



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 4RQP / pdb\_00004rqp  
Title : Crystal structure of the naturally occurring empty particle of a clinical C4 strain EV71  
Authors : Chen, R.; Lyu, K.  
Deposited on : 2014-11-04  
Resolution : 3.15 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                                                             |

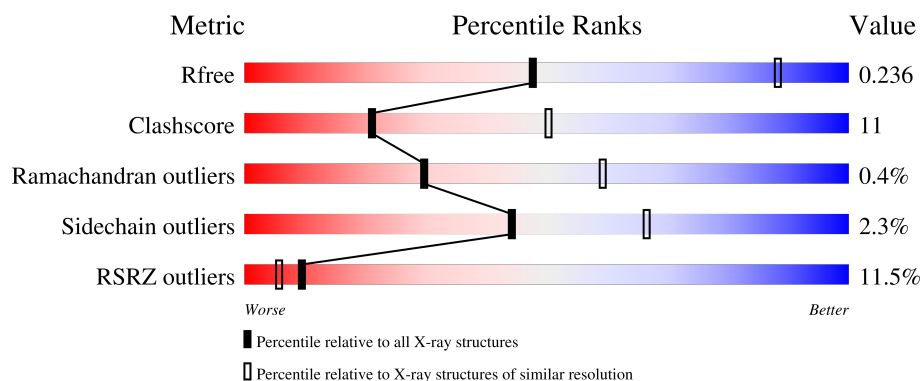
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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                      | 2361 (3.20-3.12)                                      |
| Clashscore            | 190562                      | 2486 (3.20-3.12)                                      |
| Ramachandran outliers | 187476                      | 2405 (3.20-3.12)                                      |
| Sidechain outliers    | 187428                      | 2404 (3.20-3.12)                                      |
| RSRZ outliers         | 180081                      | 2361 (3.20-3.12)                                      |

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     | 297    | <div> <div>8%</div> <div>53% 21% 25%</div> </div> |
| 1   | E     | 297    | <div> <div>7%</div> <div>55% 19% 25%</div> </div> |
| 1   | I     | 297    | <div> <div>9%</div> <div>54% 20% 25%</div> </div> |
| 1   | M     | 297    | <div> <div>7%</div> <div>54% 20% 25%</div> </div> |
| 1   | Q     | 297    | <div> <div>7%</div> <div>55% 17% 25%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B     | 242    |                  |
| 2   | F     | 242    |                  |
| 2   | J     | 242    |                  |
| 2   | N     | 242    |                  |
| 2   | R     | 242    |                  |
| 3   | C     | 323    |                  |
| 3   | G     | 323    |                  |
| 3   | K     | 323    |                  |
| 3   | O     | 323    |                  |
| 3   | S     | 323    |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26615 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 Capsid protein VP1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | E     | 223      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1764  | 1130 | 296 | 327 | 11 |         |         |       |
| 1   | Q     | 223      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1764  | 1130 | 296 | 327 | 11 |         |         |       |
| 1   | I     | 223      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1764  | 1130 | 296 | 327 | 11 |         |         |       |
| 1   | M     | 223      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1764  | 1130 | 296 | 327 | 11 |         |         |       |
| 1   | A     | 223      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1764  | 1130 | 296 | 327 | 11 |         |         |       |

- Molecule 2 is a protein called Capsid protein VP3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | F     | 225      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1718  | 1106 | 281 | 320 | 11 |         |         |       |
| 2   | R     | 225      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1718  | 1106 | 281 | 320 | 11 |         |         |       |
| 2   | J     | 225      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1718  | 1106 | 281 | 320 | 11 |         |         |       |
| 2   | N     | 225      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1718  | 1106 | 281 | 320 | 11 |         |         |       |
| 2   | B     | 225      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1718  | 1106 | 281 | 320 | 11 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| F     | 227     | GLN      | LYS    | engineered mutation | UNP F6KTB0 |
| R     | 227     | GLN      | LYS    | engineered mutation | UNP F6KTB0 |
| J     | 227     | GLN      | LYS    | engineered mutation | UNP F6KTB0 |
| N     | 227     | GLN      | LYS    | engineered mutation | UNP F6KTB0 |
| B     | 227     | GLN      | LYS    | engineered mutation | UNP F6KTB0 |

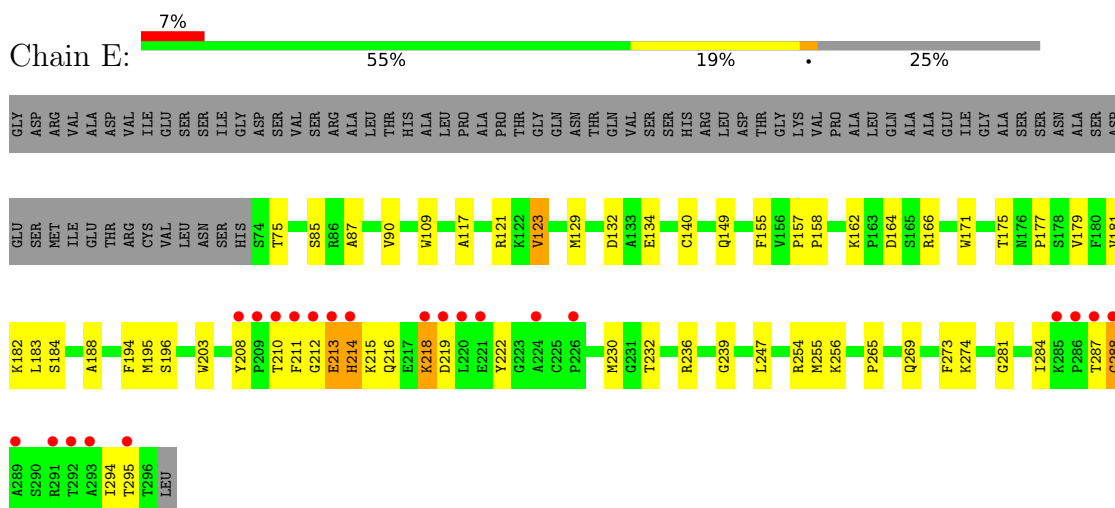
- Molecule 3 is a protein called Capsid protein VP0.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 3   | G     | 238      | Total<br>1841 | C<br>1183 | N<br>303 | O<br>347 | S<br>8 | 0       | 0       | 0     |
| 3   | S     | 238      | Total<br>1841 | C<br>1183 | N<br>303 | O<br>347 | S<br>8 | 0       | 0       | 0     |
| 3   | K     | 238      | Total<br>1841 | C<br>1183 | N<br>303 | O<br>347 | S<br>8 | 0       | 0       | 0     |
| 3   | O     | 238      | Total<br>1841 | C<br>1183 | N<br>303 | O<br>347 | S<br>8 | 0       | 0       | 0     |
| 3   | C     | 238      | Total<br>1841 | C<br>1183 | N<br>303 | O<br>347 | S<br>8 | 0       | 0       | 0     |

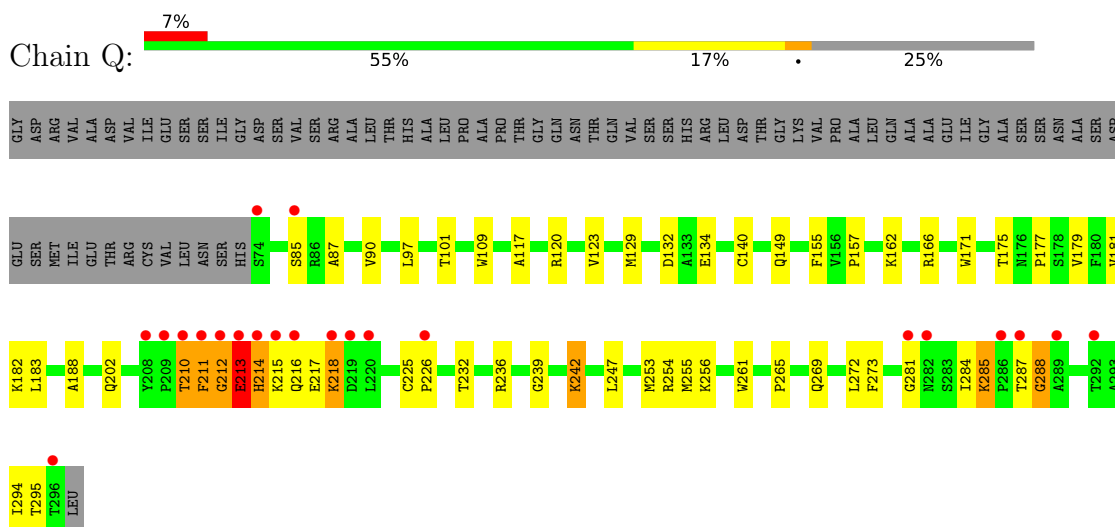
### 3 Residue-property plots [i](#)

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: Capsid protein VP1

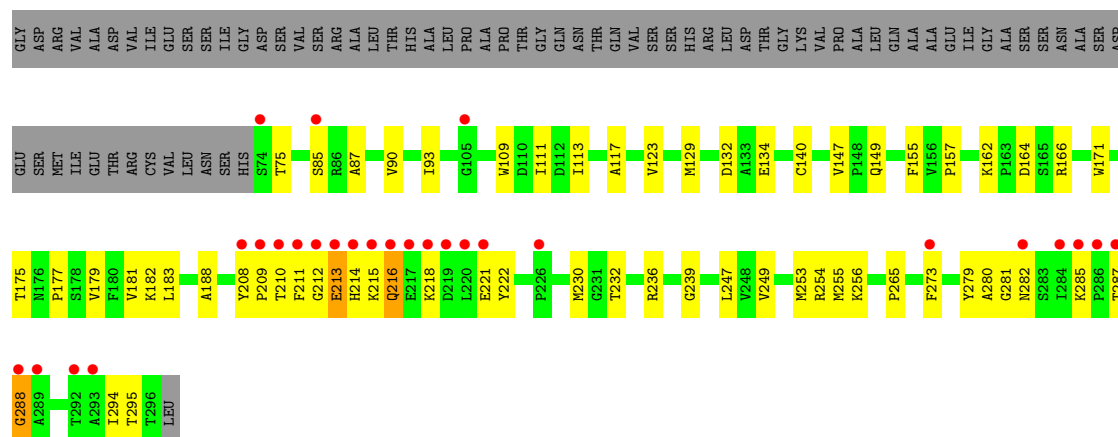


#### • Molecule 1: Capsid protein VP1

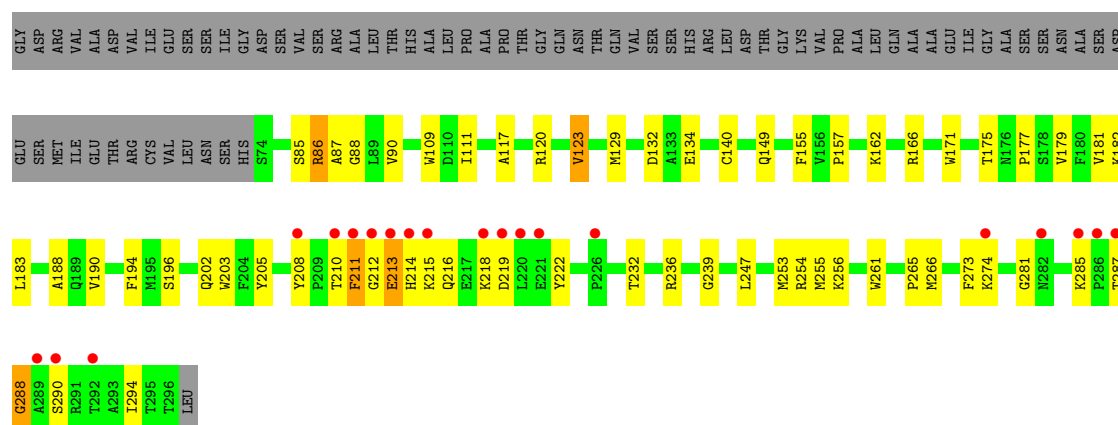


#### • Molecule 1: Capsid protein VP1

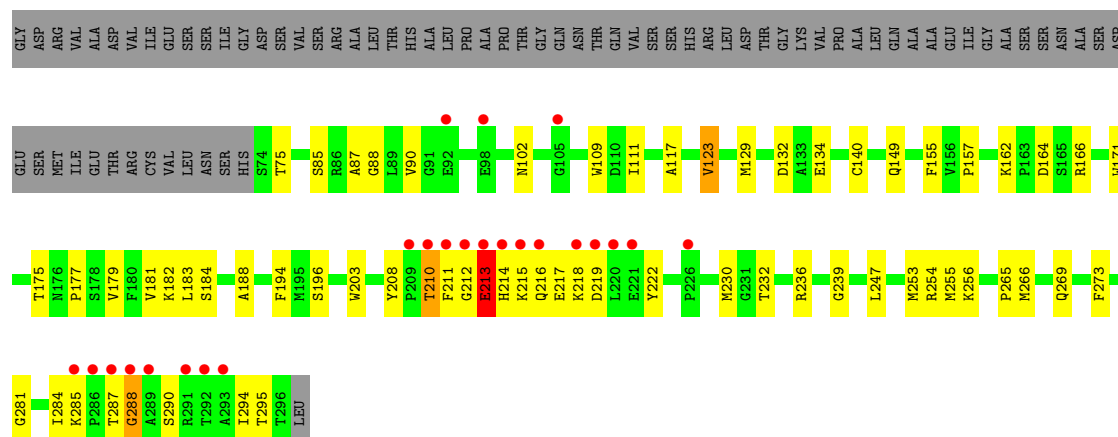




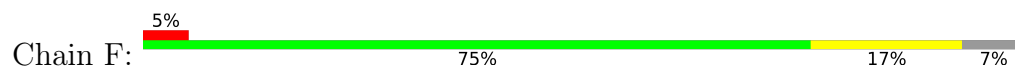
- Molecule 1: Capsid protein VP1

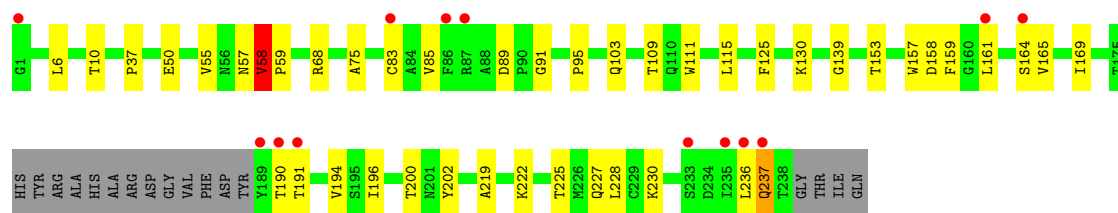


- Molecule 1: Capsid protein VP1

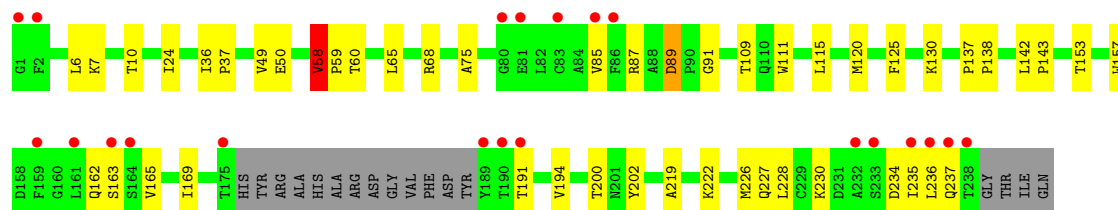
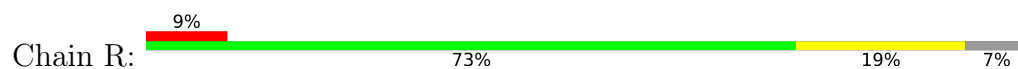


- Molecule 2: Capsid protein VP3

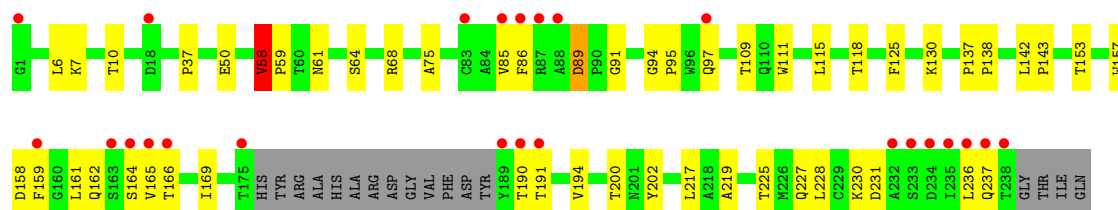




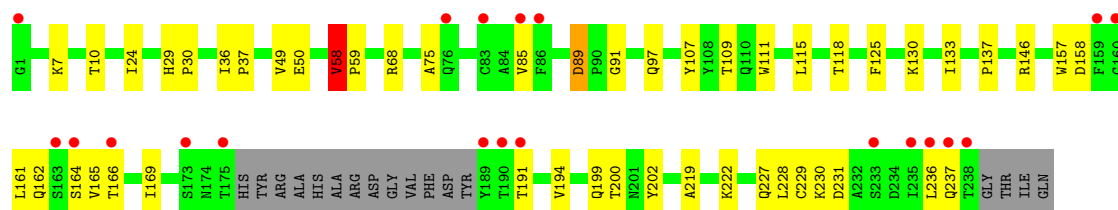
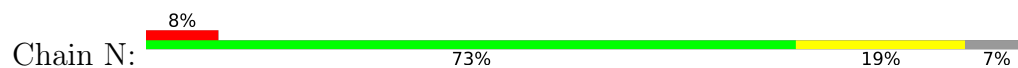
• Molecule 2: Capsid protein VP3



