



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:35 PM UTC

PDB ID : 3EEO / pdb\_00003eoo  
Title : 2.9A crystal structure of methyl-isocitrate lyase from Burkholderia pseudomallei  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2008-09-28  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

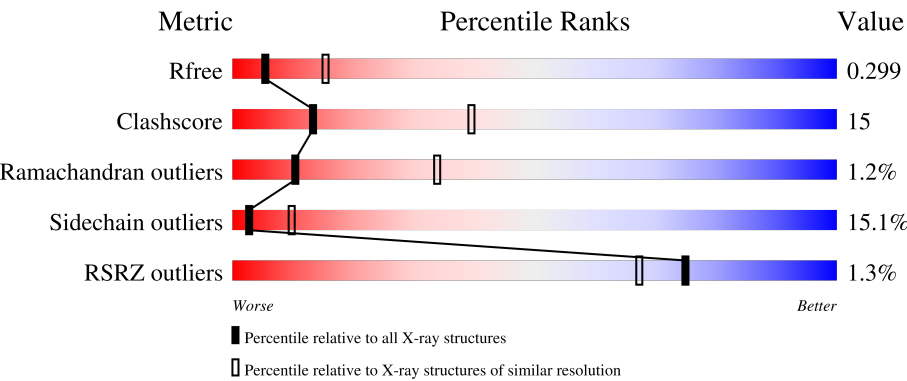
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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     | 298    | <div><div>%</div><div><div></div><div>66%</div><div>26%</div><div>5%</div><div>.</div></div></div> |
| 1   | B     | 298    | <div><div></div><div>67%</div><div>24%</div><div>.</div><div>.</div><div>.</div></div>             |
| 1   | C     | 298    | <div><div>%</div><div><div></div><div>69%</div><div>23%</div><div>.</div><div>.</div></div></div>  |
| 1   | D     | 298    | <div><div></div><div>70%</div><div>20%</div><div>6%</div><div>.</div></div>                        |
| 1   | E     | 298    | <div><div></div><div>66%</div><div>27%</div><div>.</div><div>.</div></div>                         |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 298    |                  |
| 1   | G     | 298    |                  |
| 1   | H     | 298    |                  |
| 1   | I     | 298    |                  |
| 1   | J     | 298    |                  |
| 1   | K     | 298    |                  |
| 1   | L     | 298    |                  |
| 1   | M     | 298    |                  |
| 1   | N     | 298    |                  |
| 1   | O     | 298    |                  |
| 1   | P     | 298    |                  |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 34623 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.

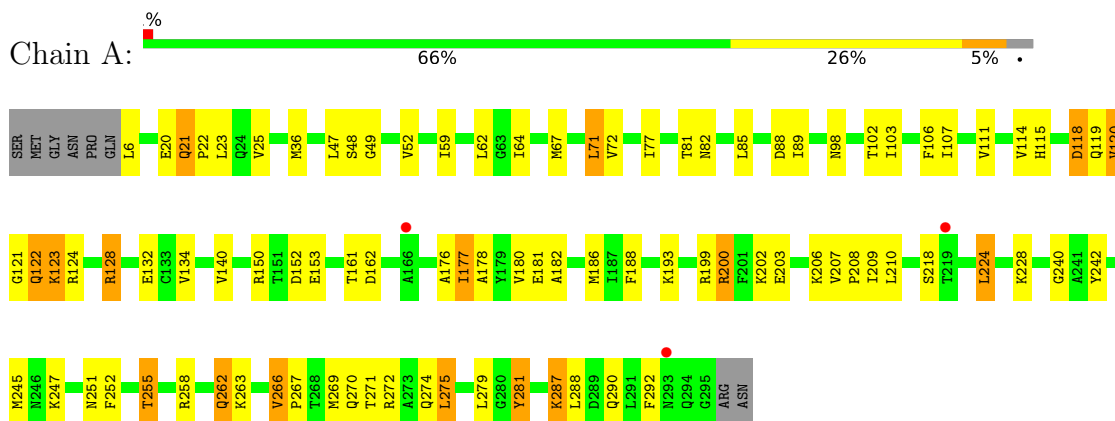
- Molecule 1 is a protein called Methylisocitrate lyase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 290      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2183  | 1379 | 376 | 416 | 12 |         |         |       |
| 1   | B     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2154  | 1362 | 370 | 410 | 12 |         |         |       |
| 1   | C     | 287      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2162  | 1366 | 372 | 412 | 12 |         |         |       |
| 1   | D     | 287      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2162  | 1368 | 371 | 411 | 12 |         |         |       |
| 1   | E     | 288      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2170  | 1372 | 373 | 413 | 12 |         |         |       |
| 1   | F     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2154  | 1362 | 370 | 410 | 12 |         |         |       |
| 1   | G     | 287      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2162  | 1368 | 371 | 411 | 12 |         |         |       |
| 1   | H     | 288      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2170  | 1372 | 373 | 413 | 12 |         |         |       |
| 1   | I     | 289      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2179  | 1377 | 375 | 415 | 12 |         |         |       |
| 1   | J     | 288      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2171  | 1373 | 373 | 413 | 12 |         |         |       |
| 1   | K     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2154  | 1362 | 370 | 410 | 12 |         |         |       |
| 1   | L     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2154  | 1362 | 370 | 410 | 12 |         |         |       |
| 1   | M     | 287      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2162  | 1366 | 372 | 412 | 12 |         |         |       |
| 1   | N     | 287      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2162  | 1368 | 371 | 411 | 12 |         |         |       |
| 1   | O     | 288      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2170  | 1372 | 373 | 413 | 12 |         |         |       |
| 1   | P     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2154  | 1362 | 370 | 410 | 12 |         |         |       |

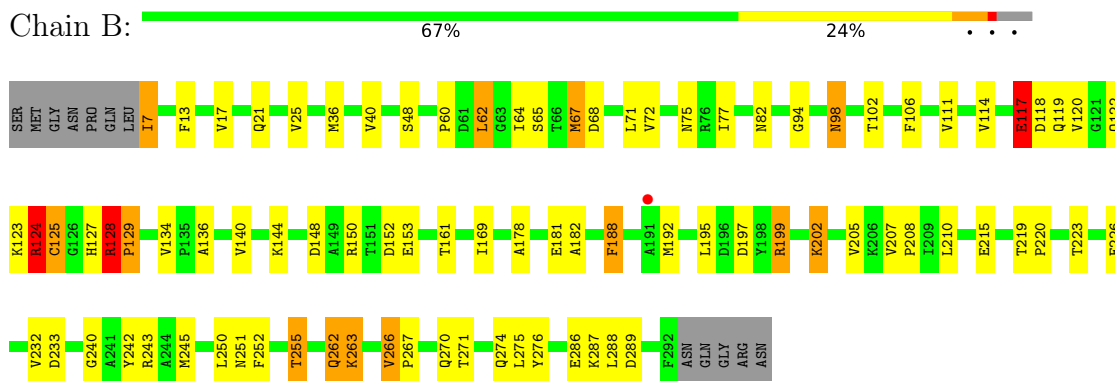
### 3 Residue-property plots [i](#)

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.

