



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 1U3H / pdb\_00001u3h  
Title : Crystal structure of mouse TCR 172.10 complexed with MHC class II I-Au molecule at 2.4 Å  
Authors : Maynard, J.; Petersson, K.; Wilson, D.H.; Adams, E.J.; Blondelle, S.E.; Boulanger, M.J.; Wilson, D.B.; Garcia, K.C.  
Deposited on : 2004-07-21  
Resolution : 2.42 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:

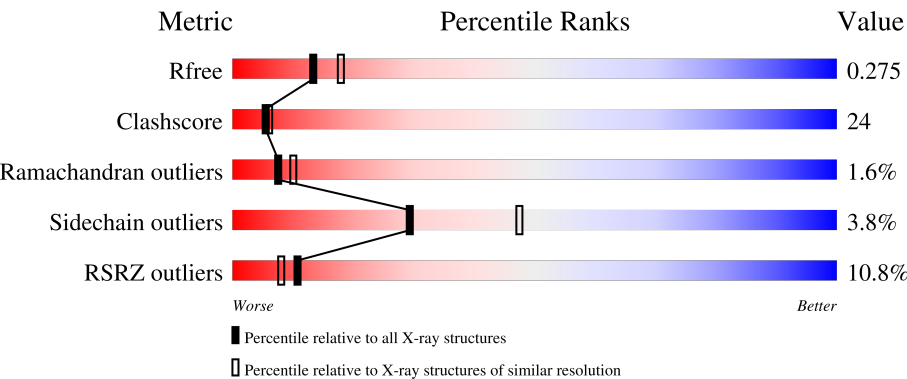
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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                      | 6062 (2.44-2.40)                                      |
| Clashscore            | 190562                      | 6562 (2.44-2.40)                                      |
| Ramachandran outliers | 187476                      | 6481 (2.44-2.40)                                      |
| Sidechain outliers    | 187428                      | 6482 (2.44-2.40)                                      |
| RSRZ outliers         | 180081                      | 6066 (2.44-2.40)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 110    |                  |
| 1   | E     | 110    |                  |
| 2   | B     | 111    |                  |
| 2   | F     | 111    |                  |
| 3   | C     | 182    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 3   | G     | 182    | <div><div>%</div><div><div></div><div>77%</div><div>20%</div><div></div></div><div></div></div>     |
| 4   | D     | 189    | <div><div>7%</div><div><div></div><div>62%</div><div>33%</div><div></div></div><div></div></div>    |
| 4   | H     | 189    | <div><div>8%</div><div><div></div><div>59%</div><div>38%</div><div></div></div><div></div></div>    |
| 5   | I     | 12     | <div><div>25%</div><div><div></div><div>67%</div><div>25%</div><div>8%</div></div><div></div></div> |
| 5   | P     | 12     | <div><div>17%</div><div><div></div><div>50%</div><div>50%</div><div></div></div><div></div></div>   |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called T-cell receptor alpha-chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 869   | 554 | 144 | 169 | 2 |         |         |       |
| 1   | E     | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 869   | 554 | 144 | 169 | 2 |         |         |       |

- Molecule 2 is a protein called Mouse TCRVbeta 172.10, extracellular variable domain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 111      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 853   | 528 | 148 | 174 | 3 |         |         |       |
| 2   | F     | 111      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 853   | 528 | 148 | 174 | 3 |         |         |       |

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-U alpha chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 182      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1464  | 946 | 233 | 282 | 3 |         |         |       |
| 3   | G     | 182      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1464  | 946 | 233 | 282 | 3 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| C     | 1       | ILE      | -      | cloning artifact | UNP P14438 |
| C     | 2       | GLU      | -      | cloning artifact | UNP P14438 |
| C     | 3       | ALA      | -      | cloning artifact | UNP P14438 |
| G     | 1       | ILE      | -      | cloning artifact | UNP P14438 |
| G     | 2       | GLU      | -      | cloning artifact | UNP P14438 |
| G     | 3       | ALA      | -      | cloning artifact | UNP P14438 |

- Molecule 4 is a protein called H-2 class II histocompatibility antigen, A-U beta chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 189      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 998 | 283 | 299 | 6 |         |         |       |
| 4   | H     | 189      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 998 | 283 | 299 | 6 |         |         |       |

- Molecule 5 is a protein called Myelin basic protein (MBP)-peptide.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 5   | P     | 12       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 91    | 52 | 20 | 19 |         |         |       |
| 5   | I     | 12       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 91    | 52 | 20 | 19 |         |         |       |

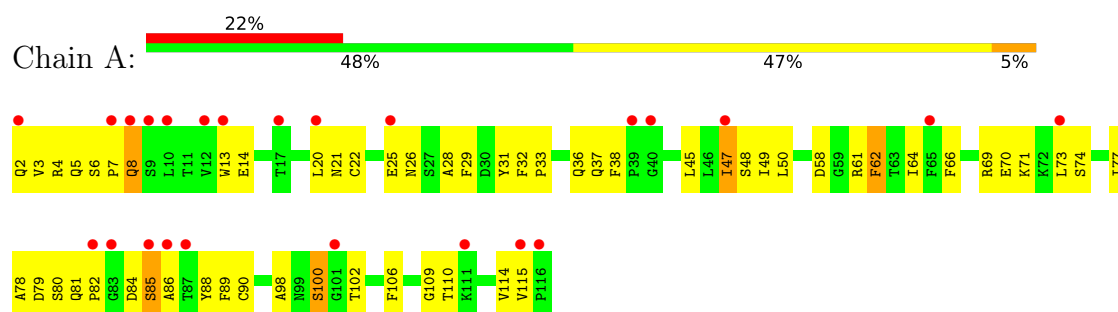
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 6   | B     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 6   | C     | 49       | Total | O  | 0       | 0       |
|     |       |          | 49    | 49 |         |         |
| 6   | D     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 6   | P     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 6   | E     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 6   | F     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 6   | G     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 6   | H     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |
| 6   | I     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

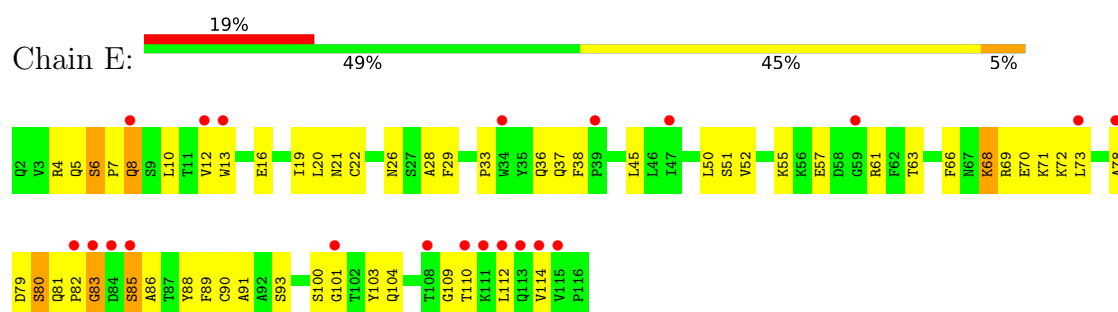
### 3 Residue-property plots [i](#)

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.

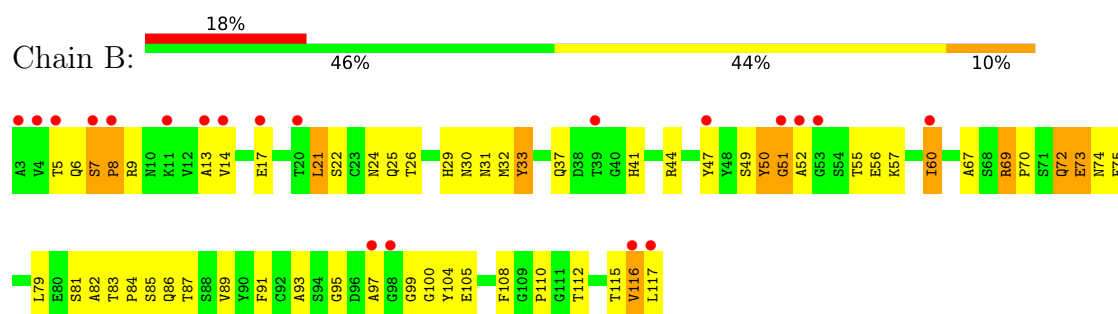
- Molecule 1: T-cell receptor alpha-chain



- Molecule 1: T-cell receptor alpha-chain

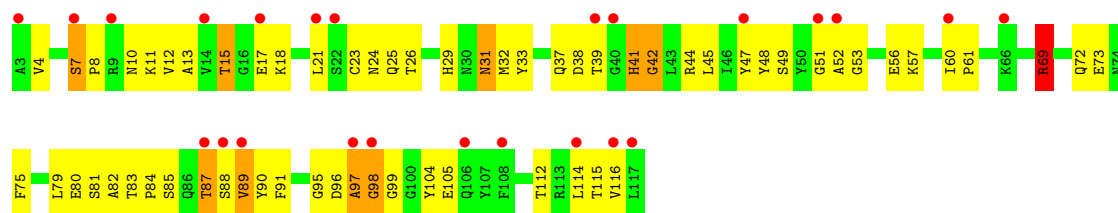


- Molecule 2: Mouse TCRVbeta 172.10, extracellular variable domain

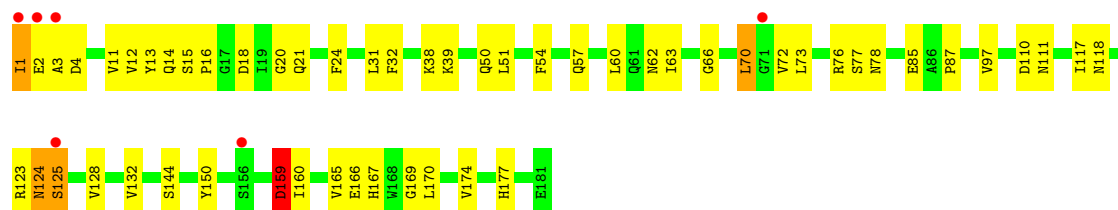


- Molecule 2: Mouse TCRVbeta 172.10, extracellular variable domain

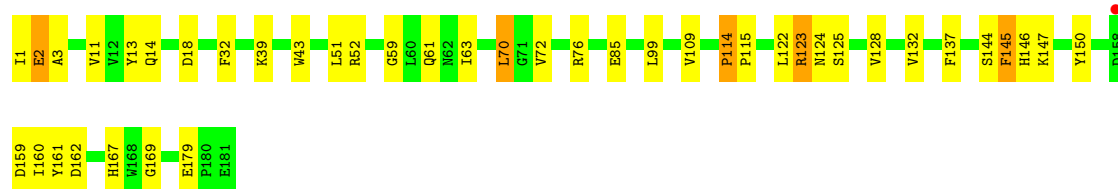
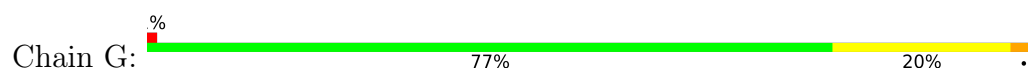