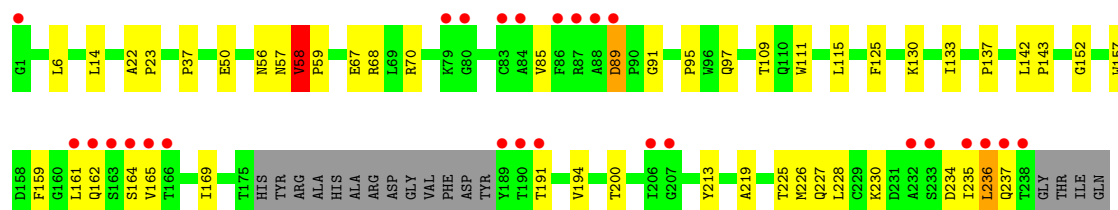
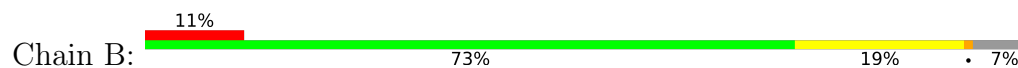
• Molecule 2: Capsid protein VP3



• Molecule 2: Capsid protein VP3

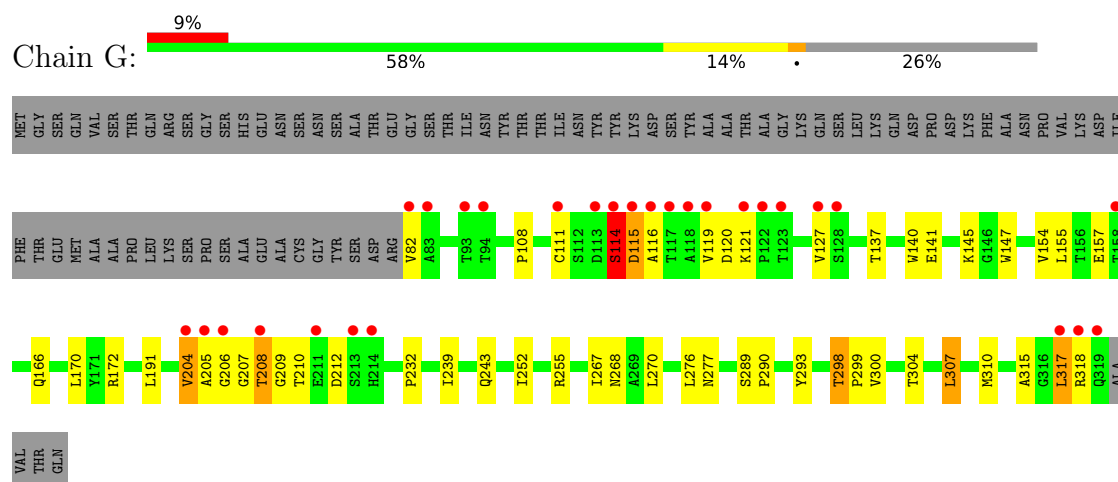


• Molecule 2: Capsid protein VP3

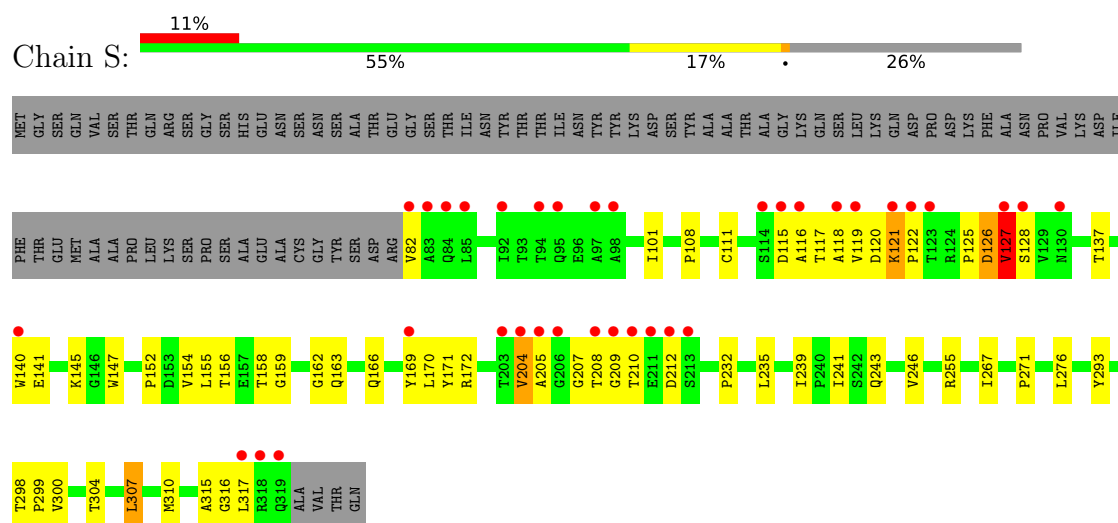




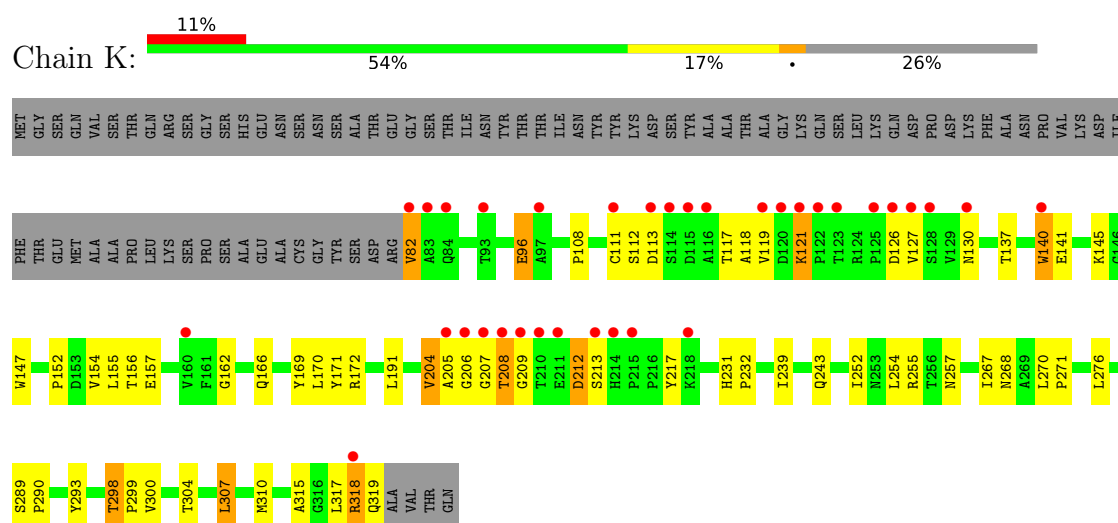
- Molecule 3: Capsid protein VP0



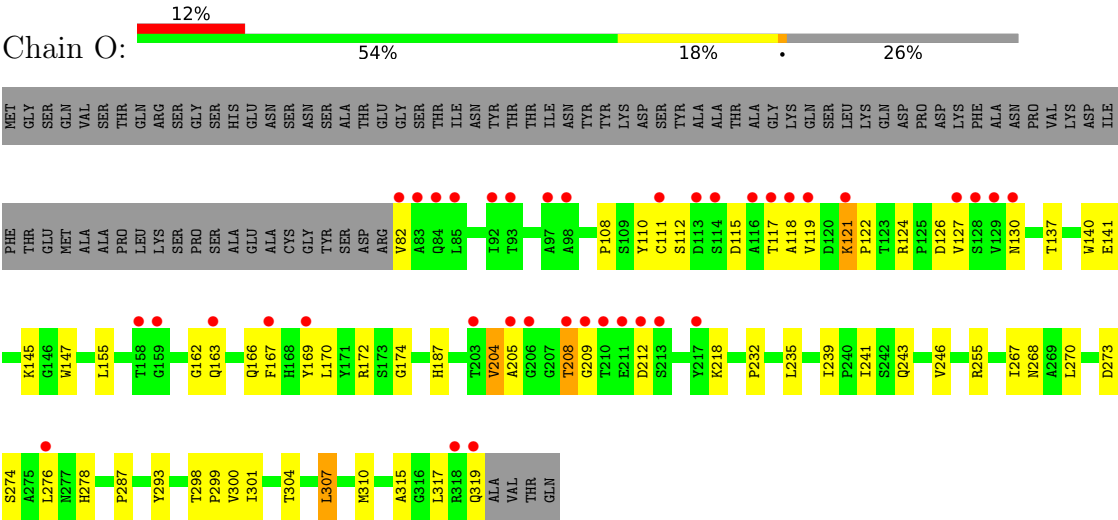
- Molecule 3: Capsid protein VP0



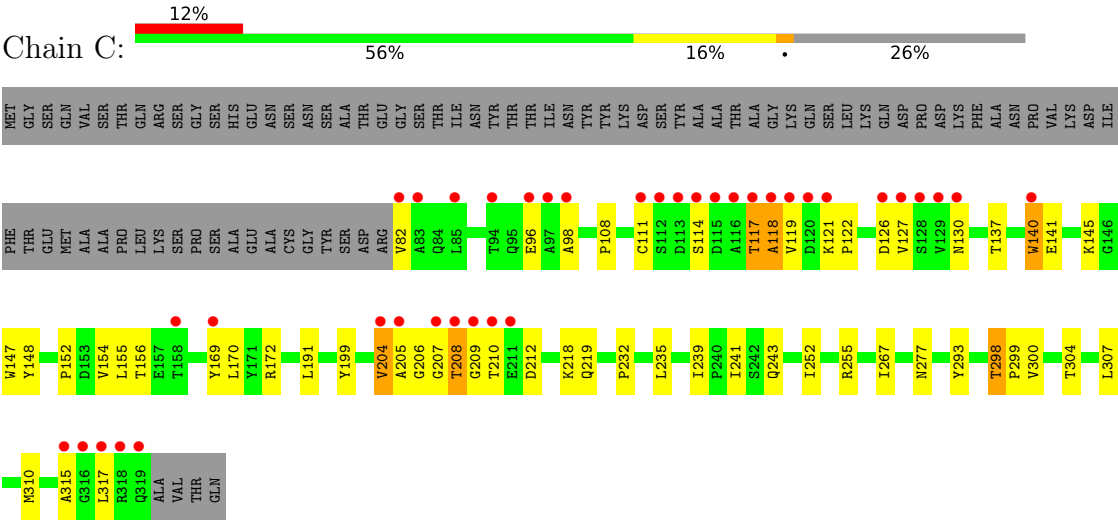
- Molecule 3: Capsid protein VP0



- Molecule 3: Capsid protein VP0



● Molecule 3: Capsid protein VP0



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 4 <sub>2</sub> 3 <sub>2</sub>                             | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 352.98Å 352.98Å 352.98Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.92 – 3.15<br>49.92 – 3.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (49.92-3.15)<br>78.4 (49.92-3.15)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.46 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.216 , 0.234<br>0.215 , 0.236                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (1.55%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 59.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.000                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 20.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 26615                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 55.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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     | 0.41         | 0/1818  | 0.83        | 6/2478 (0.2%)   |
| 1   | E     | 0.40         | 0/1818  | 0.80        | 1/2478 (0.0%)   |
| 1   | I     | 0.42         | 0/1818  | 0.85        | 2/2478 (0.1%)   |
| 1   | M     | 0.38         | 0/1818  | 0.81        | 1/2478 (0.0%)   |
| 1   | Q     | 0.43         | 0/1818  | 0.86        | 6/2478 (0.2%)   |
| 2   | B     | 0.41         | 0/1764  | 0.78        | 4/2415 (0.2%)   |
| 2   | F     | 0.37         | 0/1764  | 0.77        | 2/2415 (0.1%)   |
| 2   | J     | 0.40         | 0/1764  | 0.78        | 6/2415 (0.2%)   |
| 2   | N     | 0.38         | 0/1764  | 0.78        | 4/2415 (0.2%)   |
| 2   | R     | 0.38         | 0/1764  | 0.78        | 4/2415 (0.2%)   |
| 3   | C     | 0.40         | 0/1896  | 0.82        | 4/2602 (0.2%)   |
| 3   | G     | 0.36         | 0/1896  | 0.86        | 7/2602 (0.3%)   |
| 3   | K     | 0.38         | 0/1896  | 0.86        | 7/2602 (0.3%)   |
| 3   | O     | 0.38         | 0/1896  | 0.83        | 3/2602 (0.1%)   |
| 3   | S     | 0.39         | 0/1896  | 0.88        | 7/2602 (0.3%)   |
| All | All   | 0.39         | 0/27390 | 0.82        | 64/37475 (0.2%) |