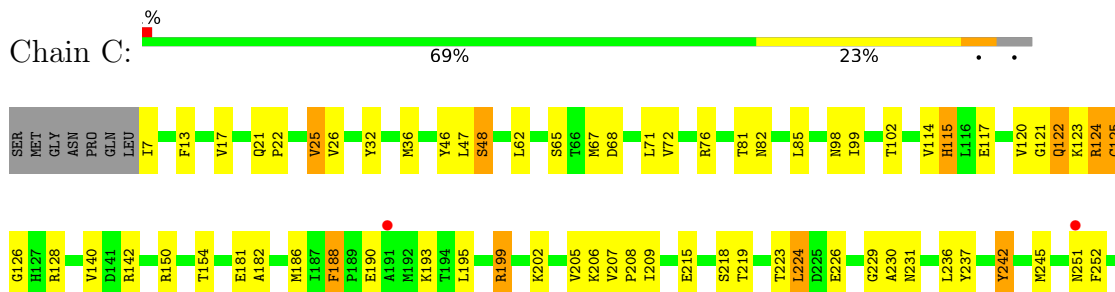
#### • Molecule 1: Methylisocitrate lyase



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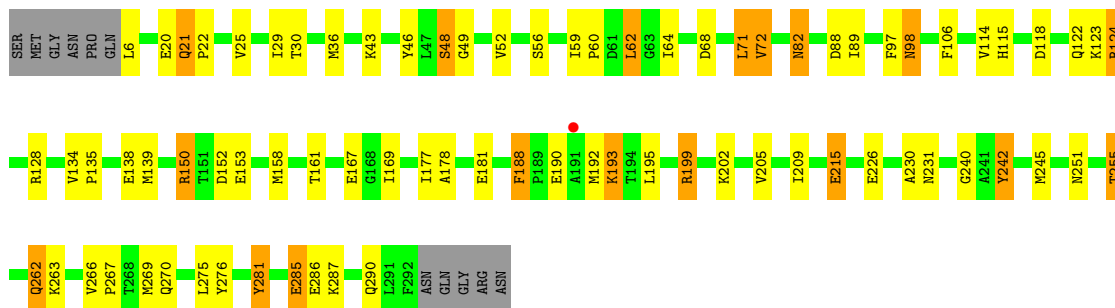


#### • Molecule 1: Methylisocitrate lyase

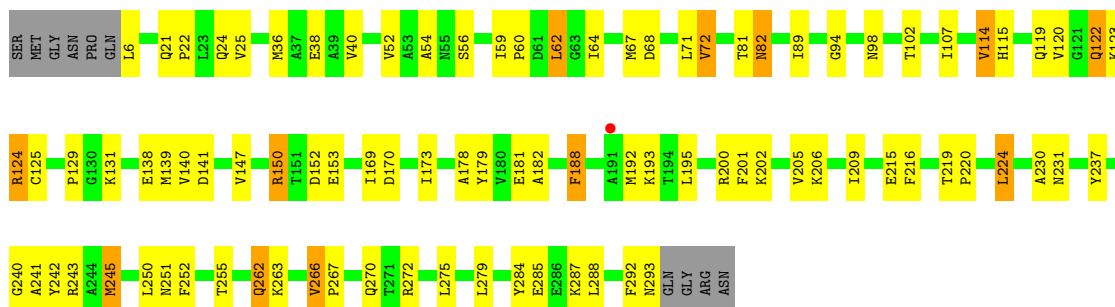




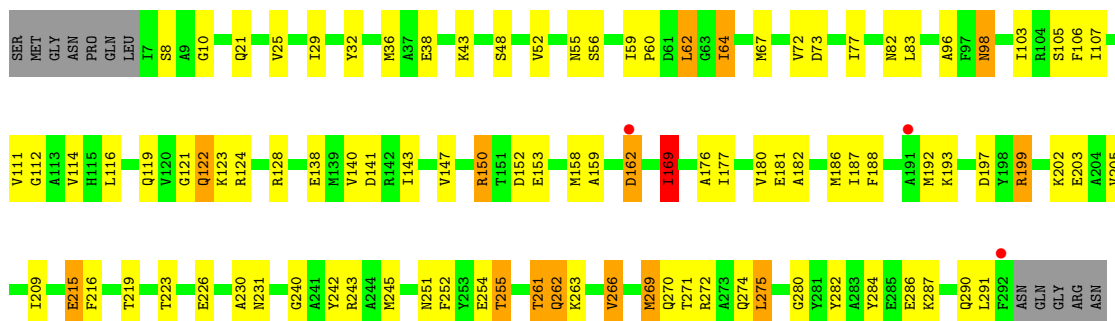
- Molecule 1: Methylisocitrate lyase



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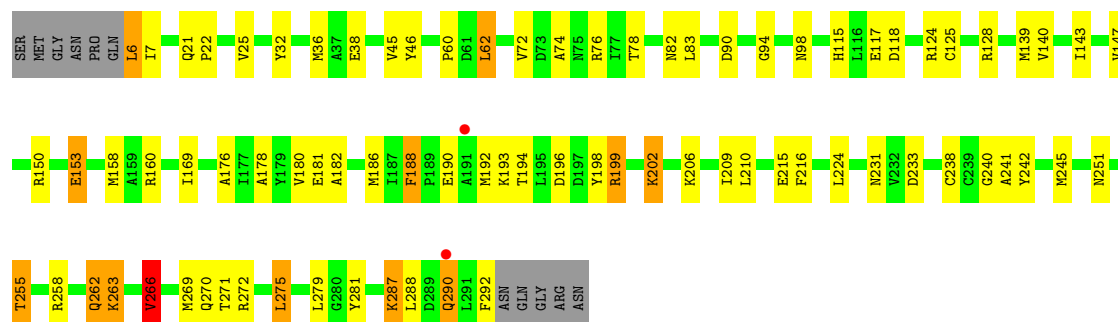