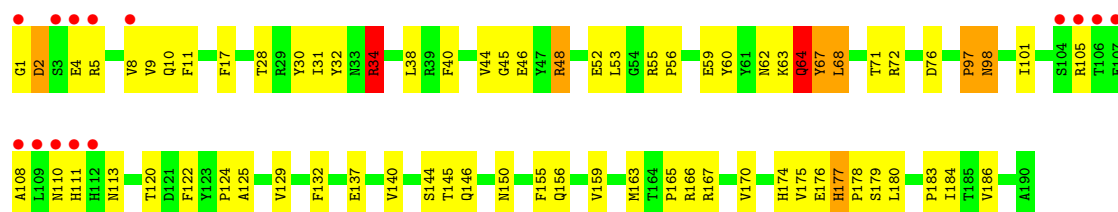
- Molecule 3: H-2 class II histocompatibility antigen, A-U alpha chain



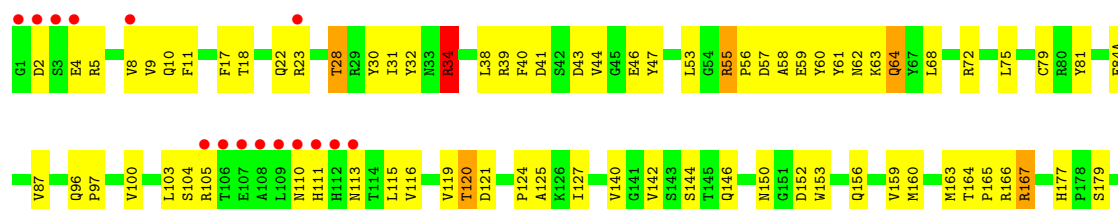
- Molecule 3: H-2 class II histocompatibility antigen, A-U alpha chain



- Molecule 4: H-2 class II histocompatibility antigen, A-U beta chain

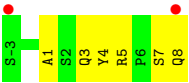


- Molecule 4: H-2 class II histocompatibility antigen, A-U beta chain

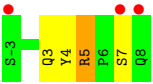




• Molecule 5: Myelin basic protein (MBP)-peptide



• Molecule 5: Myelin basic protein (MBP)-peptide



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 87.83Å 327.16Å 127.16Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 41.51 – 2.42<br>41.51 – 2.42                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.1 (41.51-2.42)<br>89.2 (41.51-2.42)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | 0.06                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.27 (at 2.42Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.232 , 0.274<br>0.235 , 0.275                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3489 reflections (5.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.898                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 56.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 9909                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.38         | 0/892         | 0.95        | 5/1208 (0.4%)   |
| 1   | E     | 0.40         | 0/892         | 0.97        | 5/1208 (0.4%)   |
| 2   | B     | 0.46         | 0/873         | 1.09        | 7/1184 (0.6%)   |
| 2   | F     | 0.44         | 0/873         | 1.00        | 6/1184 (0.5%)   |
| 3   | C     | 0.47         | 0/1509        | 1.04        | 10/2059 (0.5%)  |
| 3   | G     | 0.47         | 0/1509        | 1.03        | 5/2059 (0.2%)   |
| 4   | D     | 0.52         | 0/1625        | 1.07        | 14/2206 (0.6%)  |
| 4   | H     | 0.52         | 1/1625 (0.1%) | 1.05        | 13/2206 (0.6%)  |
| 5   | I     | 0.52         | 0/92          | 1.08        | 1/120 (0.8%)    |
| 5   | P     | 0.48         | 0/92          | 1.06        | 1/120 (0.8%)    |
| All | All   | 0.47         | 1/9982 (0.0%) | 1.03        | 67/13554 (0.5%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | H     | 87  | VAL  | CA-CB | 7.86 | 1.58        | 1.54     |