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   | I     | 0                   | 1                   |
| 3   | G     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | K     | 112 | SER  | N-CA-C | -8.34 | 102.36      | 112.54   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | J     | 58  | VAL  | CA-C-N | -7.08 | 112.64      | 120.14   |
| 2   | J     | 58  | VAL  | C-N-CA | -7.08 | 112.64      | 120.14   |
| 1   | Q     | 211 | PHE  | CA-C-N | 7.04  | 128.40      | 121.57   |
| 1   | Q     | 211 | PHE  | C-N-CA | 7.04  | 128.40      | 121.57   |
| 3   | G     | 115 | ASP  | N-CA-C | 6.90  | 125.50      | 110.80   |
| 2   | F     | 58  | VAL  | CA-C-N | -6.90 | 112.83      | 120.14   |
| 2   | F     | 58  | VAL  | C-N-CA | -6.90 | 112.83      | 120.14   |
| 2   | N     | 58  | VAL  | CA-C-N | -6.88 | 112.85      | 120.14   |
| 2   | N     | 58  | VAL  | C-N-CA | -6.88 | 112.85      | 120.14   |
| 2   | R     | 58  | VAL  | CA-C-N | -6.64 | 113.10      | 120.14   |
| 2   | R     | 58  | VAL  | C-N-CA | -6.64 | 113.10      | 120.14   |
| 1   | M     | 85  | SER  | N-CA-C | 6.62  | 120.22      | 111.75   |
| 1   | I     | 85  | SER  | N-CA-C | 6.31  | 119.83      | 111.75   |
| 2   | B     | 58  | VAL  | CA-C-N | -6.25 | 113.51      | 120.14   |
| 2   | B     | 58  | VAL  | C-N-CA | -6.25 | 113.51      | 120.14   |
| 3   | G     | 298 | THR  | CA-C-N | 6.19  | 125.81      | 119.56   |
| 3   | G     | 298 | THR  | C-N-CA | 6.19  | 125.81      | 119.56   |
| 3   | K     | 212 | ASP  | N-CA-C | 6.13  | 119.70      | 109.95   |
| 3   | G     | 127 | VAL  | N-CA-C | 6.09  | 116.25      | 110.53   |
| 3   | S     | 298 | THR  | CA-C-N | 6.03  | 125.65      | 119.56   |
| 3   | S     | 298 | THR  | C-N-CA | 6.03  | 125.65      | 119.56   |
| 2   | N     | 89  | ASP  | CA-C-N | 6.01  | 125.90      | 119.28   |
| 2   | N     | 89  | ASP  | C-N-CA | 6.01  | 125.90      | 119.28   |
| 3   | S     | 126 | ASP  | N-CA-C | -5.82 | 105.19      | 112.93   |
| 1   | E     | 85  | SER  | N-CA-C | 5.64  | 118.97      | 111.75   |
| 1   | A     | 213 | GLU  | CA-C-N | 5.56  | 131.70      | 121.70   |
| 1   | A     | 213 | GLU  | C-N-CA | 5.56  | 131.70      | 121.70   |
| 2   | B     | 89  | ASP  | CA-C-N | 5.50  | 125.33      | 119.28   |
| 2   | B     | 89  | ASP  | C-N-CA | 5.50  | 125.33      | 119.28   |
| 3   | O     | 121 | LYS  | CA-C-N | 5.43  | 125.19      | 119.76   |
| 3   | O     | 121 | LYS  | C-N-CA | 5.43  | 125.19      | 119.76   |
| 3   | O     | 112 | SER  | N-CA-C | -5.41 | 105.94      | 112.54   |
| 1   | I     | 218 | LYS  | N-CA-C | 5.39  | 116.18      | 108.74   |
| 3   | G     | 114 | SER  | N-CA-C | 5.31  | 118.05      | 110.24   |
| 3   | G     | 121 | LYS  | CA-C-N | 5.30  | 125.06      | 119.76   |
| 3   | G     | 121 | LYS  | C-N-CA | 5.30  | 125.06      | 119.76   |
| 3   | C     | 121 | LYS  | N-CA-C | 5.29  | 116.55      | 109.83   |
| 3   | K     | 298 | THR  | CA-C-N | 5.28  | 124.89      | 119.56   |
| 3   | K     | 298 | THR  | C-N-CA | 5.28  | 124.89      | 119.56   |
| 1   | Q     | 218 | LYS  | N-CA-C | 5.28  | 114.80      | 107.73   |
| 2   | J     | 94  | GLY  | CA-C-N | 5.26  | 126.42      | 119.84   |
| 2   | J     | 94  | GLY  | C-N-CA | 5.26  | 126.42      | 119.84   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Q     | 212 | GLY  | N-CA-C   | -5.26 | 102.31      | 111.62   |
| 1   | A     | 85  | SER  | N-CA-C   | 5.23  | 118.44      | 111.75   |
| 3   | K     | 121 | LYS  | CA-C-N   | 5.20  | 124.96      | 119.76   |
| 3   | K     | 121 | LYS  | C-N-CA   | 5.20  | 124.96      | 119.76   |
| 1   | Q     | 85  | SER  | N-CA-C   | 5.14  | 118.33      | 111.75   |
| 2   | J     | 89  | ASP  | CA-C-N   | 5.14  | 124.93      | 119.28   |
| 2   | J     | 89  | ASP  | C-N-CA   | 5.14  | 124.93      | 119.28   |
| 1   | A     | 210 | THR  | N-CA-C   | -5.11 | 103.66      | 110.55   |
| 1   | Q     | 213 | GLU  | CB-CA-C  | 5.11  | 119.80      | 110.10   |
| 3   | C     | 298 | THR  | CA-C-N   | 5.10  | 124.71      | 119.56   |
| 3   | C     | 298 | THR  | C-N-CA   | 5.10  | 124.71      | 119.56   |
| 3   | S     | 163 | GLN  | CA-CB-CG | -5.09 | 103.91      | 114.10   |
| 1   | A     | 102 | ASN  | CA-C-N   | 5.09  | 124.75      | 119.56   |
| 1   | A     | 102 | ASN  | C-N-CA   | 5.09  | 124.75      | 119.56   |
| 3   | S     | 127 | VAL  | N-CA-C   | 5.07  | 119.89      | 109.34   |
| 3   | C     | 140 | TRP  | CA-CB-CG | 5.07  | 123.23      | 113.60   |
| 3   | K     | 140 | TRP  | CA-CB-CG | 5.05  | 123.20      | 113.60   |
| 3   | S     | 121 | LYS  | CA-C-N   | 5.03  | 124.79      | 119.76   |
| 3   | S     | 121 | LYS  | C-N-CA   | 5.03  | 124.79      | 119.76   |
| 2   | R     | 89  | ASP  | CA-C-N   | 5.03  | 124.81      | 119.28   |
| 2   | R     | 89  | ASP  | C-N-CA   | 5.03  | 124.81      | 119.28   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | G     | 114 | SER  | Peptide |
| 1   | I     | 216 | GLN  | 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     | 1764  | 0        | 1712     | 58      | 0            |
| 1   | E     | 1764  | 0        | 1712     | 50      | 0            |
| 1   | I     | 1764  | 0        | 1712     | 48      | 0            |
| 1   | M     | 1764  | 0        | 1712     | 58      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Q     | 1764  | 0        | 1712     | 58      | 0            |
| 2   | B     | 1718  | 0        | 1707     | 34      | 0            |
| 2   | F     | 1718  | 0        | 1707     | 38      | 0            |
| 2   | J     | 1718  | 0        | 1707     | 38      | 0            |
| 2   | N     | 1718  | 0        | 1707     | 42      | 0            |
| 2   | R     | 1718  | 0        | 1707     | 42      | 0            |
| 3   | C     | 1841  | 0        | 1780     | 43      | 0            |
| 3   | G     | 1841  | 0        | 1780     | 42      | 0            |
| 3   | K     | 1841  | 0        | 1780     | 52      | 0            |
| 3   | O     | 1841  | 0        | 1780     | 46      | 0            |
| 3   | S     | 1841  | 0        | 1780     | 43      | 0            |
| All | All   | 26615 | 0        | 25995    | 576     | 0            |

