:HD21  | 1:K:199:SER:HA   | 2.02                     | 0.41              |
| 1:K:175:ARG:CZ   | 1:K:175:ARG:HB2  | 2.50                     | 0.41              |
| 1:L:146:MET:O    | 1:L:150:GLY:N    | 2.50                     | 0.41              |
| 1:I:202:TYR:C    | 1:I:202:TYR:CD1  | 2.99                     | 0.41              |
| 1:O:104:LEU:HD23 | 1:O:104:LEU:HA   | 1.89                     | 0.41              |
| 1:A:41:TYR:CD1   | 1:A:64:HIS:HB2   | 2.55                     | 0.41              |
| 1:A:72:TYR:O     | 1:B:79:ARG:HD2   | 2.20                     | 0.41              |
| 1:C:123:TRP:NE1  | 1:C:241:ASN:OD1  | 2.53                     | 0.41              |
| 1:D:51:GLN:O     | 1:D:54:HIS:CD2   | 2.74                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:239:ILE:HD13 | 1:G:275:TYR:HD2  | 1.86                     | 0.41              |
| 2:T:11:VAL:HG12  | 2:T:12:GLU:N     | 2.35                     | 0.41              |
| 1:N:98:LYS:O     | 1:N:101:ARG:O    | 2.39                     | 0.41              |
| 1:O:218:GLU:OE2  | 1:P:205:GLN:HG3  | 2.19                     | 0.41              |
| 1:A:141:LYS:HG3  | 1:A:143:THR:H    | 1.86                     | 0.41              |
| 1:C:236:ALA:O    | 1:C:239:ILE:O    | 2.38                     | 0.41              |
| 1:E:55:TYR:C     | 1:E:55:TYR:CD2   | 2.99                     | 0.41              |
| 1:F:92:ALA:O     | 1:F:93:GLU:C     | 2.63                     | 0.41              |
| 1:G:139:ALA:HB1  | 1:G:145:ILE:HG13 | 2.01                     | 0.41              |
| 1:H:119:ASN:ND2  | 1:H:233:PRO:O    | 2.40                     | 0.41              |
| 1:H:223:LEU:HD23 | 1:H:227:LEU:HD13 | 2.02                     | 0.41              |
| 2:R:55:GLU:C     | 2:R:57:SER:H     | 2.28                     | 0.41              |
| 2:U:3:ILE:HD12   | 2:U:62:ILE:HD11  | 2.02                     | 0.41              |
| 1:K:273:LYS:C    | 1:K:275:TYR:H    | 2.28                     | 0.41              |
| 1:I:317:PRO:HB2  | 1:I:319:VAL:HG23 | 2.02                     | 0.41              |
| 1:A:180:ASN:OD1  | 1:A:183:ASN:HB2  | 2.20                     | 0.41              |
| 1:B:168:PHE:CD1  | 1:B:244:VAL:HG13 | 2.56                     | 0.41              |
| 1:B:231:PHE:CD2  | 1:B:298:ILE:HD13 | 2.56                     | 0.41              |
| 1:C:265:ASP:O    | 1:C:269:LYS:HD3  | 2.21                     | 0.41              |
| 1:D:82:LEU:HB2   | 1:G:172:LYS:HE2  | 2.01                     | 0.41              |
| 1:E:129:PHE:CE1  | 1:E:155:GLU:OE2  | 2.74                     | 0.41              |
| 2:W:5:VAL:HG21   | 2:W:21:LEU:HD13  | 2.02                     | 0.41              |
| 2:W:11:VAL:C     | 2:W:13:ARG:H     | 2.29                     | 0.41              |
| 1:L:197:MET:CE   | 1:L:228:SER:HA   | 2.51                     | 0.41              |
| 1:M:17:ARG:C     | 1:M:18:GLU:O     | 2.63                     | 0.41              |
| 1:I:306:ILE:N    | 1:I:306:ILE:HD12 | 2.35                     | 0.41              |
| 1:O:194:TYR:HE1  | 1:O:224:ALA:HB3  | 1.84                     | 0.41              |
| 1:P:237:ASP:O    | 1:P:241:ASN:N    | 2.53                     | 0.41              |
| 1:A:34:ILE:O     | 1:A:37:ILE:HG12  | 2.20                     | 0.41              |
| 1:C:8:ILE:HG13   | 1:C:8:ILE:O      | 2.21                     | 0.41              |
| 1:E:181:GLU:O    | 1:E:182:MET:HB3  | 2.20                     | 0.41              |
| 1:G:99:ASN:C     | 1:G:100:LYS:HD2  | 2.45                     | 0.41              |
| 1:K:104:LEU:HD11 | 1:K:308:HIS:HD2  | 1.84                     | 0.41              |
| 1:L:115:ASN:OD1  | 1:L:234:ILE:HD11 | 2.21                     | 0.41              |
| 1:L:127:SER:O    | 1:L:128:ASP:OD1  | 2.37                     | 0.41              |
| 1:M:151:ARG:O    | 1:M:155:GLU:HB2  | 2.21                     | 0.41              |
| 1:I:98:LYS:HZ1   | 1:I:141:LYS:HG3  | 1.86                     | 0.41              |
| 1:A:57:ALA:HB1   | 1:B:73:ASP:O     | 2.21                     | 0.41              |
| 1:B:21:LEU:HD23  | 1:B:22:TYR:N     | 2.35                     | 0.41              |
| 1:B:66:PHE:CD1   | 1:B:72:TYR:HA    | 2.56                     | 0.41              |
| 1:B:120:LEU:HD22 | 1:B:125:ILE:HB   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:GLU:C    | 1:B:219:ARG:HG2  | 2.46                     | 0.41              |
| 1:C:4:LYS:HZ2    | 2:S:82:GLU:CD    | 2.29                     | 0.41              |
| 1:C:176:ARG:HA   | 1:C:177:PRO:HA   | 1.90                     | 0.41              |
| 1:E:129:PHE:CZ   | 1:E:155:GLU:OE2  | 2.74                     | 0.41              |
| 1:E:161:ASP:CG   | 1:E:170:ILE:H    | 2.25                     | 0.41              |
| 1:F:25:ASN:O     | 1:F:26:VAL:C     | 2.63                     | 0.41              |
| 1:F:34:ILE:HD12  | 1:F:59:LYS:HD3   | 2.03                     | 0.41              |
| 1:F:108:PHE:HD1  | 1:F:230:ILE:HD11 | 1.85                     | 0.41              |
| 1:F:119:ASN:OD1  | 1:F:238:ARG:NH2  | 2.54                     | 0.41              |
| 1:F:150:GLY:O    | 1:F:151:ARG:CB   | 2.68                     | 0.41              |
| 1:G:249:ILE:HD12 | 1:G:254:PHE:CE2  | 2.56                     | 0.41              |
| 1:H:53:LEU:HD11  | 1:H:76:PHE:CD1   | 2.56                     | 0.41              |
| 2:Q:4:VAL:O      | 2:Q:4:VAL:HG23   | 2.20                     | 0.41              |
| 2:Q:55:GLU:C     | 2:Q:57:SER:H     | 2.29                     | 0.41              |
| 2:W:38:THR:HG23  | 2:W:41:GLU:H     | 1.86                     | 0.41              |
| 1:K:262:LEU:C    | 1:K:262:LEU:CD1  | 2.94                     | 0.41              |
| 1:K:296:ARG:HG2  | 1:K:300:LEU:HG   | 2.02                     | 0.41              |
| 1:L:102:LEU:O    | 1:L:105:ALA:O    | 2.39                     | 0.41              |
| 1:N:123:TRP:N    | 1:N:123:TRP:CD1  | 2.89                     | 0.41              |
| 1:N:128:ASP:O    | 1:N:128:ASP:OD2  | 2.38                     | 0.41              |
| 1:I:182:MET:HE1  | 1:I:240:ALA:HB1  | 2.02                     | 0.41              |
| 1:J:43:TYR:OH    | 1:J:299:ARG:NH2  | 2.53                     | 0.41              |
| 1:O:62:LEU:CD1   | 1:O:199:SER:HA   | 2.51                     | 0.41              |
| 1:B:228:SER:O    | 1:B:232:LYS:HG3  | 2.21                     | 0.41              |
| 1:C:73:ASP:OD2   | 1:D:54:HIS:HB2   | 2.21                     | 0.41              |
| 1:C:318:LEU:HD13 | 1:C:318:LEU:C    | 2.46                     | 0.41              |
| 1:F:255:ARG:CG   | 1:F:264:THR:HG22 | 2.51                     | 0.41              |
| 1:F:303:TYR:HA   | 1:F:306:ILE:HG22 | 2.03                     | 0.41              |
| 1:G:109:VAL:HG21 | 1:G:145:ILE:CG2  | 2.51                     | 0.41              |
| 1:G:212:TYR:C    | 1:G:214:HIS:H    | 2.29                     | 0.41              |
| 1:M:55:TYR:C     | 1:M:55:TYR:CD2   | 2.99                     | 0.41              |
| 1:M:117:GLU:HG3  | 1:M:127:SER:HB2  | 2.02                     | 0.41              |
| 1:I:21:LEU:HB3   | 1:I:32:LEU:HD22  | 2.02                     | 0.41              |
| 1:I:65:PHE:CZ    | 1:J:53:LEU:HD23  | 2.57                     | 0.41              |
| 1:O:62:LEU:HD23  | 1:O:78:PRO:CD    | 2.50                     | 0.41              |
| 1:A:165:PRO:HG2  | 1:A:168:PHE:HD2  | 1.86                     | 0.40              |
| 1:A:166:GLY:O    | 1:A:169:ARG:HG2  | 2.20                     | 0.40              |
| 1:D:310:VAL:HG23 | 1:D:312:VAL:HG23 | 2.03                     | 0.40              |
| 1:E:62:LEU:HD23  | 1:E:78:PRO:CD    | 2.51                     | 0.40              |
| 1:E:102:LEU:CD2  | 1:E:145:ILE:HD11 | 2.51                     | 0.40              |
| 1:F:199:SER:O    | 1:F:203:ASN:N    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:8:ASP:O      | 2:Q:8:ASP:CG     | 2.64                     | 0.40              |
| 2:T:30:ASN:O     | 2:T:31:SER:OG    | 2.28                     | 0.40              |