- Molecule 1: Methylisocitrate lyase

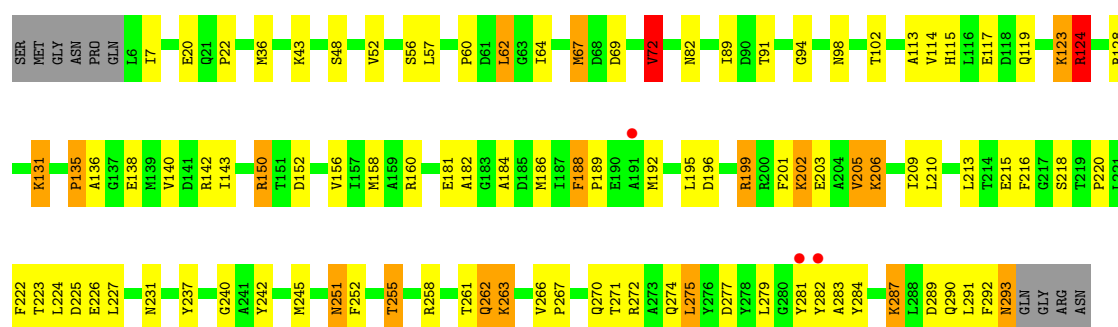


- Molecule 1: Methylisocitrate lyase

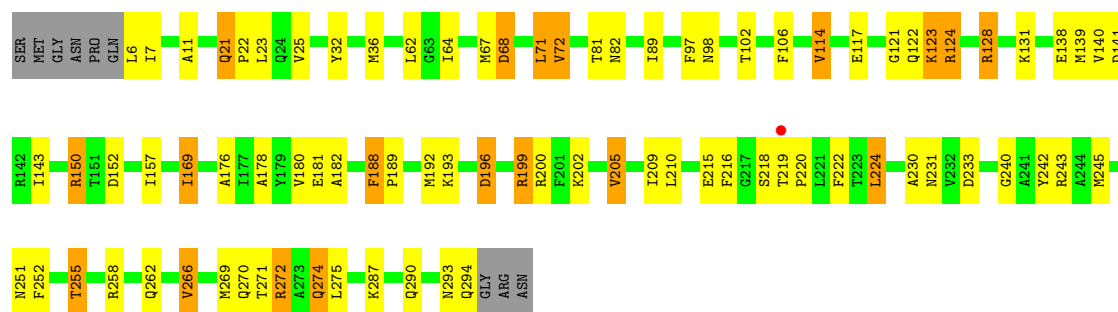




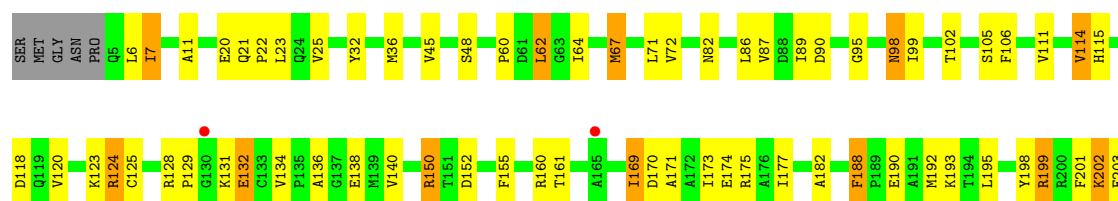
• Molecule 1: Methylisocitrate lyase



• Molecule 1: Methylisocitrate lyase

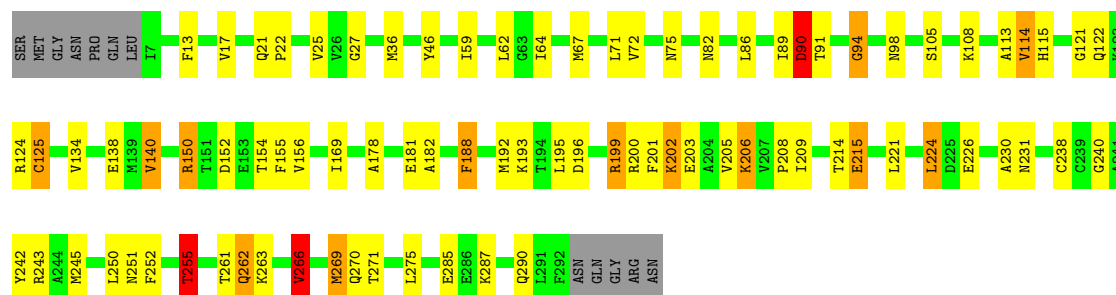


• Molecule 1: Methylisocitrate lyase

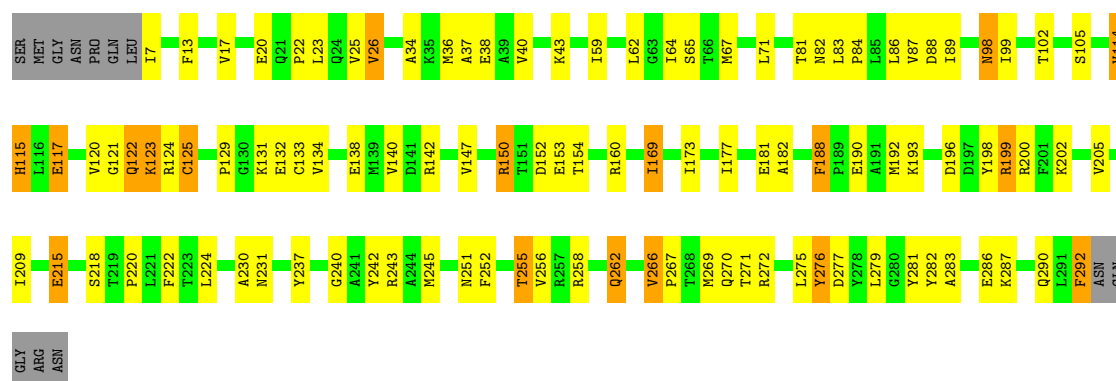




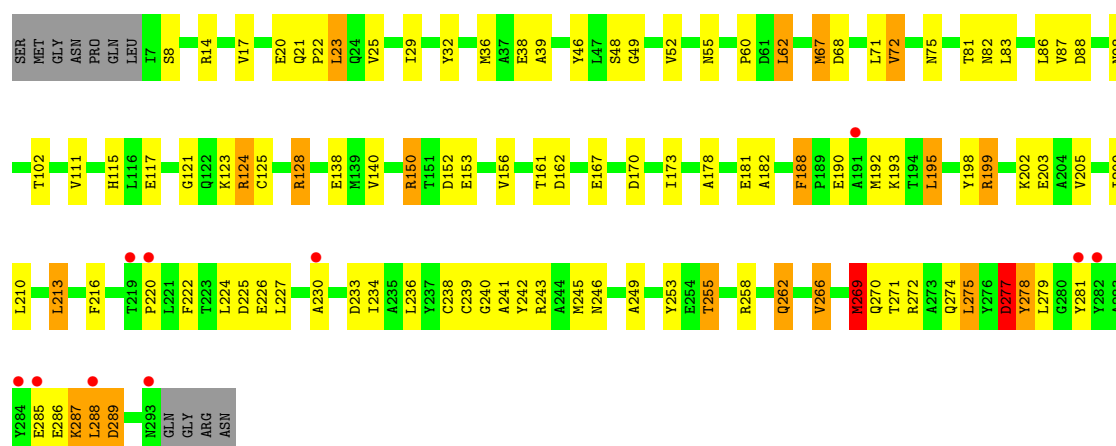
• Molecule 1: Methylisocitrate lyase



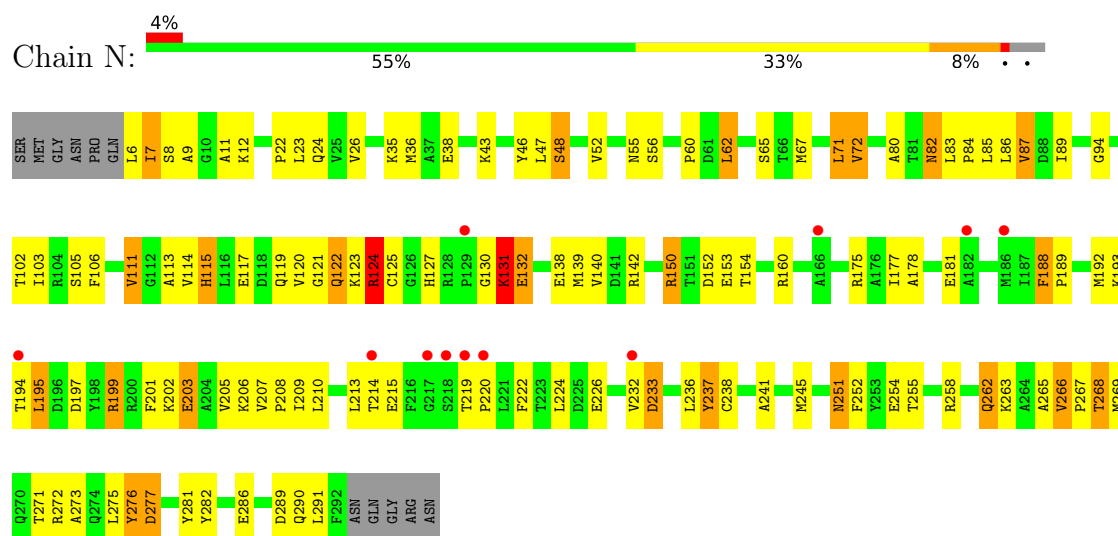