All (67) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | H     | 140 | VAL  | N-CA-C | 10.50  | 120.29      | 110.42   |
| 1   | A     | 100 | SER  | N-CA-C | -10.43 | 95.96       | 110.35   |
| 2   | F     | 52  | ALA  | N-CA-C | 9.52   | 121.60      | 111.03   |
| 3   | G     | 114 | PRO  | CA-C-N | 9.25   | 131.41      | 119.84   |
| 3   | G     | 114 | PRO  | C-N-CA | 9.25   | 131.41      | 119.84   |
| 4   | D     | 140 | VAL  | N-CA-C | 9.03   | 118.91      | 110.42   |
| 3   | G     | 70  | LEU  | N-CA-C | -8.95  | 97.03       | 110.28   |
| 4   | D     | 108 | ALA  | CA-C-N | -8.68  | 108.87      | 122.67   |
| 4   | D     | 108 | ALA  | C-N-CA | -8.68  | 108.87      | 122.67   |
| 1   | E     | 100 | SER  | N-CA-C | -8.20  | 99.95       | 110.53   |
| 4   | D     | 125 | ALA  | N-CA-C | 7.80   | 119.79      | 111.28   |
| 2   | B     | 50  | TYR  | N-CA-C | -7.47  | 104.06      | 113.02   |
| 1   | E     | 100 | SER  | O-C-N  | -7.42  | 113.53      | 122.65   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 124 | ASN  | CB-CA-C | -7.40 | 99.82       | 111.51   |
| 4   | D     | 120 | THR  | N-CA-C  | 7.34  | 120.91      | 109.52   |
| 3   | C     | 70  | LEU  | N-CA-C  | -7.32 | 100.19      | 110.50   |
| 1   | E     | 100 | SER  | CA-C-N  | -7.27 | 107.17      | 121.41   |
| 1   | E     | 100 | SER  | C-N-CA  | -7.27 | 107.17      | 121.41   |
| 4   | H     | 125 | ALA  | N-CA-C  | 7.22  | 118.79      | 111.07   |
| 2   | B     | 52  | ALA  | O-C-N   | 7.17  | 132.13      | 122.59   |
| 2   | F     | 89  | VAL  | N-CA-C  | 7.16  | 118.59      | 108.93   |
| 1   | A     | 85  | SER  | N-CA-C  | 7.08  | 125.88      | 110.80   |
| 2   | F     | 69  | ARG  | CA-C-N  | 7.08  | 126.76      | 119.82   |
| 2   | F     | 69  | ARG  | C-N-CA  | 7.08  | 126.76      | 119.82   |
| 2   | B     | 52  | ALA  | CA-C-N  | 7.03  | 135.18      | 121.41   |
| 2   | B     | 52  | ALA  | C-N-CA  | 7.03  | 135.18      | 121.41   |
| 4   | D     | 98  | ASN  | N-CA-C  | -6.97 | 98.32       | 109.76   |
| 2   | F     | 53  | GLY  | N-CA-C  | -6.92 | 96.79       | 113.18   |
| 4   | D     | 34  | ARG  | N-CA-C  | -6.85 | 104.02      | 114.16   |
| 4   | D     | 64  | GLN  | N-CA-C  | 6.69  | 118.57      | 111.28   |
| 3   | C     | 4   | ASP  | N-CA-C  | -6.63 | 105.35      | 113.50   |
| 3   | C     | 31  | LEU  | N-CA-C  | -6.60 | 103.35      | 111.40   |
| 4   | H     | 120 | THR  | N-CA-C  | 6.54  | 119.76      | 110.14   |
| 4   | H     | 146 | GLN  | N-CA-C  | -6.41 | 101.50      | 110.35   |
| 4   | H     | 34  | ARG  | N-CA-C  | -6.39 | 103.49      | 113.02   |
| 3   | G     | 144 | SER  | N-CA-C  | -6.39 | 100.52      | 110.17   |
| 3   | C     | 124 | ASN  | CA-C-N  | -6.34 | 109.44      | 121.54   |
| 3   | C     | 124 | ASN  | C-N-CA  | -6.34 | 109.44      | 121.54   |
| 4   | H     | 39  | ARG  | N-CA-C  | 6.25  | 117.90      | 108.46   |
| 4   | H     | 142 | VAL  | N-CA-C  | 6.23  | 116.84      | 108.11   |
| 2   | B     | 51  | GLY  | N-CA-C  | 6.18  | 127.83      | 113.18   |
| 3   | C     | 72  | VAL  | N-CA-C  | -5.95 | 104.71      | 110.42   |
| 1   | A     | 102 | THR  | N-CA-C  | 5.89  | 118.15      | 110.43   |
| 4   | H     | 64  | GLN  | N-CA-C  | 5.86  | 118.62      | 111.82   |
| 2   | F     | 87  | THR  | N-CA-C  | 5.84  | 118.62      | 107.75   |
| 4   | D     | 67  | TYR  | N-CA-C  | 5.82  | 121.25      | 114.04   |
| 2   | B     | 116 | VAL  | N-CA-C  | 5.64  | 116.66      | 111.81   |
| 2   | B     | 52  | ALA  | N-CA-C  | -5.58 | 98.92       | 110.80   |
| 5   | I     | 5   | ARG  | N-CA-C  | 5.53  | 117.04      | 110.07   |
| 4   | H     | 4   | GLU  | N-CA-C  | -5.52 | 105.53      | 114.09   |
| 3   | C     | 144 | SER  | N-CA-C  | -5.51 | 101.32      | 109.86   |
| 4   | D     | 145 | THR  | N-CA-C  | -5.38 | 103.79      | 110.41   |
| 1   | A     | 62  | PHE  | N-CA-C  | 5.38  | 117.47      | 109.25   |
| 1   | E     | 103 | TYR  | N-CA-C  | 5.29  | 117.52      | 110.53   |
| 3   | G     | 72  | VAL  | N-CA-C  | -5.28 | 105.56      | 110.53   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | D     | 177 | HIS  | CA-C-N | 5.23  | 125.54      | 119.47   |
| 4   | D     | 177 | HIS  | C-N-CA | 5.23  | 125.54      | 119.47   |
| 4   | D     | 170 | VAL  | N-CA-C | 5.23  | 115.38      | 107.80   |
| 3   | C     | 97  | VAL  | N-CA-C | 5.21  | 115.72      | 108.84   |
| 1   | A     | 84  | ASP  | N-CA-C | -5.18 | 106.55      | 112.92   |
| 4   | H     | 96  | GLN  | CA-C-N | 5.16  | 125.07      | 119.76   |
| 4   | H     | 96  | GLN  | C-N-CA | 5.16  | 125.07      | 119.76   |
| 4   | H     | 44  | VAL  | N-CA-C | -5.07 | 106.21      | 111.58   |
| 4   | H     | 121 | ASP  | N-CA-C | 5.04  | 118.69      | 112.24   |
| 3   | C     | 159 | ASP  | N-CA-C | 5.03  | 117.26      | 108.76   |
| 5   | P     | 5   | ARG  | N-CA-C | 5.02  | 115.98      | 109.65   |
| 4   | D     | 146 | GLN  | N-CA-C | -5.02 | 103.42      | 110.35   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 869   | 0        | 828      | 50      | 0            |
| 1   | E     | 869   | 0        | 828      | 60      | 0            |
| 2   | B     | 853   | 0        | 795      | 54      | 0            |
| 2   | F     | 853   | 0        | 795      | 79      | 0            |
| 3   | C     | 1464  | 0        | 1392     | 58      | 0            |
| 3   | G     | 1464  | 0        | 1392     | 39      | 0            |
| 4   | D     | 1586  | 0        | 1521     | 66      | 0            |
| 4   | H     | 1586  | 0        | 1521     | 68      | 0            |
| 5   | I     | 91    | 0        | 86       | 5       | 0            |
| 5   | P     | 91    | 0        | 86       | 9       | 0            |
| 6   | A     | 4     | 0        | 0        | 0       | 0            |
| 6   | B     | 4     | 0        | 0        | 1       | 0            |
| 6   | C     | 49    | 0        | 0        | 6       | 0            |
| 6   | D     | 42    | 0        | 0        | 2       | 0            |
| 6   | E     | 4     | 0        | 0        | 3       | 0            |
| 6   | F     | 3     | 0        | 0        | 2       | 0            |
| 6   | G     | 42    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | H     | 30    | 0        | 0        | 1       | 0            |
| 6   | I     | 2     | 0        | 0        | 0       | 0            |
| 6   | P     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 9909  | 0        | 9244     | 451     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (451) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:1:ILE:CG2    | 6:C:230:HOH:O    | 1.78                     | 1.26              |
| 2:F:60:ILE:HG22  | 6:F:120:HOH:O    | 1.41                     | 1.17              |
| 3:C:124:ASN:O    | 3:C:125:SER:HB2  | 1.30                     | 1.09              |
| 1:E:37:GLN:O     | 1:E:86:ALA:HB1   | 1.54                     | 1.08              |
| 3:C:124:ASN:O    | 3:C:125:SER:CB   | 2.01                     | 1.05              |
| 3:G:99:LEU:HD12  | 3:G:99:LEU:H     | 1.26                     | 0.98              |
| 1:A:37:GLN:O     | 1:A:86:ALA:HB1   | 1.63                     | 0.96              |
| 4:H:2:ASP:H      | 4:H:5:ARG:HD3    | 1.33                     | 0.93              |
| 2:B:13:ALA:HB1   | 2:B:17:GLU:OE1   | 1.69                     | 0.91              |
| 2:F:13:ALA:HB1   | 2:F:17:GLU:OE1   | 1.68                     | 0.91              |
| 1:E:6:SER:HB3    | 1:E:7:PRO:HD3    | 1.52                     | 0.90              |
| 2:B:41:HIS:HB3   | 2:B:44:ARG:HD2   | 1.52                     | 0.90              |
| 3:C:62:ASN:HD21  | 5:P:3:GLN:NE2    | 1.70                     | 0.89              |
| 1:A:6:SER:HB3    | 1:A:21:ASN:HB2   | 1.54                     | 0.88              |
| 2:F:47:TYR:CE1   | 2:F:61:PRO:HB2   | 2.08                     | 0.88              |
| 4:H:167:ARG:HH11 | 4:H:167:ARG:HB3  | 1.40                     | 0.87              |
| 2:F:7:SER:HB3    | 2:F:8:PRO:HD3    | 1.58                     | 0.86              |
| 1:E:37:GLN:HE22  | 2:F:37:GLN:HE22  | 1.25                     | 0.85              |
| 4:H:59:GLU:HG2   | 4:H:63:LYS:HE2   | 1.60                     | 0.84              |
| 4:H:68:LEU:HD22  | 4:H:72:ARG:HE    | 1.44                     | 0.82              |
| 4:H:150:ASN:HD21 | 4:H:156:GLN:HE21 | 1.23                     | 0.82              |
| 3:C:62:ASN:HD21  | 5:P:3:GLN:HE22   | 1.23                     | 0.82              |
| 2:B:84:PRO:HA    | 2:B:116:VAL:HG21 | 1.61                     | 0.81              |
| 3:C:1:ILE:HG22   | 6:C:230:HOH:O    | 1.60                     | 0.80              |
| 1:A:47:ILE:HD11  | 1:A:58:ASP:HB3   | 1.64                     | 0.79              |
| 4:D:34:ARG:HG3   | 4:D:34:ARG:O     | 1.81                     | 0.79              |
| 2:B:84:PRO:HA    | 2:B:116:VAL:CG2  | 2.12                     | 0.79              |
| 4:D:150:ASN:HD21 | 4:D:156:GLN:HE21 | 1.28                     | 0.79              |
| 1:A:6:SER:HB3    | 1:A:7:PRO:HD3    | 1.66                     | 0.78              |
| 1:E:85:SER:HB2   | 6:E:118:HOH:O    | 1.83                     | 0.78              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:25:GLU:HA    | 1:A:71:LYS:HD3  | 1.65                     | 0.77              |
| 2:B:7:SER:OG     | 2:B:8:PRO:HD2   | 1.84                     | 0.77              |
| 2:F:47:TYR:CE1   | 2:F:61:PRO:CB   | 2.69                     | 0.75              |
| 1:E:6:SER:HB3    | 1:E:21:ASN:HB2  | 1.67                     | 0.75              |
| 4:D:28:THR:HG21  | 6:D:194:HOH:O   | 1.86                     | 0.74              |
| 2:F:31:ASN:HB2   | 2:F:49:SER:O    | 1.86                     | 0.74              |
| 1:E:5:GLN:HE22   | 1:E:89:PHE:HA   | 1.52                     | 0.74              |
| 4:H:2:ASP:H      | 4:H:5:ARG:CD    | 1.99                     | 0.74              |
| 1:A:47:ILE:HG22  | 1:A:64:ILE:HD11 | 1.70                     | 0.74              |
| 2:F:37:GLN:HE21  | 2:F:91:PHE:HE2  | 1.34                     | 0.73              |
| 2:F:13:ALA:CB    | 2:F:17:GLU:OE1  | 2.37                     | 0.73              |
| 2:B:37:GLN:HE21  | 2:B:91:PHE:HE2  | 1.35                     | 0.73              |
| 4:D:59:GLU:HG2   | 4:D:63:LYS:HE2  | 1.69                     | 0.73              |
| 2:B:73:GLU:H     | 2:B:73:GLU:CD   | 1.97                     | 0.71              |