| 1:L:296:ARG:O    | 1:L:299:ARG:N    | 2.54                     | 0.40              |
| 1:M:110:VAL:O    | 1:M:114:LYS:HB2  | 2.21                     | 0.40              |
| 1:M:182:MET:CE   | 1:M:244:VAL:HG21 | 2.51                     | 0.40              |
| 1:B:82:LEU:O     | 1:B:83:LEU:C     | 2.65                     | 0.40              |
| 1:B:168:PHE:HB3  | 1:B:182:MET:HB2  | 2.04                     | 0.40              |
| 1:D:95:TYR:C     | 1:D:95:TYR:CD2   | 2.99                     | 0.40              |
| 1:D:115:ASN:ND2  | 1:D:318:LEU:O    | 2.52                     | 0.40              |
| 1:D:181:GLU:HB3  | 1:D:254:PHE:CE1  | 2.56                     | 0.40              |
| 1:E:65:PHE:CZ    | 1:F:53:LEU:HD23  | 2.57                     | 0.40              |
| 2:Q:2:TYR:CD2    | 2:Q:68:MET:HA    | 2.57                     | 0.40              |
| 2:R:4:VAL:O      | 2:R:4:VAL:HG23   | 2.21                     | 0.40              |
| 2:V:83:GLU:HG2   | 2:V:84:ILE:HG23  | 2.03                     | 0.40              |
| 2:W:28:VAL:HG12  | 2:X:61:ILE:CD1   | 2.51                     | 0.40              |
| 1:K:64:HIS:ND1   | 1:K:75:THR:HG23  | 2.36                     | 0.40              |
| 1:L:209:THR:HG23 | 1:L:210:ILE:HD12 | 2.02                     | 0.40              |
| 1:I:43:TYR:OH    | 1:I:188:PHE:HE1  | 2.04                     | 0.40              |
| 1:O:108:PHE:CD2  | 1:O:226:ASP:OD2  | 2.74                     | 0.40              |
| 1:P:292:VAL:O    | 1:P:293:THR:C    | 2.65                     | 0.40              |
| 1:A:34:ILE:HD13  | 1:A:55:TYR:HE2   | 1.87                     | 0.40              |
| 1:A:157:TYR:O    | 1:A:170:ILE:HD11 | 2.21                     | 0.40              |
| 1:A:174:THR:CG2  | 1:A:178:PRO:HA   | 2.51                     | 0.40              |
| 1:B:25:ASN:OD1   | 1:B:26:VAL:N     | 2.54                     | 0.40              |
| 1:E:85:GLY:HA3   | 1:F:216:PRO:HB2  | 2.03                     | 0.40              |
| 1:E:182:MET:HE1  | 1:E:240:ALA:O    | 2.21                     | 0.40              |
| 1:F:140:LYS:HD2  | 1:F:141:LYS:HD3  | 2.03                     | 0.40              |
| 1:M:197:MET:HE3  | 1:M:227:LEU:HG   | 2.04                     | 0.40              |
| 1:M:313:GLU:O    | 1:M:313:GLU:HG2  | 2.22                     | 0.40              |
| 1:J:214:HIS:N    | 1:J:226:ASP:OD1  | 2.52                     | 0.40              |
| 1:J:219:ARG:O    | 1:J:220:ARG:CG   | 2.69                     | 0.40              |
| 1:O:83:LEU:HD21  | 1:P:221:PHE:CE1  | 2.57                     | 0.40              |
| 1:O:281:LYS:HG2  | 1:O:282:THR:H    | 1.86                     | 0.40              |
| 1:C:29:ARG:O     | 1:C:31:PRO:HD3   | 2.21                     | 0.40              |
| 1:D:125:ILE:HD11 | 1:D:163:SER:HB2  | 2.02                     | 0.40              |
| 1:E:8:ILE:HA     | 2:U:84:ILE:C     | 2.46                     | 0.40              |
| 1:E:26:VAL:O     | 1:E:26:VAL:HG23  | 2.21                     | 0.40              |
| 1:E:31:PRO:CB    | 2:U:68:MET:HB2   | 2.51                     | 0.40              |
| 1:G:239:ILE:CD1  | 1:G:275:TYR:HD2  | 2.34                     | 0.40              |
| 1:M:307:LYS:O    | 1:M:312:VAL:N    | 2.48                     | 0.40              |
| 1:O:83:LEU:HD21  | 1:P:221:PHE:HE1  | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:114:LYS:HE2  | 1:O:319:VAL:HG22 | 2.03                     | 0.40              |
| 1:P:182:MET:CE   | 1:P:244:VAL:HG21 | 2.51                     | 0.40              |
| 1:C:29:ARG:HG2   | 1:C:29:ARG:O     | 2.22                     | 0.40              |
| 1:C:261:VAL:C    | 1:C:262:LEU:HD12 | 2.46                     | 0.40              |
| 1:D:193:LEU:O    | 1:D:197:MET:HG2  | 2.21                     | 0.40              |
| 1:D:303:TYR:O    | 1:D:306:ILE:N    | 2.54                     | 0.40              |
| 1:E:100:LYS:HA   | 1:E:103:PHE:HB3  | 2.03                     | 0.40              |
| 1:F:140:LYS:CD   | 1:F:141:LYS:NZ   | 2.85                     | 0.40              |
| 1:F:219:ARG:O    | 1:F:219:ARG:CG   | 2.69                     | 0.40              |
| 2:S:7:TYR:CD1    | 2:S:9:VAL:HG23   | 2.57                     | 0.40              |
| 2:U:11:VAL:HG12  | 2:U:12:GLU:N     | 2.36                     | 0.40              |
| 2:U:17:VAL:HG11  | 2:U:53:ILE:HG12  | 2.04                     | 0.40              |
| 1:K:71:TYR:CE1   | 1:K:178:PRO:HG3  | 2.57                     | 0.40              |
| 1:M:25:ASN:OD1   | 1:M:27:ASN:O     | 2.39                     | 0.40              |
| 1:N:123:TRP:CH2  | 1:N:241:ASN:HB2  | 2.57                     | 0.40              |
| 1:I:69:TYR:CD1   | 1:I:69:TYR:N     | 2.88                     | 0.40              |
| 1:I:154:GLN:O    | 1:I:157:TYR:O    | 2.39                     | 0.40              |
| 1:I:197:MET:O    | 1:I:201:ILE:HG12 | 2.21                     | 0.40              |
| 1:I:275:TYR:O    | 1:I:279:LEU:N    | 2.53                     | 0.40              |
| 1:I:279:LEU:HD22 | 1:I:295:ARG:HB3  | 2.02                     | 0.40              |
| 1:O:29:ARG:HD3   | 1:O:29:ARG:N     | 2.36                     | 0.40              |
| 1:O:181:GLU:C    | 1:O:183:ASN:H    | 2.30                     | 0.40              |
| 1:P:185:LEU:O    | 1:P:189:LEU:HB2  | 2.21                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 1:N:252:ASP:O    | 1:J:219:ARG:NH1[1_455] | 1.86                     | 0.34              |
| 1:B:187:SER:OG   | 1:F:259:ASN:ND2[1_655] | 2.06                     | 0.14              |
| 1:D:259:ASN:HD21 | 1:H:187:SER:O[1_455]   | 1.57                     | 0.03              |
| 1:L:259:ASN:HD21 | 1:P:187:SER:O[1_455]   | 1.58                     | 0.02              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 307/322 (95%)   | 285 (93%)  | 21 (7%)  | 1 (0%)   | 36          | 69  |
| 1   | B     | 302/322 (94%)   | 275 (91%)  | 25 (8%)  | 2 (1%)   | 18          | 53  |
| 1   | C     | 308/322 (96%)   | 278 (90%)  | 26 (8%)  | 4 (1%)   | 9           | 40  |
| 1   | D     | 302/322 (94%)   | 274 (91%)  | 21 (7%)  | 7 (2%)   | 5           | 30  |
| 1   | E     | 308/322 (96%)   | 288 (94%)  | 19 (6%)  | 1 (0%)   | 36          | 69  |
| 1   | F     | 302/322 (94%)   | 273 (90%)  | 28 (9%)  | 1 (0%)   | 36          | 69  |
| 1   | G     | 308/322 (96%)   | 279 (91%)  | 27 (9%)  | 2 (1%)   | 21          | 55  |
| 1   | H     | 300/322 (93%)   | 287 (96%)  | 12 (4%)  | 1 (0%)   | 36          | 69  |
| 1   | I     | 308/322 (96%)   | 282 (92%)  | 21 (7%)  | 5 (2%)   | 7           | 36  |
| 1   | J     | 301/322 (94%)   | 279 (93%)  | 22 (7%)  | 0        | 100         | 100 |
| 1   | K     | 306/322 (95%)   | 279 (91%)  | 26 (8%)  | 1 (0%)   | 36          | 69  |
| 1   | L     | 302/322 (94%)   | 267 (88%)  | 32 (11%) | 3 (1%)   | 12          | 45  |
| 1   | M     | 310/322 (96%)   | 275 (89%)  | 34 (11%) | 1 (0%)   | 36          | 69  |
| 1   | N     | 297/322 (92%)   | 273 (92%)  | 24 (8%)  | 0        | 100         | 100 |
| 1   | O     | 307/322 (95%)   | 282 (92%)  | 24 (8%)  | 1 (0%)   | 36          | 69  |
| 1   | P     | 300/322 (93%)   | 283 (94%)  | 16 (5%)  | 1 (0%)   | 36          | 69  |
| 2   | Q     | 82/85 (96%)     | 76 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 2   | R     | 82/85 (96%)     | 74 (90%)   | 8 (10%)  | 0        | 100         | 100 |
| 2   | S     | 82/85 (96%)     | 75 (92%)   | 7 (8%)   | 0        | 100         | 100 |
| 2   | T     | 82/85 (96%)     | 77 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 2   | U     | 82/85 (96%)     | 77 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 2   | V     | 82/85 (96%)     | 76 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 2   | W     | 82/85 (96%)     | 71 (87%)   | 11 (13%) | 0        | 100         | 100 |
| 2   | X     | 82/85 (96%)     | 81 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| All | All   | 5524/5832 (95%) | 5066 (92%) | 427 (8%) | 31 (1%)  | 21          | 55  |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | GLU  |