• Molecule 1: Methylisocitrate lyase



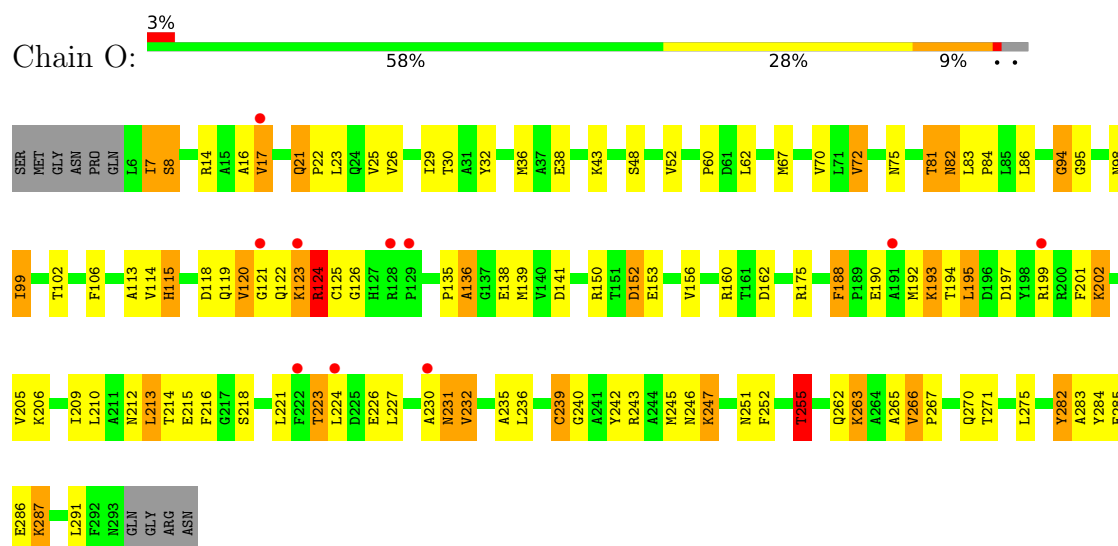
• Molecule 1: Methylisocitrate lyase



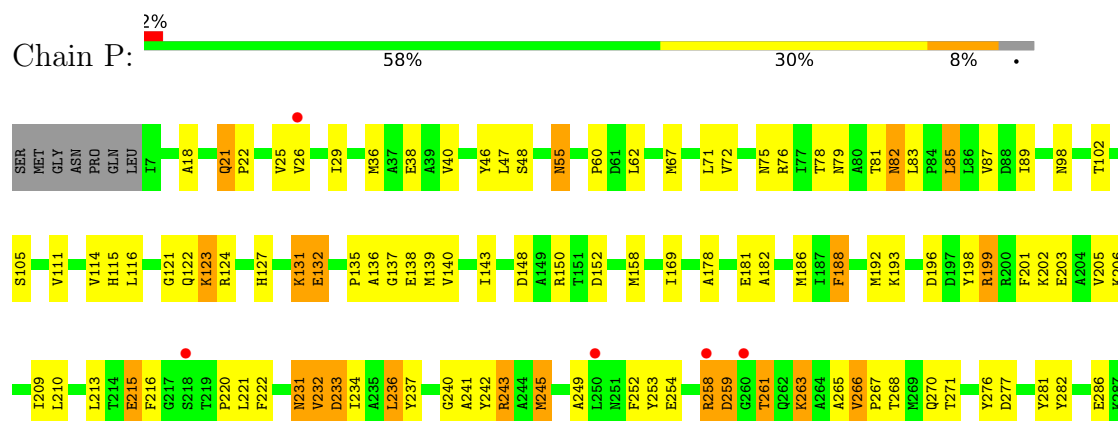
• Molecule 1: Methylisocitrate lyase



• Molecule 1: Methylisocitrate lyase



• Molecule 1: Methylisocitrate lyase



|      |      |      |      |      |     |     |     |     |     |
|------|------|------|------|------|-----|-----|-----|-----|-----|
| L288 | D289 | Q290 | L291 | F292 | ASN | GLN | GLY | ARG | ASN |
|------|------|------|------|------|-----|-----|-----|-----|-----|