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

All (576) 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:I:210:THR:HG22 | 1:I:211:PHE:HA   | 1.29                     | 1.15              |
| 1:Q:213:GLU:HB2  | 1:Q:214:HIS:HA   | 1.34                     | 1.05              |
| 1:A:215:LYS:H    | 1:A:216:GLN:HA   | 1.29                     | 0.96              |
| 1:M:86:ARG:NH2   | 2:N:229:CYS:SG   | 2.42                     | 0.92              |
| 1:Q:213:GLU:CB   | 1:Q:214:HIS:HA   | 2.03                     | 0.88              |
| 1:I:287:THR:O    | 2:J:68:ARG:NH2   | 2.11                     | 0.83              |
| 1:I:210:THR:CG2  | 1:I:211:PHE:HA   | 2.09                     | 0.80              |
| 2:N:89:ASP:HB2   | 2:N:191:THR:HG21 | 1.63                     | 0.80              |
| 1:M:181:VAL:HG21 | 1:M:188:ALA:HB2  | 1.64                     | 0.79              |
| 1:M:287:THR:O    | 2:N:68:ARG:NH2   | 2.15                     | 0.79              |
| 3:C:208:THR:OG1  | 3:C:209:GLY:N    | 2.13                     | 0.79              |
| 2:R:89:ASP:HB2   | 2:R:191:THR:HG21 | 1.64                     | 0.79              |
| 1:E:181:VAL:HG21 | 1:E:188:ALA:HB2  | 1.65                     | 0.78              |
| 2:F:89:ASP:HB2   | 2:F:191:THR:HG21 | 1.66                     | 0.78              |
| 3:S:119:VAL:HG13 | 3:S:120:ASP:HB3  | 1.65                     | 0.77              |
| 1:A:181:VAL:HG21 | 1:A:188:ALA:HB2  | 1.67                     | 0.76              |
| 2:B:89:ASP:HB2   | 2:B:191:THR:HG21 | 1.66                     | 0.76              |
| 3:S:208:THR:HG22 | 3:S:209:GLY:N    | 2.00                     | 0.76              |
| 1:E:287:THR:O    | 2:F:68:ARG:NH2   | 2.18                     | 0.76              |
| 1:Q:215:LYS:H    | 1:Q:216:GLN:HA   | 1.52                     | 0.75              |
| 1:A:218:LYS:HG2  | 1:A:219:ASP:H    | 1.51                     | 0.75              |
| 1:A:215:LYS:N    | 1:A:216:GLN:HA   | 1.94                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:181:VAL:HG21 | 1:I:188:ALA:HB2  | 1.67                     | 0.74              |
| 1:Q:210:THR:HG22 | 1:Q:211:PHE:HB3  | 1.68                     | 0.74              |
| 3:K:318:ARG:HG2  | 3:K:319:GLN:N    | 2.01                     | 0.74              |
| 2:J:109:THR:HB   | 2:J:228:LEU:HB3  | 1.69                     | 0.74              |
| 1:A:287:THR:O    | 2:B:68:ARG:NH2   | 2.20                     | 0.74              |
| 1:Q:287:THR:O    | 2:R:68:ARG:NH2   | 2.21                     | 0.73              |
| 1:E:117:ALA:HA   | 2:F:236:LEU:HD22 | 1.70                     | 0.73              |
| 3:G:317:LEU:HB2  | 2:B:137:PRO:HG3  | 1.68                     | 0.73              |
| 1:Q:181:VAL:HG21 | 1:Q:188:ALA:HB2  | 1.69                     | 0.73              |
| 1:E:213:GLU:HB2  | 1:E:214:HIS:HA   | 1.71                     | 0.71              |
| 1:M:215:LYS:H    | 1:M:216:GLN:HA   | 1.53                     | 0.71              |
| 1:A:117:ALA:HA   | 2:B:236:LEU:HD22 | 1.72                     | 0.71              |
| 2:F:109:THR:HB   | 2:F:228:LEU:HB3  | 1.73                     | 0.71              |
| 1:Q:117:ALA:HA   | 2:R:236:LEU:HD22 | 1.71                     | 0.71              |
| 3:G:208:THR:OG1  | 3:G:209:GLY:N    | 2.22                     | 0.70              |
| 2:F:236:LEU:HG   | 2:F:237:GLN:H    | 1.56                     | 0.70              |
| 2:J:236:LEU:HG   | 2:J:237:GLN:H    | 1.57                     | 0.70              |
| 3:G:115:ASP:CG   | 3:G:116:ALA:H    | 1.99                     | 0.70              |
| 1:Q:285:LYS:H    | 1:Q:285:LYS:CD   | 2.03                     | 0.70              |
| 1:M:117:ALA:HA   | 2:N:236:LEU:HD22 | 1.73                     | 0.70              |
| 3:K:140:TRP:HB2  | 3:K:147:TRP:HH2  | 1.57                     | 0.69              |
| 2:R:236:LEU:HG   | 2:R:237:GLN:H    | 1.56                     | 0.69              |
| 3:O:140:TRP:HB2  | 3:O:147:TRP:HH2  | 1.55                     | 0.69              |
| 1:E:216:GLN:HE21 | 3:G:277:ASN:HD21 | 1.40                     | 0.69              |
| 3:G:140:TRP:HB2  | 3:G:147:TRP:HH2  | 1.56                     | 0.69              |
| 2:N:109:THR:HB   | 2:N:228:LEU:HB3  | 1.73                     | 0.69              |
| 3:S:140:TRP:HB2  | 3:S:147:TRP:HH2  | 1.55                     | 0.69              |
| 2:N:236:LEU:HG   | 2:N:237:GLN:H    | 1.56                     | 0.69              |
| 3:G:141:GLU:HG2  | 3:G:300:VAL:HG12 | 1.74                     | 0.68              |
| 1:M:211:PHE:HE1  | 3:O:274:SER:HB2  | 1.57                     | 0.68              |
| 2:J:89:ASP:HB2   | 2:J:191:THR:HG21 | 1.75                     | 0.68              |
| 3:S:126:ASP:OD1  | 3:S:127:VAL:N    | 2.26                     | 0.68              |
| 3:K:141:GLU:HG2  | 3:K:300:VAL:HG12 | 1.74                     | 0.68              |
| 3:C:140:TRP:HB2  | 3:C:147:TRP:HH2  | 1.56                     | 0.68              |
| 1:I:117:ALA:HA   | 2:J:236:LEU:HD22 | 1.76                     | 0.68              |
| 2:B:85:VAL:HB    | 2:B:194:VAL:HB   | 1.75                     | 0.67              |
| 3:K:208:THR:OG1  | 3:K:209:GLY:N    | 2.27                     | 0.67              |
| 2:R:109:THR:HB   | 2:R:228:LEU:HB3  | 1.76                     | 0.67              |
| 2:J:37:PRO:HG2   | 3:K:267:ILE:HG12 | 1.77                     | 0.67              |
| 1:A:210:THR:OG1  | 1:A:211:PHE:HA   | 1.94                     | 0.67              |
| 1:A:213:GLU:HG3  | 1:A:215:LYS:N    | 2.10                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:141:GLU:HG2  | 3:S:300:VAL:HG12 | 1.76                     | 0.66              |
| 2:R:37:PRO:HG2   | 3:S:267:ILE:HG12 | 1.77                     | 0.66              |
| 1:E:213:GLU:HB2  | 1:E:214:HIS:CA   | 2.28                     | 0.64              |
| 2:B:37:PRO:HG2   | 3:C:267:ILE:HG12 | 1.79                     | 0.64              |
| 1:M:213:GLU:HB2  | 1:M:214:HIS:CA   | 2.29                     | 0.63              |
| 1:Q:210:THR:HG22 | 1:Q:211:PHE:CB   | 2.28                     | 0.63              |
| 3:C:141:GLU:HG2  | 3:C:300:VAL:HG12 | 1.80                     | 0.62              |
| 1:I:265:PRO:HG2  | 3:K:239:ILE:HD12 | 1.81                     | 0.62              |
| 2:N:85:VAL:HB    | 2:N:194:VAL:HB   | 1.80                     | 0.62              |
| 1:E:162:LYS:HD3  | 1:E:232:THR:HG21 | 1.81                     | 0.62              |
| 2:F:236:LEU:HG   | 2:F:237:GLN:HG3  | 1.82                     | 0.62              |
| 2:J:161:LEU:HD23 | 2:J:164:SER:HB2  | 1.82                     | 0.62              |
| 1:A:273:PHE:CE2  | 3:C:212:ASP:HB3  | 2.35                     | 0.61              |
| 1:E:215:LYS:H    | 1:E:216:GLN:HA   | 1.65                     | 0.61              |
| 1:A:162:LYS:HD3  | 1:A:232:THR:HG21 | 1.81                     | 0.61              |
| 2:F:75:ALA:HA    | 2:F:202:TYR:HB3  | 1.83                     | 0.61              |
| 1:M:134:GLU:HB2  | 1:M:256:LYS:HE3  | 1.81                     | 0.61              |
| 1:M:213:GLU:HB2  | 1:M:214:HIS:C    | 2.26                     | 0.61              |
| 2:R:130:LYS:HB2  | 2:R:200:THR:HG23 | 1.82                     | 0.61              |
| 1:E:132:ASP:HB2  | 1:E:256:LYS:HB2  | 1.83                     | 0.61              |
| 1:M:202:GLN:NE2  | 1:M:205:TYR:HD1  | 1.98                     | 0.61              |
| 2:F:236:LEU:HG   | 2:F:237:GLN:CG   | 2.31                     | 0.60              |
| 1:Q:162:LYS:HD3  | 1:Q:232:THR:HG21 | 1.82                     | 0.60              |
| 1:M:162:LYS:HD3  | 1:M:232:THR:HG21 | 1.83                     | 0.60              |
| 2:R:137:PRO:HD3  | 3:K:317:LEU:HD22 | 1.83                     | 0.60              |
| 1:E:210:THR:HB   | 1:E:211:PHE:HA   | 1.83                     | 0.60              |
| 1:E:218:LYS:HG3  | 1:E:219:ASP:H    | 1.66                     | 0.60              |
| 1:A:216:GLN:HG2  | 1:A:217:GLU:H    | 1.67                     | 0.60              |
| 2:B:50:GLU:HA    | 2:B:219:ALA:HB2  | 1.84                     | 0.60              |
| 2:B:109:THR:HB   | 2:B:228:LEU:HB3  | 1.83                     | 0.60              |
| 2:B:236:LEU:HG   | 2:B:237:GLN:H    | 1.65                     | 0.60              |
| 1:I:213:GLU:HB2  | 1:I:214:HIS:C    | 2.27                     | 0.59              |
| 1:Q:269:GLN:NE2  | 1:Q:284:ILE:O    | 2.33                     | 0.59              |
| 3:K:204:VAL:HG12 | 3:K:206:GLY:H    | 1.68                     | 0.59              |
| 3:G:115:ASP:CG   | 3:G:116:ALA:N    | 2.60                     | 0.59              |
| 1:I:166:ARG:NH2  | 1:I:239:GLY:O    | 2.34                     | 0.59              |
| 1:I:281:GLY:N    | 3:K:204:VAL:HG11 | 2.18                     | 0.59              |
| 2:R:115:LEU:HB2  | 2:R:169:ILE:HB   | 1.84                     | 0.59              |
| 1:A:273:PHE:CZ   | 3:C:212:ASP:HB3  | 2.38                     | 0.59              |
| 1:Q:217:GLU:O    | 1:Q:218:LYS:HG3  | 2.02                     | 0.59              |
| 1:I:213:GLU:HB2  | 1:I:214:HIS:CA   | 2.33                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:82:VAL:N     | 3:K:96:GLU:OE2   | 2.35                     | 0.59              |
| 3:O:208:THR:OG1  | 3:O:209:GLY:N    | 2.35                     | 0.59              |
| 2:F:10:THR:HG23  | 2:B:6:LEU:H      | 1.68                     | 0.58              |
| 2:N:50:GLU:HA    | 2:N:219:ALA:HB2  | 1.85                     | 0.58              |
| 1:E:281:GLY:N    | 3:G:204:VAL:HG11 | 2.18                     | 0.58              |
| 1:I:281:GLY:H    | 3:K:204:VAL:HG11 | 1.69                     | 0.58              |
| 1:M:166:ARG:NH2  | 1:M:239:GLY:O    | 2.37                     | 0.58              |
| 1:E:265:PRO:HG2  | 3:G:239:ILE:HD12 | 1.86                     | 0.57              |
| 1:Q:213:GLU:HB2  | 1:Q:214:HIS:CA   | 2.23                     | 0.57              |
| 1:A:265:PRO:HB3  | 3:C:243:GLN:HB2  | 1.86                     | 0.57              |
| 2:N:7:LYS:O      | 2:N:10:THR:OG1   | 2.21                     | 0.57              |
| 2:N:161:LEU:HD13 | 2:N:164:SER:HB2  | 1.86                     | 0.57              |
| 3:K:108:PRO:HG2  | 3:K:310:MET:HG3  | 1.86                     | 0.57              |
| 1:M:211:PHE:CE1  | 3:O:274:SER:HB2  | 2.38                     | 0.57              |
| 2:F:139:GLY:HA2  | 1:Q:211:PHE:HE1  | 1.67                     | 0.57              |
| 1:A:213:GLU:HG3  | 1:A:214:HIS:C    | 2.29                     | 0.57              |
| 1:Q:273:PHE:CZ   | 3:S:212:ASP:HB3  | 2.39                     | 0.57              |
| 2:B:115:LEU:HB2  | 2:B:169:ILE:HB   | 1.87                     | 0.57              |
| 2:J:137:PRO:HD3  | 3:O:317:LEU:HD22 | 1.85                     | 0.57              |
| 2:R:85:VAL:HB    | 2:R:194:VAL:HB   | 1.87                     | 0.57              |
| 1:E:273:PHE:CE2  | 3:G:212:ASP:HB3  | 2.40                     | 0.56              |
| 2:J:85:VAL:HB    | 2:J:194:VAL:HB   | 1.86                     | 0.56              |
| 1:E:166:ARG:NH2  | 1:E:239:GLY:O    | 2.38                     | 0.56              |
| 1:E:273:PHE:CZ   | 3:G:212:ASP:HB3  | 2.40                     | 0.56              |
| 2:F:85:VAL:HB    | 2:F:194:VAL:HB   | 1.86                     | 0.56              |
| 2:F:190:THR:HB   | 1:Q:211:PHE:CZ   | 2.40                     | 0.56              |
| 2:J:91:GLY:HA3   | 2:J:111:TRP:CZ2  | 2.41                     | 0.56              |
| 3:S:145:LYS:HB3  | 3:S:232:PRO:HG3  | 1.87                     | 0.56              |
| 2:F:115:LEU:HB2  | 2:F:169:ILE:HB   | 1.87                     | 0.56              |
| 1:A:281:GLY:N    | 3:C:204:VAL:HG11 | 2.21                     | 0.56              |
| 2:N:137:PRO:HG3  | 3:C:317:LEU:HB2  | 1.88                     | 0.56              |
| 1:A:166:ARG:NH2  | 1:A:239:GLY:O    | 2.39                     | 0.56              |
| 3:O:141:GLU:HG2  | 3:O:300:VAL:HG12 | 1.87                     | 0.56              |
| 3:C:126:ASP:OD1  | 3:C:127:VAL:N    | 2.38                     | 0.56              |
| 1:I:294:ILE:HG13 | 1:I:295:THR:HG23 | 1.87                     | 0.55              |
| 2:J:50:GLU:HA    | 2:J:219:ALA:HB2  | 1.87                     | 0.55              |
| 1:Q:285:LYS:H    | 1:Q:285:LYS:HD2  | 1.69                     | 0.55              |
| 2:N:130:LYS:HB2  | 2:N:200:THR:HG23 | 1.87                     | 0.55              |
| 3:O:108:PRO:HG2  | 3:O:310:MET:HG3  | 1.87                     | 0.55              |
| 1:I:287:THR:OG1  | 1:I:288:GLY:N    | 2.39                     | 0.55              |
| 2:R:75:ALA:HA    | 2:R:202:TYR:HB3  | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:108:PRO:HG2  | 3:S:310:MET:HG3  | 1.89                     | 0.55              |
| 3:O:126:ASP:OD1  | 3:O:127:VAL:N    | 2.40                     | 0.54              |
| 3:K:145:LYS:HB3  | 3:K:232:PRO:HG3  | 1.90                     | 0.54              |
| 2:J:130:LYS:HB2  | 2:J:200:THR:HG23 | 1.89                     | 0.54              |
| 3:C:108:PRO:HG2  | 3:C:310:MET:HG3  | 1.88                     | 0.54              |
| 1:I:140:CYS:HA   | 1:I:183:LEU:HD21 | 1.90                     | 0.54              |
| 2:B:157:TRP:CG   | 2:B:165:VAL:HG21 | 2.42                     | 0.54              |
| 1:Q:211:PHE:HD1  | 1:Q:212:GLY:O    | 1.89                     | 0.54              |
| 1:M:287:THR:OG1  | 1:M:288:GLY:N    | 2.41                     | 0.54              |
| 1:A:140:CYS:HA   | 1:A:183:LEU:HD21 | 1.89                     | 0.54              |
| 2:R:143:PRO:HB3  | 3:K:318:ARG:NH2  | 2.23                     | 0.54              |
| 2:J:125:PHE:HA   | 3:K:255:ARG:HG3  | 1.90                     | 0.54              |
| 1:Q:273:PHE:CE2  | 3:S:212:ASP:HB3  | 2.43                     | 0.54              |
| 1:E:149:GLN:HG2  | 1:E:247:LEU:HD11 | 1.88                     | 0.54              |
| 1:M:213:GLU:HB2  | 1:M:214:HIS:HA   | 1.90                     | 0.54              |
| 1:A:166:ARG:HG2  | 1:A:236:ARG:HH21 | 1.72                     | 0.53              |
| 2:R:6:LEU:H      | 2:J:10:THR:HG23  | 1.73                     | 0.53              |
| 2:F:37:PRO:HG2   | 3:G:267:ILE:HG12 | 1.89                     | 0.53              |
| 2:R:143:PRO:HB3  | 3:K:318:ARG:HH22 | 1.74                     | 0.53              |
| 1:E:182:LYS:HE2  | 1:A:184:SER:O    | 2.09                     | 0.53              |
| 1:M:90:VAL:HG21  | 1:M:253:MET:HB3  | 1.89                     | 0.53              |
| 1:A:265:PRO:HG2  | 3:C:239:ILE:HD12 | 1.91                     | 0.53              |
| 3:C:191:LEU:HB2  | 3:C:252:ILE:HB   | 1.91                     | 0.53              |
| 1:E:117:ALA:O    | 2:F:236:LEU:HD13 | 2.08                     | 0.53              |
| 1:Q:285:LYS:HE2  | 2:R:60:THR:O     | 2.09                     | 0.53              |
| 2:R:222:LYS:H    | 2:R:222:LYS:HD2  | 1.73                     | 0.53              |
| 3:G:204:VAL:HG12 | 3:G:206:GLY:H    | 1.73                     | 0.52              |
| 3:O:166:GLN:HG3  | 3:O:276:LEU:HD21 | 1.90                     | 0.52              |
| 3:O:140:TRP:HB2  | 3:O:147:TRP:CH2  | 2.42                     | 0.52              |
| 1:Q:294:ILE:HG13 | 1:Q:295:THR:HG23 | 1.90                     | 0.52              |
| 1:I:162:LYS:HD3  | 1:I:232:THR:HG21 | 1.91                     | 0.52              |
| 1:A:287:THR:OG1  | 1:A:288:GLY:N    | 2.40                     | 0.52              |
| 1:Q:90:VAL:HG12  | 1:Q:109:TRP:CZ2  | 2.45                     | 0.52              |
| 2:B:125:PHE:HA   | 3:C:255:ARG:HG3  | 1.90                     | 0.52              |
| 2:R:50:GLU:HA    | 2:R:219:ALA:HB2  | 1.90                     | 0.52              |
| 2:R:125:PHE:HA   | 3:S:255:ARG:HG3  | 1.92                     | 0.52              |
| 2:N:125:PHE:HA   | 3:O:255:ARG:HG3  | 1.90                     | 0.52              |
| 2:F:222:LYS:H    | 2:F:222:LYS:HD2  | 1.74                     | 0.52              |
| 1:M:273:PHE:CZ   | 3:O:212:ASP:HB3  | 2.44                     | 0.52              |
| 3:K:126:ASP:O    | 3:K:130:ASN:HB2  | 2.10                     | 0.52              |
| 2:J:75:ALA:HA    | 2:J:202:TYR:HB3  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:115:LEU:HB2  | 2:J:169:ILE:HB   | 1.92                     | 0.52              |
| 1:Q:287:THR:OG1  | 1:Q:288:GLY:N    | 2.43                     | 0.51              |
| 1:M:265:PRO:HB3  | 3:O:243:GLN:HB2  | 1.91                     | 0.51              |
| 2:R:120:MET:HA   | 2:R:163:SER:HB2  | 1.93                     | 0.51              |
| 2:R:91:GLY:HA3   | 2:R:111:TRP:CZ2  | 2.44                     | 0.51              |
| 2:F:190:THR:O    | 1:Q:211:PHE:HE2  | 1.93                     | 0.51              |
| 2:F:6:LEU:H      | 2:R:10:THR:HG23  | 1.75                     | 0.51              |
| 1:M:86:ARG:HE    | 1:A:175:THR:HG22 | 1.74                     | 0.51              |
| 1:M:273:PHE:CE2  | 3:O:212:ASP:HB3  | 2.46                     | 0.51              |
| 3:K:204:VAL:HG12 | 3:K:205:ALA:H    | 1.75                     | 0.51              |
| 1:M:149:GLN:HG2  | 1:M:247:LEU:HD11 | 1.93                     | 0.51              |
| 1:I:90:VAL:HG12  | 1:I:109:TRP:CZ2  | 2.45                     | 0.51              |
| 2:F:50:GLU:HA    | 2:F:219:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:181:VAL:HG12 | 1:A:182:LYS:O    | 2.11                     | 0.51              |
| 3:S:170:LEU:HB2  | 3:S:315:ALA:HB3  | 1.93                     | 0.51              |
| 3:C:111:CYS:SG   | 3:C:172:ARG:HD3  | 2.50                     | 0.51              |
| 3:C:218:LYS:HD3  | 3:C:218:LYS:N    | 2.25                     | 0.51              |