| 1   | B     | 128 | ASP  |
| 1   | D     | 25  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 26  | VAL  |
| 1   | D     | 257 | ASP  |
| 1   | G     | 18  | GLU  |
| 1   | G     | 173 | ARG  |
| 1   | H     | 129 | PHE  |
| 1   | K     | 262 | LEU  |
| 1   | L     | 25  | ASN  |
| 1   | L     | 26  | VAL  |
| 1   | M     | 18  | GLU  |
| 1   | I     | 18  | GLU  |
| 1   | I     | 319 | VAL  |
| 1   | C     | 321 | TRP  |
| 1   | D     | 27  | ASN  |
| 1   | D     | 128 | ASP  |
| 1   | F     | 180 | ASN  |
| 1   | I     | 17  | ARG  |
| 1   | P     | 294 | ARG  |
| 1   | C     | 29  | ARG  |
| 1   | D     | 24  | GLU  |
| 1   | E     | 31  | PRO  |
| 1   | L     | 24  | GLU  |
| 1   | I     | 32  | LEU  |
| 1   | C     | 320 | ALA  |
| 1   | D     | 19  | ASN  |
| 1   | I     | 31  | PRO  |
| 1   | B     | 85  | GLY  |
| 1   | C     | 30  | LYS  |
| 1   | O     | 177 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 275/284 (97%) | 274 (100%) | 1 (0%)   | 84          | 83  |
| 1   | B     | 272/284 (96%) | 272 (100%) | 0        | 100         | 100 |
| 1   | C     | 276/284 (97%) | 276 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | D     | 272/284 (96%)   | 272 (100%)  | 0        | 100         | 100 |
| 1   | E     | 276/284 (97%)   | 276 (100%)  | 0        | 100         | 100 |
| 1   | F     | 272/284 (96%)   | 272 (100%)  | 0        | 100         | 100 |
| 1   | G     | 276/284 (97%)   | 276 (100%)  | 0        | 100         | 100 |
| 1   | H     | 270/284 (95%)   | 270 (100%)  | 0        | 100         | 100 |
| 1   | I     | 276/284 (97%)   | 276 (100%)  | 0        | 100         | 100 |
| 1   | J     | 271/284 (95%)   | 271 (100%)  | 0        | 100         | 100 |
| 1   | K     | 274/284 (96%)   | 274 (100%)  | 0        | 100         | 100 |
| 1   | L     | 272/284 (96%)   | 272 (100%)  | 0        | 100         | 100 |
| 1   | M     | 278/284 (98%)   | 278 (100%)  | 0        | 100         | 100 |
| 1   | N     | 269/284 (95%)   | 269 (100%)  | 0        | 100         | 100 |
| 1   | O     | 275/284 (97%)   | 275 (100%)  | 0        | 100         | 100 |
| 1   | P     | 270/284 (95%)   | 270 (100%)  | 0        | 100         | 100 |
| 2   | Q     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | R     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | S     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | T     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | U     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | V     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | W     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| 2   | X     | 79/80 (99%)     | 79 (100%)   | 0        | 100         | 100 |
| All | All   | 5006/5184 (97%) | 5005 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | HIS  |
| 1   | B     | 45  | HIS  |
| 1   | B     | 64  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 253 | HIS  |
| 1   | B     | 308 | HIS  |
| 1   | C     | 47  | ASN  |
| 1   | C     | 119 | ASN  |
| 1   | C     | 190 | ASN  |
| 1   | C     | 214 | HIS  |
| 1   | D     | 54  | HIS  |
| 1   | D     | 68  | HIS  |
| 1   | D     | 205 | GLN  |
| 1   | D     | 308 | HIS  |
| 1   | E     | 68  | HIS  |
| 1   | E     | 122 | ASN  |
| 1   | E     | 132 | HIS  |
| 1   | F     | 122 | ASN  |
| 1   | F     | 308 | HIS  |
| 1   | G     | 19  | ASN  |
| 1   | H     | 68  | HIS  |
| 1   | H     | 132 | HIS  |
| 2   | Q     | 24  | HIS  |
| 2   | T     | 30  | ASN  |
| 2   | V     | 24  | HIS  |
| 1   | K     | 54  | HIS  |
| 1   | K     | 68  | HIS  |
| 1   | K     | 308 | HIS  |
| 1   | L     | 64  | HIS  |
| 1   | L     | 94  | HIS  |
| 1   | L     | 131 | ASN  |
| 1   | L     | 241 | ASN  |
| 1   | L     | 276 | ASN  |
| 1   | L     | 308 | HIS  |
| 1   | M     | 19  | ASN  |
| 1   | M     | 91  | GLN  |
| 1   | M     | 115 | ASN  |
| 1   | M     | 214 | HIS  |
| 1   | N     | 308 | HIS  |
| 1   | I     | 45  | HIS  |
| 1   | I     | 91  | GLN  |
| 1   | I     | 132 | HIS  |
| 1   | I     | 308 | HIS  |
| 1   | J     | 131 | ASN  |
| 1   | J     | 308 | HIS  |
| 1   | O     | 19  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 45  | HIS  |
| 1   | O     | 205 | GLN  |
| 1   | O     | 241 | ASN  |
| 1   | O     | 276 | ASN  |
| 1   | P     | 25  | ASN  |
| 1   | P     | 27  | ASN  |
| 1   | P     | 308 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 311/322 (96%) | 1.48   | 83 (26%) 1 3  | 16, 55, 106, 134      | 0     |
| 1   | B     | 308/322 (95%) | 1.14   | 42 (13%) 7 10 | 17, 47, 85, 127       | 0     |
| 1   | C     | 312/322 (96%) | 1.41   | 72 (23%) 2 4  | 12, 48, 102, 125      | 0     |
| 1   | D     | 308/322 (95%) | 0.94   | 28 (9%) 15 16 | 15, 41, 78, 115       | 0     |
| 1   | E     | 312/322 (96%) | 1.45   | 77 (24%) 2 4  | 9, 52, 98, 142        | 0     |
| 1   | F     | 308/322 (95%) | 1.27   | 56 (18%) 3 6  | 18, 66, 104, 119      | 0     |
| 1   | G     | 312/322 (96%) | 1.29   | 58 (18%) 3 6  | 9, 46, 94, 137        | 0     |
| 1   | H     | 306/322 (95%) | 1.18   | 52 (16%) 4 7  | 13, 60, 102, 121      | 0     |
| 1   | I     | 312/322 (96%) | 1.42   | 73 (23%) 2 4  | 13, 52, 89, 107       | 0     |
| 1   | J     | 307/322 (95%) | 1.24   | 51 (16%) 4 7  | 24, 63, 95, 117       | 0     |
| 1   | K     | 310/322 (96%) | 1.29   | 50 (16%) 4 7  | 11, 45, 87, 115       | 0     |
| 1   | L     | 308/322 (95%) | 1.24   | 61 (19%) 3 5  | 14, 56, 94, 114       | 0     |
| 1   | M     | 314/322 (97%) | 1.49   | 80 (25%) 1 4  | 14, 58, 98, 144       | 0     |
| 1   | N     | 305/322 (94%) | 1.48   | 74 (24%) 2 4  | 31, 79, 109, 127      | 0     |
| 1   | O     | 311/322 (96%) | 1.38   | 68 (21%) 2 4  | 10, 51, 97, 128       | 0     |
| 1   | P     | 306/322 (95%) | 1.40   | 68 (22%) 2 4  | 22, 72, 105, 134      | 0     |
| 2   | Q     | 84/85 (98%)   | 1.12   | 9 (10%) 11 14 | 18, 54, 91, 101       | 0     |
| 2   | R     | 84/85 (98%)   | 1.08   | 12 (14%) 6 9  | 13, 47, 85, 112       | 0     |
| 2   | S     | 84/85 (98%)   | 1.08   | 11 (13%) 7 10 | 12, 49, 86, 119       | 0     |
| 2   | T     | 84/85 (98%)   | 1.10   | 12 (14%) 6 9  | 9, 45, 72, 99         | 0     |
| 2   | U     | 84/85 (98%)   | 1.29   | 15 (17%) 3 6  | 17, 50, 97, 119       | 0     |
| 2   | V     | 84/85 (98%)   | 1.21   | 14 (16%) 4 7  | 16, 52, 83, 91        | 0     |
| 2   | W     | 84/85 (98%)   | 1.06   | 14 (16%) 4 7  | 16, 43, 87, 117       | 0     |
| 2   | X     | 84/85 (98%)   | 1.15   | 13 (15%) 5 8  | 13, 47, 83, 112       | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|------------------------------|-----------------------|-------|
| All | All   | 5622/5832 (96%) | 1.30   | 1093 (19%) <b>3</b> <b>5</b> | 9, 55, 99, 144        | 0     |

All (1093) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 218 | GLU  | 7.4  |
| 1   | M     | 286 | PRO  | 7.0  |
| 1   | C     | 292 | VAL  | 6.6  |
| 1   | N     | 68  | HIS  | 6.6  |
| 1   | C     | 218 | GLU  | 6.6  |
| 1   | A     | 311 | GLY  | 6.6  |
| 1   | K     | 161 | ASP  | 6.6  |
| 1   | J     | 178 | PRO  | 6.6  |
| 1   | G     | 218 | GLU  | 6.5  |
| 1   | G     | 217 | SER  | 6.4  |
| 1   | O     | 142 | VAL  | 6.4  |
| 1   | P     | 162 | GLU  | 6.0  |
| 1   | C     | 158 | ALA  | 5.9  |
| 1   | C     | 150 | GLY  | 5.7  |
| 1   | H     | 153 | ARG  | 5.6  |
| 1   | F     | 82  | LEU  | 5.5  |
| 1   | F     | 148 | VAL  | 5.4  |
| 1   | L     | 218 | GLU  | 5.3  |
| 1   | A     | 262 | LEU  | 5.3  |
| 1   | N     | 82  | LEU  | 5.3  |
| 1   | I     | 33  | ALA  | 5.2  |
| 1   | M     | 218 | GLU  | 5.2  |
| 1   | G     | 144 | GLU  | 5.1  |
| 1   | M     | 34  | ILE  | 5.1  |
| 1   | I     | 135 | GLU  | 5.1  |
| 1   | A     | 261 | VAL  | 5.1  |
| 1   | O     | 36  | GLY  | 5.0  |
| 2   | X     | 12  | GLU  | 5.0  |
| 1   | F     | 283 | VAL  | 5.0  |
| 1   | A     | 292 | VAL  | 5.0  |
| 1   | G     | 117 | GLU  | 4.9  |
| 2   | U     | 53  | ILE  | 4.9  |
| 1   | O     | 33  | ALA  | 4.9  |
| 1   | H     | 80  | GLU  | 4.9  |
| 1   | I     | 158 | ALA  | 4.9  |
| 1   | O     | 35  | GLU  | 4.9  |