| 2:F:41:HIS:H     | 2:F:41:HIS:CD2  | 2.08                     | 0.71              |
| 3:G:14:GLN:HB3   | 4:H:8:VAL:HG23  | 1.71                     | 0.71              |
| 4:H:28:THR:CG2   | 4:H:30:TYR:HE1  | 2.03                     | 0.71              |
| 4:D:105:ARG:HB2  | 4:D:113:ASN:OD1 | 1.91                     | 0.71              |
| 4:H:10:GLN:HB2   | 4:H:31:ILE:HB   | 1.72                     | 0.71              |
| 3:G:99:LEU:HD12  | 3:G:99:LEU:N    | 2.01                     | 0.70              |
| 4:H:28:THR:HG21  | 6:H:199:HOH:O   | 1.92                     | 0.70              |
| 2:F:41:HIS:H     | 2:F:41:HIS:HD2  | 1.38                     | 0.69              |
| 4:H:68:LEU:HD22  | 4:H:72:ARG:NE   | 2.06                     | 0.69              |
| 2:F:87:THR:HG23  | 2:F:114:LEU:O   | 1.92                     | 0.69              |
| 4:H:104:SER:O    | 4:H:105:ARG:HG2 | 1.92                     | 0.69              |
| 2:F:11:LYS:NZ    | 2:F:13:ALA:HB2  | 2.08                     | 0.68              |
| 3:G:99:LEU:H     | 3:G:99:LEU:CD1  | 2.03                     | 0.68              |
| 4:D:124:PRO:O    | 4:D:177:HIS:HE1 | 1.77                     | 0.68              |
| 2:F:41:HIS:CD2   | 2:F:41:HIS:N    | 2.58                     | 0.68              |
| 4:H:8:VAL:O      | 4:H:32:TYR:O    | 2.10                     | 0.68              |
| 3:C:160:ILE:HG23 | 3:C:177:HIS:CE1 | 2.29                     | 0.67              |
| 4:H:18:THR:HB    | 4:H:23:ARG:HB3  | 1.76                     | 0.67              |
| 4:D:167:ARG:NH1  | 4:D:167:ARG:HB3 | 2.09                     | 0.67              |
| 2:B:50:TYR:OH    | 3:C:57:GLN:HG3  | 1.95                     | 0.67              |
| 3:C:1:ILE:HG22   | 3:C:2:GLU:N     | 2.10                     | 0.67              |
| 1:A:37:GLN:O     | 1:A:86:ALA:CB   | 2.39                     | 0.66              |
| 2:F:11:LYS:HZ2   | 2:F:13:ALA:HB2  | 1.61                     | 0.66              |
| 3:C:160:ILE:HG23 | 3:C:177:HIS:HE1 | 1.58                     | 0.65              |
| 2:F:51:GLY:O     | 2:F:69:ARG:HD2  | 1.97                     | 0.65              |
| 4:D:10:GLN:HB2   | 4:D:31:ILE:HB   | 1.77                     | 0.65              |
| 2:B:69:ARG:HG3   | 2:B:69:ARG:HH11 | 1.60                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:9:ARG:NH2    | 2:B:110:PRO:HB2   | 2.11                     | 0.65              |
| 2:B:32:MET:HG3   | 2:B:69:ARG:NH2    | 2.11                     | 0.65              |
| 2:B:97:ALA:O     | 2:B:104:TYR:CE2   | 2.50                     | 0.65              |
| 1:E:13:TRP:HB2   | 1:E:16:GLU:OE2    | 1.97                     | 0.64              |
| 2:F:7:SER:CB     | 2:F:8:PRO:HD3     | 2.26                     | 0.64              |
| 2:B:21:LEU:H     | 2:B:21:LEU:HD12   | 1.63                     | 0.64              |
| 2:F:88:SER:O     | 2:F:90:TYR:CD1    | 2.50                     | 0.64              |
| 1:E:6:SER:HB3    | 1:E:7:PRO:CD      | 2.27                     | 0.64              |
| 2:F:24:ASN:HA    | 2:F:73:GLU:O      | 1.97                     | 0.63              |
| 3:C:117:ILE:HD11 | 3:C:165:VAL:CG1   | 2.28                     | 0.63              |
| 4:D:11:PHE:CE1   | 4:D:28:THR:HG23   | 2.33                     | 0.63              |
| 1:A:69:ARG:O     | 1:A:70:GLU:HB2    | 1.97                     | 0.63              |
| 4:D:2:ASP:H      | 4:D:5:ARG:HD3     | 1.64                     | 0.63              |
| 4:D:177:HIS:HD2  | 4:D:179:SER:OG    | 1.82                     | 0.63              |
| 2:B:13:ALA:CB    | 2:B:17:GLU:OE1    | 2.45                     | 0.62              |
| 2:B:84:PRO:CA    | 2:B:116:VAL:HG21  | 2.28                     | 0.62              |
| 1:E:8:GLN:CD     | 1:E:8:GLN:H       | 2.07                     | 0.62              |
| 3:C:160:ILE:CG2  | 3:C:177:HIS:HE1   | 2.12                     | 0.62              |
| 2:F:11:LYS:HD3   | 2:F:12:VAL:N      | 2.14                     | 0.62              |
| 2:F:38:ASP:OD1   | 2:F:88:SER:CB     | 2.48                     | 0.62              |
| 2:B:51:GLY:HA2   | 2:B:69:ARG:NH1    | 2.14                     | 0.62              |
| 2:B:79:LEU:N     | 2:B:79:LEU:HD12   | 2.14                     | 0.62              |
| 2:B:21:LEU:HD12  | 2:B:21:LEU:N      | 2.14                     | 0.62              |
| 2:F:7:SER:HB3    | 2:F:8:PRO:CD      | 2.27                     | 0.62              |
| 2:F:11:LYS:O     | 2:F:114:LEU:HD12  | 1.99                     | 0.62              |
| 4:D:8:VAL:O      | 4:D:32:TYR:O      | 2.16                     | 0.62              |
| 1:E:6:SER:CB     | 1:E:7:PRO:HD3     | 2.26                     | 0.62              |
| 1:E:26:ASN:C     | 1:E:26:ASN:HD22   | 2.07                     | 0.62              |
| 1:A:47:ILE:HG22  | 1:A:64:ILE:CD1    | 2.29                     | 0.61              |
| 3:C:1:ILE:HD12   | 3:C:1:ILE:N       | 2.15                     | 0.61              |
| 3:C:167:HIS:CD2  | 3:C:169:GLY:H     | 2.18                     | 0.61              |
| 1:E:66:PHE:HD1   | 1:E:73:LEU:HD13   | 1.65                     | 0.61              |
| 4:H:81:TYR:O     | 4:H:84(A):GLU:HB2 | 2.00                     | 0.61              |
| 2:B:41:HIS:HB3   | 2:B:44:ARG:CD     | 2.28                     | 0.61              |
| 4:D:97:PRO:HD3   | 4:D:122:PHE:CB    | 2.31                     | 0.61              |
| 4:D:167:ARG:HB3  | 4:D:167:ARG:HH11  | 1.64                     | 0.60              |
| 1:E:7:PRO:HD3    | 1:E:21:ASN:HD22   | 1.67                     | 0.60              |
| 3:G:1:ILE:HG22   | 3:G:2:GLU:N       | 2.16                     | 0.60              |
| 4:H:177:HIS:HD2  | 4:H:179:SER:OG    | 1.84                     | 0.60              |
| 3:C:1:ILE:HG23   | 6:C:230:HOH:O     | 1.68                     | 0.60              |
| 2:F:73:GLU:CD    | 2:F:73:GLU:H      | 2.09                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:14:GLN:HB3   | 4:H:8:VAL:CG2    | 2.31                     | 0.60              |
| 1:A:66:PHE:HD1   | 1:A:73:LEU:HD13  | 1.67                     | 0.60              |
| 2:F:83:THR:HG23  | 2:F:84:PRO:HD2   | 1.84                     | 0.60              |
| 1:E:69:ARG:C     | 1:E:71:LYS:H     | 2.10                     | 0.59              |
| 2:B:7:SER:CB     | 2:B:8:PRO:CD     | 2.80                     | 0.59              |
| 2:F:88:SER:O     | 2:F:90:TYR:CE1   | 2.56                     | 0.59              |
| 2:B:51:GLY:CA    | 2:B:69:ARG:NH1   | 2.66                     | 0.59              |
| 2:B:30:ASN:HA    | 2:B:72:GLN:HE22  | 1.68                     | 0.58              |
| 1:A:25:GLU:HA    | 1:A:71:LYS:CD    | 2.33                     | 0.58              |
| 2:F:15:THR:HG23  | 2:F:84:PRO:HD3   | 1.85                     | 0.58              |
| 3:C:167:HIS:HD2  | 3:C:169:GLY:H    | 1.51                     | 0.58              |
| 4:D:62:ASN:O     | 4:D:68:LEU:HB2   | 2.03                     | 0.58              |
| 2:F:26:THR:HG22  | 2:F:26:THR:O     | 2.03                     | 0.58              |
| 2:F:87:THR:HG23  | 2:F:115:THR:HA   | 1.85                     | 0.58              |
| 4:H:116:VAL:HG22 | 4:H:160:MET:HG3  | 1.86                     | 0.58              |
| 2:F:21:LEU:N     | 2:F:21:LEU:HD12  | 2.18                     | 0.58              |
| 2:B:73:GLU:CD    | 2:B:73:GLU:N     | 2.62                     | 0.58              |
| 3:C:123:ARG:HB2  | 3:C:128:VAL:HG21 | 1.86                     | 0.58              |
| 1:A:45:LEU:HB3   | 2:B:105:GLU:OE2  | 2.03                     | 0.58              |
| 3:C:123:ARG:HD3  | 3:C:159:ASP:OD2  | 2.04                     | 0.58              |
| 2:F:84:PRO:HA    | 2:F:116:VAL:CG2  | 2.34                     | 0.58              |
| 4:D:55:ARG:HB3   | 4:D:56:PRO:HD3   | 1.86                     | 0.58              |
| 2:F:87:THR:OG1   | 2:F:116:VAL:HG22 | 2.03                     | 0.57              |
| 3:C:1:ILE:HD12   | 3:C:1:ILE:H1     | 1.70                     | 0.57              |
| 5:P:3:GLN:NE2    | 5:P:3:GLN:HA     | 2.19                     | 0.57              |
| 2:F:89:VAL:HA    | 2:F:112:THR:O    | 2.05                     | 0.57              |
| 4:D:163:MET:HE1  | 4:D:165:PRO:HB3  | 1.86                     | 0.56              |
| 1:E:38:PHE:CD1   | 1:E:86:ALA:HB2   | 2.40                     | 0.56              |
| 3:G:114:PRO:O    | 3:G:167:HIS:HE1  | 1.88                     | 0.56              |
| 4:H:28:THR:CG2   | 4:H:30:TYR:CE1   | 2.87                     | 0.56              |
| 3:C:3:ALA:HB1    | 4:D:17:PHE:O     | 2.05                     | 0.56              |
| 2:F:60:ILE:CG2   | 6:F:120:HOH:O    | 2.18                     | 0.56              |
| 2:B:7:SER:HG     | 2:B:22:SER:H     | 1.54                     | 0.56              |
| 1:E:19:ILE:O     | 1:E:20:LEU:HD23  | 2.06                     | 0.56              |
| 3:G:1:ILE:N      | 3:G:1:ILE:HD12   | 2.21                     | 0.56              |
| 3:G:76:ARG:HD2   | 4:H:53:LEU:HD23  | 1.88                     | 0.56              |
| 2:F:32:MET:HG3   | 2:F:69:ARG:NH2   | 2.20                     | 0.56              |
| 1:A:8:GLN:CD     | 1:A:8:GLN:H      | 2.13                     | 0.56              |
| 1:E:20:LEU:HD22  | 1:E:110:THR:HG21 | 1.88                     | 0.56              |
| 2:F:79:LEU:HD12  | 2:F:79:LEU:N     | 2.20                     | 0.56              |
| 3:G:85:GLU:O     | 3:G:169:GLY:HA3  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:111:HIS:O    | 4:D:165:PRO:HD2  | 2.05                     | 0.55              |
| 1:A:13:TRP:HD1   | 1:A:115:VAL:HB   | 1.70                     | 0.55              |
| 4:D:52:GLU:HG2   | 4:D:55:ARG:HH21  | 1.71                     | 0.55              |
| 4:H:30:TYR:HB2   | 4:H:38:LEU:HB3   | 1.88                     | 0.55              |
| 3:C:170:LEU:HD13 | 3:C:174:VAL:HG23 | 1.89                     | 0.55              |
| 4:D:9:VAL:HA     | 4:D:32:TYR:O     | 2.06                     | 0.55              |
| 1:A:7:PRO:HD3    | 1:A:21:ASN:HB2   | 1.89                     | 0.55              |
| 2:F:31:ASN:C     | 2:F:31:ASN:HD22  | 2.15                     | 0.55              |
| 1:A:89:PHE:CE1   | 1:A:109:GLY:HA3  | 2.41                     | 0.55              |
| 2:B:83:THR:HG22  | 2:B:85:SER:H     | 1.71                     | 0.54              |
| 4:H:167:ARG:HB3  | 4:H:167:ARG:NH1  | 2.17                     | 0.54              |