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 163.81Å 172.40Å 179.28Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 48.00 – 2.90<br>48.00 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (48.00-2.90)<br>98.4 (48.00-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.49 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.237 , 0.299<br>0.237 , 0.299                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5514 reflections (4.89%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.069                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 23.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 34623                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 48.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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     | 0.87         | 1/2218 (0.0%)   | 1.04        | 5/3005 (0.2%)   |
| 1   | B     | 0.85         | 1/2189 (0.0%)   | 1.07        | 5/2966 (0.2%)   |
| 1   | C     | 0.83         | 0/2197          | 1.04        | 1/2977 (0.0%)   |
| 1   | D     | 0.80         | 0/2197          | 1.02        | 1/2977 (0.0%)   |
| 1   | E     | 0.84         | 0/2205          | 1.07        | 2/2988 (0.1%)   |
| 1   | F     | 0.83         | 1/2189 (0.0%)   | 1.04        | 7/2966 (0.2%)   |
| 1   | G     | 0.80         | 1/2197 (0.0%)   | 1.06        | 2/2977 (0.1%)   |
| 1   | H     | 0.84         | 1/2205 (0.0%)   | 1.04        | 0/2988          |
| 1   | I     | 0.80         | 0/2214          | 1.05        | 3/3000 (0.1%)   |
| 1   | J     | 0.81         | 0/2206          | 1.05        | 5/2989 (0.2%)   |
| 1   | K     | 0.86         | 2/2189 (0.1%)   | 1.08        | 10/2966 (0.3%)  |
| 1   | L     | 0.85         | 1/2189 (0.0%)   | 1.08        | 6/2966 (0.2%)   |
| 1   | M     | 0.90         | 2/2197 (0.1%)   | 1.10        | 6/2977 (0.2%)   |
| 1   | N     | 0.92         | 3/2197 (0.1%)   | 1.15        | 9/2977 (0.3%)   |
| 1   | O     | 0.94         | 4/2205 (0.2%)   | 1.09        | 5/2988 (0.2%)   |
| 1   | P     | 0.89         | 1/2189 (0.0%)   | 1.05        | 3/2966 (0.1%)   |
| All | All   | 0.85         | 18/35183 (0.1%) | 1.07        | 70/47673 (0.1%) |

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

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

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | L     | 266 | VAL  | CA-CB | 10.11 | 1.59        | 1.54     |
| 1   | K     | 266 | VAL  | CA-CB | 8.56  | 1.59        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | N     | 232 | VAL  | CA-CB | 6.57  | 1.61        | 1.54     |
| 1   | O     | 255 | THR  | CA-CB | 6.40  | 1.63        | 1.53     |
| 1   | A     | 120 | VAL  | CA-CB | 6.21  | 1.61        | 1.54     |
| 1   | H     | 72  | VAL  | CA-CB | 5.83  | 1.61        | 1.54     |
| 1   | O     | 214 | THR  | CA-CB | 5.70  | 1.62        | 1.53     |
| 1   | K     | 255 | THR  | CA-CB | 5.66  | 1.62        | 1.53     |
| 1   | M     | 255 | THR  | CA-CB | 5.63  | 1.62        | 1.53     |
| 1   | F     | 266 | VAL  | CA-CB | 5.58  | 1.61        | 1.54     |
| 1   | P     | 40  | VAL  | CA-CB | 5.42  | 1.61        | 1.54     |
| 1   | N     | 72  | VAL  | CA-CB | 5.31  | 1.61        | 1.54     |
| 1   | M     | 266 | VAL  | CA-CB | 5.18  | 1.57        | 1.53     |
| 1   | G     | 266 | VAL  | CA-CB | 5.10  | 1.57        | 1.53     |
| 1   | O     | 223 | THR  | CA-CB | 5.10  | 1.61        | 1.53     |
| 1   | N     | 255 | THR  | CA-CB | 5.06  | 1.61        | 1.53     |
| 1   | B     | 266 | VAL  | CA-CB | 5.04  | 1.60        | 1.54     |
| 1   | O     | 239 | CYS  | CB-SG | -5.02 | 1.64        | 1.81     |