| 1   | O     | 255 | ARG  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 34  | ILE  | 4.9  |
| 1   | F     | 71  | TYR  | 4.8  |
| 1   | F     | 51  | GLN  | 4.8  |
| 1   | B     | 68  | HIS  | 4.8  |
| 1   | N     | 17  | ARG  | 4.8  |
| 1   | F     | 149 | GLU  | 4.8  |
| 1   | M     | 33  | ALA  | 4.8  |
| 1   | I     | 136 | LEU  | 4.8  |
| 1   | F     | 80  | GLU  | 4.7  |
| 2   | Q     | 36  | GLU  | 4.7  |
| 1   | A     | 154 | GLN  | 4.7  |
| 1   | C     | 256 | GLU  | 4.6  |
| 1   | H     | 68  | HIS  | 4.6  |
| 1   | J     | 162 | GLU  | 4.5  |
| 1   | K     | 72  | TYR  | 4.5  |
| 1   | A     | 293 | THR  | 4.5  |
| 1   | G     | 25  | ASN  | 4.5  |
| 1   | H     | 178 | PRO  | 4.5  |
| 1   | A     | 219 | ARG  | 4.5  |
| 1   | A     | 218 | GLU  | 4.4  |
| 1   | F     | 178 | PRO  | 4.4  |
| 1   | P     | 321 | TRP  | 4.4  |
| 2   | Q     | 77  | GLU  | 4.3  |
| 1   | E     | 258 | LEU  | 4.3  |
| 1   | L     | 117 | GLU  | 4.3  |
| 1   | G     | 27  | ASN  | 4.3  |
| 1   | N     | 313 | GLU  | 4.3  |
| 1   | G     | 147 | ASN  | 4.3  |
| 1   | H     | 129 | PHE  | 4.3  |
| 1   | K     | 203 | ASN  | 4.3  |
| 1   | L     | 178 | PRO  | 4.3  |
| 2   | S     | 36  | GLU  | 4.3  |
| 1   | C     | 169 | ARG  | 4.2  |
| 1   | E     | 292 | VAL  | 4.2  |
| 1   | K     | 153 | ARG  | 4.2  |
| 1   | G     | 320 | ALA  | 4.2  |
| 1   | M     | 35  | GLU  | 4.2  |
| 1   | E     | 117 | GLU  | 4.2  |
| 1   | P     | 144 | GLU  | 4.2  |
| 1   | E     | 217 | SER  | 4.2  |
| 1   | A     | 149 | GLU  | 4.2  |
| 1   | I     | 29  | ARG  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 219 | ARG  | 4.2  |
| 1   | A     | 181 | GLU  | 4.2  |
| 1   | M     | 258 | LEU  | 4.2  |
| 1   | M     | 97  | ASP  | 4.1  |
| 1   | A     | 217 | SER  | 4.1  |
| 1   | D     | 173 | ARG  | 4.1  |
| 1   | O     | 218 | GLU  | 4.1  |
| 1   | P     | 80  | GLU  | 4.1  |
| 1   | M     | 219 | ARG  | 4.1  |
| 1   | O     | 262 | LEU  | 4.1  |
| 1   | N     | 157 | TYR  | 4.1  |
| 1   | C     | 217 | SER  | 4.1  |
| 1   | H     | 255 | ARG  | 4.1  |
| 1   | N     | 255 | ARG  | 4.1  |
| 1   | K     | 33  | ALA  | 4.1  |
| 1   | I     | 36  | GLY  | 4.1  |
| 1   | I     | 67  | ASN  | 4.1  |
| 1   | J     | 173 | ARG  | 4.1  |
| 1   | B     | 38  | TYR  | 4.0  |
| 1   | N     | 161 | ASP  | 4.0  |
| 1   | N     | 71  | TYR  | 4.0  |
| 1   | N     | 69  | TYR  | 4.0  |
| 1   | C     | 174 | THR  | 4.0  |
| 1   | C     | 171 | GLY  | 4.0  |
| 1   | F     | 174 | THR  | 4.0  |
| 1   | M     | 221 | PHE  | 4.0  |
| 1   | N     | 83  | LEU  | 4.0  |
| 2   | Q     | 39  | LEU  | 4.0  |
| 1   | J     | 68  | HIS  | 4.0  |
| 1   | K     | 171 | GLY  | 4.0  |
| 1   | A     | 33  | ALA  | 4.0  |
| 1   | I     | 70  | GLY  | 3.9  |
| 1   | O     | 97  | ASP  | 3.9  |
| 1   | C     | 33  | ALA  | 3.9  |
| 1   | H     | 173 | ARG  | 3.9  |
| 1   | I     | 153 | ARG  | 3.9  |
| 1   | K     | 30  | LYS  | 3.9  |
| 2   | R     | 78  | LYS  | 3.9  |
| 1   | E     | 143 | THR  | 3.9  |
| 1   | F     | 293 | THR  | 3.9  |
| 1   | O     | 112 | GLY  | 3.9  |
| 1   | K     | 82  | LEU  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 83  | LEU  | 3.8  |
| 1   | H     | 259 | ASN  | 3.8  |
| 1   | N     | 283 | VAL  | 3.8  |
| 1   | M     | 322 | PHE  | 3.8  |
| 1   | P     | 158 | ALA  | 3.8  |
| 2   | S     | 56  | ASN  | 3.8  |
| 1   | C     | 18  | GLU  | 3.8  |
| 1   | H     | 71  | TYR  | 3.8  |
| 1   | E     | 179 | LYS  | 3.8  |
| 1   | C     | 258 | LEU  | 3.8  |
| 1   | E     | 219 | ARG  | 3.8  |
| 1   | E     | 266 | GLU  | 3.7  |
| 1   | E     | 283 | VAL  | 3.7  |
| 1   | H     | 69  | TYR  | 3.7  |
| 1   | P     | 69  | TYR  | 3.7  |
| 2   | S     | 12  | GLU  | 3.7  |
| 1   | G     | 219 | ARG  | 3.7  |
| 1   | K     | 144 | GLU  | 3.7  |
| 1   | C     | 35  | GLU  | 3.7  |
| 1   | K     | 27  | ASN  | 3.7  |
| 1   | P     | 99  | ASN  | 3.7  |
| 1   | K     | 36  | GLY  | 3.7  |
| 1   | K     | 128 | ASP  | 3.7  |
| 1   | J     | 129 | PHE  | 3.7  |
| 1   | I     | 204 | THR  | 3.6  |
| 1   | H     | 283 | VAL  | 3.6  |
| 1   | C     | 117 | GLU  | 3.6  |
| 1   | K     | 218 | GLU  | 3.6  |
| 1   | J     | 80  | GLU  | 3.6  |
| 1   | B     | 26  | VAL  | 3.6  |
| 1   | P     | 178 | PRO  | 3.6  |
| 1   | A     | 39  | ASP  | 3.6  |
| 1   | H     | 320 | ALA  | 3.6  |
| 1   | J     | 85  | GLY  | 3.6  |
| 1   | K     | 29  | ARG  | 3.6  |
| 1   | K     | 219 | ARG  | 3.6  |
| 1   | O     | 203 | ASN  | 3.6  |
| 1   | N     | 277 | GLN  | 3.6  |
| 2   | R     | 36  | GLU  | 3.6  |
| 1   | N     | 33  | ALA  | 3.6  |
| 1   | B     | 83  | LEU  | 3.6  |
| 1   | M     | 262 | LEU  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 314 | GLU  | 3.6  |
| 1   | I     | 218 | GLU  | 3.6  |
| 1   | O     | 135 | GLU  | 3.6  |
| 2   | T     | 36  | GLU  | 3.6  |
| 1   | H     | 166 | GLY  | 3.5  |
| 1   | M     | 203 | ASN  | 3.5  |
| 1   | J     | 146 | MET  | 3.5  |
| 1   | D     | 71  | TYR  | 3.5  |
| 1   | M     | 84  | SER  | 3.5  |
| 2   | U     | 68  | MET  | 3.5  |
| 2   | T     | 78  | LYS  | 3.5  |
| 1   | A     | 153 | ARG  | 3.5  |
| 1   | L     | 128 | ASP  | 3.5  |
| 1   | M     | 255 | ARG  | 3.5  |
| 1   | F     | 166 | GLY  | 3.5  |
| 1   | K     | 292 | VAL  | 3.5  |
| 1   | J     | 292 | VAL  | 3.5  |
| 1   | H     | 136 | LEU  | 3.5  |
| 1   | D     | 54  | HIS  | 3.5  |
| 1   | N     | 153 | ARG  | 3.5  |
| 1   | H     | 127 | SER  | 3.5  |
| 1   | M     | 217 | SER  | 3.5  |
| 1   | L     | 69  | TYR  | 3.4  |
| 2   | V     | 83  | GLU  | 3.4  |
| 1   | O     | 28  | GLY  | 3.4  |
| 1   | M     | 180 | ASN  | 3.4  |
| 1   | G     | 36  | GLY  | 3.4  |
| 1   | G     | 140 | LYS  | 3.4  |
| 1   | O     | 27  | ASN  | 3.4  |
| 1   | F     | 68  | HIS  | 3.4  |
| 1   | E     | 257 | ASP  | 3.4  |
| 1   | I     | 159 | ARG  | 3.4  |
| 1   | C     | 113 | ALA  | 3.4  |
| 1   | F     | 129 | PHE  | 3.4  |
| 1   | N     | 97  | ASP  | 3.4  |
| 1   | D     | 83  | LEU  | 3.4  |
| 1   | B     | 71  | TYR  | 3.4  |
| 1   | G     | 71  | TYR  | 3.4  |
| 1   | F     | 17  | ARG  | 3.4  |
| 1   | K     | 124 | GLY  | 3.4  |
| 1   | M     | 153 | ARG  | 3.4  |
| 1   | L     | 124 | GLY  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 18  | GLU  | 3.3  |
| 1   | E     | 136 | LEU  | 3.3  |
| 1   | H     | 86  | ASP  | 3.3  |
| 1   | L     | 217 | SER  | 3.3  |
| 1   | M     | 36  | GLY  | 3.3  |
| 1   | L     | 148 | VAL  | 3.3  |
| 1   | M     | 98  | LYS  | 3.3  |
| 1   | E     | 153 | ARG  | 3.3  |
| 1   | O     | 143 | THR  | 3.3  |
| 1   | H     | 252 | ASP  | 3.3  |
| 1   | L     | 172 | LYS  | 3.3  |
| 1   | B     | 33  | ALA  | 3.3  |
| 1   | A     | 176 | ARG  | 3.3  |
| 1   | B     | 128 | ASP  | 3.3  |
| 1   | C     | 82  | LEU  | 3.3  |
| 1   | E     | 296 | ARG  | 3.3  |
| 1   | O     | 181 | GLU  | 3.3  |
| 1   | P     | 132 | HIS  | 3.3  |
| 1   | B     | 178 | PRO  | 3.3  |
| 1   | N     | 190 | ASN  | 3.3  |
| 1   | P     | 150 | GLY  | 3.3  |
| 1   | P     | 174 | THR  | 3.3  |
| 1   | P     | 314 | GLU  | 3.3  |
| 1   | M     | 32  | LEU  | 3.2  |
| 1   | N     | 79  | ARG  | 3.2  |
| 1   | P     | 159 | ARG  | 3.2  |
| 1   | O     | 217 | SER  | 3.2  |
| 1   | A     | 117 | GLU  | 3.2  |
| 1   | F     | 297 | LEU  | 3.2  |
| 1   | A     | 173 | ARG  | 3.2  |
| 1   | A     | 255 | ARG  | 3.2  |
| 1   | O     | 219 | ARG  | 3.2  |
| 1   | A     | 150 | GLY  | 3.2  |
| 1   | F     | 220 | ARG  | 3.2  |
| 1   | F     | 292 | VAL  | 3.2  |
| 1   | P     | 84  | SER  | 3.2  |
| 1   | A     | 172 | LYS  | 3.2  |
| 1   | E     | 251 | LYS  | 3.2  |
| 1   | C     | 160 | TRP  | 3.2  |
| 1   | A     | 260 | GLY  | 3.2  |
| 1   | P     | 71  | TYR  | 3.2  |
| 1   | O     | 153 | ARG  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 26  | VAL  | 3.2  |
| 2   | W     | 78  | LYS  | 3.2  |
| 1   | M     | 136 | LEU  | 3.2  |
| 1   | J     | 70  | GLY  | 3.2  |
| 1   | D     | 27  | ASN  | 3.2  |
| 1   | M     | 55  | TYR  | 3.2  |
| 1   | O     | 29  | ARG  | 3.2  |
| 1   | J     | 280 | GLU  | 3.2  |