| 4:H:2:ASP:N      | 4:H:5:ARG:HD3    | 2.13                     | 0.54              |
| 2:B:69:ARG:HG3   | 2:B:69:ARG:NH1   | 2.23                     | 0.54              |
| 3:G:159:ASP:O    | 3:G:160:ILE:HD12 | 2.07                     | 0.54              |
| 2:B:56:GLU:CD    | 3:C:39:LYS:HZ2   | 2.15                     | 0.54              |
| 4:H:60:TYR:CZ    | 4:H:64:GLN:HG3   | 2.43                     | 0.54              |
| 2:F:56:GLU:OE1   | 3:G:39:LYS:HE2   | 2.08                     | 0.53              |
| 2:B:93:ALA:HB2   | 2:B:108:PHE:CD1  | 2.43                     | 0.53              |
| 1:E:101:GLY:HA3  | 5:I:3:GLN:HE22   | 1.73                     | 0.53              |
| 1:E:81:GLN:N     | 1:E:114:VAL:HG11 | 2.23                     | 0.53              |
| 1:E:81:GLN:C     | 1:E:114:VAL:HG11 | 2.33                     | 0.53              |
| 3:G:167:HIS:CD2  | 3:G:169:GLY:H    | 2.27                     | 0.53              |
| 4:H:55:ARG:HB3   | 4:H:56:PRO:HD3   | 1.91                     | 0.53              |
| 3:C:1:ILE:HG22   | 3:C:2:GLU:H      | 1.73                     | 0.53              |
| 4:D:166:ARG:HH11 | 4:D:166:ARG:HG2  | 1.73                     | 0.53              |
| 4:D:11:PHE:HE1   | 4:D:28:THR:HG23  | 1.72                     | 0.53              |
| 3:G:3:ALA:HB1    | 4:H:17:PHE:O     | 2.09                     | 0.53              |
| 4:H:111:HIS:O    | 4:H:164:THR:HA   | 2.09                     | 0.53              |
| 3:C:57:GLN:NE2   | 3:C:60:LEU:HD12  | 2.23                     | 0.53              |
| 3:C:70:LEU:HD13  | 4:D:9:VAL:HG13   | 1.90                     | 0.53              |
| 3:G:123:ARG:HG3  | 3:G:161:TYR:CE2  | 2.43                     | 0.53              |
| 5:P:7:SER:O      | 5:P:8:GLN:HB2    | 2.08                     | 0.52              |
| 4:H:150:ASN:ND2  | 4:H:156:GLN:HE21 | 2.02                     | 0.52              |
| 1:A:69:ARG:C     | 1:A:71:LYS:H     | 2.18                     | 0.52              |
| 2:F:37:GLN:NE2   | 2:F:91:PHE:HE2   | 2.06                     | 0.52              |
| 2:B:97:ALA:O     | 2:B:104:TYR:HE2  | 1.92                     | 0.52              |
| 1:E:80:SER:O     | 1:E:81:GLN:HB2   | 2.10                     | 0.52              |
| 2:F:11:LYS:O     | 2:F:114:LEU:HA   | 2.09                     | 0.52              |
| 1:E:55:LYS:HE2   | 1:E:57:GLU:OE2   | 2.09                     | 0.52              |
| 2:F:47:TYR:CZ    | 2:F:57:LYS:HG2   | 2.45                     | 0.52              |
| 4:H:41:ASP:OD1   | 4:H:43:ASP:HB2   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:81:GLN:C     | 1:A:114:VAL:HG11 | 2.35                     | 0.52              |
| 1:E:57:GLU:HB3   | 1:E:63:THR:HG23  | 1.90                     | 0.52              |
| 4:D:11:PHE:HB2   | 5:P:4:TYR:CE1    | 2.45                     | 0.52              |
| 4:H:55:ARG:CB    | 4:H:56:PRO:HD3   | 2.39                     | 0.52              |
| 2:F:41:HIS:O     | 2:F:42:GLY:O     | 2.27                     | 0.52              |
| 3:G:115:PRO:HG3  | 3:G:145:PHE:CE1  | 2.44                     | 0.52              |
| 4:D:11:PHE:HE1   | 4:D:28:THR:CG2   | 2.23                     | 0.51              |
| 4:D:28:THR:HG22  | 4:D:30:TYR:CE1   | 2.45                     | 0.51              |
| 2:F:29:HIS:HB3   | 2:F:95:GLY:O     | 2.10                     | 0.51              |
| 4:H:104:SER:C    | 4:H:105:ARG:HG2  | 2.36                     | 0.51              |
| 1:A:31:TYR:CD2   | 2:B:100:GLY:HA2  | 2.46                     | 0.51              |
| 3:C:51:LEU:N     | 3:C:51:LEU:HD12  | 2.25                     | 0.51              |
| 4:H:53:LEU:HD23  | 4:H:53:LEU:O     | 2.11                     | 0.51              |
| 3:C:24:PHE:HZ    | 5:P:1:ALA:HB2    | 1.76                     | 0.51              |
| 4:D:97:PRO:HD3   | 4:D:122:PHE:HB2  | 1.92                     | 0.51              |
| 1:E:38:PHE:HD1   | 1:E:86:ALA:HB2   | 1.75                     | 0.51              |
| 1:A:85:SER:OG    | 1:A:114:VAL:N    | 2.37                     | 0.51              |
| 1:E:101:GLY:HA3  | 5:I:3:GLN:NE2    | 2.25                     | 0.51              |
| 4:D:45:GLY:O     | 4:D:72:ARG:NH1   | 2.44                     | 0.51              |
| 4:H:61:TYR:CE2   | 5:I:5:ARG:HB2    | 2.46                     | 0.51              |
| 2:B:89:VAL:HA    | 2:B:112:THR:O    | 2.11                     | 0.50              |
| 1:E:66:PHE:CE2   | 1:E:68:LYS:HA    | 2.46                     | 0.50              |
| 2:F:97:ALA:HB1   | 3:G:61:GLN:NE2   | 2.26                     | 0.50              |
| 3:G:137:PHE:CE1  | 3:G:147:LYS:HE3  | 2.46                     | 0.50              |
| 2:B:31:ASN:OD1   | 2:B:97:ALA:HA    | 2.11                     | 0.50              |
| 4:D:111:HIS:HB2  | 4:D:113:ASN:HD21 | 1.77                     | 0.50              |
| 2:B:24:ASN:HA    | 2:B:73:GLU:O     | 2.12                     | 0.50              |
| 4:D:97:PRO:HD3   | 4:D:122:PHE:HB3  | 1.92                     | 0.50              |
| 2:B:37:GLN:NE2   | 2:B:91:PHE:CE2   | 2.78                     | 0.50              |
| 1:E:10:LEU:O     | 1:E:112:LEU:HA   | 2.12                     | 0.50              |
| 1:A:4:ARG:HG2    | 1:A:4:ARG:HH11   | 1.77                     | 0.50              |
| 1:E:50:LEU:C     | 1:E:52:VAL:H     | 2.20                     | 0.50              |
| 4:D:177:HIS:CG   | 4:D:178:PRO:HD2  | 2.46                     | 0.49              |
| 2:F:32:MET:HE2   | 2:F:72:GLN:O     | 2.12                     | 0.49              |
| 1:A:14:GLU:HB2   | 1:A:82:PRO:HD3   | 1.94                     | 0.49              |
| 4:D:174:HIS:HD2  | 6:D:225:HOH:O    | 1.95                     | 0.49              |
| 1:E:81:GLN:O     | 1:E:83:GLY:N     | 2.41                     | 0.49              |
| 2:B:60:ILE:HG22  | 6:B:121:HOH:O    | 2.11                     | 0.49              |
| 4:D:67:TYR:O     | 4:D:68:LEU:C     | 2.54                     | 0.49              |
| 3:C:32:PHE:CD1   | 3:C:32:PHE:C     | 2.90                     | 0.49              |
| 4:D:167:ARG:HH11 | 4:D:167:ARG:CB   | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:41:HIS:HB2   | 2:F:44:ARG:HD2   | 1.94                     | 0.49              |
| 3:C:62:ASN:ND2   | 5:P:3:GLN:HE22   | 2.00                     | 0.49              |
| 4:H:40:PHE:HB2   | 4:H:47:TYR:CE1   | 2.47                     | 0.49              |
| 1:E:45:LEU:HD22  | 2:F:105:GLU:HB2  | 1.95                     | 0.49              |
| 4:H:110:ASN:OD1  | 4:H:166:ARG:NH1  | 2.47                     | 0.48              |
| 1:A:38:PHE:HD1   | 1:A:86:ALA:HB2   | 1.79                     | 0.48              |
| 1:A:61:ARG:HD2   | 1:A:79:ASP:O     | 2.13                     | 0.48              |
| 2:F:7:SER:CB     | 2:F:8:PRO:CD     | 2.87                     | 0.48              |
| 2:F:7:SER:O      | 2:F:8:PRO:C      | 2.54                     | 0.48              |
| 3:G:1:ILE:CG2    | 3:G:2:GLU:N      | 2.77                     | 0.48              |
| 4:H:167:ARG:HH11 | 4:H:167:ARG:CB   | 2.20                     | 0.48              |
| 4:D:8:VAL:HG22   | 4:D:9:VAL:N      | 2.29                     | 0.48              |
| 1:A:26:ASN:HB3   | 1:A:29:PHE:CD2   | 2.48                     | 0.48              |
| 3:C:77:SER:O     | 3:C:78:ASN:HB2   | 2.13                     | 0.48              |
| 4:H:163:MET:HE1  | 4:H:165:PRO:HB3  | 1.94                     | 0.48              |
| 2:B:49:SER:HB3   | 2:B:69:ARG:NH1   | 2.29                     | 0.48              |
| 3:G:122:LEU:HB2  | 3:G:162:ASP:HB2  | 1.96                     | 0.48              |
| 4:D:28:THR:HB    | 4:D:40:PHE:HB3   | 1.95                     | 0.48              |
| 1:E:26:ASN:C     | 1:E:26:ASN:ND2   | 2.72                     | 0.48              |
| 1:E:61:ARG:HB3   | 1:E:78:ALA:O     | 2.13                     | 0.48              |
| 3:G:85:GLU:CD    | 4:H:34:ARG:HH21  | 2.22                     | 0.48              |
| 4:H:144:SER:CB   | 4:H:159:VAL:HG22 | 2.44                     | 0.48              |
| 2:B:87:THR:HG23  | 2:B:115:THR:HA   | 1.95                     | 0.47              |
| 1:A:26:ASN:HD21  | 1:A:28:ALA:HB3   | 1.79                     | 0.47              |
| 1:A:31:TYR:CE1   | 1:A:48:SER:HB2   | 2.48                     | 0.47              |
| 1:A:38:PHE:CD1   | 1:A:86:ALA:HB2   | 2.49                     | 0.47              |
| 2:B:29:HIS:HB3   | 2:B:95:GLY:O     | 2.14                     | 0.47              |
| 2:B:33:TYR:CD1   | 2:B:33:TYR:N     | 2.81                     | 0.47              |
| 3:G:123:ARG:HG3  | 3:G:123:ARG:HH11 | 1.79                     | 0.47              |
| 3:C:1:ILE:CG2    | 3:C:2:GLU:N      | 2.75                     | 0.47              |
| 4:D:97:PRO:CD    | 4:D:122:PHE:HB3  | 2.44                     | 0.47              |
| 1:E:37:GLN:HA    | 6:E:119:HOH:O    | 2.14                     | 0.47              |
| 4:D:60:TYR:CZ    | 4:D:64:GLN:HG3   | 2.50                     | 0.47              |
| 1:E:26:ASN:HB3   | 1:E:29:PHE:CE2   | 2.49                     | 0.47              |
| 1:E:83:GLY:C     | 1:E:85:SER:H     | 2.22                     | 0.47              |
| 4:H:9:VAL:HA     | 4:H:32:TYR:O     | 2.15                     | 0.47              |
| 3:C:70:LEU:CD1   | 4:D:9:VAL:HG13   | 2.44                     | 0.47              |
| 2:F:47:TYR:HE1   | 2:F:61:PRO:HB2   | 1.72                     | 0.47              |
| 1:A:26:ASN:HB3   | 1:A:29:PHE:CE2   | 2.50                     | 0.47              |
| 2:B:9:ARG:CZ     | 2:B:110:PRO:HB2  | 2.44                     | 0.47              |
| 3:C:123:ARG:HG3  | 3:C:123:ARG:HH11 | 1.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:5:GLN:NE2    | 1:E:109:GLY:HA2  | 2.30                     | 0.47              |
| 4:D:46:GLU:HG3   | 4:D:62:ASN:OD1   | 2.15                     | 0.47              |
| 2:F:83:THR:HG22  | 2:F:85:SER:H     | 1.79                     | 0.46              |
| 3:G:70:LEU:HD13  | 4:H:9:VAL:HG13   | 1.96                     | 0.46              |
| 1:E:37:GLN:NE2   | 2:F:37:GLN:HE22  | 2.03                     | 0.46              |
| 4:D:111:HIS:HB2  | 4:D:113:ASN:ND2  | 2.30                     | 0.46              |
| 2:F:84:PRO:HA    | 2:F:116:VAL:HG21 | 1.97                     | 0.46              |
| 3:C:50:GLN:HB2   | 3:C:51:LEU:HD12  | 1.97                     | 0.46              |