| 1:Q:272:LEU:HD22 | 3:S:208:THR:HG21 | 1.93                     | 0.51              |
| 2:N:91:GLY:HA3   | 2:N:111:TRP:CZ2  | 2.46                     | 0.51              |
| 2:N:222:LYS:H    | 2:N:222:LYS:HD2  | 1.75                     | 0.51              |
| 1:M:194:PHE:CZ   | 1:M:196:SER:HB3  | 2.46                     | 0.51              |
| 3:S:117:THR:HG22 | 3:S:121:LYS:HG2  | 1.93                     | 0.51              |
| 1:I:215:LYS:HB3  | 1:I:216:GLN:O    | 2.11                     | 0.51              |
| 1:Q:281:GLY:N    | 3:S:204:VAL:HG11 | 2.26                     | 0.50              |
| 2:F:58:VAL:HG22  | 2:F:59:PRO:HD3   | 1.93                     | 0.50              |
| 2:F:130:LYS:HB2  | 2:F:200:THR:HG23 | 1.92                     | 0.50              |
| 3:G:108:PRO:HG2  | 3:G:310:MET:HG3  | 1.92                     | 0.50              |
| 2:N:75:ALA:HA    | 2:N:202:TYR:HB3  | 1.92                     | 0.50              |
| 3:S:127:VAL:HG23 | 3:S:128:SER:H    | 1.76                     | 0.50              |
| 1:A:269:GLN:NE2  | 1:A:284:ILE:O    | 2.41                     | 0.50              |
| 1:A:213:GLU:OE1  | 3:C:277:ASN:ND2  | 2.43                     | 0.50              |
| 1:Q:129:MET:HE1  | 1:Q:255:MET:HE1  | 1.94                     | 0.50              |
| 2:B:130:LYS:HB2  | 2:B:200:THR:HG23 | 1.93                     | 0.50              |
| 1:I:129:MET:HE1  | 1:I:255:MET:HE1  | 1.94                     | 0.50              |
| 2:J:153:THR:H    | 3:O:317:LEU:CD2  | 2.24                     | 0.50              |
| 1:I:273:PHE:CE2  | 3:K:212:ASP:HB3  | 2.46                     | 0.50              |
| 2:N:130:LYS:NZ   | 2:N:158:ASP:OD2  | 2.38                     | 0.50              |
| 3:O:163:GLN:OE1  | 3:O:167:PHE:HE2  | 1.94                     | 0.50              |
| 1:Q:179:VAL:HG12 | 1:Q:181:VAL:HG23 | 1.94                     | 0.50              |
| 2:J:7:LYS:O      | 2:J:10:THR:OG1   | 2.23                     | 0.50              |
| 2:J:58:VAL:HG22  | 2:J:59:PRO:HD3   | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:140:CYS:HA   | 1:E:183:LEU:HD21 | 1.94                     | 0.49              |
| 3:G:293:TYR:CZ   | 3:G:299:PRO:HA   | 2.47                     | 0.49              |
| 3:C:152:PRO:O    | 3:C:156:THR:HG23 | 2.11                     | 0.49              |
| 1:I:90:VAL:HG21  | 1:I:253:MET:HB3  | 1.93                     | 0.49              |
| 2:J:118:THR:HG23 | 2:J:217:LEU:HB2  | 1.93                     | 0.49              |
| 1:Q:90:VAL:HG12  | 1:Q:109:TRP:HZ2  | 1.78                     | 0.49              |
| 1:M:177:PRO:HB2  | 2:N:24:ILE:HG12  | 1.93                     | 0.49              |
| 1:A:132:ASP:HB2  | 1:A:256:LYS:HB2  | 1.93                     | 0.49              |
| 2:N:37:PRO:HG2   | 3:O:267:ILE:HG12 | 1.95                     | 0.49              |
| 1:Q:215:LYS:HB3  | 1:Q:216:GLN:O    | 2.12                     | 0.49              |
| 2:F:59:PRO:HD2   | 2:F:68:ARG:HG2   | 1.95                     | 0.49              |
| 1:Q:149:GLN:HG2  | 1:Q:247:LEU:HD11 | 1.95                     | 0.49              |
| 2:F:125:PHE:HA   | 3:G:255:ARG:HG3  | 1.94                     | 0.49              |
| 2:B:111:TRP:HB3  | 2:B:226:MET:HG2  | 1.95                     | 0.49              |
| 2:F:157:TRP:CG   | 2:F:165:VAL:HG21 | 2.48                     | 0.48              |
| 1:I:216:GLN:HG2  | 3:K:217:TYR:OH   | 2.13                     | 0.48              |
| 2:R:137:PRO:HG3  | 3:K:317:LEU:HB2  | 1.95                     | 0.48              |
| 2:R:142:LEU:HD12 | 2:R:143:PRO:HD2  | 1.93                     | 0.48              |
| 3:K:126:ASP:OD1  | 3:K:127:VAL:N    | 2.44                     | 0.48              |
| 3:C:204:VAL:HG12 | 3:C:205:ALA:H    | 1.77                     | 0.48              |
| 1:E:265:PRO:HB3  | 3:G:243:GLN:HB2  | 1.93                     | 0.48              |
| 1:E:129:MET:HE1  | 1:E:255:MET:HE1  | 1.94                     | 0.48              |
| 2:N:133:ILE:HD12 | 2:N:165:VAL:HG11 | 1.95                     | 0.48              |
| 3:K:117:THR:HG22 | 3:K:121:LYS:HG2  | 1.96                     | 0.48              |
| 3:C:235:LEU:HD21 | 3:C:241:ILE:HG13 | 1.95                     | 0.48              |
| 2:F:91:GLY:HA3   | 2:F:111:TRP:CZ2  | 2.48                     | 0.48              |
| 1:Q:181:VAL:HG12 | 1:Q:182:LYS:O    | 2.14                     | 0.48              |
| 3:S:207:GLY:HA2  | 3:S:208:THR:OG1  | 2.14                     | 0.48              |
| 1:M:215:LYS:N    | 1:M:216:GLN:HA   | 2.22                     | 0.48              |
| 1:M:285:LYS:HD2  | 1:M:287:THR:O    | 2.13                     | 0.48              |
| 2:B:58:VAL:HG22  | 2:B:59:PRO:HD3   | 1.96                     | 0.48              |
| 3:O:162:GLY:O    | 3:O:166:GLN:HB2  | 2.14                     | 0.48              |
| 3:C:204:VAL:HG12 | 3:C:206:GLY:H    | 1.77                     | 0.48              |
| 1:E:134:GLU:HB2  | 1:E:256:LYS:HE3  | 1.96                     | 0.48              |
| 1:Q:272:LEU:HD13 | 3:S:208:THR:HG21 | 1.95                     | 0.48              |
| 3:K:140:TRP:HB2  | 3:K:147:TRP:CH2  | 2.42                     | 0.48              |
| 1:E:87:ALA:HB2   | 1:E:254:ARG:HB2  | 1.96                     | 0.48              |
| 1:M:281:GLY:N    | 3:O:204:VAL:HG11 | 2.28                     | 0.48              |
| 2:J:6:LEU:H      | 2:N:10:THR:HG23  | 1.78                     | 0.48              |
| 3:S:204:VAL:HG12 | 3:S:205:ALA:H    | 1.78                     | 0.48              |
| 3:K:166:GLN:HG3  | 3:K:276:LEU:HD21 | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:145:LYS:HB3  | 3:G:232:PRO:HG3  | 1.96                     | 0.48              |
| 3:G:204:VAL:HG12 | 3:G:205:ALA:H    | 1.78                     | 0.48              |
| 1:A:230:MET:HE3  | 1:A:230:MET:HB2  | 1.74                     | 0.48              |
| 3:C:126:ASP:O    | 3:C:130:ASN:HB2  | 2.13                     | 0.48              |
| 2:F:153:THR:H    | 3:S:317:LEU:CD1  | 2.26                     | 0.47              |
| 1:Q:175:THR:O    | 1:Q:177:PRO:HD3  | 2.14                     | 0.47              |
| 1:Q:265:PRO:HB3  | 3:S:243:GLN:HB2  | 1.95                     | 0.47              |
| 2:N:58:VAL:HG22  | 2:N:59:PRO:HD3   | 1.96                     | 0.47              |
| 3:S:293:TYR:CZ   | 3:S:299:PRO:HA   | 2.49                     | 0.47              |
| 3:K:204:VAL:HG12 | 3:K:205:ALA:N    | 2.29                     | 0.47              |
| 3:O:204:VAL:HG12 | 3:O:205:ALA:H    | 1.78                     | 0.47              |
| 1:Q:87:ALA:HB2   | 1:Q:254:ARG:HB2  | 1.95                     | 0.47              |
| 1:M:265:PRO:HG2  | 3:O:239:ILE:HD12 | 1.97                     | 0.47              |
| 1:M:132:ASP:HB2  | 1:M:256:LYS:HB2  | 1.96                     | 0.47              |
| 1:A:90:VAL:HG21  | 1:A:253:MET:HB3  | 1.97                     | 0.47              |
| 2:N:137:PRO:HD3  | 3:C:317:LEU:HD22 | 1.95                     | 0.47              |
| 1:E:179:VAL:HG12 | 1:E:181:VAL:HG23 | 1.96                     | 0.47              |
| 3:G:154:VAL:HG13 | 3:G:155:LEU:HG   | 1.95                     | 0.47              |
| 3:G:207:GLY:HA2  | 3:G:208:THR:HA   | 1.69                     | 0.47              |
| 1:I:213:GLU:HB2  | 1:I:214:HIS:HA   | 1.96                     | 0.47              |
| 2:R:59:PRO:HD2   | 2:R:68:ARG:HG2   | 1.97                     | 0.47              |
| 2:N:115:LEU:HB2  | 2:N:169:ILE:HB   | 1.97                     | 0.47              |
| 3:O:117:THR:HG22 | 3:O:121:LYS:HG2  | 1.96                     | 0.47              |
| 3:C:207:GLY:HA2  | 3:C:208:THR:HA   | 1.63                     | 0.47              |
| 1:A:117:ALA:O    | 2:B:236:LEU:HD13 | 2.14                     | 0.47              |
| 2:R:153:THR:H    | 3:K:317:LEU:CD2  | 2.28                     | 0.47              |
| 2:J:157:TRP:CG   | 2:J:165:VAL:HG21 | 2.49                     | 0.47              |
| 3:O:169:TYR:CD2  | 3:O:170:LEU:HG   | 2.49                     | 0.47              |
| 1:E:294:ILE:HG13 | 1:E:295:THR:HG23 | 1.97                     | 0.47              |
| 2:B:161:LEU:HD13 | 2:B:164:SER:HB2  | 1.96                     | 0.47              |
| 3:S:156:THR:HA   | 3:S:162:GLY:HA2  | 1.95                     | 0.47              |
| 3:K:111:CYS:SG   | 3:K:172:ARG:HD3  | 2.54                     | 0.47              |
| 1:E:90:VAL:HG12  | 1:E:109:TRP:CZ2  | 2.50                     | 0.47              |
| 1:I:208:TYR:CE2  | 1:I:222:TYR:HB2  | 2.50                     | 0.47              |
| 1:M:166:ARG:HG2  | 1:M:236:ARG:HH21 | 1.78                     | 0.47              |
| 1:A:212:GLY:HA2  | 1:A:213:GLU:HA   | 1.47                     | 0.47              |
| 3:C:122:PRO:HB3  | 3:C:315:ALA:HB2  | 1.96                     | 0.47              |
| 1:Q:212:GLY:HA2  | 1:Q:213:GLU:O    | 2.15                     | 0.47              |
| 1:A:294:ILE:HG13 | 1:A:295:THR:HG23 | 1.96                     | 0.47              |
| 3:K:191:LEU:HB2  | 3:K:252:ILE:HB   | 1.97                     | 0.47              |
| 3:G:114:SER:HG   | 3:G:115:ASP:CG   | 2.23                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:218:LYS:CG   | 1:E:219:ASP:H    | 2.29                     | 0.46              |
| 3:G:209:GLY:HA3  | 3:G:210:THR:HA   | 1.74                     | 0.46              |
| 1:I:175:THR:O    | 1:I:177:PRO:HD3  | 2.16                     | 0.46              |
| 1:M:90:VAL:HG12  | 1:M:109:TRP:CZ2  | 2.49                     | 0.46              |
| 2:R:49:VAL:HG11  | 3:S:246:VAL:HA   | 1.96                     | 0.46              |
| 1:E:181:VAL:HG12 | 1:E:182:LYS:O    | 2.15                     | 0.46              |
| 1:A:215:LYS:HB3  | 1:A:216:GLN:O    | 2.15                     | 0.46              |
| 2:J:166:THR:O    | 2:J:166:THR:OG1  | 2.29                     | 0.46              |
| 1:Q:140:CYS:HA   | 1:Q:183:LEU:HD21 | 1.96                     | 0.46              |
| 1:A:87:ALA:HB2   | 1:A:254:ARG:HB2  | 1.95                     | 0.46              |
| 3:C:111:CYS:HB3  | 3:C:172:ARG:CZ   | 2.45                     | 0.46              |
| 1:I:181:VAL:HG12 | 1:I:182:LYS:O    | 2.15                     | 0.46              |
| 1:M:155:PHE:O    | 1:M:157:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:90:VAL:HG12  | 1:A:109:TRP:CZ2  | 2.50                     | 0.46              |
| 1:E:194:PHE:CZ   | 1:E:196:SER:HB3  | 2.51                     | 0.46              |
| 3:G:317:LEU:HD21 | 2:B:152:GLY:HA3  | 1.97                     | 0.46              |
| 3:O:111:CYS:SG   | 3:O:172:ARG:HD3  | 2.55                     | 0.46              |
| 1:Q:155:PHE:O    | 1:Q:157:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:129:MET:HE1  | 1:A:255:MET:HE1  | 1.98                     | 0.46              |
| 2:J:142:LEU:HD12 | 2:J:143:PRO:HD2  | 1.96                     | 0.46              |
| 1:E:230:MET:HE3  | 1:E:230:MET:HB2  | 1.71                     | 0.46              |
| 1:I:87:ALA:HB2   | 1:I:254:ARG:HB2  | 1.98                     | 0.46              |
| 1:M:179:VAL:HG12 | 1:M:181:VAL:HG23 | 1.97                     | 0.46              |
| 2:N:49:VAL:HG11  | 3:O:246:VAL:HA   | 1.98                     | 0.46              |
| 1:I:117:ALA:O    | 2:J:236:LEU:HD13 | 2.16                     | 0.46              |
| 1:I:265:PRO:HB3  | 3:K:243:GLN:HB2  | 1.98                     | 0.46              |
| 1:A:194:PHE:CZ   | 1:A:196:SER:HB3  | 2.51                     | 0.46              |
| 3:C:118:ALA:HA   | 3:C:119:VAL:HA   | 1.52                     | 0.46              |
| 1:E:287:THR:OG1  | 1:E:288:GLY:N    | 2.49                     | 0.46              |
| 3:O:126:ASP:O    | 3:O:130:ASN:HB2  | 2.16                     | 0.46              |
| 3:C:96:GLU:O     | 3:C:98:ALA:N     | 2.45                     | 0.46              |
| 3:C:293:TYR:CZ   | 3:C:299:PRO:HA   | 2.51                     | 0.46              |
| 1:I:166:ARG:HG2  | 1:I:236:ARG:HH21 | 1.80                     | 0.45              |
| 2:N:157:TRP:CG   | 2:N:165:VAL:HG21 | 2.51                     | 0.45              |
| 3:C:117:THR:O    | 3:C:118:ALA:C    | 2.58                     | 0.45              |
| 3:G:170:LEU:HB2  | 3:G:315:ALA:HB3  | 1.97                     | 0.45              |
| 1:I:134:GLU:HB2  | 1:I:256:LYS:HE3  | 1.98                     | 0.45              |
| 1:A:149:GLN:HG2  | 1:A:247:LEU:HD11 | 1.97                     | 0.45              |
| 1:I:230:MET:HE3  | 1:I:230:MET:HB2  | 1.82                     | 0.45              |
| 1:M:87:ALA:HB2   | 1:M:254:ARG:HB2  | 1.99                     | 0.45              |
| 1:M:109:TRP:CZ3  | 1:M:111:ILE:HA   | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:222:LYS:H    | 2:R:222:LYS:CD   | 2.30                     | 0.45              |
| 2:J:86:PHE:HB3   | 2:J:95:PRO:HG2   | 1.98                     | 0.45              |
| 2:J:138:PRO:HB3  | 2:J:191:THR:HA   | 1.97                     | 0.45              |
| 3:S:111:CYS:SG   | 3:S:172:ARG:HD3  | 2.56                     | 0.45              |
| 3:O:268:ASN:HD22 | 3:O:270:LEU:H    | 1.63                     | 0.45              |
| 1:E:164:ASP:OD1  | 1:E:164:ASP:N    | 2.49                     | 0.45              |
| 1:E:166:ARG:HG2  | 1:E:236:ARG:HH21 | 1.80                     | 0.45              |
| 1:Q:132:ASP:HB2  | 1:Q:256:LYS:HB2  | 1.99                     | 0.45              |
| 1:I:147:VAL:H    | 1:I:183:LEU:HD22 | 1.81                     | 0.45              |
| 1:A:285:LYS:HD2  | 1:A:287:THR:O    | 2.16                     | 0.45              |
| 2:R:58:VAL:HG22  | 2:R:59:PRO:HD3   | 1.99                     | 0.45              |
| 3:K:154:VAL:HG13 | 3:K:155:LEU:HG   | 1.98                     | 0.45              |
| 3:O:122:PRO:HB3  | 3:O:315:ALA:HB2  | 1.99                     | 0.45              |
| 1:E:212:GLY:HA2  | 1:E:213:GLU:HA   | 1.58                     | 0.45              |
| 1:M:175:THR:HG21 | 2:J:231:ASP:H    | 1.82                     | 0.45              |
| 1:M:211:PHE:CG   | 1:M:212:GLY:N    | 2.85                     | 0.45              |
| 1:M:218:LYS:HG3  | 1:M:219:ASP:H    | 1.82                     | 0.45              |
| 1:A:109:TRP:CZ3  | 1:A:111:ILE:HA   | 2.51                     | 0.45              |
| 2:B:162:GLN:CD   | 2:B:162:GLN:H    | 2.24                     | 0.45              |
| 1:E:158:PRO:HD2  | 1:E:195:MET:HE2  | 1.99                     | 0.45              |
| 1:Q:117:ALA:O    | 2:R:236:LEU:HD13 | 2.17                     | 0.45              |
| 1:I:279:TYR:OH   | 3:K:231:HIS:ND1  | 2.35                     | 0.45              |
| 1:M:88:GLY:O     | 1:M:90:VAL:HG23  | 2.17                     | 0.45              |
| 3:G:137:THR:HG22 | 3:G:304:THR:HG23 | 1.97                     | 0.45              |
| 1:Q:210:THR:HA   | 1:Q:211:PHE:HA   | 1.44                     | 0.45              |
| 1:M:171:TRP:CE3  | 1:M:236:ARG:HD2  | 2.51                     | 0.45              |
| 2:B:59:PRO:HD2   | 2:B:68:ARG:HG2   | 1.99                     | 0.45              |
| 3:S:122:PRO:HB3  | 3:S:315:ALA:HB2  | 1.98                     | 0.45              |
| 3:C:137:THR:HG22 | 3:C:304:THR:HG23 | 1.99                     | 0.45              |
| 1:E:208:TYR:CE2  | 1:E:222:TYR:HB2  | 2.52                     | 0.45              |
| 3:G:111:CYS:SG   | 3:G:172:ARG:HD3  | 2.56                     | 0.45              |
| 1:Q:129:MET:HE2  | 1:Q:129:MET:HB3  | 1.82                     | 0.45              |
| 3:S:169:TYR:CD2  | 3:S:170:LEU:HG   | 2.52                     | 0.45              |
| 1:Q:134:GLU:HB2  | 1:Q:256:LYS:HE3  | 1.99                     | 0.44              |
| 1:I:155:PHE:O    | 1:I:157:PRO:HD3  | 2.16                     | 0.44              |
| 1:I:212:GLY:HA2  | 1:I:213:GLU:HA   | 1.51                     | 0.44              |
| 1:A:171:TRP:CE3  | 1:A:236:ARG:HD2  | 2.53                     | 0.44              |
| 2:J:118:THR:HA   | 2:J:166:THR:HA   | 1.98                     | 0.44              |
| 3:S:152:PRO:HG3  | 3:S:171:TYR:CE2  | 2.52                     | 0.44              |
| 1:E:274:LYS:HA   | 2:F:237:GLN:OE1  | 2.17                     | 0.44              |
| 1:I:273:PHE:CZ   | 3:K:212:ASP:HB3  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:236:LEU:HG   | 2:N:237:GLN:N    | 2.30                     | 0.44              |
| 1:M:212:GLY:HA2  | 1:M:213:GLU:HA   | 1.50                     | 0.44              |
| 3:K:172:ARG:HD2  | 3:K:271:PRO:O    | 2.18                     | 0.44              |
| 1:Q:225:CYS:HA   | 1:Q:226:PRO:HD3  | 1.87                     | 0.44              |
| 1:A:179:VAL:HG12 | 1:A:181:VAL:HG23 | 1.99                     | 0.44              |
| 2:R:162:GLN:H    | 2:R:162:GLN:CD   | 2.26                     | 0.44              |
| 2:J:59:PRO:HD2   | 2:J:68:ARG:HG2   | 1.99                     | 0.44              |
| 3:O:137:THR:HG22 | 3:O:304:THR:HG23 | 2.00                     | 0.44              |
| 1:E:215:LYS:HG2  | 1:E:216:GLN:O    | 2.18                     | 0.44              |
| 1:M:285:LYS:NZ   | 1:M:288:GLY:HA3  | 2.32                     | 0.44              |
| 3:S:209:GLY:HA3  | 3:S:210:THR:HA   | 1.89                     | 0.44              |
| 3:S:316:GLY:O    | 3:S:317:LEU:HD23 | 2.17                     | 0.44              |
| 3:C:209:GLY:HA3  | 3:C:210:THR:HA   | 1.63                     | 0.44              |
| 2:F:161:LEU:HD13 | 2:F:164:SER:HB2  | 2.00                     | 0.44              |
| 3:G:155:LEU:HD21 | 3:G:307:LEU:HD11 | 2.00                     | 0.44              |
| 1:Q:90:VAL:HG21  | 1:Q:253:MET:HB3  | 2.00                     | 0.44              |