All (70) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 266 | VAL  | N-CA-CB | 8.99  | 116.16      | 110.50   |
| 1   | J     | 90  | ASP  | CB-CA-C | -7.24 | 108.21      | 116.54   |
| 1   | F     | 59  | ILE  | CA-C-N  | 7.17  | 127.21      | 119.89   |
| 1   | F     | 59  | ILE  | C-N-CA  | 7.17  | 127.21      | 119.89   |
| 1   | E     | 292 | PHE  | N-CA-C  | 6.90  | 118.72      | 110.44   |
| 1   | J     | 134 | VAL  | CA-C-N  | -6.85 | 113.25      | 120.03   |
| 1   | J     | 134 | VAL  | C-N-CA  | -6.85 | 113.25      | 120.03   |
| 1   | O     | 115 | HIS  | N-CA-C  | 6.56  | 119.10      | 108.41   |
| 1   | L     | 266 | VAL  | N-CA-CB | 6.55  | 115.56      | 110.45   |
| 1   | K     | 266 | VAL  | N-CA-CB | 6.46  | 114.57      | 110.50   |
| 1   | K     | 269 | MET  | N-CA-C  | 6.36  | 119.26      | 108.90   |
| 1   | I     | 266 | VAL  | CA-C-N  | -6.35 | 113.40      | 120.45   |
| 1   | I     | 266 | VAL  | C-N-CA  | -6.35 | 113.40      | 120.45   |
| 1   | M     | 117 | GLU  | N-CA-C  | 6.30  | 119.29      | 109.52   |
| 1   | B     | 117 | GLU  | N-CA-C  | 6.30  | 119.80      | 109.85   |
| 1   | L     | 169 | ILE  | N-CA-C  | 6.29  | 117.79      | 110.62   |
| 1   | P     | 115 | HIS  | N-CA-C  | 6.29  | 118.70      | 108.26   |
| 1   | A     | 287 | LYS  | N-CA-C  | -6.26 | 105.67      | 113.55   |
| 1   | E     | 115 | HIS  | N-CA-C  | 6.16  | 118.44      | 108.34   |
| 1   | N     | 189 | PRO  | CB-CA-C | -6.12 | 106.73      | 111.87   |
| 1   | L     | 272 | ARG  | N-CA-C  | -6.11 | 104.73      | 111.82   |
| 1   | N     | 72  | VAL  | N-CA-CB | 6.05  | 118.77      | 110.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 200 | ARG  | CB-CA-C | -6.04 | 101.40      | 110.88   |
| 1   | J     | 115 | HIS  | N-CA-C  | 5.99  | 118.69      | 108.02   |
| 1   | I     | 293 | ASN  | N-CA-C  | 5.98  | 116.98      | 108.54   |
| 1   | N     | 117 | GLU  | N-CA-C  | 5.95  | 118.45      | 109.41   |
| 1   | O     | 83  | LEU  | CA-C-N  | -5.92 | 113.87      | 119.85   |
| 1   | O     | 83  | LEU  | C-N-CA  | -5.92 | 113.87      | 119.85   |
| 1   | N     | 266 | VAL  | CA-C-N  | -5.83 | 113.97      | 120.45   |
| 1   | N     | 266 | VAL  | C-N-CA  | -5.83 | 113.97      | 120.45   |
| 1   | K     | 94  | GLY  | N-CA-C  | 5.78  | 119.17      | 110.97   |
| 1   | N     | 115 | HIS  | N-CA-C  | 5.68  | 118.80      | 107.62   |
| 1   | K     | 266 | VAL  | CA-C-N  | -5.66 | 114.28      | 119.82   |
| 1   | K     | 266 | VAL  | C-N-CA  | -5.66 | 114.28      | 119.82   |
| 1   | L     | 115 | HIS  | N-CA-C  | 5.59  | 118.00      | 108.90   |
| 1   | M     | 115 | HIS  | N-CA-C  | 5.57  | 117.97      | 108.90   |
| 1   | A     | 281 | TYR  | N-CA-C  | 5.52  | 118.01      | 111.33   |
| 1   | N     | 87  | VAL  | N-CA-C  | 5.50  | 115.82      | 108.11   |
| 1   | F     | 266 | VAL  | CA-C-N  | -5.50 | 113.95      | 119.56   |
| 1   | F     | 266 | VAL  | C-N-CA  | -5.50 | 113.95      | 119.56   |
| 1   | L     | 131 | LYS  | N-CA-C  | 5.46  | 117.54      | 110.65   |
| 1   | B     | 77  | ILE  | N-CA-C  | 5.45  | 115.65      | 110.42   |
| 1   | P     | 169 | ILE  | N-CA-C  | 5.41  | 116.78      | 110.62   |
| 1   | O     | 94  | GLY  | N-CA-C  | 5.35  | 118.57      | 110.97   |
| 1   | K     | 59  | ILE  | CA-C-N  | 5.34  | 125.64      | 119.92   |
| 1   | K     | 59  | ILE  | C-N-CA  | 5.34  | 125.64      | 119.92   |
| 1   | F     | 8   | SER  | N-CA-C  | 5.32  | 116.95      | 110.41   |
| 1   | N     | 127 | HIS  | N-CA-C  | 5.31  | 117.15      | 110.24   |
| 1   | M     | 266 | VAL  | CA-C-N  | -5.30 | 114.36      | 119.87   |
| 1   | M     | 266 | VAL  | C-N-CA  | -5.30 | 114.36      | 119.87   |
| 1   | D     | 169 | ILE  | N-CA-C  | 5.29  | 116.65      | 110.62   |
| 1   | B     | 128 | ARG  | CA-C-N  | -5.28 | 113.24      | 119.84   |
| 1   | B     | 128 | ARG  | C-N-CA  | -5.28 | 113.24      | 119.84   |
| 1   | F     | 169 | ILE  | N-CA-C  | 5.22  | 117.57      | 111.05   |
| 1   | N     | 111 | VAL  | N-CA-C  | -5.19 | 104.40      | 110.05   |
| 1   | O     | 291 | LEU  | N-CA-C  | 5.18  | 116.73      | 111.14   |
| 1   | A     | 115 | HIS  | N-CA-C  | 5.16  | 116.82      | 108.26   |
| 1   | J     | 169 | ILE  | N-CA-C  | 5.13  | 116.47      | 110.62   |
| 1   | C     | 281 | TYR  | N-CA-C  | 5.12  | 121.70      | 110.80   |
| 1   | M     | 8   | SER  | N-CA-C  | 5.10  | 117.63      | 110.23   |
| 1   | K     | 115 | HIS  | N-CA-C  | 5.09  | 116.71      | 108.41   |
| 1   | G     | 94  | GLY  | N-CA-C  | 5.08  | 118.02      | 110.60   |
| 1   | K     | 169 | ILE  | N-CA-C  | 5.08  | 116.41      | 110.62   |
| 1   | P     | 127 | HIS  | N-CA-C  | 5.08  | 117.41      | 110.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 153 | GLU  | N-CA-C  | 5.08  | 117.55      | 111.71   |
| 1   | F     | 123 | LYS  | N-CA-C  | -5.08 | 102.64      | 109.95   |
| 1   | A     | 77  | ILE  | N-CA-C  | 5.03  | 115.25      | 110.53   |
| 1   | L     | 132 | GLU  | N-CA-C  | 5.01  | 117.57      | 110.50   |
| 1   | K     | 90  | ASP  | CB-CA-C | -5.01 | 110.78      | 116.54   |
| 1   | M     | 266 | VAL  | N-CA-CB | 5.01  | 113.66      | 110.50   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | C     | 121 | GLY  | Peptide |
| 1   | N     | 122 | 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     | 2183  | 0        | 2179     | 57      | 0            |
| 1   | B     | 2154  | 0        | 2151     | 62      | 0            |
| 1   | C     | 2162  | 0        | 2157     | 53      | 0            |
| 1   | D     | 2162  | 0        | 2162     | 60      | 0            |
| 1   | E     | 2170  | 0        | 2168     | 66      | 0            |
| 1   | F     | 2154  | 0        | 2151     | 74      | 0            |
| 1   | G     | 2162  | 0        | 2162     | 64      | 0            |
| 1   | H     | 2170  | 0        | 2168     | 76      | 0            |
| 1   | I     | 2179  | 0        | 2176     | 60      | 0            |
| 1   | J     | 2171  | 0        | 2170     | 68      | 0            |
| 1   | K     | 2154  | 0        | 2151     | 62      | 0            |
| 1   | L     | 2154  | 0        | 2151     | 64      | 0            |
| 1   | M     | 2162  | 0        | 2157     | 97      | 0            |
| 1   | N     | 2162  | 0        | 2162     | 102     | 0            |
| 1   | O     | 2170  | 0        | 2168     | 96      | 0            |
| 1   | P     | 2154  | 0        | 2151     | 85      | 0            |
| All | All   | 34623 | 0        | 34584    | 1023    | 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 15.