| 1:A:5:GLN:NE2    | 1:A:90:CYS:H     | 2.13                     | 0.46              |
| 4:D:1:GLY:N      | 4:D:5:ARG:HD3    | 2.30                     | 0.46              |
| 4:D:101:ILE:HD12 | 4:D:186:VAL:HG12 | 1.98                     | 0.46              |
| 4:D:166:ARG:HG2  | 4:D:166:ARG:NH1  | 2.30                     | 0.46              |
| 1:E:4:ARG:HG2    | 1:E:4:ARG:HH11   | 1.79                     | 0.46              |
| 2:F:4:VAL:HG13   | 2:F:25:GLN:HB3   | 1.96                     | 0.46              |
| 2:F:11:LYS:HB3   | 2:F:114:LEU:HD13 | 1.97                     | 0.46              |
| 1:E:69:ARG:C     | 1:E:71:LYS:N     | 2.74                     | 0.46              |
| 3:C:117:ILE:HD11 | 3:C:165:VAL:HG13 | 1.98                     | 0.46              |
| 1:E:12:VAL:HG13  | 1:E:16:GLU:CD    | 2.40                     | 0.46              |
| 4:H:11:PHE:HB2   | 5:I:4:TYR:CE1    | 2.51                     | 0.46              |
| 3:C:15:SER:HA    | 3:C:16:PRO:C     | 2.41                     | 0.46              |
| 4:D:132:PHE:CE2  | 4:D:137:GLU:HB2  | 2.51                     | 0.46              |
| 1:E:70:GLU:HG2   | 1:E:72:LYS:HE2   | 1.98                     | 0.46              |
| 4:H:62:ASN:O     | 4:H:68:LEU:HB2   | 2.15                     | 0.46              |
| 1:A:38:PHE:HA    | 1:A:86:ALA:HB2   | 1.97                     | 0.45              |
| 1:E:26:ASN:HB3   | 1:E:29:PHE:CD2   | 2.51                     | 0.45              |
| 4:H:144:SER:HB2  | 4:H:159:VAL:HG22 | 1.97                     | 0.45              |
| 1:A:62:PHE:HD1   | 1:A:77:ILE:HG12  | 1.81                     | 0.45              |
| 3:C:14:GLN:HB3   | 4:D:8:VAL:HB     | 1.99                     | 0.45              |
| 3:C:50:GLN:C     | 3:C:51:LEU:HD12  | 2.42                     | 0.45              |
| 1:E:5:GLN:NE2    | 1:E:90:CYS:H     | 2.15                     | 0.45              |
| 3:G:32:PHE:CD1   | 3:G:32:PHE:C     | 2.94                     | 0.45              |
| 2:F:33:TYR:CD1   | 2:F:33:TYR:N     | 2.84                     | 0.45              |
| 2:F:96:ASP:HB3   | 2:F:104:TYR:CD2  | 2.52                     | 0.45              |
| 4:H:119:VAL:HG11 | 4:H:127:ILE:HD11 | 1.99                     | 0.45              |
| 2:B:7:SER:HG     | 2:B:22:SER:N     | 2.14                     | 0.45              |
| 3:C:15:SER:HB2   | 3:C:16:PRO:HA    | 1.98                     | 0.45              |
| 1:E:61:ARG:HD2   | 1:E:79:ASP:O     | 2.17                     | 0.45              |
| 2:F:23:CYS:SG    | 2:F:24:ASN:N     | 2.90                     | 0.45              |
| 4:D:31:ILE:N     | 4:D:31:ILE:HD12  | 2.32                     | 0.45              |
| 1:E:26:ASN:ND2   | 1:E:28:ALA:H     | 2.15                     | 0.45              |
| 1:A:4:ARG:O      | 1:A:22:CYS:HA    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:31:ASN:CB    | 2:F:49:SER:O     | 2.62                     | 0.45              |
| 4:D:144:SER:HB3  | 4:D:159:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:6:SER:CB     | 1:A:7:PRO:HD3    | 2.40                     | 0.44              |
| 3:C:167:HIS:HD2  | 3:C:169:GLY:N    | 2.14                     | 0.44              |
| 4:H:177:HIS:CD2  | 4:H:179:SER:H    | 2.35                     | 0.44              |
| 3:C:85:GLU:HG3   | 4:D:34:ARG:NH2   | 2.32                     | 0.44              |
| 4:H:40:PHE:HB2   | 4:H:47:TYR:CD1   | 2.52                     | 0.44              |
| 1:E:66:PHE:CD1   | 1:E:73:LEU:HD13  | 2.50                     | 0.44              |
| 3:G:43:TRP:CH2   | 3:G:52:ARG:HG3   | 2.52                     | 0.44              |
| 2:B:79:LEU:HD23  | 2:B:86:GLN:CD    | 2.42                     | 0.44              |
| 1:E:81:GLN:CA    | 1:E:114:VAL:HG11 | 2.47                     | 0.44              |
| 3:G:160:ILE:HG13 | 3:G:179:GLU:HB3  | 1.99                     | 0.44              |
| 4:H:8:VAL:HG22   | 4:H:9:VAL:N      | 2.32                     | 0.44              |
| 4:D:97:PRO:HG3   | 4:D:122:PHE:HB3  | 1.99                     | 0.44              |
| 1:A:85:SER:HG    | 1:A:114:VAL:H    | 1.61                     | 0.44              |
| 4:D:2:ASP:N      | 4:D:5:ARG:HD3    | 2.30                     | 0.44              |
| 2:B:14:VAL:HA    | 2:B:116:VAL:O    | 2.18                     | 0.44              |
| 3:C:110:ASP:OD1  | 3:C:111:ASN:N    | 2.47                     | 0.43              |
| 3:C:132:VAL:HA   | 3:C:150:TYR:O    | 2.18                     | 0.43              |
| 4:H:5:ARG:HH11   | 4:H:5:ARG:HG2    | 1.83                     | 0.43              |
| 4:H:31:ILE:HD12  | 4:H:31:ILE:N     | 2.33                     | 0.43              |
| 1:A:2:GLN:HG2    | 1:A:3:VAL:N      | 2.32                     | 0.43              |
| 1:A:7:PRO:O      | 1:A:110:THR:HG23 | 2.18                     | 0.43              |
| 1:E:10:LEU:HA    | 6:E:117:HOH:O    | 2.18                     | 0.43              |
| 3:G:132:VAL:HA   | 3:G:150:TYR:O    | 2.19                     | 0.43              |
| 3:G:137:PHE:CZ   | 3:G:147:LYS:HE3  | 2.53                     | 0.43              |
| 4:H:58:ALA:O     | 4:H:62:ASN:ND2   | 2.51                     | 0.43              |
| 3:C:1:ILE:CG2    | 3:C:2:GLU:H      | 2.30                     | 0.43              |
| 1:E:104:GLN:HG3  | 2:F:99:GLY:O     | 2.18                     | 0.43              |
| 2:F:41:HIS:O     | 2:F:42:GLY:C     | 2.62                     | 0.43              |
| 4:H:105:ARG:HG3  | 4:H:113:ASN:HA   | 1.99                     | 0.43              |
| 1:E:81:GLN:H     | 1:E:114:VAL:HG11 | 1.84                     | 0.43              |
| 2:F:32:MET:HE3   | 2:F:75:PHE:HB2   | 2.00                     | 0.43              |
| 3:C:118:ASN:HB2  | 3:C:166:GLU:HB2  | 2.00                     | 0.43              |
| 2:F:47:TYR:OH    | 2:F:57:LYS:HE2   | 2.19                     | 0.43              |
| 4:D:1:GLY:H2     | 4:D:5:ARG:HD3    | 1.83                     | 0.43              |
| 2:F:73:GLU:CD    | 2:F:73:GLU:N     | 2.76                     | 0.43              |
| 3:C:13:TYR:OH    | 3:C:18:ASP:HB3   | 2.19                     | 0.43              |
| 3:G:11:VAL:HB    | 4:H:11:PHE:HB3   | 1.99                     | 0.43              |
| 2:B:67:ALA:HB1   | 2:B:75:PHE:CE1   | 2.53                     | 0.43              |
| 4:D:44:VAL:HG13  | 4:D:48:ARG:NH2   | 2.34                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:H:5:ARG:H     | 4:H:5:ARG:HG3   | 1.57                     | 0.43              |
| 1:A:32:PHE:CD1  | 1:A:32:PHE:N    | 2.87                     | 0.43              |
| 4:H:57:ASP:OD1  | 5:I:7:SER:HB2   | 2.19                     | 0.43              |
| 1:A:38:PHE:HA   | 1:A:86:ALA:CB   | 2.48                     | 0.42              |
| 2:B:70:PRO:HD2  | 2:B:74:ASN:O    | 2.18                     | 0.42              |
| 4:H:188:TRP:CH2 | 4:H:190:ALA:HA  | 2.54                     | 0.42              |
| 1:A:98:ALA:O    | 1:A:100:SER:O   | 2.37                     | 0.42              |
| 3:C:21:GLN:HG2  | 6:C:204:HOH:O   | 2.18                     | 0.42              |
| 1:E:50:LEU:C    | 1:E:52:VAL:N    | 2.76                     | 0.42              |
| 3:G:59:GLY:O    | 3:G:63:ILE:HG12 | 2.18                     | 0.42              |
| 2:B:47:TYR:CZ   | 2:B:57:LYS:HG2  | 2.54                     | 0.42              |
| 4:D:122:PHE:CE1 | 4:D:155:PHE:HB2 | 2.54                     | 0.42              |
| 2:F:87:THR:O    | 2:F:87:THR:HG22 | 2.19                     | 0.42              |
| 1:A:20:LEU:O    | 1:A:74:SER:HB2  | 2.19                     | 0.42              |
| 1:A:61:ARG:HB3  | 1:A:78:ALA:O    | 2.19                     | 0.42              |
| 3:C:12:VAL:O    | 3:C:20:GLY:HA2  | 2.19                     | 0.42              |
| 2:F:15:THR:O    | 2:F:15:THR:HG22 | 2.19                     | 0.42              |
| 2:F:69:ARG:HG3  | 2:F:69:ARG:HH11 | 1.83                     | 0.42              |
| 3:C:76:ARG:C    | 3:C:78:ASN:H    | 2.26                     | 0.42              |
| 3:C:87:PRO:HG3  | 6:C:196:HOH:O   | 2.18                     | 0.42              |
| 4:D:177:HIS:ND1 | 4:D:178:PRO:HD2 | 2.35                     | 0.42              |
| 1:E:22:CYS:N    | 1:E:73:LEU:O    | 2.52                     | 0.42              |
| 2:F:45:LEU:HD21 | 2:F:48:TYR:CD2  | 2.55                     | 0.42              |
| 2:F:81:SER:O    | 2:F:82:ALA:C    | 2.62                     | 0.42              |
| 1:E:6:SER:CB    | 1:E:21:ASN:HB2  | 2.43                     | 0.42              |
| 4:H:28:THR:HG21 | 4:H:30:TYR:HE1  | 1.83                     | 0.42              |
| 3:C:73:LEU:HB3  | 4:D:32:TYR:CD1  | 2.54                     | 0.42              |
| 1:A:31:TYR:HE1  | 1:A:48:SER:HB2  | 1.85                     | 0.42              |
| 1:A:61:ARG:HD2  | 1:A:78:ALA:O    | 2.19                     | 0.42              |
| 4:D:55:ARG:CB   | 4:D:56:PRO:HD3  | 2.50                     | 0.42              |
| 1:A:33:PRO:HB2  | 1:A:45:LEU:CD1  | 2.50                     | 0.42              |
| 4:D:46:GLU:OE1  | 4:D:48:ARG:NH1  | 2.52                     | 0.42              |
| 2:F:32:MET:CE   | 2:F:69:ARG:NE   | 2.82                     | 0.42              |
| 3:G:123:ARG:HB2 | 3:G:128:VAL:CG2 | 2.50                     | 0.42              |
| 1:A:49:ILE:HG12 | 1:A:50:LEU:N    | 2.35                     | 0.42              |
| 4:D:30:TYR:HB2  | 4:D:38:LEU:HB3  | 2.01                     | 0.42              |
| 2:F:25:GLN:O    | 2:F:73:GLU:HB2  | 2.20                     | 0.42              |
| 3:G:1:ILE:HD12  | 3:G:1:ILE:H1    | 1.84                     | 0.42              |
| 4:H:152:ASP:O   | 4:H:153:TRP:HB2 | 2.19                     | 0.42              |
| 2:B:26:THR:O    | 2:B:26:THR:HG22 | 2.20                     | 0.41              |
| 1:E:19:ILE:HG22 | 1:E:20:LEU:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:76:ARG:HD2   | 4:H:53:LEU:CD2   | 2.49                     | 0.41              |
| 1:A:36:GLN:HB2   | 1:A:88:TYR:HE1   | 1.85                     | 0.41              |
| 2:F:17:GLU:HG2   | 2:F:18:LYS:N     | 2.35                     | 0.41              |
| 3:G:124:ASN:O    | 3:G:125:SER:HB2  | 2.21                     | 0.41              |
| 4:H:75:LEU:O     | 4:H:79:CYS:HB2   | 2.19                     | 0.41              |