| 1   | N     | 179 | LYS  | 3.2  |
| 1   | D     | 187 | SER  | 3.2  |
| 1   | M     | 102 | LEU  | 3.2  |
| 2   | W     | 84  | ILE  | 3.1  |
| 1   | E     | 267 | GLY  | 3.1  |
| 1   | I     | 173 | ARG  | 3.1  |
| 1   | L     | 190 | ASN  | 3.1  |
| 1   | J     | 71  | TYR  | 3.1  |
| 2   | X     | 19  | LYS  | 3.1  |
| 1   | A     | 102 | LEU  | 3.1  |
| 1   | F     | 133 | LEU  | 3.1  |
| 1   | L     | 83  | LEU  | 3.1  |
| 1   | F     | 219 | ARG  | 3.1  |
| 1   | L     | 141 | LYS  | 3.1  |
| 1   | B     | 69  | TYR  | 3.1  |
| 1   | H     | 218 | GLU  | 3.1  |
| 1   | O     | 127 | SER  | 3.1  |
| 2   | R     | 12  | GLU  | 3.1  |
| 2   | U     | 55  | GLU  | 3.1  |
| 1   | I     | 322 | PHE  | 3.1  |
| 1   | E     | 70  | GLY  | 3.1  |
| 1   | I     | 81  | THR  | 3.1  |
| 1   | J     | 69  | TYR  | 3.1  |
| 1   | M     | 181 | GLU  | 3.1  |
| 1   | I     | 215 | GLU  | 3.1  |
| 1   | A     | 216 | PRO  | 3.1  |
| 1   | M     | 141 | LYS  | 3.1  |
| 1   | C     | 293 | THR  | 3.1  |
| 1   | C     | 47  | ASN  | 3.1  |
| 2   | R     | 56  | ASN  | 3.1  |
| 1   | L     | 157 | TYR  | 3.1  |
| 1   | K     | 294 | ARG  | 3.1  |
| 1   | P     | 68  | HIS  | 3.1  |
| 1   | P     | 225 | LEU  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 259 | ASN  | 3.1  |
| 1   | M     | 69  | TYR  | 3.1  |
| 2   | U     | 52  | ILE  | 3.1  |
| 1   | I     | 256 | GLU  | 3.1  |
| 1   | P     | 281 | LYS  | 3.1  |
| 1   | F     | 86  | ASP  | 3.1  |
| 1   | P     | 320 | ALA  | 3.0  |
| 1   | B     | 43  | TYR  | 3.0  |
| 1   | C     | 180 | ASN  | 3.0  |
| 1   | N     | 180 | ASN  | 3.0  |
| 1   | J     | 67  | ASN  | 3.0  |
| 1   | P     | 300 | LEU  | 3.0  |
| 1   | M     | 37  | ILE  | 3.0  |
| 1   | H     | 139 | ALA  | 3.0  |
| 1   | I     | 68  | HIS  | 3.0  |
| 1   | C     | 159 | ARG  | 3.0  |
| 1   | C     | 155 | GLU  | 3.0  |
| 1   | D     | 280 | GLU  | 3.0  |
| 1   | C     | 70  | GLY  | 3.0  |
| 1   | G     | 28  | GLY  | 3.0  |
| 1   | C     | 58  | GLN  | 3.0  |
| 1   | K     | 173 | ARG  | 3.0  |
| 1   | I     | 219 | ARG  | 3.0  |
| 2   | V     | 39  | LEU  | 3.0  |
| 1   | G     | 259 | ASN  | 3.0  |
| 1   | J     | 156 | TYR  | 3.0  |
| 1   | F     | 280 | GLU  | 3.0  |
| 1   | C     | 154 | GLN  | 3.0  |
| 1   | C     | 126 | SER  | 3.0  |
| 1   | L     | 110 | VAL  | 3.0  |
| 2   | S     | 11  | VAL  | 3.0  |
| 1   | A     | 119 | ASN  | 3.0  |
| 1   | M     | 99  | ASN  | 3.0  |
| 1   | N     | 165 | PRO  | 3.0  |
| 1   | E     | 83  | LEU  | 3.0  |
| 1   | I     | 154 | GLN  | 3.0  |
| 1   | I     | 265 | ASP  | 3.0  |
| 2   | W     | 58  | ASP  | 3.0  |
| 1   | A     | 266 | GLU  | 2.9  |
| 1   | P     | 18  | GLU  | 2.9  |
| 1   | E     | 185 | LEU  | 2.9  |
| 1   | M     | 17  | ARG  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 211 | SER  | 2.9  |
| 1   | J     | 79  | ARG  | 2.9  |
| 1   | A     | 158 | ALA  | 2.9  |
| 1   | A     | 71  | TYR  | 2.9  |
| 1   | G     | 69  | TYR  | 2.9  |
| 1   | M     | 71  | TYR  | 2.9  |
| 1   | N     | 178 | PRO  | 2.9  |
| 1   | N     | 322 | PHE  | 2.9  |
| 1   | C     | 173 | ARG  | 2.9  |
| 1   | E     | 36  | GLY  | 2.9  |
| 1   | E     | 184 | ALA  | 2.9  |
| 1   | P     | 121 | LYS  | 2.9  |
| 1   | N     | 170 | ILE  | 2.9  |
| 1   | F     | 155 | GLU  | 2.9  |
| 2   | W     | 36  | GLU  | 2.9  |
| 1   | O     | 81  | THR  | 2.9  |
| 1   | C     | 100 | LYS  | 2.9  |
| 1   | M     | 313 | GLU  | 2.9  |
| 1   | D     | 150 | GLY  | 2.9  |
| 1   | H     | 70  | GLY  | 2.9  |
| 1   | L     | 154 | GLN  | 2.9  |
| 1   | C     | 32  | LEU  | 2.9  |
| 1   | E     | 93  | GLU  | 2.9  |
| 1   | H     | 155 | GLU  | 2.9  |
| 1   | O     | 54  | HIS  | 2.9  |
| 1   | I     | 110 | VAL  | 2.9  |
| 1   | P     | 112 | GLY  | 2.9  |
| 2   | S     | 10  | GLY  | 2.9  |
| 2   | X     | 78  | LYS  | 2.9  |
| 1   | P     | 102 | LEU  | 2.9  |
| 1   | N     | 159 | ARG  | 2.9  |
| 1   | P     | 43  | TYR  | 2.9  |
| 1   | C     | 183 | ASN  | 2.9  |
| 1   | I     | 141 | LYS  | 2.9  |
| 1   | P     | 190 | ASN  | 2.9  |
| 1   | D     | 85  | GLY  | 2.8  |
| 1   | E     | 28  | GLY  | 2.8  |
| 1   | O     | 312 | VAL  | 2.8  |
| 1   | H     | 83  | LEU  | 2.8  |
| 1   | N     | 160 | TRP  | 2.8  |
| 1   | G     | 176 | ARG  | 2.8  |
| 1   | P     | 238 | ARG  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 130 | SER  | 2.8  |
| 1   | K     | 28  | GLY  | 2.8  |
| 1   | M     | 86  | ASP  | 2.8  |
| 1   | I     | 161 | ASP  | 2.8  |
| 1   | A     | 159 | ARG  | 2.8  |
| 1   | N     | 173 | ARG  | 2.8  |
| 1   | E     | 312 | VAL  | 2.8  |
| 1   | N     | 80  | GLU  | 2.8  |
| 1   | L     | 68  | HIS  | 2.8  |
| 1   | I     | 112 | GLY  | 2.8  |
| 1   | J     | 171 | GLY  | 2.8  |
| 1   | C     | 252 | ASP  | 2.8  |
| 1   | G     | 158 | ALA  | 2.8  |
| 1   | I     | 174 | THR  | 2.8  |
| 1   | I     | 255 | ARG  | 2.8  |
| 1   | M     | 127 | SER  | 2.8  |
| 1   | M     | 157 | TYR  | 2.8  |
| 1   | A     | 314 | GLU  | 2.8  |
| 1   | B     | 205 | GLN  | 2.8  |
| 1   | G     | 18  | GLU  | 2.8  |
| 1   | N     | 70  | GLY  | 2.8  |
| 2   | Q     | 56  | ASN  | 2.8  |
| 2   | U     | 26  | ASN  | 2.8  |
| 1   | L     | 106 | LYS  | 2.8  |
| 1   | L     | 151 | ARG  | 2.8  |
| 1   | F     | 26  | VAL  | 2.8  |
| 2   | V     | 37  | VAL  | 2.8  |
| 1   | E     | 35  | GLU  | 2.8  |
| 1   | E     | 203 | ASN  | 2.8  |
| 1   | I     | 58  | GLN  | 2.8  |
| 1   | P     | 266 | GLU  | 2.8  |
| 1   | K     | 7   | THR  | 2.8  |
| 1   | A     | 177 | PRO  | 2.8  |
| 1   | H     | 217 | SER  | 2.8  |
| 1   | O     | 71  | TYR  | 2.8  |
| 1   | H     | 146 | MET  | 2.8  |
| 1   | I     | 117 | GLU  | 2.8  |
| 1   | P     | 200 | GLU  | 2.8  |
| 1   | P     | 179 | LYS  | 2.8  |
| 1   | D     | 73  | ASP  | 2.7  |
| 1   | P     | 128 | ASP  | 2.7  |
| 1   | G     | 321 | TRP  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 22  | TYR  | 2.7  |
| 1   | C     | 181 | GLU  | 2.7  |
| 1   | F     | 124 | GLY  | 2.7  |
| 1   | F     | 162 | GLU  | 2.7  |
| 2   | U     | 77  | GLU  | 2.7  |
| 1   | O     | 82  | LEU  | 2.7  |
| 1   | M     | 125 | ILE  | 2.7  |
| 2   | T     | 53  | ILE  | 2.7  |
| 1   | O     | 86  | ASP  | 2.7  |
| 1   | C     | 222 | SER  | 2.7  |
| 1   | I     | 222 | SER  | 2.7  |
| 1   | G     | 31  | PRO  | 2.7  |
| 1   | J     | 314 | GLU  | 2.7  |
| 1   | O     | 102 | LEU  | 2.7  |
| 2   | S     | 77  | GLU  | 2.7  |
| 1   | N     | 119 | ASN  | 2.7  |
| 1   | I     | 169 | ARG  | 2.7  |
| 1   | D     | 68  | HIS  | 2.7  |
| 1   | E     | 126 | SER  | 2.7  |
| 2   | U     | 31  | SER  | 2.7  |
| 1   | E     | 142 | VAL  | 2.7  |
| 1   | A     | 29  | ARG  | 2.7  |
| 1   | N     | 144 | GLU  | 2.7  |
| 1   | N     | 149 | GLU  | 2.7  |
| 1   | N     | 282 | THR  | 2.7  |
| 1   | G     | 30  | LYS  | 2.7  |
| 1   | M     | 312 | VAL  | 2.7  |
| 2   | W     | 11  | VAL  | 2.7  |
| 1   | F     | 15  | LEU  | 2.7  |
| 2   | X     | 39  | LEU  | 2.7  |
| 1   | N     | 51  | GLN  | 2.7  |
| 1   | G     | 72  | TYR  | 2.7  |
| 1   | I     | 320 | ALA  | 2.7  |
| 1   | A     | 35  | GLU  | 2.7  |
| 1   | L     | 174 | THR  | 2.7  |
| 1   | N     | 181 | GLU  | 2.7  |
| 1   | J     | 256 | GLU  | 2.7  |
| 1   | M     | 131 | ASN  | 2.7  |
| 1   | C     | 161 | ASP  | 2.7  |
| 1   | E     | 265 | ASP  | 2.7  |
| 1   | E     | 158 | ALA  | 2.7  |
| 1   | H     | 85  | GLY  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 158 | ALA  | 2.7  |
| 2   | S     | 83  | GLU  | 2.7  |
| 2   | U     | 43  | GLU  | 2.7  |
| 1   | H     | 122 | ASN  | 2.7  |
| 1   | N     | 27  | ASN  | 2.7  |
| 1   | J     | 259 | ASN  | 2.7  |
| 1   | P     | 115 | ASN  | 2.7  |
| 2   | W     | 16  | LYS  | 2.7  |
| 1   | L     | 82  | LEU  | 2.7  |
| 2   | S     | 57  | SER  | 2.7  |
| 1   | B     | 148 | VAL  | 2.6  |
| 1   | P     | 255 | ARG  | 2.6  |
| 1   | P     | 277 | GLN  | 2.6  |
| 2   | V     | 52  | ILE  | 2.6  |
| 1   | L     | 166 | GLY  | 2.6  |
| 1   | M     | 28  | GLY  | 2.6  |
| 1   | F     | 38  | TYR  | 2.6  |
| 1   | G     | 35  | GLU  | 2.6  |
| 1   | J     | 241 | ASN  | 2.6  |