| 1:M:129:MET:HE1  | 1:M:255:MET:HE1  | 2.00                     | 0.44              |
| 1:M:210:THR:HA   | 1:M:211:PHE:HA   | 1.63                     | 0.44              |
| 3:S:235:LEU:HD21 | 3:S:241:ILE:HG13 | 2.00                     | 0.44              |
| 3:K:118:ALA:HA   | 3:K:119:VAL:HA   | 1.77                     | 0.44              |
| 3:G:204:VAL:HG12 | 3:G:205:ALA:N    | 2.33                     | 0.43              |
| 1:Q:120:ARG:HH11 | 2:R:237:GLN:HG2  | 1.83                     | 0.43              |
| 1:M:208:TYR:CE2  | 1:M:222:TYR:HB2  | 2.53                     | 0.43              |
| 2:J:158:ASP:OD1  | 2:J:159:PHE:N    | 2.51                     | 0.43              |
| 2:J:162:GLN:CD   | 2:J:162:GLN:H    | 2.26                     | 0.43              |
| 2:B:133:ILE:HD12 | 2:B:165:VAL:HG11 | 2.00                     | 0.43              |
| 3:K:169:TYR:CD2  | 3:K:170:LEU:HG   | 2.53                     | 0.43              |
| 3:C:111:CYS:HB2  | 3:C:114:SER:OG   | 2.18                     | 0.43              |
| 3:G:298:THR:HA   | 3:G:299:PRO:HD3  | 1.72                     | 0.43              |
| 1:I:113:ILE:HD11 | 1:I:230:MET:HE1  | 1.99                     | 0.43              |
| 3:S:154:VAL:HG13 | 3:S:155:LEU:HG   | 2.00                     | 0.43              |
| 3:G:268:ASN:HD22 | 3:G:270:LEU:H    | 1.65                     | 0.43              |
| 1:Q:171:TRP:CE3  | 1:Q:236:ARG:HD2  | 2.53                     | 0.43              |
| 1:I:179:VAL:HG12 | 1:I:181:VAL:HG23 | 2.00                     | 0.43              |
| 1:M:117:ALA:O    | 2:N:236:LEU:HD13 | 2.18                     | 0.43              |
| 1:A:164:ASP:OD1  | 1:A:164:ASP:N    | 2.50                     | 0.43              |
| 3:O:293:TYR:CZ   | 3:O:299:PRO:HA   | 2.54                     | 0.43              |
| 1:E:269:GLN:NE2  | 1:E:284:ILE:O    | 2.39                     | 0.43              |
| 2:F:55:VAL:HG13  | 2:F:85:VAL:HA    | 1.99                     | 0.43              |
| 2:F:236:LEU:HG   | 2:F:237:GLN:HG2  | 1.99                     | 0.43              |
| 3:G:119:VAL:HA   | 3:G:120:ASP:HA   | 1.76                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:140:CYS:HA   | 1:M:183:LEU:HD21 | 2.00                     | 0.43              |
| 2:B:70:ARG:HB2   | 2:B:213:TYR:HB3  | 2.00                     | 0.43              |
| 3:K:254:LEU:HD23 | 3:K:254:LEU:HA   | 1.88                     | 0.43              |
| 3:O:298:THR:HA   | 3:O:299:PRO:HD3  | 1.78                     | 0.43              |
| 3:K:155:LEU:HD21 | 3:K:307:LEU:HD11 | 2.01                     | 0.43              |
| 3:C:148:TYR:OH   | 3:C:219:GLN:O    | 2.25                     | 0.43              |
| 3:G:166:GLN:HG3  | 3:G:276:LEU:HD21 | 1.99                     | 0.43              |
| 1:I:75:THR:HG22  | 2:J:225:THR:HG22 | 2.01                     | 0.43              |
| 1:A:175:THR:HG21 | 2:N:231:ASP:H    | 1.84                     | 0.43              |
| 1:A:218:LYS:HG2  | 1:A:219:ASP:N    | 2.27                     | 0.43              |
| 2:J:153:THR:H    | 3:O:317:LEU:HD21 | 1.83                     | 0.43              |
| 2:B:91:GLY:HA3   | 2:B:111:TRP:CZ2  | 2.54                     | 0.43              |
| 1:E:184:SER:O    | 1:Q:182:LYS:HE2  | 2.19                     | 0.43              |
| 1:I:171:TRP:CE3  | 1:I:236:ARG:HD2  | 2.53                     | 0.43              |
| 1:I:280:ALA:C    | 1:I:282:ASN:H    | 2.26                     | 0.43              |
| 1:M:120:ARG:NH1  | 2:N:237:GLN:HG2  | 2.34                     | 0.43              |
| 1:A:155:PHE:O    | 1:A:157:PRO:HD3  | 2.19                     | 0.43              |
| 1:E:123:VAL:HG13 | 1:E:203:TRP:NE1  | 2.33                     | 0.43              |
| 2:F:139:GLY:HA2  | 1:Q:211:PHE:CE1  | 2.52                     | 0.43              |
| 1:M:120:ARG:HH11 | 2:N:237:GLN:HG2  | 1.83                     | 0.43              |
| 3:C:154:VAL:HG13 | 3:C:155:LEU:HG   | 2.01                     | 0.43              |
| 3:G:140:TRP:HB2  | 3:G:147:TRP:CH2  | 2.44                     | 0.43              |
| 3:G:155:LEU:C    | 3:G:157:GLU:H    | 2.26                     | 0.43              |
| 3:G:191:LEU:HB2  | 3:G:252:ILE:HB   | 2.00                     | 0.43              |
| 1:M:181:VAL:HG12 | 1:M:182:LYS:O    | 2.18                     | 0.43              |
| 3:K:155:LEU:HD11 | 3:K:307:LEU:HD13 | 2.00                     | 0.43              |
| 1:Q:261:TRP:CD1  | 2:R:36:ILE:HB    | 2.54                     | 0.43              |
| 3:S:115:ASP:CG   | 3:S:116:ALA:H    | 2.26                     | 0.43              |
| 1:I:209:PRO:HD2  | 1:I:221:GLU:HB3  | 2.01                     | 0.42              |
| 3:K:137:THR:HG22 | 3:K:304:THR:HG23 | 2.01                     | 0.42              |
| 3:K:207:GLY:HA2  | 3:K:208:THR:HA   | 1.74                     | 0.42              |
| 3:O:187:HIS:CD2  | 3:O:301:ILE:HD11 | 2.54                     | 0.42              |
| 1:E:171:TRP:CE3  | 1:E:236:ARG:HD2  | 2.54                     | 0.42              |
| 1:M:266:MET:HE1  | 2:N:107:TYR:CE2  | 2.54                     | 0.42              |
| 3:K:156:THR:HA   | 3:K:162:GLY:HA2  | 2.00                     | 0.42              |
| 1:E:281:GLY:H    | 3:G:204:VAL:HG11 | 1.81                     | 0.42              |
| 2:N:222:LYS:H    | 2:N:222:LYS:CD   | 2.32                     | 0.42              |
| 2:B:159:PHE:HB3  | 3:C:255:ARG:NH2  | 2.33                     | 0.42              |
| 3:S:166:GLN:HG3  | 3:S:276:LEU:HD21 | 2.01                     | 0.42              |
| 3:O:140:TRP:CZ3  | 3:O:287:PRO:HB3  | 2.55                     | 0.42              |
| 3:C:298:THR:HA   | 3:C:299:PRO:HD3  | 1.74                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:222:LYS:H    | 2:F:222:LYS:CD   | 2.31                     | 0.42              |
| 1:A:208:TYR:CE2  | 1:A:222:TYR:HB2  | 2.54                     | 0.42              |
| 3:K:155:LEU:C    | 3:K:157:GLU:H    | 2.27                     | 0.42              |
| 3:C:145:LYS:HB3  | 3:C:232:PRO:HG3  | 2.00                     | 0.42              |
| 3:C:199:TYR:OH   | 3:C:235:LEU:O    | 2.33                     | 0.42              |
| 3:G:155:LEU:HD11 | 3:G:307:LEU:HD13 | 2.02                     | 0.42              |
| 1:M:123:VAL:HG13 | 1:M:203:TRP:NE1  | 2.34                     | 0.42              |
| 1:A:266:MET:HE2  | 1:A:266:MET:HB3  | 1.96                     | 0.42              |
| 3:S:119:VAL:HA   | 3:S:120:ASP:HA   | 1.84                     | 0.42              |
| 3:K:268:ASN:HD22 | 3:K:270:LEU:H    | 1.65                     | 0.42              |
| 1:A:134:GLU:HB2  | 1:A:256:LYS:HE3  | 2.02                     | 0.42              |
| 2:R:138:PRO:HB3  | 2:R:191:THR:HA   | 2.02                     | 0.42              |
| 2:N:162:GLN:CD   | 2:N:162:GLN:H    | 2.27                     | 0.42              |
| 2:B:57:ASN:ND2   | 2:B:95:PRO:HD3   | 2.35                     | 0.42              |
| 1:I:149:GLN:HG2  | 1:I:247:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:123:VAL:HG13 | 1:A:203:TRP:NE1  | 2.34                     | 0.42              |
| 1:A:281:GLY:H    | 3:C:204:VAL:HG11 | 1.85                     | 0.42              |
| 2:N:157:TRP:HB2  | 2:N:165:VAL:HG21 | 2.01                     | 0.42              |
| 3:K:170:LEU:HB2  | 3:K:315:ALA:HB3  | 2.01                     | 0.42              |
| 2:F:158:ASP:OD1  | 2:F:159:PHE:N    | 2.52                     | 0.42              |
| 1:M:261:TRP:CD1  | 2:N:36:ILE:HB    | 2.55                     | 0.42              |
| 3:S:204:VAL:HG12 | 3:S:205:ALA:N    | 2.34                     | 0.42              |
| 3:O:115:ASP:O    | 3:O:117:THR:N    | 2.53                     | 0.42              |
| 1:M:190:VAL:HG21 | 2:N:24:ILE:HD12  | 2.01                     | 0.42              |
| 1:M:211:PHE:CE2  | 3:O:169:TYR:CE1  | 3.07                     | 0.42              |
| 3:S:155:LEU:HD11 | 3:S:307:LEU:HD13 | 2.02                     | 0.42              |
| 2:F:57:ASN:ND2   | 2:F:95:PRO:HD3   | 2.35                     | 0.42              |
| 1:I:171:TRP:CZ3  | 1:I:236:ARG:HD2  | 2.55                     | 0.42              |
| 2:R:234:ASP:CG   | 2:R:235:ILE:H    | 2.28                     | 0.42              |
| 2:J:61:ASN:ND2   | 2:J:64:SER:OG    | 2.53                     | 0.42              |
| 1:E:216:GLN:HE21 | 3:G:277:ASN:ND2  | 2.13                     | 0.41              |
| 1:Q:265:PRO:HG2  | 3:S:239:ILE:HD12 | 2.02                     | 0.41              |
| 2:B:142:LEU:HD12 | 2:B:143:PRO:HD2  | 2.02                     | 0.41              |
| 3:O:273:ASP:OD2  | 3:O:278:HIS:ND1  | 2.37                     | 0.41              |
| 1:E:155:PHE:O    | 1:E:157:PRO:HD3  | 2.19                     | 0.41              |
| 2:F:153:THR:OG1  | 3:S:317:LEU:HD11 | 2.20                     | 0.41              |
| 3:G:289:SER:HA   | 3:G:290:PRO:HD3  | 1.82                     | 0.41              |
| 1:A:287:THR:HG22 | 2:B:97:GLN:HB2   | 2.02                     | 0.41              |
| 3:K:293:TYR:CZ   | 3:K:299:PRO:HA   | 2.55                     | 0.41              |
| 3:C:169:TYR:CD2  | 3:C:170:LEU:HG   | 2.54                     | 0.41              |
| 3:G:317:LEU:HB3  | 3:G:318:ARG:H    | 1.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:215:LYS:N    | 1:Q:216:GLN:HA   | 2.21                     | 0.41              |
| 2:J:137:PRO:HG3  | 3:O:317:LEU:HB2  | 2.03                     | 0.41              |
| 3:S:172:ARG:HD2  | 3:S:271:PRO:O    | 2.20                     | 0.41              |
| 1:I:164:ASP:OD1  | 1:I:164:ASP:N    | 2.50                     | 0.41              |
| 3:K:152:PRO:HG3  | 3:K:171:TYR:CE2  | 2.55                     | 0.41              |
| 1:E:121:ARG:NH2  | 2:F:103:GLN:OE1  | 2.52                     | 0.41              |
| 1:E:175:THR:O    | 1:E:177:PRO:HD3  | 2.20                     | 0.41              |
| 1:Q:166:ARG:NH2  | 1:Q:239:GLY:O    | 2.53                     | 0.41              |
| 1:M:175:THR:O    | 1:M:177:PRO:HD3  | 2.21                     | 0.41              |
| 2:R:7:LYS:O      | 2:R:10:THR:OG1   | 2.29                     | 0.41              |
| 3:K:257:ASN:OD1  | 3:K:257:ASN:N    | 2.53                     | 0.41              |
| 1:E:75:THR:HG22  | 2:F:225:THR:HG22 | 2.01                     | 0.41              |
| 1:I:132:ASP:HB2  | 1:I:256:LYS:HB2  | 2.02                     | 0.41              |
| 1:M:266:MET:HE2  | 1:M:266:MET:HB3  | 1.93                     | 0.41              |
| 1:A:88:GLY:O     | 1:A:90:VAL:HG23  | 2.20                     | 0.41              |
| 3:S:115:ASP:OD1  | 3:S:115:ASP:N    | 2.52                     | 0.41              |
| 3:O:108:PRO:HB3  | 3:O:174:GLY:HA3  | 2.02                     | 0.41              |
| 3:C:204:VAL:HG12 | 3:C:205:ALA:N    | 2.34                     | 0.41              |
| 1:A:175:THR:O    | 1:A:177:PRO:HD3  | 2.20                     | 0.41              |
| 3:K:111:CYS:HB3  | 3:K:172:ARG:CZ   | 2.51                     | 0.41              |
| 1:Q:120:ARG:NH1  | 2:R:237:GLN:HG2  | 2.36                     | 0.41              |
| 2:R:111:TRP:HB3  | 2:R:226:MET:HG2  | 2.03                     | 0.41              |
| 2:N:97:GLN:HE21  | 2:N:97:GLN:HB3   | 1.74                     | 0.41              |
| 2:B:22:ALA:HA    | 2:B:23:PRO:HD2   | 1.94                     | 0.41              |
| 3:K:289:SER:HA   | 3:K:290:PRO:HD3  | 1.89                     | 0.41              |
| 3:O:111:CYS:HB3  | 3:O:172:ARG:CZ   | 2.51                     | 0.41              |
| 3:O:145:LYS:HB3  | 3:O:232:PRO:HG3  | 2.03                     | 0.41              |
| 1:Q:97:LEU:O     | 1:Q:242:LYS:NZ   | 2.45                     | 0.41              |
| 1:M:215:LYS:HB3  | 1:M:216:GLN:O    | 2.21                     | 0.41              |
| 2:N:29:HIS:HA    | 2:N:30:PRO:HD2   | 1.97                     | 0.41              |
| 2:B:56:ASN:ND2   | 2:B:67:GLU:O     | 2.53                     | 0.41              |
| 3:O:155:LEU:HD21 | 3:O:307:LEU:HD11 | 2.03                     | 0.41              |
| 3:O:235:LEU:HD21 | 3:O:241:ILE:HG13 | 2.03                     | 0.41              |
| 2:F:83:CYS:SG    | 2:F:196:ILE:HD12 | 2.61                     | 0.41              |
| 1:I:93:ILE:HB    | 1:I:249:VAL:HB   | 2.02                     | 0.41              |
| 1:A:75:THR:HG22  | 2:B:225:THR:HG22 | 2.03                     | 0.41              |
| 1:A:129:MET:HE2  | 1:A:129:MET:HB3  | 1.90                     | 0.41              |
| 1:A:285:LYS:NZ   | 1:A:288:GLY:HA3  | 2.36                     | 0.41              |
| 2:R:120:MET:HA   | 2:R:163:SER:CB   | 2.50                     | 0.41              |
| 2:B:234:ASP:CG   | 2:B:235:ILE:H    | 2.28                     | 0.41              |
| 3:S:137:THR:HG22 | 3:S:304:THR:HG23 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:298:THR:HA   | 3:K:299:PRO:HD3  | 1.77                     | 0.41              |
| 3:O:110:TYR:HB3  | 3:O:124:ARG:NH1  | 2.36                     | 0.41              |
| 3:O:204:VAL:HG12 | 3:O:205:ALA:N    | 2.36                     | 0.41              |
| 3:C:210:THR:HG22 | 3:C:210:THR:O    | 2.21                     | 0.41              |
| 2:N:59:PRO:HD2   | 2:N:68:ARG:HG2   | 2.04                     | 0.40              |
| 3:S:158:THR:HB   | 3:S:159:GLY:H    | 1.74                     | 0.40              |
| 1:Q:177:PRO:HB2  | 2:R:24:ILE:HG12  | 2.02                     | 0.40              |
| 1:M:288:GLY:O    | 1:M:290:SER:N    | 2.54                     | 0.40              |
| 2:R:87:ARG:H     | 2:R:87:ARG:HG3   | 1.65                     | 0.40              |
| 2:R:157:TRP:CG   | 2:R:165:VAL:HG21 | 2.57                     | 0.40              |
| 2:N:146:ARG:NH1  | 2:N:199:GLN:OE1  | 2.53                     | 0.40              |
| 1:E:179:VAL:HG22 | 2:B:14:LEU:HD13  | 2.03                     | 0.40              |
| 3:G:317:LEU:HB2  | 2:B:137:PRO:CG   | 2.45                     | 0.40              |
| 1:Q:285:LYS:HG3  | 2:R:65:LEU:HD21  | 2.02                     | 0.40              |
| 1:A:288:GLY:O    | 1:A:290:SER:N    | 2.53                     | 0.40              |
| 2:J:159:PHE:HB3  | 3:K:255:ARG:NH2  | 2.37                     | 0.40              |
| 2:N:118:THR:HA   | 2:N:166:THR:HA   | 2.03                     | 0.40              |
| 1:I:109:TRP:CZ3  | 1:I:111:ILE:HA   | 2.56                     | 0.40              |
| 1:A:213:GLU:OE1  | 1:A:213:GLU:HA   | 2.22                     | 0.40              |
| 2:J:97:GLN:HE21  | 2:J:97:GLN:HB3   | 1.74                     | 0.40              |
| 3:O:118:ALA:HA   | 3:O:119:VAL:HA   | 1.77                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1   | A     | 221/297 (74%) | 207 (94%) | 13 (6%) | 1 (0%)   | 24 55       |
| 1   | E     | 221/297 (74%) | 206 (93%) | 14 (6%) | 1 (0%)   | 24 55       |
| 1   | I     | 221/297 (74%) | 208 (94%) | 12 (5%) | 1 (0%)   | 24 55       |
| 1   | M     | 221/297 (74%) | 207 (94%) | 13 (6%) | 1 (0%)   | 24 55       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | Q     | 221/297 (74%)   | 207 (94%)  | 12 (5%)  | 2 (1%)   | 14          | 43  |
| 2   | B     | 221/242 (91%)   | 202 (91%)  | 18 (8%)  | 1 (0%)   | 24          | 55  |
| 2   | F     | 221/242 (91%)   | 201 (91%)  | 20 (9%)  | 0        | 100         | 100 |
| 2   | J     | 221/242 (91%)   | 201 (91%)  | 20 (9%)  | 0        | 100         | 100 |
| 2   | N     | 221/242 (91%)   | 200 (90%)  | 21 (10%) | 0        | 100         | 100 |
| 2   | R     | 221/242 (91%)   | 201 (91%)  | 20 (9%)  | 0        | 100         | 100 |
| 3   | C     | 236/323 (73%)   | 219 (93%)  | 16 (7%)  | 1 (0%)   | 30          | 59  |
| 3   | G     | 236/323 (73%)   | 219 (93%)  | 17 (7%)  | 0        | 100         | 100 |
| 3   | K     | 236/323 (73%)   | 220 (93%)  | 15 (6%)  | 1 (0%)   | 30          | 59  |
| 3   | O     | 236/323 (73%)   | 219 (93%)  | 17 (7%)  | 0        | 100         | 100 |
| 3   | S     | 236/323 (73%)   | 218 (92%)  | 15 (6%)  | 3 (1%)   | 9           | 36  |
| All | All   | 3390/4310 (79%) | 3135 (92%) | 243 (7%) | 12 (0%)  | 30          | 59  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | S     | 127 | VAL  |
| 1   | Q     | 288 | GLY  |
| 1   | M     | 288 | GLY  |
| 1   | A     | 288 | GLY  |
| 3   | K     | 113 | ASP  |
| 3   | C     | 118 | ALA  |
| 1   | E     | 288 | GLY  |
| 2   | B     | 236 | LEU  |
| 3   | S     | 118 | ALA  |
| 1   | Q     | 101 | THR  |
| 1   | I     | 288 | GLY  |
| 3   | S     | 125 | 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     | 191/251 (76%)   | 189 (99%)  | 2 (1%)   | 68          | 76 |
| 1   | E     | 191/251 (76%)   | 187 (98%)  | 4 (2%)   | 47          | 67 |
| 1   | I     | 191/251 (76%)   | 188 (98%)  | 3 (2%)   | 55          | 71 |
| 1   | M     | 191/251 (76%)   | 185 (97%)  | 6 (3%)   | 35          | 61 |
| 1   | Q     | 191/251 (76%)   | 184 (96%)  | 7 (4%)   | 30          | 58 |
| 2   | B     | 189/202 (94%)   | 186 (98%)  | 3 (2%)   | 55          | 71 |
| 2   | F     | 189/202 (94%)   | 185 (98%)  | 4 (2%)   | 47          | 67 |
| 2   | J     | 189/202 (94%)   | 185 (98%)  | 4 (2%)   | 47          | 67 |
| 2   | N     | 189/202 (94%)   | 186 (98%)  | 3 (2%)   | 55          | 71 |
| 2   | R     | 189/202 (94%)   | 186 (98%)  | 3 (2%)   | 55          | 71 |
| 3   | C     | 202/272 (74%)   | 197 (98%)  | 5 (2%)   | 42          | 65 |
| 3   | G     | 202/272 (74%)   | 197 (98%)  | 5 (2%)   | 42          | 65 |
| 3   | K     | 202/272 (74%)   | 195 (96%)  | 7 (4%)   | 32          | 59 |
| 3   | O     | 202/272 (74%)   | 196 (97%)  | 6 (3%)   | 36          | 62 |
| 3   | S     | 202/272 (74%)   | 198 (98%)  | 4 (2%)   | 48          | 68 |
| All | All   | 2910/3625 (80%) | 2844 (98%) | 66 (2%)  | 44          | 66 |