| 2:B:7:SER:HB2    | 2:B:8:PRO:HD3    | 2.01                     | 0.41              |
| 3:C:123:ARG:CD   | 3:C:159:ASP:OD2  | 2.68                     | 0.41              |
| 1:E:82:PRO:HA    | 1:E:114:VAL:HB   | 2.03                     | 0.41              |
| 3:C:38:LYS:O     | 3:C:39:LYS:HB2   | 2.20                     | 0.41              |
| 4:D:97:PRO:CG    | 4:D:122:PHE:HB3  | 2.50                     | 0.41              |
| 2:F:96:ASP:O     | 2:F:98:GLY:N     | 2.53                     | 0.41              |
| 2:F:21:LEU:N     | 2:F:21:LEU:CD1   | 2.82                     | 0.41              |
| 4:H:34:ARG:O     | 4:H:34:ARG:HG3   | 2.20                     | 0.41              |
| 4:H:57:ASP:O     | 4:H:58:ALA:C     | 2.64                     | 0.41              |
| 1:E:29:PHE:HD1   | 1:E:93:SER:C     | 2.29                     | 0.41              |
| 1:E:70:GLU:CD    | 1:E:72:LYS:HE2   | 2.45                     | 0.41              |
| 4:H:124:PRO:O    | 4:H:177:HIS:HE1  | 2.03                     | 0.41              |
| 4:D:59:GLU:O     | 4:D:63:LYS:HG3   | 2.21                     | 0.41              |
| 4:D:129:VAL:HG13 | 4:D:175:VAL:HG22 | 2.03                     | 0.41              |
| 2:F:82:ALA:HB1   | 2:F:116:VAL:CG1  | 2.51                     | 0.41              |
| 4:H:103:LEU:HD13 | 4:H:115:LEU:HD23 | 2.02                     | 0.41              |
| 4:D:180:LEU:HD13 | 4:D:184:ILE:HG13 | 2.02                     | 0.41              |
| 1:E:6:SER:CB     | 1:E:7:PRO:CD     | 2.91                     | 0.41              |
| 1:A:36:GLN:HB2   | 1:A:88:TYR:CE1   | 2.55                     | 0.41              |
| 1:A:106:PHE:CD1  | 1:A:106:PHE:N    | 2.89                     | 0.41              |
| 2:B:7:SER:HB2    | 2:B:8:PRO:CD     | 2.51                     | 0.41              |
| 3:C:1:ILE:N      | 3:C:1:ILE:CD1    | 2.82                     | 0.41              |
| 1:E:33:PRO:HG2   | 1:E:91:ALA:HB3   | 2.03                     | 0.41              |
| 3:G:109:VAL:O    | 3:G:146:HIS:HA   | 2.20                     | 0.41              |
| 4:H:163:MET:SD   | 4:H:165:PRO:HD3  | 2.61                     | 0.41              |
| 1:A:69:ARG:C     | 1:A:71:LYS:N     | 2.79                     | 0.41              |
| 1:E:36:GLN:HB2   | 1:E:88:TYR:HE1   | 1.86                     | 0.41              |
| 2:F:13:ALA:O     | 2:F:116:VAL:HA   | 2.21                     | 0.41              |
| 4:H:111:HIS:O    | 4:H:164:THR:HG23 | 2.20                     | 0.41              |
| 3:C:11:VAL:HG13  | 3:C:63:ILE:HD13  | 2.03                     | 0.40              |
| 3:C:66:GLY:HA2   | 5:P:4:TYR:HE2    | 1.86                     | 0.40              |
| 6:G:183:HOH:O    | 4:H:120:THR:HB   | 2.21                     | 0.40              |
| 2:B:5:THR:HG22   | 2:B:6:GLN:N      | 2.37                     | 0.40              |
| 2:B:25:GLN:HG2   | 2:B:32:MET:SD    | 2.62                     | 0.40              |
| 3:C:62:ASN:ND2   | 5:P:3:GLN:NE2    | 2.53                     | 0.40              |
| 2:F:32:MET:CE    | 2:F:75:PHE:HB2   | 2.52                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:83:THR:C     | 2:F:116:VAL:HG21 | 2.45                     | 0.40              |
| 3:G:70:LEU:CD1   | 4:H:9:VAL:HG13   | 2.50                     | 0.40              |
| 2:B:116:VAL:HG23 | 2:B:117:LEU:N    | 2.37                     | 0.40              |
| 3:C:54:PHE:HA    | 6:C:220:HOH:O    | 2.21                     | 0.40              |
| 2:B:79:LEU:HD23  | 2:B:86:GLN:OE1   | 2.22                     | 0.40              |
| 4:D:71:THR:O     | 4:D:72:ARG:C     | 2.63                     | 0.40              |
| 4:D:176:GLU:HG2  | 4:D:183:PRO:HG3  | 2.04                     | 0.40              |
| 2:F:8:PRO:O      | 2:F:112:THR:HG23 | 2.21                     | 0.40              |
| 3:G:13:TYR:OH    | 3:G:18:ASP:HB3   | 2.21                     | 0.40              |
| 3:G:63:ILE:HD13  | 3:G:63:ILE:HA    | 1.95                     | 0.40              |
| 3:G:145:PHE:N    | 3:G:145:PHE:CD1  | 2.89                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 108/110 (98%)   | 90 (83%)   | 17 (16%)  | 1 (1%)   | 14          | 20  |
| 1   | E     | 108/110 (98%)   | 89 (82%)   | 14 (13%)  | 5 (5%)   | 2           | 1   |
| 2   | B     | 109/111 (98%)   | 94 (86%)   | 11 (10%)  | 4 (4%)   | 2           | 2   |
| 2   | F     | 109/111 (98%)   | 89 (82%)   | 15 (14%)  | 5 (5%)   | 2           | 1   |
| 3   | C     | 180/182 (99%)   | 169 (94%)  | 10 (6%)   | 1 (1%)   | 21          | 30  |
| 3   | G     | 180/182 (99%)   | 174 (97%)  | 6 (3%)    | 0        | 100         | 100 |
| 4   | D     | 187/189 (99%)   | 171 (91%)  | 14 (8%)   | 2 (1%)   | 11          | 16  |
| 4   | H     | 187/189 (99%)   | 161 (86%)  | 25 (13%)  | 1 (0%)   | 24          | 35  |
| 5   | I     | 10/12 (83%)     | 10 (100%)  | 0         | 0        | 100         | 100 |
| 5   | P     | 10/12 (83%)     | 9 (90%)    | 1 (10%)   | 0        | 100         | 100 |
| All | All   | 1188/1208 (98%) | 1056 (89%) | 113 (10%) | 19 (2%)  | 7           | 10  |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 80  | SER  |
| 2   | F     | 7   | SER  |
| 2   | F     | 42  | GLY  |
| 2   | F     | 97  | ALA  |
| 1   | A     | 80  | SER  |
| 2   | B     | 82  | ALA  |
| 4   | D     | 2   | ASP  |
| 4   | D     | 110 | ASN  |
| 1   | E     | 51  | SER  |
| 1   | E     | 68  | LYS  |
| 2   | F     | 15  | THR  |
| 2   | B     | 81  | SER  |
| 2   | B     | 99  | GLY  |
| 1   | E     | 6   | SER  |
| 1   | E     | 83  | GLY  |
| 3   | C     | 125 | SER  |
| 4   | H     | 22  | GLN  |
| 2   | B     | 7   | SER  |
| 2   | F     | 98  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | A     | 94/94 (100%)   | 92 (98%)  | 2 (2%)   | 47          | 67  |
| 1   | E     | 94/94 (100%)   | 92 (98%)  | 2 (2%)   | 47          | 67  |
| 2   | B     | 91/91 (100%)   | 83 (91%)  | 8 (9%)   | 9           | 14  |
| 2   | F     | 91/91 (100%)   | 85 (93%)  | 6 (7%)   | 15          | 25  |
| 3   | C     | 163/163 (100%) | 161 (99%) | 2 (1%)   | 63          | 79  |
| 3   | G     | 163/163 (100%) | 159 (98%) | 4 (2%)   | 42          | 62  |
| 4   | D     | 175/175 (100%) | 166 (95%) | 9 (5%)   | 21          | 35  |
| 4   | H     | 175/175 (100%) | 168 (96%) | 7 (4%)   | 28          | 45  |
| 5   | I     | 9/9 (100%)     | 9 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 5   | P     | 9/9 (100%)       | 9 (100%)   | 0        | 100         | 100 |
| All | All   | 1064/1064 (100%) | 1024 (96%) | 40 (4%)  | 29          | 47  |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | GLN  |
| 1   | A     | 47  | ILE  |
| 2   | B     | 8   | PRO  |
| 2   | B     | 21  | LEU  |
| 2   | B     | 33  | TYR  |
| 2   | B     | 55  | THR  |
| 2   | B     | 60  | ILE  |
| 2   | B     | 69  | ARG  |
| 2   | B     | 72  | GLN  |
| 2   | B     | 73  | GLU  |
| 3   | C     | 1   | ILE  |
| 3   | C     | 159 | ASP  |
| 4   | D     | 4   | GLU  |
| 4   | D     | 34  | ARG  |
| 4   | D     | 48  | ARG  |
| 4   | D     | 53  | LEU  |
| 4   | D     | 64  | GLN  |
| 4   | D     | 68  | LEU  |
| 4   | D     | 76  | ASP  |
| 4   | D     | 97  | PRO  |
| 4   | D     | 98  | ASN  |
| 1   | E     | 8   | GLN  |
| 1   | E     | 85  | SER  |
| 2   | F     | 10  | ASN  |
| 2   | F     | 31  | ASN  |
| 2   | F     | 39  | THR  |
| 2   | F     | 41  | HIS  |
| 2   | F     | 69  | ARG  |
| 2   | F     | 80  | GLU  |
| 3   | G     | 2   | GLU  |
| 3   | G     | 51  | LEU  |
| 3   | G     | 123 | ARG  |
| 3   | G     | 145 | PHE  |
| 4   | H     | 28  | THR  |
| 4   | H     | 34  | ARG  |
| 4   | H     | 46  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 55  | ARG  |
| 4   | H     | 97  | PRO  |
| 4   | H     | 100 | VAL  |
| 4   | H     | 167 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | GLN  |
| 1   | A     | 26  | ASN  |
| 1   | A     | 67  | ASN  |
| 1   | A     | 81  | GLN  |
| 1   | A     | 104 | GLN  |
| 1   | A     | 113 | GLN  |
| 2   | B     | 24  | ASN  |
| 2   | B     | 28  | ASN  |
| 2   | B     | 37  | GLN  |
| 2   | B     | 72  | GLN  |
| 2   | B     | 74  | ASN  |
| 2   | B     | 106 | GLN  |
| 3   | C     | 84  | ASN  |
| 3   | C     | 124 | ASN  |
| 3   | C     | 167 | HIS  |
| 4   | D     | 33  | ASN  |
| 4   | D     | 64  | GLN  |
| 4   | D     | 111 | HIS  |
| 4   | D     | 146 | GLN  |
| 4   | D     | 150 | ASN  |
| 4   | D     | 177 | HIS  |
| 5   | P     | 3   | GLN  |
| 1   | E     | 5   | GLN  |
| 1   | E     | 21  | ASN  |
| 1   | E     | 26  | ASN  |
| 1   | E     | 36  | GLN  |
| 1   | E     | 67  | ASN  |
| 1   | E     | 76  | HIS  |
| 1   | E     | 81  | GLN  |
| 1   | E     | 113 | GLN  |
| 2   | F     | 24  | ASN  |
| 2   | F     | 28  | ASN  |
| 2   | F     | 31  | ASN  |
| 2   | F     | 37  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 41  | HIS  |
| 2   | F     | 72  | GLN  |
| 2   | F     | 74  | ASN  |
| 3   | G     | 14  | GLN  |
| 3   | G     | 101 | GLN  |
| 3   | G     | 118 | ASN  |
| 3   | G     | 167 | HIS  |
| 4   | H     | 64  | GLN  |
| 4   | H     | 111 | HIS  |
| 4   | H     | 150 | ASN  |
| 4   | H     | 174 | HIS  |
| 4   | H     | 177 | HIS  |
| 5   | I     | 3   | GLN  |
| 5   | I     | 8   | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2   |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|-----------|-------|-----------------------|-------|
| 1   | A     | 110/110 (100%)   | 1.30   | 24 (21%)  | 2 2   | 47, 78, 102, 112      | 0     |
| 1   | E     | 110/110 (100%)   | 1.33   | 21 (19%)  | 3 2   | 51, 80, 100, 110      | 0     |
| 2   | B     | 111/111 (100%)   | 1.25   | 20 (18%)  | 3 3   | 48, 74, 92, 101       | 0     |
| 2   | F     | 111/111 (100%)   | 1.41   | 24 (21%)  | 2 2   | 52, 78, 97, 104       | 0     |
| 3   | C     | 182/182 (100%)   | -0.03  | 6 (3%)    | 49 45 | 27, 46, 79, 107       | 0     |
| 3   | G     | 182/182 (100%)   | -0.08  | 1 (0%)    | 87 86 | 28, 45, 74, 102       | 0     |
| 4   | D     | 189/189 (100%)   | 0.33   | 14 (7%)   | 20 17 | 25, 49, 119, 154      | 0     |
| 4   | H     | 189/189 (100%)   | 0.34   | 15 (7%)   | 18 15 | 24, 50, 120, 155      | 0     |
| 5   | I     | 12/12 (100%)     | 0.78   | 3 (25%)   | 2 1   | 45, 52, 83, 96        | 0     |
| 5   | P     | 12/12 (100%)     | 0.57   | 2 (16%)   | 4 3   | 38, 48, 71, 84        | 0     |
| All | All   | 1208/1208 (100%) | 0.58   | 130 (10%) | 11 8  | 24, 60, 99, 155       | 0     |