| 1   | O     | 164 | LEU  | 2.6  |
| 1   | P     | 83  | LEU  | 2.6  |
| 1   | F     | 52  | ALA  | 2.6  |
| 1   | I     | 106 | LYS  | 2.6  |
| 1   | P     | 311 | GLY  | 2.6  |
| 1   | L     | 11  | ASP  | 2.6  |
| 1   | N     | 81  | THR  | 2.6  |
| 1   | O     | 128 | ASP  | 2.6  |
| 1   | I     | 155 | GLU  | 2.6  |
| 2   | U     | 12  | GLU  | 2.6  |
| 1   | E     | 262 | LEU  | 2.6  |
| 2   | V     | 53  | ILE  | 2.6  |
| 1   | E     | 178 | PRO  | 2.6  |
| 1   | F     | 154 | GLN  | 2.6  |
| 1   | I     | 216 | PRO  | 2.6  |
| 1   | N     | 43  | TYR  | 2.6  |
| 1   | B     | 97  | ASP  | 2.6  |
| 1   | B     | 93  | GLU  | 2.6  |
| 1   | D     | 218 | GLU  | 2.6  |
| 1   | E     | 322 | PHE  | 2.6  |
| 1   | K     | 149 | GLU  | 2.6  |
| 1   | L     | 256 | GLU  | 2.6  |
| 1   | A     | 25  | ASN  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 276 | ASN  | 2.6  |
| 1   | E     | 5   | SER  | 2.6  |
| 1   | J     | 163 | SER  | 2.6  |
| 1   | P     | 180 | ASN  | 2.6  |
| 1   | P     | 319 | VAL  | 2.6  |
| 1   | F     | 29  | ARG  | 2.6  |
| 1   | A     | 30  | LYS  | 2.6  |
| 1   | E     | 33  | ALA  | 2.6  |
| 1   | I     | 184 | ALA  | 2.6  |
| 1   | A     | 82  | LEU  | 2.6  |
| 1   | C     | 28  | GLY  | 2.6  |
| 1   | C     | 102 | LEU  | 2.6  |
| 1   | D     | 70  | GLY  | 2.6  |
| 1   | G     | 150 | GLY  | 2.6  |
| 1   | B     | 161 | ASP  | 2.6  |
| 1   | E     | 278 | GLU  | 2.6  |
| 2   | T     | 54  | ASP  | 2.6  |
| 2   | X     | 58  | ASP  | 2.6  |
| 2   | X     | 83  | GLU  | 2.6  |
| 1   | K     | 259 | ASN  | 2.6  |
| 1   | J     | 147 | ASN  | 2.6  |
| 1   | P     | 27  | ASN  | 2.6  |
| 2   | R     | 15  | ASN  | 2.6  |
| 1   | J     | 141 | LYS  | 2.6  |
| 1   | H     | 300 | LEU  | 2.6  |
| 1   | C     | 36  | GLY  | 2.6  |
| 1   | M     | 68  | HIS  | 2.6  |
| 1   | M     | 285 | HIS  | 2.6  |
| 1   | I     | 28  | GLY  | 2.6  |
| 1   | A     | 156 | TYR  | 2.6  |
| 1   | D     | 256 | GLU  | 2.6  |
| 1   | I     | 127 | SER  | 2.6  |
| 1   | J     | 230 | ILE  | 2.6  |
| 1   | A     | 161 | ASP  | 2.6  |
| 1   | K     | 11  | ASP  | 2.6  |
| 1   | B     | 27  | ASN  | 2.6  |
| 1   | F     | 121 | LYS  | 2.6  |
| 1   | G     | 131 | ASN  | 2.6  |
| 1   | L     | 319 | VAL  | 2.6  |
| 1   | M     | 159 | ARG  | 2.6  |
| 1   | I     | 238 | ARG  | 2.6  |
| 2   | R     | 19  | LYS  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | S     | 39  | LEU  | 2.6  |
| 1   | B     | 165 | PRO  | 2.6  |
| 1   | N     | 317 | PRO  | 2.6  |
| 1   | A     | 44  | GLY  | 2.6  |
| 1   | F     | 311 | GLY  | 2.6  |
| 1   | K     | 311 | GLY  | 2.6  |
| 1   | P     | 322 | PHE  | 2.6  |
| 1   | K     | 68  | HIS  | 2.5  |
| 1   | E     | 264 | THR  | 2.5  |
| 1   | B     | 40  | ILE  | 2.5  |
| 1   | C     | 135 | GLU  | 2.5  |
| 1   | H     | 121 | LYS  | 2.5  |
| 1   | M     | 266 | GLU  | 2.5  |
| 1   | G     | 310 | VAL  | 2.5  |
| 1   | L     | 136 | LEU  | 2.5  |
| 1   | K     | 112 | GLY  | 2.5  |
| 1   | N     | 171 | GLY  | 2.5  |
| 2   | Q     | 10  | GLY  | 2.5  |
| 1   | B     | 159 | ARG  | 2.5  |
| 1   | C     | 127 | SER  | 2.5  |
| 1   | M     | 130 | SER  | 2.5  |
| 1   | E     | 256 | GLU  | 2.5  |
| 1   | K     | 135 | GLU  | 2.5  |
| 2   | Q     | 12  | GLU  | 2.5  |
| 1   | C     | 262 | LEU  | 2.5  |
| 1   | O     | 225 | LEU  | 2.5  |
| 1   | L     | 241 | ASN  | 2.5  |
| 1   | M     | 67  | ASN  | 2.5  |
| 1   | E     | 137 | GLN  | 2.5  |
| 1   | O     | 260 | GLY  | 2.5  |
| 1   | A     | 125 | ILE  | 2.5  |
| 1   | A     | 72  | TYR  | 2.5  |
| 1   | E     | 29  | ARG  | 2.5  |
| 1   | M     | 192 | ARG  | 2.5  |
| 1   | C     | 314 | GLU  | 2.5  |
| 1   | C     | 27  | ASN  | 2.5  |
| 1   | H     | 25  | ASN  | 2.5  |
| 1   | O     | 158 | ALA  | 2.5  |
| 1   | D     | 145 | ILE  | 2.5  |
| 1   | K     | 260 | GLY  | 2.5  |
| 1   | G     | 169 | ARG  | 2.5  |
| 2   | T     | 66  | ARG  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 22  | TYR  | 2.5  |
| 1   | F     | 126 | SER  | 2.5  |
| 1   | N     | 132 | HIS  | 2.5  |
| 1   | I     | 217 | SER  | 2.5  |
| 1   | J     | 136 | LEU  | 2.5  |
| 1   | A     | 144 | GLU  | 2.5  |
| 1   | F     | 218 | GLU  | 2.5  |
| 1   | H     | 313 | GLU  | 2.5  |
| 2   | X     | 36  | GLU  | 2.5  |
| 1   | H     | 131 | ASN  | 2.5  |
| 1   | N     | 131 | ASN  | 2.5  |
| 1   | B     | 320 | ALA  | 2.5  |
| 1   | E     | 140 | LYS  | 2.5  |
| 1   | F     | 304 | LYS  | 2.5  |
| 1   | K     | 121 | LYS  | 2.5  |
| 1   | M     | 134 | LYS  | 2.5  |
| 1   | O     | 251 | LYS  | 2.5  |
| 1   | C     | 166 | GLY  | 2.5  |
| 1   | E     | 85  | GLY  | 2.5  |
| 1   | B     | 292 | VAL  | 2.5  |
| 1   | J     | 54  | HIS  | 2.5  |
| 1   | J     | 148 | VAL  | 2.5  |
| 1   | F     | 181 | GLU  | 2.5  |
| 1   | O     | 266 | GLU  | 2.5  |
| 1   | P     | 155 | GLU  | 2.5  |
| 1   | N     | 321 | TRP  | 2.5  |
| 1   | C     | 118 | LYS  | 2.5  |
| 1   | G     | 241 | ASN  | 2.5  |
| 1   | L     | 304 | LYS  | 2.5  |
| 1   | P     | 106 | LYS  | 2.5  |
| 1   | A     | 224 | ALA  | 2.5  |
| 1   | O     | 270 | ILE  | 2.5  |
| 1   | P     | 113 | ALA  | 2.5  |
| 1   | L     | 309 | LEU  | 2.5  |
| 1   | M     | 138 | GLY  | 2.5  |
| 2   | V     | 54  | ASP  | 2.5  |
| 1   | A     | 209 | THR  | 2.5  |
| 1   | D     | 84  | SER  | 2.5  |
| 1   | K     | 146 | MET  | 2.5  |
| 1   | H     | 244 | VAL  | 2.5  |
| 1   | P     | 142 | VAL  | 2.5  |
| 1   | B     | 18  | GLU  | 2.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | H            | 93         | GLU         | 2.4         |
| 1          | L            | 129        | PHE         | 2.4         |
| 2          | W            | 83         | GLU         | 2.4         |
| 1          | E            | 34         | ILE         | 2.4         |
| 1          | M            | 321        | TRP         | 2.4         |
| 2          | X            | 40         | ALA         | 2.4         |
| 1          | F            | 112        | GLY         | 2.4         |
| 1          | F            | 237        | ASP         | 2.4         |
| 1          | L            | 252        | ASP         | 2.4         |
| 1          | K            | 81         | THR         | 2.4         |
| 1          | K            | 293        | THR         | 2.4         |
| 1          | M            | 293        | THR         | 2.4         |
| 1          | O            | 310        | VAL         | 2.4         |
| 2          | W            | 6          | VAL         | 2.4         |
| 1          | A            | 38         | TYR         | 2.4         |
| 1          | A            | 179        | LYS         | 2.4         |
| 1          | C            | 140        | LYS         | 2.4         |
| 1          | E            | 269        | LYS         | 2.4         |
| 1          | H            | 232        | LYS         | 2.4         |
| 2          | U            | 51         | LYS         | 2.4         |
| 1          | M            | 135        | GLU         | 2.4         |
| 2          | W            | 77         | GLU         | 2.4         |
| 1          | F            | 321        | TRP         | 2.4         |
| 1          | G            | 123        | TRP         | 2.4         |
| 1          | A            | 113        | ALA         | 2.4         |
| 1          | G            | 203        | ASN         | 2.4         |
| 1          | L            | 159        | ARG         | 2.4         |
| 1          | N            | 220        | ARG         | 2.4         |
| 1          | I            | 183        | ASN         | 2.4         |
| 1          | M            | 311        | GLY         | 2.4         |
| 1          | A            | 134        | LYS         | 2.4         |
| 1          | G            | 142        | VAL         | 2.4         |
| 1          | A            | 34         | ILE         | 2.4         |
| 1          | M            | 156        | TYR         | 2.4         |
| 1          | N            | 212        | TYR         | 2.4         |
| 1          | P            | 239        | ILE         | 2.4         |