All (1023) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:67:MET:HE3   | 1:A:102:THR:HA   | 1.24                     | 1.19              |
| 1:C:67:MET:HE3   | 1:C:102:THR:HA   | 1.27                     | 1.15              |
| 1:I:67:MET:HE3   | 1:I:102:THR:HA   | 1.23                     | 1.14              |
| 1:E:67:MET:HE3   | 1:E:102:THR:HA   | 1.25                     | 1.10              |
| 1:L:199:ARG:HH11 | 1:L:199:ARG:HB2  | 1.14                     | 1.07              |
| 1:I:123:LYS:HD2  | 1:I:124:ARG:H    | 1.12                     | 1.07              |
| 1:I:67:MET:CE    | 1:I:102:THR:HA   | 1.85                     | 1.05              |
| 1:G:199:ARG:HH11 | 1:G:199:ARG:HB2  | 0.88                     | 1.03              |
| 1:G:199:ARG:HB2  | 1:G:199:ARG:NH1  | 1.74                     | 1.02              |
| 1:B:67:MET:HE2   | 1:B:102:THR:HA   | 1.37                     | 1.01              |
| 1:H:199:ARG:HB2  | 1:H:199:ARG:HH11 | 1.25                     | 1.00              |
| 1:G:199:ARG:HH11 | 1:G:199:ARG:CB   | 1.75                     | 0.99              |
| 1:L:67:MET:HE3   | 1:L:102:THR:HA   | 1.43                     | 0.99              |
| 1:O:67:MET:CE    | 1:O:102:THR:HA   | 1.92                     | 0.99              |
| 1:N:67:MET:HE3   | 1:N:102:THR:HA   | 1.41                     | 0.99              |
| 1:J:160:ARG:NH2  | 1:J:190:GLU:HG3  | 1.79                     | 0.98              |
| 1:C:67:MET:CE    | 1:C:102:THR:HA   | 1.96                     | 0.96              |
| 1:H:67:MET:CE    | 1:H:102:THR:HA   | 1.95                     | 0.95              |
| 1:C:223:THR:OG1  | 1:C:226:GLU:HG3  | 1.66                     | 0.95              |
| 1:I:245:MET:HB2  | 1:J:245:MET:HB2  | 1.48                     | 0.93              |
| 1:I:128:ARG:H    | 1:I:128:ARG:HD2  | 1.29                     | 0.93              |
| 1:H:262:GLN:H    | 1:H:262:GLN:HE21 | 0.99                     | 0.93              |
| 1:B:148:ASP:OD2  | 1:D:287:LYS:HE2  | 1.70                     | 0.92              |
| 1:L:262:GLN:H    | 1:L:262:GLN:HE21 | 1.03                     | 0.92              |
| 1:G:251:ASN:O    | 1:G:255:THR:HG23 | 1.70                     | 0.91              |
| 1:C:245:MET:HB2  | 1:D:245:MET:HB2  | 1.51                     | 0.91              |
| 1:A:245:MET:HB2  | 1:B:245:MET:HB2  | 1.52                     | 0.89              |
| 1:O:252:PHE:CE1  | 1:P:240:GLY:HA3  | 2.07                     | 0.89              |
| 1:I:199:ARG:HH11 | 1:I:199:ARG:HB2  | 1.36                     | 0.89              |
| 1:O:67:MET:HE3   | 1:O:102:THR:HA   | 1.55                     | 0.88              |
| 1:N:199:ARG:CB   | 1:N:199:ARG:HH11 | 1.86                     | 0.88              |
| 1:H:20:GLU:OE1   | 1:H:43:LYS:HE3   | 1.74                     | 0.88              |
| 1:P:242:TYR:HA   | 1:P:245:MET:HG3  | 1.54                     | 0.88              |
| 1:E:250:LEU:HD22 | 1:F:36:MET:HE2   | 1.56                     | 0.88              |
| 1:C:122:GLN:HG2  | 1:C:123:LYS:N    | 1.89                     | 0.88              |
| 1:L:199:ARG:HB2  | 1:L:199:ARG:NH1  | 1.88                     | 0.87              |
| 1:I:271:THR:OG1  | 1:I:274:GLN:HG3  | 1.74                     | 0.86              |
| 1:K:245:MET:HB2  | 1:L:245:MET:HB2  | 1.54                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:199:ARG:HH11 | 1:F:199:ARG:HB2  | 1.39                     | 0.86              |
| 1:E:216:PHE:HB2  | 1:F:272:ARG:HG3  | 1.57                     | 0.86              |
| 1:H:22:PRO:HG2   | 1:H:224:LEU:CD2  | 2.06                     | 0.85              |
| 1:A:242:TYR:HA   | 1:A:245:MET:HG2  | 1.57                     | 0.85              |
| 1:G:245:MET:HB2  | 1:H:245:MET:HB2  | 1.58                     | 0.85              |
| 1:E:67:MET:CE    | 1:E:102:THR:HA   | 2.07                     | 0.84              |
| 1:F:251:ASN:O    | 1:F:255:THR:HG23 | 1.77                     | 0.84              |
| 1:A:271:THR:OG1  | 1:A:274:GLN:HG3  | 1.76                     | 0.84              |
| 1:N:205:VAL:HG21 | 1:N:209:ILE:HD11 | 1.57                     | 0.84              |
| 1:B:262:GLN:H    | 1:B:262:GLN:HE21 | 1.23                     | 0.84              |
| 1:H:203:GLU:O    | 1:H:206:LYS:HE3  | 1.77                     | 0.84              |
| 1:N:67:MET:CE    | 1:N:102:THR:HA   | 2.07                     | 0.84              |
| 1:O:160:ARG:HH21 | 1:O:190:GLU:HG3  | 1.42                     | 0.84              |
| 1:F:242:TYR:HA   | 1:F:245:MET:HG2  | 1.57                     | 0.84              |
| 1:O:188:PHE:HZ   | 1:O:212:ASN:HD22 | 1.23                     | 0.84              |
| 1:G:262:GLN:H    | 1:G:262:GLN:HE21 | 1.22                     | 0.84              |
| 1:P:258:ARG:HA   | 1:P:258:ARG:NE   | 1.93                     | 0.83              |
| 1:F:215:GLU:HG2  | 1:F:243:ARG:HH21 | 1.40                     | 0.83              |
| 1:J:275:LEU:HD22 | 1:J:279:LEU:HD22 | 1.60                     | 0.83              |
| 1:N:177:ILE:O    | 1:N:181:GLU:HG2  | 1.79                     | 0.83              |
| 1:A:67:MET:CE    | 1:A:102:THR:HA   | 2.06                     | 0.83              |
| 1:M:67:MET:HE2   | 1:M:102:THR:HA   | 1.60                     | 0.83              |
| 1:C:122:GLN:HG2  | 1:C:123:LYS:H    | 1.40                     | 0.83              |
| 1:E:36:MET:CE    | 1:E:270:GLN:HE22 | 1.92                     | 0.82              |
| 1:J:67:MET:CE    | 1:J:102:THR:HA   | 2.09                     | 0.82              |
| 1:L:22:PRO:HG2   | 1:L:224:LEU:HD22 | 1.62                     | 0.82              |
| 1:B:67:MET:HE2   | 1:B:102:THR:CA   | 2.10                     | 0.82              |