All (66) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 123 | VAL  |
| 1   | E     | 213 | GLU  |
| 1   | E     | 214 | HIS  |
| 1   | E     | 218 | LYS  |
| 2   | F     | 58  | VAL  |
| 2   | F     | 227 | GLN  |
| 2   | F     | 230 | LYS  |
| 2   | F     | 237 | GLN  |
| 3   | G     | 82  | VAL  |
| 3   | G     | 204 | VAL  |
| 3   | G     | 208 | THR  |
| 3   | G     | 307 | LEU  |
| 3   | G     | 317 | LEU  |
| 1   | Q     | 123 | VAL  |
| 1   | Q     | 202 | GLN  |
| 1   | Q     | 210 | THR  |
| 1   | Q     | 213 | GLU  |
| 1   | Q     | 214 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 242 | LYS  |
| 1   | Q     | 285 | LYS  |
| 1   | I     | 123 | VAL  |
| 1   | I     | 213 | GLU  |
| 1   | I     | 285 | LYS  |
| 1   | M     | 86  | ARG  |
| 1   | M     | 123 | VAL  |
| 1   | M     | 211 | PHE  |
| 1   | M     | 213 | GLU  |
| 1   | M     | 274 | LYS  |
| 1   | M     | 294 | ILE  |
| 1   | A     | 123 | VAL  |
| 1   | A     | 213 | GLU  |
| 2   | R     | 58  | VAL  |
| 2   | R     | 227 | GLN  |
| 2   | R     | 230 | LYS  |
| 2   | J     | 58  | VAL  |
| 2   | J     | 190 | THR  |
| 2   | J     | 227 | GLN  |
| 2   | J     | 230 | LYS  |
| 2   | N     | 58  | VAL  |
| 2   | N     | 227 | GLN  |
| 2   | N     | 230 | LYS  |
| 2   | B     | 58  | VAL  |
| 2   | B     | 227 | GLN  |
| 2   | B     | 230 | LYS  |
| 3   | S     | 82  | VAL  |
| 3   | S     | 101 | ILE  |
| 3   | S     | 204 | VAL  |
| 3   | S     | 307 | LEU  |
| 3   | K     | 82  | VAL  |
| 3   | K     | 96  | GLU  |
| 3   | K     | 204 | VAL  |
| 3   | K     | 208 | THR  |
| 3   | K     | 213 | SER  |
| 3   | K     | 307 | LEU  |
| 3   | K     | 318 | ARG  |
| 3   | O     | 82  | VAL  |
| 3   | O     | 204 | VAL  |
| 3   | O     | 208 | THR  |
| 3   | O     | 218 | LYS  |
| 3   | O     | 307 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | O     | 319 | GLN  |
| 3   | C     | 82  | VAL  |
| 3   | C     | 117 | THR  |
| 3   | C     | 204 | VAL  |
| 3   | C     | 208 | THR  |
| 3   | C     | 307 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 189 | GLN  |
| 1   | E     | 202 | GLN  |
| 3   | G     | 214 | HIS  |
| 3   | G     | 250 | GLN  |
| 3   | G     | 277 | ASN  |
| 1   | Q     | 189 | GLN  |
| 1   | I     | 202 | GLN  |
| 1   | A     | 189 | GLN  |
| 1   | A     | 202 | GLN  |
| 2   | J     | 56  | ASN  |
| 2   | B     | 110 | GLN  |
| 3   | S     | 250 | GLN  |
| 3   | K     | 250 | GLN  |
| 3   | K     | 280 | ASN  |
| 3   | O     | 214 | HIS  |
| 3   | O     | 250 | GLN  |
| 3   | O     | 319 | GLN  |
| 3   | C     | 214 | HIS  |
| 3   | C     | 258 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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     | 223/297 (75%)   | 0.36   | 24 (10%) 11 6 | 28, 37, 132, 220      | 0     |
| 1   | E     | 223/297 (75%)   | 0.21   | 22 (9%) 13 7  | 27, 37, 133, 222      | 0     |
| 1   | I     | 223/297 (75%)   | 0.38   | 28 (12%) 8 5  | 29, 38, 132, 219      | 0     |
| 1   | M     | 223/297 (75%)   | 0.19   | 20 (8%) 15 9  | 28, 38, 132, 219      | 0     |
| 1   | Q     | 223/297 (75%)   | 0.24   | 22 (9%) 13 7  | 28, 38, 133, 219      | 0     |
| 2   | B     | 225/242 (92%)   | 0.40   | 26 (11%) 9 6  | 30, 42, 79, 153       | 0     |
| 2   | F     | 225/242 (92%)   | 0.14   | 13 (5%) 29 16 | 30, 41, 77, 151       | 0     |
| 2   | J     | 225/242 (92%)   | 0.39   | 24 (10%) 11 6 | 30, 42, 79, 153       | 0     |
| 2   | N     | 225/242 (92%)   | 0.24   | 20 (8%) 15 9  | 30, 42, 81, 155       | 0     |
| 2   | R     | 225/242 (92%)   | 0.30   | 21 (9%) 14 8  | 30, 42, 79, 152       | 0     |
| 3   | C     | 238/323 (73%)   | 0.63   | 38 (15%) 5 3  | 30, 50, 166, 220      | 0     |
| 3   | G     | 238/323 (73%)   | 0.45   | 28 (11%) 9 5  | 30, 49, 161, 218      | 0     |
| 3   | K     | 238/323 (73%)   | 0.58   | 34 (14%) 6 4  | 30, 50, 163, 218      | 0     |
| 3   | O     | 238/323 (73%)   | 0.57   | 38 (15%) 5 3  | 30, 50, 163, 217      | 0     |
| 3   | S     | 238/323 (73%)   | 0.62   | 35 (14%) 6 3  | 31, 52, 164, 221      | 0     |
| All | All   | 3430/4310 (79%) | 0.38   | 393 (11%) 9 6 | 27, 42, 137, 222      | 0     |