| 1          | K            | 35         | GLU         | 2.4         |
| 1          | M            | 214        | HIS         | 2.4         |
| 1          | M            | 314        | GLU         | 2.4         |
| 1          | J            | 214        | HIS         | 2.4         |
| 1          | O            | 155        | GLU         | 2.4         |
| 1          | D            | 259        | ASN         | 2.4         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 259 | ASN  | 2.4  |
| 1   | F     | 165 | PRO  | 2.4  |
| 1   | G     | 257 | ASP  | 2.4  |
| 2   | R     | 54  | ASP  | 2.4  |
| 1   | K     | 262 | LEU  | 2.4  |
| 1   | I     | 120 | LEU  | 2.4  |
| 1   | O     | 38  | TYR  | 2.4  |
| 1   | O     | 258 | LEU  | 2.4  |
| 1   | H     | 135 | GLU  | 2.4  |
| 1   | A     | 169 | ARG  | 2.4  |
| 1   | G     | 159 | ARG  | 2.4  |
| 1   | L     | 158 | ALA  | 2.4  |
| 1   | M     | 175 | ARG  | 2.4  |
| 1   | O     | 159 | ARG  | 2.4  |
| 2   | T     | 56  | ASN  | 2.4  |
| 2   | V     | 15  | ASN  | 2.4  |
| 1   | B     | 166 | GLY  | 2.4  |
| 1   | C     | 172 | LYS  | 2.4  |
| 1   | E     | 111 | GLY  | 2.4  |
| 1   | G     | 179 | LYS  | 2.4  |
| 1   | H     | 179 | LYS  | 2.4  |
| 2   | X     | 10  | GLY  | 2.4  |
| 1   | B     | 283 | VAL  | 2.4  |
| 1   | H     | 26  | VAL  | 2.4  |
| 1   | I     | 310 | VAL  | 2.4  |
| 1   | A     | 270 | ILE  | 2.4  |
| 1   | L     | 258 | LEU  | 2.4  |
| 1   | G     | 161 | ASP  | 2.4  |
| 1   | I     | 226 | ASP  | 2.4  |
| 2   | R     | 66  | ARG  | 2.4  |
| 1   | M     | 113 | ALA  | 2.4  |
| 1   | E     | 147 | ASN  | 2.4  |
| 1   | P     | 122 | ASN  | 2.4  |
| 1   | B     | 49  | THR  | 2.4  |
| 1   | N     | 133 | LEU  | 2.4  |
| 1   | I     | 270 | ILE  | 2.4  |
| 1   | J     | 83  | LEU  | 2.4  |
| 1   | J     | 283 | VAL  | 2.4  |
| 1   | E     | 43  | TYR  | 2.4  |
| 1   | F     | 69  | TYR  | 2.4  |
| 1   | H     | 11  | ASP  | 2.4  |
| 1   | M     | 257 | ASP  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 52  | ALA  | 2.4  |
| 1   | J     | 117 | GLU  | 2.4  |
| 1   | O     | 144 | GLU  | 2.4  |
| 2   | V     | 82  | GLU  | 2.4  |
| 1   | F     | 246 | LYS  | 2.4  |
| 1   | O     | 141 | LYS  | 2.4  |
| 1   | P     | 172 | LYS  | 2.4  |
| 1   | A     | 112 | GLY  | 2.3  |
| 1   | A     | 321 | TRP  | 2.3  |
| 1   | K     | 150 | GLY  | 2.3  |
| 1   | L     | 126 | SER  | 2.3  |
| 1   | C     | 264 | THR  | 2.3  |
| 1   | M     | 143 | THR  | 2.3  |
| 1   | I     | 319 | VAL  | 2.3  |
| 1   | O     | 26  | VAL  | 2.3  |
| 1   | G     | 17  | ARG  | 2.3  |
| 1   | O     | 175 | ARG  | 2.3  |
| 1   | I     | 38  | TYR  | 2.3  |
| 1   | B     | 265 | ASP  | 2.3  |
| 1   | E     | 30  | LYS  | 2.3  |
| 1   | L     | 269 | LYS  | 2.3  |
| 1   | I     | 179 | LYS  | 2.3  |
| 2   | V     | 19  | LYS  | 2.3  |
| 1   | L     | 162 | GLU  | 2.3  |
| 1   | A     | 308 | HIS  | 2.3  |
| 1   | D     | 217 | SER  | 2.3  |
| 1   | E     | 216 | PRO  | 2.3  |
| 1   | E     | 248 | ILE  | 2.3  |
| 1   | J     | 166 | GLY  | 2.3  |
| 1   | G     | 143 | THR  | 2.3  |
| 1   | G     | 319 | VAL  | 2.3  |
| 1   | K     | 20  | THR  | 2.3  |
| 1   | K     | 272 | THR  | 2.3  |
| 1   | L     | 13  | THR  | 2.3  |
| 1   | L     | 282 | THR  | 2.3  |
| 2   | S     | 44  | ARG  | 2.3  |
| 1   | K     | 179 | LYS  | 2.3  |
| 2   | V     | 40  | ALA  | 2.3  |
| 1   | C     | 257 | ASP  | 2.3  |
| 1   | I     | 144 | GLU  | 2.3  |
| 1   | E     | 270 | ILE  | 2.3  |
| 1   | O     | 136 | LEU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 132 | HIS  | 2.3  |
| 1   | H     | 317 | PRO  | 2.3  |
| 1   | L     | 127 | SER  | 2.3  |
| 1   | I     | 126 | SER  | 2.3  |
| 1   | I     | 214 | HIS  | 2.3  |
| 1   | O     | 130 | SER  | 2.3  |
| 1   | P     | 111 | GLY  | 2.3  |
| 1   | O     | 180 | ASN  | 2.3  |
| 1   | N     | 174 | THR  | 2.3  |
| 1   | A     | 121 | LYS  | 2.3  |
| 1   | I     | 100 | LYS  | 2.3  |
| 2   | T     | 18  | LYS  | 2.3  |
| 1   | G     | 258 | LEU  | 2.3  |
| 1   | N     | 320 | ALA  | 2.3  |
| 1   | A     | 265 | ASP  | 2.3  |
| 2   | V     | 36  | GLU  | 2.3  |
| 2   | W     | 12  | GLU  | 2.3  |
| 1   | N     | 126 | SER  | 2.3  |
| 1   | G     | 171 | GLY  | 2.3  |
| 2   | R     | 80  | PRO  | 2.3  |
| 1   | D     | 292 | VAL  | 2.3  |
| 1   | E     | 68  | HIS  | 2.3  |
| 1   | M     | 26  | VAL  | 2.3  |
| 1   | F     | 25  | ASN  | 2.3  |
| 1   | A     | 118 | LYS  | 2.3  |
| 1   | H     | 123 | TRP  | 2.3  |
| 1   | O     | 134 | LYS  | 2.3  |
| 2   | T     | 27  | TRP  | 2.3  |
| 1   | P     | 133 | LEU  | 2.3  |
| 1   | C     | 71  | TYR  | 2.3  |
| 1   | G     | 156 | TYR  | 2.3  |
| 1   | M     | 129 | PHE  | 2.3  |
| 1   | N     | 239 | ILE  | 2.3  |
| 1   | L     | 51  | GLN  | 2.3  |
| 1   | D     | 141 | LYS  | 2.3  |
| 1   | A     | 17  | ARG  | 2.3  |
| 1   | B     | 81  | THR  | 2.3  |
| 1   | E     | 255 | ARG  | 2.3  |
| 1   | F     | 67  | ASN  | 2.3  |
| 1   | M     | 183 | ASN  | 2.3  |
| 1   | I     | 143 | THR  | 2.3  |
| 1   | J     | 15  | LEU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 210 | ILE  | 2.3  |
| 2   | X     | 84  | ILE  | 2.3  |
| 1   | M     | 38  | TYR  | 2.3  |
| 1   | E     | 149 | GLU  | 2.3  |
| 1   | I     | 181 | GLU  | 2.3  |
| 1   | N     | 216 | PRO  | 2.3  |
| 2   | U     | 10  | GLY  | 2.3  |
| 2   | U     | 69  | PRO  | 2.3  |
| 1   | I     | 7   | THR  | 2.2  |
| 1   | H     | 15  | LEU  | 2.2  |
| 1   | O     | 32  | LEU  | 2.2  |
| 1   | K     | 34  | ILE  | 2.2  |
| 1   | B     | 127 | SER  | 2.2  |
| 2   | X     | 16  | LYS  | 2.2  |
| 1   | C     | 80  | GLU  | 2.2  |
| 1   | D     | 80  | GLU  | 2.2  |
| 1   | I     | 93  | GLU  | 2.2  |
| 1   | J     | 93  | GLU  | 2.2  |
| 2   | U     | 83  | GLU  | 2.2  |
| 1   | E     | 146 | MET  | 2.2  |
| 1   | B     | 79  | ARG  | 2.2  |
| 1   | B     | 296 | ARG  | 2.2  |
| 1   | C     | 153 | ARG  | 2.2  |
| 1   | E     | 173 | ARG  | 2.2  |
| 1   | K     | 151 | ARG  | 2.2  |
| 1   | M     | 148 | VAL  | 2.2  |
| 1   | O     | 254 | PHE  | 2.2  |
| 1   | O     | 321 | TRP  | 2.2  |
| 1   | N     | 91  | GLN  | 2.2  |
| 1   | N     | 141 | LYS  | 2.2  |
| 1   | P     | 251 | LYS  | 2.2  |
| 2   | X     | 51  | LYS  | 2.2  |
| 1   | A     | 162 | GLU  | 2.2  |
| 1   | B     | 278 | GLU  | 2.2  |
| 1   | F     | 35  | GLU  | 2.2  |
| 1   | G     | 266 | GLU  | 2.2  |
| 1   | M     | 82  | LEU  | 2.2  |
| 1   | A     | 264 | THR  | 2.2  |
| 1   | A     | 282 | THR  | 2.2  |
| 1   | A     | 37  | ILE  | 2.2  |
| 1   | E     | 129 | PHE  | 2.2  |
| 1   | K     | 183 | ASN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 276 | ASN  | 2.2  |
| 1   | P     | 125 | ILE  | 2.2  |
| 1   | P     | 253 | HIS  | 2.2  |
| 1   | E     | 274 | ALA  | 2.2  |
| 1   | G     | 134 | LYS  | 2.2  |
| 1   | L     | 321 | TRP  | 2.2  |
| 1   | N     | 123 | TRP  | 2.2  |
| 1   | P     | 250 | LYS  | 2.2  |
| 2   | Q     | 16  | LYS  | 2.2  |
| 1   | E     | 72  | TYR  | 2.2  |
| 1   | B     | 261 | VAL  | 2.2  |
| 1   | D     | 26  | VAL  | 2.2  |
| 1   | L     | 213 | LEU  | 2.2  |
| 1   | O     | 169 | ARG  | 2.2  |
| 1   | H     | 28  | GLY  | 2.2  |
| 1   | I     | 171 | GLY  | 2.2  |
| 1   | J     | 35  | GLU  | 2.2  |
| 1   | O     | 24  | GLU  | 2.2  |
| 1   | P     | 35  | GLU  | 2.2  |
| 1   | P     | 124 | GLY  | 2.2  |
| 1   | L     | 259 | ASN  | 2.2  |
| 1   | A     | 273 | LYS  | 2.2  |
| 1   | E     | 172 | LYS  | 2.2  |
| 1   | L     | 273 | LYS  | 2.2  |
| 1   | M     | 39  | ASP  | 2.2  |
| 1   | I     | 281 | LYS  | 2.2  |
| 1   | O     | 281 | LYS  | 2.2  |
| 1   | A     | 184 | ALA  | 2.2  |
| 1   | C     | 184 | ALA  | 2.2  |
| 1   | P     | 146 | MET  | 2.2  |
| 1   | N     | 130 | SER  | 2.2  |
| 1   | A     | 192 | ARG  | 2.2  |
| 1   | C     | 29  | ARG  | 2.2  |
| 1   | G     | 153 | ARG  | 2.2  |
| 1   | M     | 295 | ARG  | 2.2  |
| 1   | N     | 296 | ARG  | 2.2  |
| 2   | W     | 28  | VAL  | 2.2  |
| 1   | L     | 18  | GLU  | 2.2  |
| 1   | E     | 204 | THR  | 2.2  |
| 1   | M     | 172 | LYS  | 2.2  |
| 1   | P     | 141 | LYS  | 2.2  |