All (130) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | H     | 109 | LEU  | 7.9  |
| 4   | D     | 109 | LEU  | 6.7  |
| 2   | B     | 52  | ALA  | 5.9  |
| 2   | B     | 3   | ALA  | 5.5  |
| 2   | F     | 3   | ALA  | 5.4  |
| 4   | D     | 106 | THR  | 5.4  |
| 4   | H     | 106 | THR  | 5.4  |
| 4   | D     | 108 | ALA  | 5.3  |
| 2   | F     | 47  | TYR  | 5.2  |
| 1   | E     | 101 | GLY  | 5.1  |
| 4   | H     | 111 | HIS  | 4.9  |
| 4   | D     | 111 | HIS  | 4.8  |
| 4   | H     | 112 | HIS  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 17  | GLU  | 4.5  |
| 4   | H     | 108 | ALA  | 4.2  |
| 2   | B     | 47  | TYR  | 4.1  |
| 2   | F     | 14  | VAL  | 4.1  |
| 2   | F     | 52  | ALA  | 4.0  |
| 2   | B     | 4   | VAL  | 4.0  |
| 4   | H     | 1   | GLY  | 3.9  |
| 3   | C     | 3   | ALA  | 3.9  |
| 2   | B     | 98  | GLY  | 3.8  |
| 4   | D     | 110 | ASN  | 3.7  |
| 4   | H     | 110 | ASN  | 3.7  |
| 4   | H     | 107 | GLU  | 3.7  |
| 1   | E     | 108 | THR  | 3.6  |
| 1   | E     | 112 | LEU  | 3.6  |
| 1   | A     | 85  | SER  | 3.5  |
| 2   | B     | 17  | GLU  | 3.5  |
| 4   | D     | 3   | SER  | 3.5  |
| 2   | B     | 97  | ALA  | 3.4  |
| 4   | D     | 112 | HIS  | 3.4  |
| 2   | B     | 51  | GLY  | 3.3  |
| 2   | B     | 53  | GLY  | 3.3  |
| 4   | D     | 1   | GLY  | 3.3  |
| 4   | H     | 4   | GLU  | 3.2  |
| 1   | A     | 13  | TRP  | 3.2  |
| 1   | A     | 101 | GLY  | 3.2  |
| 4   | D     | 105 | ARG  | 3.2  |
| 2   | F     | 98  | GLY  | 3.2  |
| 4   | H     | 3   | SER  | 3.1  |
| 4   | H     | 105 | ARG  | 3.1  |
| 2   | F     | 89  | VAL  | 3.0  |
| 2   | F     | 88  | SER  | 3.0  |
| 1   | E     | 115 | VAL  | 2.9  |
| 1   | E     | 111 | LYS  | 2.9  |
| 5   | I     | 8   | GLN  | 2.9  |
| 2   | F     | 117 | LEU  | 2.9  |
| 2   | B     | 5   | THR  | 2.8  |
| 2   | B     | 8   | PRO  | 2.8  |
| 1   | A     | 65  | PHE  | 2.8  |
| 1   | A     | 9   | SER  | 2.8  |
| 5   | I     | -3  | SER  | 2.8  |
| 3   | C     | 2   | GLU  | 2.8  |
| 2   | B     | 20  | THR  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | G     | 158 | ASP  | 2.8  |
| 4   | D     | 107 | GLU  | 2.7  |
| 3   | C     | 125 | SER  | 2.7  |
| 5   | P     | -3  | SER  | 2.7  |
| 1   | A     | 25  | GLU  | 2.7  |
| 4   | H     | 113 | ASN  | 2.7  |
| 3   | C     | 156 | SER  | 2.7  |
| 3   | C     | 1   | ILE  | 2.6  |
| 1   | A     | 12  | VAL  | 2.6  |
| 2   | F     | 22  | SER  | 2.6  |
| 1   | A     | 86  | ALA  | 2.6  |
| 2   | F     | 51  | GLY  | 2.6  |
| 4   | H     | 8   | VAL  | 2.6  |
| 2   | F     | 7   | SER  | 2.6  |
| 1   | A     | 8   | GLN  | 2.6  |
| 2   | B     | 116 | VAL  | 2.6  |
| 2   | F     | 116 | VAL  | 2.6  |
| 1   | E     | 85  | SER  | 2.5  |
| 2   | B     | 7   | SER  | 2.5  |
| 1   | E     | 13  | TRP  | 2.5  |
| 2   | B     | 60  | ILE  | 2.5  |
| 1   | A     | 7   | PRO  | 2.5  |
| 1   | A     | 83  | GLY  | 2.5  |
| 1   | E     | 78  | ALA  | 2.4  |
| 2   | B     | 117 | LEU  | 2.4  |
| 1   | A     | 87  | THR  | 2.4  |
| 1   | E     | 83  | GLY  | 2.4  |
| 1   | A     | 10  | LEU  | 2.4  |
| 1   | A     | 20  | LEU  | 2.3  |
| 4   | D     | 4   | GLU  | 2.3  |
| 1   | E     | 82  | PRO  | 2.3  |
| 2   | F     | 39  | THR  | 2.3  |
| 4   | H     | 2   | ASP  | 2.3  |
| 1   | E     | 12  | VAL  | 2.3  |
| 2   | B     | 13  | ALA  | 2.2  |
| 1   | E     | 113 | GLN  | 2.2  |
| 1   | E     | 73  | LEU  | 2.2  |
| 2   | F     | 108 | PHE  | 2.2  |
| 1   | E     | 39  | PRO  | 2.2  |
| 4   | D     | 8   | VAL  | 2.2  |
| 2   | F     | 97  | ALA  | 2.2  |
| 1   | E     | 110 | THR  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 115 | VAL  | 2.2  |
| 1   | A     | 2   | GLN  | 2.2  |
| 2   | B     | 11  | LYS  | 2.2  |
| 5   | P     | 8   | GLN  | 2.2  |
| 2   | B     | 39  | THR  | 2.2  |
| 2   | F     | 60  | ILE  | 2.2  |
| 1   | A     | 39  | PRO  | 2.2  |
| 1   | A     | 82  | PRO  | 2.2  |
| 1   | E     | 114 | VAL  | 2.1  |
| 2   | B     | 14  | VAL  | 2.1  |
| 1   | A     | 17  | THR  | 2.1  |
| 1   | A     | 73  | LEU  | 2.1  |
| 2   | F     | 9   | ARG  | 2.1  |
| 1   | A     | 116 | PRO  | 2.1  |
| 5   | I     | 7   | SER  | 2.1  |
| 1   | A     | 111 | LYS  | 2.1  |
| 1   | A     | 40  | GLY  | 2.1  |
| 2   | F     | 114 | LEU  | 2.1  |
| 4   | D     | 5   | ARG  | 2.1  |
| 1   | A     | 47  | ILE  | 2.1  |
| 2   | F     | 66  | LYS  | 2.1  |
| 1   | E     | 34  | TRP  | 2.1  |
| 2   | F     | 40  | GLY  | 2.1  |
| 1   | E     | 47  | ILE  | 2.1  |
| 1   | E     | 8   | GLN  | 2.0  |
| 2   | F     | 21  | LEU  | 2.0  |
| 1   | E     | 59  | GLY  | 2.0  |
| 3   | C     | 71  | GLY  | 2.0  |
| 2   | F     | 87  | THR  | 2.0  |
| 4   | D     | 104 | SER  | 2.0  |
| 2   | F     | 106 | GLN  | 2.0  |
| 4   | H     | 23  | ARG  | 2.0  |
| 1   | E     | 84  | ASP  | 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.