All (393) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 116 | ALA  | 10.9 |
| 3   | C     | 119 | VAL  | 9.1  |
| 1   | E     | 220 | LEU  | 8.3  |
| 1   | A     | 212 | GLY  | 7.9  |
| 2   | F     | 164 | SER  | 7.2  |
| 2   | B     | 164 | SER  | 7.1  |
| 2   | R     | 190 | THR  | 6.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 210 | THR  | 6.8  |
| 2   | R     | 86  | PHE  | 6.6  |
| 3   | S     | 116 | ALA  | 6.6  |
| 3   | K     | 127 | VAL  | 6.4  |
| 1   | Q     | 212 | GLY  | 6.4  |
| 3   | O     | 210 | THR  | 6.3  |
| 1   | E     | 211 | PHE  | 6.1  |
| 1   | A     | 289 | ALA  | 5.9  |
| 2   | B     | 83  | CYS  | 5.8  |
| 1   | Q     | 74  | SER  | 5.8  |
| 2   | N     | 1   | GLY  | 5.8  |
| 1   | E     | 210 | THR  | 5.8  |
| 3   | C     | 210 | THR  | 5.8  |
| 3   | O     | 213 | SER  | 5.7  |
| 3   | G     | 116 | ALA  | 5.6  |
| 3   | K     | 116 | ALA  | 5.6  |
| 1   | Q     | 210 | THR  | 5.4  |
| 2   | R     | 175 | THR  | 5.4  |
| 1   | Q     | 211 | PHE  | 5.3  |
| 1   | A     | 209 | PRO  | 5.2  |
| 3   | C     | 127 | VAL  | 5.1  |
| 1   | A     | 211 | PHE  | 5.0  |
| 3   | S     | 127 | VAL  | 4.9  |
| 3   | S     | 119 | VAL  | 4.9  |
| 1   | I     | 287 | THR  | 4.8  |
| 3   | C     | 117 | THR  | 4.8  |
| 1   | I     | 213 | GLU  | 4.8  |
| 3   | O     | 97  | ALA  | 4.8  |
| 3   | C     | 118 | ALA  | 4.7  |
| 3   | G     | 115 | ASP  | 4.7  |
| 1   | E     | 212 | GLY  | 4.7  |
| 1   | I     | 208 | TYR  | 4.7  |
| 1   | I     | 289 | ALA  | 4.7  |
| 2   | J     | 164 | SER  | 4.6  |
| 2   | B     | 190 | THR  | 4.6  |
| 2   | B     | 232 | ALA  | 4.6  |
| 3   | O     | 211 | GLU  | 4.6  |
| 1   | M     | 286 | PRO  | 4.6  |
| 2   | J     | 237 | GLN  | 4.6  |
| 2   | J     | 18  | ASP  | 4.5  |
| 3   | G     | 127 | VAL  | 4.5  |
| 2   | J     | 83  | CYS  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | N     | 86  | PHE  | 4.4  |
| 3   | G     | 205 | ALA  | 4.4  |
| 2   | N     | 175 | THR  | 4.4  |
| 1   | I     | 212 | GLY  | 4.3  |
| 1   | Q     | 209 | PRO  | 4.3  |
| 2   | J     | 238 | THR  | 4.3  |
| 3   | K     | 119 | VAL  | 4.3  |
| 2   | R     | 189 | TYR  | 4.3  |
| 2   | F     | 83  | CYS  | 4.3  |
| 3   | G     | 119 | VAL  | 4.3  |
| 3   | S     | 169 | TYR  | 4.2  |
| 2   | N     | 85  | VAL  | 4.2  |
| 3   | K     | 128 | SER  | 4.2  |
| 1   | M     | 289 | ALA  | 4.2  |
| 3   | S     | 204 | VAL  | 4.1  |
| 1   | A     | 220 | LEU  | 4.1  |
| 2   | J     | 86  | PHE  | 4.1  |
| 3   | K     | 213 | SER  | 4.1  |
| 3   | S     | 205 | ALA  | 4.1  |
| 1   | I     | 286 | PRO  | 4.1  |
| 3   | G     | 122 | PRO  | 4.1  |
| 1   | I     | 219 | ASP  | 4.1  |
| 2   | B     | 1   | GLY  | 4.1  |
| 3   | S     | 115 | ASP  | 4.1  |
| 3   | S     | 210 | THR  | 4.1  |
| 1   | E     | 221 | GLU  | 4.0  |
| 3   | S     | 83  | ALA  | 4.0  |
| 2   | J     | 1   | GLY  | 4.0  |
| 2   | J     | 236 | LEU  | 4.0  |
| 1   | A     | 285 | LYS  | 4.0  |
| 3   | K     | 205 | ALA  | 4.0  |
| 3   | O     | 111 | CYS  | 4.0  |
| 1   | I     | 288 | GLY  | 3.9  |
| 3   | G     | 123 | THR  | 3.9  |
| 3   | K     | 208 | THR  | 3.9  |
| 2   | F     | 233 | SER  | 3.9  |
| 3   | C     | 114 | SER  | 3.9  |
| 2   | N     | 236 | LEU  | 3.9  |
| 3   | S     | 85  | LEU  | 3.9  |
| 1   | M     | 213 | GLU  | 3.8  |
| 2   | R     | 238 | THR  | 3.8  |
| 2   | R     | 164 | SER  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | G     | 82  | VAL  | 3.8  |
| 2   | R     | 235 | ILE  | 3.7  |
| 3   | S     | 206 | GLY  | 3.7  |
| 2   | J     | 191 | THR  | 3.7  |
| 3   | K     | 97  | ALA  | 3.7  |
| 2   | J     | 234 | ASP  | 3.6  |
| 1   | E     | 292 | THR  | 3.6  |
| 3   | C     | 120 | ASP  | 3.6  |
| 2   | N     | 190 | THR  | 3.6  |
| 1   | E     | 286 | PRO  | 3.6  |
| 3   | O     | 319 | GLN  | 3.5  |
| 1   | E     | 285 | LYS  | 3.5  |
| 3   | G     | 128 | SER  | 3.5  |
| 3   | K     | 210 | THR  | 3.5  |
| 3   | S     | 203 | THR  | 3.5  |
| 3   | O     | 158 | THR  | 3.5  |
| 1   | I     | 220 | LEU  | 3.5  |
| 1   | A     | 218 | LYS  | 3.5  |
| 3   | S     | 82  | VAL  | 3.5  |
| 3   | K     | 206 | GLY  | 3.5  |
| 3   | S     | 97  | ALA  | 3.5  |
| 3   | K     | 214 | HIS  | 3.5  |
| 1   | M     | 226 | PRO  | 3.5  |
| 3   | K     | 120 | ASP  | 3.5  |
| 3   | C     | 82  | VAL  | 3.4  |
| 1   | I     | 211 | PHE  | 3.4  |
| 3   | C     | 97  | ALA  | 3.4  |
| 3   | C     | 318 | ARG  | 3.4  |
| 2   | B     | 166 | THR  | 3.4  |
| 1   | I     | 218 | LYS  | 3.4  |
| 1   | I     | 285 | LYS  | 3.4  |
| 3   | O     | 114 | SER  | 3.4  |
| 3   | C     | 317 | LEU  | 3.4  |
| 1   | M     | 220 | LEU  | 3.4  |
| 3   | O     | 127 | VAL  | 3.4  |
| 3   | O     | 217 | TYR  | 3.4  |
| 3   | G     | 206 | GLY  | 3.4  |
| 1   | M     | 212 | GLY  | 3.3  |
| 2   | R     | 236 | LEU  | 3.3  |
| 3   | O     | 128 | SER  | 3.3  |
| 1   | E     | 219 | ASP  | 3.3  |
| 1   | A     | 226 | PRO  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | S     | 118 | ALA  | 3.3  |
| 1   | Q     | 219 | ASP  | 3.3  |
| 3   | O     | 119 | VAL  | 3.3  |
| 3   | G     | 114 | SER  | 3.3  |
| 1   | E     | 226 | PRO  | 3.3  |
| 2   | J     | 190 | THR  | 3.3  |
| 1   | Q     | 218 | LYS  | 3.3  |
| 3   | G     | 121 | LYS  | 3.3  |
| 3   | G     | 318 | ARG  | 3.2  |
| 2   | N     | 164 | SER  | 3.2  |
| 3   | C     | 208 | THR  | 3.2  |
| 2   | J     | 235 | ILE  | 3.2  |
| 3   | O     | 116 | ALA  | 3.2  |
| 3   | G     | 317 | LEU  | 3.2  |
| 3   | G     | 111 | CYS  | 3.2  |
| 1   | Q     | 226 | PRO  | 3.2  |
| 1   | Q     | 286 | PRO  | 3.2  |
| 1   | M     | 211 | PHE  | 3.2  |
| 1   | I     | 282 | ASN  | 3.2  |
| 3   | S     | 319 | GLN  | 3.2  |
| 2   | N     | 166 | THR  | 3.2  |
| 3   | G     | 83  | ALA  | 3.2  |
| 1   | E     | 218 | LYS  | 3.2  |
| 3   | C     | 207 | GLY  | 3.2  |
| 1   | Q     | 220 | LEU  | 3.2  |
| 2   | F     | 236 | LEU  | 3.2  |
| 1   | I     | 226 | PRO  | 3.2  |
| 1   | E     | 214 | HIS  | 3.2  |
| 2   | B     | 163 | SER  | 3.2  |
| 1   | A     | 292 | THR  | 3.2  |
| 2   | J     | 189 | TYR  | 3.1  |
| 1   | E     | 287 | THR  | 3.1  |
| 3   | S     | 94  | THR  | 3.1  |
| 3   | S     | 213 | SER  | 3.1  |
| 2   | R     | 237 | GLN  | 3.1  |
| 2   | F     | 190 | THR  | 3.1  |
| 2   | R     | 191 | THR  | 3.1  |
| 3   | K     | 114 | SER  | 3.1  |
| 3   | O     | 159 | GLY  | 3.1  |
| 3   | K     | 140 | TRP  | 3.1  |
| 3   | K     | 318 | ARG  | 3.1  |
| 1   | A     | 286 | PRO  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 208 | TYR  | 3.1  |
| 2   | N     | 189 | TYR  | 3.1  |
| 1   | Q     | 292 | THR  | 3.1  |
| 3   | O     | 93  | THR  | 3.1  |
| 1   | I     | 74  | SER  | 3.1  |
| 3   | O     | 212 | ASP  | 3.1  |
| 1   | M     | 282 | ASN  | 3.1  |
| 3   | O     | 208 | THR  | 3.1  |
| 3   | O     | 169 | TYR  | 3.1  |
| 1   | M     | 285 | LYS  | 3.0  |
| 1   | A     | 213 | GLU  | 3.0  |
| 1   | A     | 293 | ALA  | 3.0  |
| 3   | G     | 117 | THR  | 3.0  |
| 1   | Q     | 213 | GLU  | 3.0  |
| 3   | S     | 211 | GLU  | 3.0  |
| 3   | S     | 128 | SER  | 3.0  |
| 2   | R     | 83  | CYS  | 3.0  |
| 2   | N     | 160 | GLY  | 3.0  |
| 3   | O     | 318 | ARG  | 3.0  |
| 3   | K     | 126 | ASP  | 3.0  |
| 1   | A     | 214 | HIS  | 3.0  |
| 3   | K     | 111 | CYS  | 3.0  |
| 1   | E     | 213 | GLU  | 3.0  |
| 3   | K     | 83  | ALA  | 3.0  |
| 2   | B     | 189 | TYR  | 3.0  |
| 3   | C     | 316 | GLY  | 3.0  |
| 1   | A     | 219 | ASP  | 2.9  |
| 1   | I     | 210 | THR  | 2.9  |
| 1   | A     | 98  | GLU  | 2.9  |
| 2   | R     | 81  | GLU  | 2.9  |
| 1   | Q     | 208 | TYR  | 2.9  |
| 3   | C     | 209 | GLY  | 2.9  |
| 1   | Q     | 287 | THR  | 2.9  |
| 3   | S     | 123 | THR  | 2.9  |
| 2   | B     | 235 | ILE  | 2.9  |
| 3   | C     | 205 | ALA  | 2.9  |
| 2   | R     | 85  | VAL  | 2.9  |
| 1   | I     | 209 | PRO  | 2.8  |
| 3   | S     | 122 | PRO  | 2.8  |
| 3   | C     | 98  | ALA  | 2.8  |
| 1   | M     | 210 | THR  | 2.8  |
| 1   | A     | 288 | GLY  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 85  | LEU  | 2.8  |
| 2   | R     | 233 | SER  | 2.8  |
| 3   | O     | 83  | ALA  | 2.8  |
| 2   | J     | 175 | THR  | 2.8  |
| 3   | S     | 208 | THR  | 2.8  |
| 3   | C     | 111 | CYS  | 2.8  |
| 3   | S     | 95  | GLN  | 2.8  |
| 3   | K     | 84  | GLN  | 2.8  |
| 3   | C     | 115 | ASP  | 2.8  |
| 2   | B     | 86  | PHE  | 2.8  |
| 1   | M     | 208 | TYR  | 2.8  |
| 1   | I     | 293 | ALA  | 2.8  |
| 3   | O     | 163 | GLN  | 2.8  |
| 1   | I     | 292 | THR  | 2.8  |
| 3   | C     | 94  | THR  | 2.8  |
| 1   | M     | 214 | HIS  | 2.8  |
| 2   | R     | 2   | PHE  | 2.7  |
| 3   | G     | 208 | THR  | 2.8  |
| 3   | G     | 113 | ASP  | 2.7  |
| 1   | Q     | 214 | HIS  | 2.7  |
| 3   | G     | 93  | THR  | 2.7  |
| 3   | G     | 118 | ALA  | 2.7  |
| 3   | O     | 167 | PHE  | 2.7  |
| 2   | R     | 163 | SER  | 2.7  |
| 3   | C     | 113 | ASP  | 2.7  |
| 1   | I     | 216 | GLN  | 2.7  |
| 3   | K     | 211 | GLU  | 2.7  |
| 3   | S     | 140 | TRP  | 2.7  |
| 1   | Q     | 282 | ASN  | 2.7  |
| 1   | M     | 290 | SER  | 2.7  |
| 3   | S     | 212 | ASP  | 2.7  |
| 2   | F     | 235 | ILE  | 2.6  |
| 2   | B     | 87  | ARG  | 2.6  |
| 3   | S     | 318 | ARG  | 2.6  |
| 1   | A     | 215 | LYS  | 2.6  |
| 3   | K     | 93  | THR  | 2.6  |
| 2   | B     | 206 | ILE  | 2.6  |
| 2   | F     | 237 | GLN  | 2.6  |
| 1   | A     | 287 | THR  | 2.6  |
| 3   | G     | 158 | THR  | 2.6  |
| 3   | C     | 128 | SER  | 2.6  |
| 1   | Q     | 215 | LYS  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | O     | 130 | ASN  | 2.6  |
| 3   | O     | 206 | GLY  | 2.6  |
| 2   | B     | 238 | THR  | 2.6  |
| 3   | O     | 203 | THR  | 2.6  |
| 3   | C     | 158 | THR  | 2.6  |
| 2   | J     | 163 | SER  | 2.6  |
| 3   | G     | 213 | SER  | 2.6  |
| 2   | B     | 161 | LEU  | 2.6  |
| 3   | S     | 98  | ALA  | 2.6  |
| 3   | K     | 160 | VAL  | 2.6  |
| 3   | K     | 121 | LYS  | 2.6  |
| 1   | E     | 293 | ALA  | 2.6  |
| 3   | O     | 82  | VAL  | 2.6  |
| 1   | A     | 291 | ARG  | 2.5  |
| 1   | A     | 221 | GLU  | 2.5  |
| 2   | N     | 191 | THR  | 2.5  |
| 3   | O     | 117 | THR  | 2.5  |
| 1   | E     | 209 | PRO  | 2.5  |
| 1   | Q     | 216 | GLN  | 2.5  |
| 1   | I     | 215 | LYS  | 2.5  |
| 2   | B     | 84  | ALA  | 2.5  |
| 3   | K     | 113 | ASP  | 2.5  |
| 1   | E     | 288 | GLY  | 2.5  |
| 3   | O     | 121 | LYS  | 2.5  |
| 2   | B     | 162 | GLN  | 2.5  |
| 2   | B     | 233 | SER  | 2.5  |
| 3   | C     | 204 | VAL  | 2.5  |
| 1   | M     | 218 | LYS  | 2.5  |
| 2   | J     | 87  | ARG  | 2.5  |
| 2   | J     | 85  | VAL  | 2.5  |
| 2   | B     | 165 | VAL  | 2.5  |
| 3   | S     | 84  | GLN  | 2.5  |
| 3   | O     | 205 | ALA  | 2.5  |
| 2   | N     | 235 | ILE  | 2.5  |
| 1   | I     | 273 | PHE  | 2.5  |
| 1   | I     | 217 | GLU  | 2.4  |
| 3   | C     | 96  | GLU  | 2.4  |
| 2   | N     | 159 | PHE  | 2.4  |
| 3   | C     | 126 | ASP  | 2.4  |
| 3   | C     | 319 | GLN  | 2.4  |
| 3   | K     | 218 | LYS  | 2.4  |
| 1   | I     | 85  | SER  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 236 | LEU  | 2.4  |
| 3   | O     | 98  | ALA  | 2.4  |
| 1   | Q     | 296 | THR  | 2.4  |
| 2   | J     | 165 | VAL  | 2.4  |
| 3   | G     | 204 | VAL  | 2.4  |
| 3   | O     | 209 | GLY  | 2.4  |
| 1   | Q     | 289 | ALA  | 2.4  |
| 3   | C     | 121 | LYS  | 2.4  |
| 2   | J     | 166 | THR  | 2.3  |
| 2   | N     | 238 | THR  | 2.3  |
| 3   | S     | 209 | GLY  | 2.3  |
| 2   | B     | 88  | ALA  | 2.3  |
| 1   | M     | 219 | ASP  | 2.3  |
| 2   | F     | 161 | LEU  | 2.3  |
| 2   | N     | 237 | GLN  | 2.3  |
| 1   | E     | 224 | ALA  | 2.3  |
| 1   | M     | 215 | LYS  | 2.3  |
| 1   | M     | 287 | THR  | 2.3  |
| 1   | I     | 214 | HIS  | 2.3  |
| 3   | S     | 130 | ASN  | 2.3  |
| 1   | M     | 274 | LYS  | 2.3  |
| 1   | Q     | 281 | GLY  | 2.3  |
| 3   | S     | 317 | LEU  | 2.3  |
| 3   | O     | 85  | LEU  | 2.3  |
| 2   | N     | 233 | SER  | 2.3  |
| 1   | M     | 221 | GLU  | 2.2  |
| 2   | B     | 80  | GLY  | 2.2  |
| 2   | B     | 79  | LYS  | 2.2  |
| 3   | O     | 84  | GLN  | 2.2  |
| 3   | C     | 129 | VAL  | 2.2  |
| 3   | C     | 130 | ASN  | 2.2  |
| 2   | R     | 80  | GLY  | 2.2  |
| 3   | O     | 118 | ALA  | 2.2  |
| 3   | S     | 121 | LYS  | 2.2  |
| 2   | F     | 189 | TYR  | 2.2  |
| 2   | N     | 173 | SER  | 2.2  |
| 2   | F     | 191 | THR  | 2.2  |
| 3   | C     | 169 | TYR  | 2.2  |
| 1   | Q     | 85  | SER  | 2.2  |
| 3   | C     | 112 | SER  | 2.2  |
| 3   | G     | 211 | GLU  | 2.2  |
| 2   | R     | 232 | ALA  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | N     | 83  | CYS  | 2.2  |
| 2   | B     | 207 | GLY  | 2.2  |
| 2   | B     | 89  | ASP  | 2.2  |
| 2   | F     | 86  | PHE  | 2.2  |
| 3   | G     | 94  | THR  | 2.2  |
| 3   | O     | 113 | ASP  | 2.2  |
| 3   | K     | 82  | VAL  | 2.1  |
| 3   | O     | 129 | VAL  | 2.1  |
| 2   | N     | 163 | SER  | 2.1  |
| 3   | K     | 115 | ASP  | 2.1  |
| 2   | R     | 161 | LEU  | 2.1  |
| 1   | E     | 291 | ARG  | 2.1  |
| 1   | A     | 216 | GLN  | 2.1  |
| 3   | S     | 114 | SER  | 2.1  |
| 3   | K     | 207 | GLY  | 2.1  |
| 1   | M     | 292 | THR  | 2.1  |
| 3   | S     | 92  | ILE  | 2.1  |
| 3   | O     | 92  | ILE  | 2.1  |
| 1   | E     | 289 | ALA  | 2.1  |
| 1   | A     | 105 | GLY  | 2.1  |
| 2   | F     | 1   | GLY  | 2.1  |
| 3   | K     | 209 | GLY  | 2.1  |
| 3   | K     | 215 | PRO  | 2.1  |
| 2   | J     | 233 | SER  | 2.1  |
| 3   | K     | 130 | ASN  | 2.1  |
| 2   | F     | 87  | ARG  | 2.1  |
| 2   | B     | 191 | THR  | 2.1  |
| 2   | J     | 97  | GLN  | 2.1  |
| 2   | B     | 237 | GLN  | 2.1  |
| 1   | I     | 105 | GLY  | 2.1  |
| 2   | R     | 1   | GLY  | 2.1  |
| 1   | I     | 221 | GLU  | 2.1  |
| 3   | C     | 140 | TRP  | 2.1  |
| 3   | K     | 123 | THR  | 2.1  |
| 2   | J     | 232 | ALA  | 2.1  |
| 3   | C     | 315 | ALA  | 2.1  |
| 3   | G     | 319 | GLN  | 2.1  |
| 2   | R     | 159 | PHE  | 2.1  |
| 3   | K     | 122 | PRO  | 2.1  |
| 3   | K     | 125 | PRO  | 2.1  |
| 3   | C     | 211 | GLU  | 2.1  |
| 3   | G     | 214 | HIS  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 88  | ALA  | 2.0  |
| 3   | C     | 83  | ALA  | 2.0  |
| 2   | J     | 159 | PHE  | 2.0  |
| 1   | A     | 92  | GLU  | 2.0  |
| 3   | O     | 276 | LEU  | 2.0  |
| 1   | E     | 295 | THR  | 2.0  |
| 2   | N     | 76  | GLN  | 2.0  |
| 1   | I     | 284 | ILE  | 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.