| 1   | A     | 147 | ASN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | T     | 15  | ASN  | 2.2  |
| 1   | A     | 257 | ASP  | 2.2  |
| 1   | G     | 33  | ALA  | 2.2  |
| 1   | G     | 184 | ALA  | 2.2  |
| 1   | C     | 151 | ARG  | 2.2  |
| 1   | H     | 321 | TRP  | 2.2  |
| 1   | I     | 133 | LEU  | 2.2  |
| 1   | N     | 299 | ARG  | 2.2  |
| 1   | F     | 110 | VAL  | 2.2  |
| 1   | L     | 72  | TYR  | 2.2  |
| 1   | I     | 69  | TYR  | 2.2  |
| 1   | N     | 201 | ILE  | 2.2  |
| 1   | E     | 229 | GLU  | 2.2  |
| 1   | L     | 24  | GLU  | 2.2  |
| 1   | N     | 167 | GLU  | 2.2  |
| 1   | N     | 256 | GLU  | 2.2  |
| 1   | I     | 233 | PRO  | 2.2  |
| 1   | L     | 140 | LYS  | 2.2  |
| 1   | M     | 273 | LYS  | 2.2  |
| 1   | E     | 180 | ASN  | 2.2  |
| 1   | H     | 27  | ASN  | 2.2  |
| 1   | B     | 82  | LEU  | 2.2  |
| 1   | M     | 133 | LEU  | 2.2  |
| 1   | N     | 300 | LEU  | 2.2  |
| 1   | J     | 120 | LEU  | 2.2  |
| 2   | R     | 39  | LEU  | 2.2  |
| 1   | A     | 151 | ARG  | 2.1  |
| 1   | C     | 68  | HIS  | 2.1  |
| 1   | C     | 295 | ARG  | 2.1  |
| 1   | G     | 214 | HIS  | 2.1  |
| 1   | H     | 54  | HIS  | 2.1  |
| 1   | L     | 132 | HIS  | 2.1  |
| 1   | M     | 94  | HIS  | 2.1  |
| 1   | N     | 217 | SER  | 2.1  |
| 1   | I     | 71  | TYR  | 2.1  |
| 2   | U     | 9   | VAL  | 2.1  |
| 2   | V     | 84  | ILE  | 2.1  |
| 1   | G     | 216 | PRO  | 2.1  |
| 1   | L     | 266 | GLU  | 2.1  |
| 1   | M     | 100 | LYS  | 2.1  |
| 1   | I     | 35  | GLU  | 2.1  |
| 1   | B     | 174 | THR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 282 | THR  | 2.1  |
| 1   | L     | 81  | THR  | 2.1  |
| 1   | J     | 133 | LEU  | 2.1  |
| 1   | O     | 83  | LEU  | 2.1  |
| 1   | J     | 236 | ALA  | 2.1  |
| 2   | V     | 56  | ASN  | 2.1  |
| 2   | X     | 44  | ARG  | 2.1  |
| 1   | A     | 211 | SER  | 2.1  |
| 1   | D     | 191 | SER  | 2.1  |
| 1   | P     | 163 | SER  | 2.1  |
| 1   | D     | 86  | ASP  | 2.1  |
| 1   | K     | 257 | ASP  | 2.1  |
| 1   | G     | 283 | VAL  | 2.1  |
| 1   | I     | 34  | ILE  | 2.1  |
| 1   | P     | 123 | TRP  | 2.1  |
| 1   | B     | 95  | TYR  | 2.1  |
| 1   | D     | 43  | TYR  | 2.1  |
| 1   | N     | 121 | LYS  | 2.1  |
| 1   | I     | 157 | TYR  | 2.1  |
| 2   | R     | 18  | LYS  | 2.1  |
| 1   | M     | 177 | PRO  | 2.1  |
| 1   | J     | 124 | GLY  | 2.1  |
| 1   | F     | 135 | GLU  | 2.1  |
| 2   | R     | 77  | GLU  | 2.1  |
| 2   | U     | 36  | GLU  | 2.1  |
| 1   | H     | 293 | THR  | 2.1  |
| 1   | K     | 174 | THR  | 2.1  |
| 1   | A     | 136 | LEU  | 2.1  |
| 1   | K     | 120 | LEU  | 2.1  |
| 1   | H     | 224 | ALA  | 2.1  |
| 1   | L     | 67  | ASN  | 2.1  |
| 1   | E     | 84  | SER  | 2.1  |
| 1   | E     | 37  | ILE  | 2.1  |
| 1   | L     | 170 | ILE  | 2.1  |
| 1   | C     | 319 | VAL  | 2.1  |
| 1   | A     | 86  | ASP  | 2.1  |
| 1   | A     | 245 | LYS  | 2.1  |
| 1   | C     | 97  | ASP  | 2.1  |
| 1   | F     | 54  | HIS  | 2.1  |
| 1   | I     | 97  | ASP  | 2.1  |
| 1   | K     | 38  | TYR  | 2.1  |
| 1   | P     | 171 | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 256 | GLU  | 2.1  |
| 1   | F     | 93  | GLU  | 2.1  |
| 1   | L     | 80  | GLU  | 2.1  |
| 1   | P     | 167 | GLU  | 2.1  |
| 1   | P     | 213 | LEU  | 2.1  |
| 1   | B     | 151 | ARG  | 2.1  |
| 1   | G     | 151 | ARG  | 2.1  |
| 2   | Q     | 13  | ARG  | 2.1  |
| 2   | S     | 66  | ARG  | 2.1  |
| 1   | C     | 186 | ILE  | 2.1  |
| 1   | N     | 19  | ASN  | 2.1  |
| 1   | O     | 211 | SER  | 2.1  |
| 1   | A     | 269 | LYS  | 2.1  |
| 1   | F     | 179 | LYS  | 2.1  |
| 1   | F     | 205 | GLN  | 2.1  |
| 1   | A     | 271 | VAL  | 2.1  |
| 1   | C     | 261 | VAL  | 2.1  |
| 2   | T     | 6   | VAL  | 2.1  |
| 1   | A     | 267 | GLY  | 2.1  |
| 1   | E     | 150 | GLY  | 2.1  |
| 1   | L     | 71  | TYR  | 2.1  |
| 1   | L     | 135 | GLU  | 2.1  |
| 1   | N     | 35  | GLU  | 2.1  |
| 1   | N     | 93  | GLU  | 2.1  |
| 1   | J     | 293 | THR  | 2.1  |
| 1   | O     | 18  | GLU  | 2.1  |
| 1   | H     | 219 | ARG  | 2.1  |
| 1   | J     | 220 | ARG  | 2.1  |
| 1   | B     | 187 | SER  | 2.1  |
| 1   | F     | 134 | LYS  | 2.1  |
| 1   | M     | 191 | SER  | 2.1  |
| 1   | J     | 179 | LYS  | 2.1  |
| 2   | T     | 40  | ALA  | 2.1  |
| 1   | P     | 130 | SER  | 2.1  |
| 1   | M     | 25  | ASN  | 2.1  |
| 1   | D     | 283 | VAL  | 2.1  |
| 1   | H     | 261 | VAL  | 2.1  |
| 1   | N     | 292 | VAL  | 2.1  |
| 1   | E     | 69  | TYR  | 2.1  |
| 1   | E     | 182 | MET  | 2.1  |
| 1   | G     | 43  | TYR  | 2.1  |
| 1   | M     | 212 | TYR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 86  | ASP  | 2.1  |
| 1   | N     | 73  | ASP  | 2.1  |
| 1   | N     | 257 | ASP  | 2.1  |
| 1   | B     | 7   | THR  | 2.1  |
| 1   | K     | 117 | GLU  | 2.1  |
| 1   | N     | 293 | THR  | 2.1  |
| 1   | C     | 17  | ARG  | 2.1  |
| 1   | C     | 219 | ARG  | 2.1  |
| 1   | H     | 220 | ARG  | 2.1  |
| 1   | L     | 153 | ARG  | 2.1  |
| 1   | E     | 250 | LYS  | 2.1  |
| 1   | H     | 126 | SER  | 2.1  |
| 1   | O     | 84  | SER  | 2.1  |
| 1   | O     | 195 | ALA  | 2.1  |
| 1   | E     | 23  | PHE  | 2.1  |
| 1   | A     | 203 | ASN  | 2.1  |
| 1   | C     | 147 | ASN  | 2.1  |
| 1   | C     | 259 | ASN  | 2.1  |
| 1   | M     | 58  | GLN  | 2.1  |
| 1   | J     | 262 | LEU  | 2.1  |
| 1   | A     | 54  | HIS  | 2.0  |
| 1   | C     | 156 | TYR  | 2.0  |
| 1   | H     | 311 | GLY  | 2.0  |
| 1   | I     | 45  | HIS  | 2.0  |
| 1   | J     | 132 | HIS  | 2.0  |
| 1   | O     | 138 | GLY  | 2.0  |
| 1   | C     | 123 | TRP  | 2.0  |
| 1   | E     | 160 | TRP  | 2.0  |
| 1   | E     | 177 | PRO  | 2.0  |
| 1   | O     | 177 | PRO  | 2.0  |
| 1   | K     | 265 | ASP  | 2.0  |
| 1   | A     | 24  | GLU  | 2.0  |
| 1   | B     | 186 | ILE  | 2.0  |
| 1   | E     | 18  | GLU  | 2.0  |
| 1   | G     | 155 | GLU  | 2.0  |
| 1   | M     | 90  | LYS  | 2.0  |
| 1   | N     | 230 | ILE  | 2.0  |
| 1   | I     | 167 | GLU  | 2.0  |
| 1   | J     | 215 | GLU  | 2.0  |
| 2   | V     | 12  | GLU  | 2.0  |
| 1   | E     | 163 | SER  | 2.0  |
| 1   | E     | 316 | SER  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 187 | SER  | 2.0  |
| 1   | G     | 120 | LEU  | 2.0  |
| 1   | F     | 244 | VAL  | 2.0  |
| 1   | G     | 292 | VAL  | 2.0  |
| 1   | I     | 142 | VAL  | 2.0  |
| 1   | B     | 190 | ASN  | 2.0  |
| 1   | L     | 122 | ASN  | 2.0  |
| 1   | I     | 27  | ASN  | 2.0  |
| 1   | O     | 147 | ASN  | 2.0  |
| 1   | C     | 267 | GLY  | 2.0  |
| 1   | A     | 157 | TYR  | 2.0  |
| 1   | K     | 55  | TYR  | 2.0  |
| 1   | E     | 299 | ARG  | 2.0  |
| 1   | N     | 54  | HIS  | 2.0  |
| 1   | I     | 177 | PRO  | 2.0  |
| 1   | O     | 30  | LYS  | 2.0  |
| 1   | O     | 273 | LYS  | 2.0  |
| 2   | Q     | 46  | LYS  | 2.0  |
| 2   | T     | 22  | ARG  | 2.0  |
| 1   | P     | 81  | THR  | 2.0  |
| 1   | B     | 35  | GLU  | 2.0  |
| 1   | G     | 215 | GLU  | 2.0  |
| 1   | L     | 155 | GLU  | 2.0  |
| 1   | I     | 18  | GLU  | 2.0  |
| 2   | W     | 8   | ASP  | 2.0  |
| 1   | A     | 221 | PHE  | 2.0  |
| 1   | L     | 320 | ALA  | 2.0  |
| 1   | L     | 292 | VAL  | 2.0  |
| 1   | O     | 183 | ASN  | 2.0  |
| 1   | P     | 276 | ASN  | 2.0  |
| 1   | C     | 60  | GLY  | 2.0  |
| 1   | M     | 247 | GLY  | 2.0  |
| 1   | J     | 311 | GLY  | 2.0  |
| 1   | C     | 61  | ILE  | 2.0  |
| 1   | C     | 315 | TYR  | 2.0  |
| 1   | P     | 17  | ARG  | 2.0  |
| 1   | D     | 174 | THR  | 2.0  |
| 1   | P     | 143 | THR  | 2.0  |
| 1   | A     | 155 | GLU  | 2.0  |
| 1   | G     | 133 | LEU  | 2.0  |
| 1   | K     | 280 | GLU  | 2.0  |
| 1   | N     | 309 | LEU  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | W     | 82  | GLU  | 2.0  |
| 1   | J     | 84  | SER  | 2.0  |
| 1   | J     | 257 | ASP  | 2.0  |
| 1   | J     | 320 | ALA  | 2.0  |
| 2   | W     | 59  | SER  | 2.0  |
| 1   | P     | 109 | VAL  | 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 oligosaccharides 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.