| 1:I:67:MET:HE3   | 1:I:102:THR:CA   | 2.06                     | 0.82              |
| 1:F:223:THR:OG1  | 1:F:226:GLU:HG3  | 1.80                     | 0.81              |
| 1:F:60:PRO:HB2   | 1:F:62:LEU:HD22  | 1.62                     | 0.81              |
| 1:C:242:TYR:HA   | 1:C:245:MET:HG2  | 1.60                     | 0.81              |
| 1:A:262:GLN:H    | 1:A:262:GLN:HE21 | 1.26                     | 0.81              |
| 1:O:205:VAL:HG21 | 1:O:209:ILE:HD11 | 1.61                     | 0.81              |
| 1:N:199:ARG:HH11 | 1:N:199:ARG:HB2  | 1.46                     | 0.80              |
| 1:L:251:ASN:O    | 1:L:255:THR:HG23 | 1.82                     | 0.80              |
| 1:J:98:ASN:N     | 1:J:98:ASN:HD22  | 1.79                     | 0.80              |
| 1:N:219:THR:HG23 | 1:N:222:PHE:HE1  | 1.47                     | 0.80              |
| 1:M:32:TYR:HE2   | 1:M:36:MET:HE3   | 1.47                     | 0.79              |
| 1:N:35:LYS:HE2   | 1:N:80:ALA:O     | 1.82                     | 0.79              |
| 1:K:89:ILE:HD13  | 1:K:114:VAL:HG21 | 1.65                     | 0.79              |
| 1:D:98:ASN:N     | 1:D:98:ASN:HD22  | 1.79                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:46:TYR:HD1   | 1:N:86:LEU:HD23  | 1.47                     | 0.79              |
| 1:G:6:LEU:HD12   | 1:G:7:ILE:H      | 1.45                     | 0.79              |
| 1:E:122:GLN:NE2  | 1:N:94:GLY:HA2   | 1.98                     | 0.79              |
| 1:H:67:MET:HE3   | 1:H:102:THR:HA   | 1.63                     | 0.79              |
| 1:I:252:PHE:CE1  | 1:J:240:GLY:HA3  | 2.19                     | 0.78              |
| 1:M:67:MET:CE    | 1:M:102:THR:HA   | 2.13                     | 0.78              |
| 1:M:238:CYS:HG   | 1:M:239:CYS:HG   | 1.32                     | 0.78              |
| 1:E:252:PHE:CE1  | 1:F:240:GLY:HA3  | 2.19                     | 0.78              |
| 1:K:250:LEU:HB2  | 1:L:36:MET:HE2   | 1.65                     | 0.77              |
| 1:F:36:MET:HE3   | 1:F:270:GLN:HE22 | 1.48                     | 0.77              |
| 1:H:262:GLN:H    | 1:H:262:GLN:NE2  | 1.80                     | 0.77              |
| 1:B:128:ARG:HG2  | 1:B:129:PRO:HD3  | 1.66                     | 0.77              |
| 1:M:241:ALA:O    | 1:M:245:MET:HG2  | 1.84                     | 0.77              |
| 1:C:67:MET:HE3   | 1:C:102:THR:CA   | 2.13                     | 0.76              |
| 1:H:242:TYR:HA   | 1:H:245:MET:HG2  | 1.67                     | 0.76              |
| 1:M:245:MET:HE3  | 1:N:245:MET:HE2  | 1.67                     | 0.76              |
| 1:E:242:TYR:HA   | 1:E:245:MET:HG3  | 1.66                     | 0.76              |
| 1:F:262:GLN:H    | 1:F:262:GLN:HE21 | 1.33                     | 0.76              |
| 1:K:199:ARG:HG2  | 1:K:199:ARG:HH11 | 1.51                     | 0.76              |
| 1:M:22:PRO:HG2   | 1:M:224:LEU:HD23 | 1.66                     | 0.76              |
| 1:M:32:TYR:CE2   | 1:M:36:MET:HE3   | 2.20                     | 0.76              |
| 1:I:36:MET:CE    | 1:I:270:GLN:HE22 | 1.98                     | 0.76              |
| 1:O:192:MET:HE1  | 1:O:201:PHE:CD1  | 2.21                     | 0.76              |
| 1:E:22:PRO:HG2   | 1:E:224:LEU:HD22 | 1.66                     | 0.76              |
| 1:C:262:GLN:H    | 1:C:262:GLN:HE21 | 1.34                     | 0.76              |
| 1:K:242:TYR:HA   | 1:K:245:MET:HG2  | 1.66                     | 0.76              |
| 1:A:36:MET:CE    | 1:A:270:GLN:HE22 | 2.00                     | 0.75              |
| 1:N:130:GLY:O    | 1:N:131:LYS:HB2  | 1.85                     | 0.75              |
| 1:E:293:ASN:HB2  | 1:H:272:ARG:NH2  | 2.02                     | 0.75              |
| 1:B:192:MET:HE3  | 1:B:197:ASP:HB3  | 1.67                     | 0.75              |
| 1:F:98:ASN:H     | 1:F:98:ASN:HD22  | 1.33                     | 0.74              |
| 1:G:240:GLY:HA3  | 1:H:252:PHE:CE1  | 2.22                     | 0.74              |
| 1:J:98:ASN:HD22  | 1:J:98:ASN:H     | 1.35                     | 0.74              |
| 1:A:36:MET:HE2   | 1:B:250:LEU:HB2  | 1.70                     | 0.73              |
| 1:I:199:ARG:HB2  | 1:I:199:ARG:NH1  | 2.02                     | 0.73              |
| 1:M:281:TYR:HD2  | 1:M:281:TYR:O    | 1.70                     | 0.73              |
| 1:G:262:GLN:H    | 1:G:262:GLN:NE2  | 1.87                     | 0.73              |
| 1:E:288:LEU:HD13 | 1:F:128:ARG:HG3  | 1.70                     | 0.73              |
| 1:K:36:MET:CE    | 1:K:270:GLN:HE22 | 2.02                     | 0.73              |
| 1:L:64:ILE:HA    | 1:P:98:ASN:HD21  | 1.54                     | 0.73              |
| 1:D:205:VAL:HG21 | 1:D:209:ILE:HD11 | 1.70                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:98:ASN:HD22  | 1:F:98:ASN:N     | 1.86                     | 0.73              |
| 1:G:6:LEU:HD12   | 1:G:7:ILE:N      | 2.03                     | 0.73              |
| 1:J:242:TYR:HA   | 1:J:245:MET:HG2  | 1.70                     | 0.73              |
| 1:E:241:ALA:O    | 1:E:245:MET:HG2  | 1.88                     | 0.72              |
| 1:F:177:ILE:O    | 1:F:181:GLU:HG2  | 1.88                     | 0.72              |
| 1:I:22:PRO:HG2   | 1:I:224:LEU:HD22 | 1.71                     | 0.72              |
| 1:J:160:ARG:HH21 | 1:J:190:GLU:HG3  | 1.52                     | 0.72              |
| 1:H:251:ASN:O    | 1:H:255:THR:HG23 | 1.90                     | 0.72              |
| 1:O:201:PHE:O    | 1:O:205:VAL:HG22 | 1.89                     | 0.72              |
| 1:A:251:ASN:O    | 1:A:255:THR:HG23 | 1.90                     | 0.72              |
| 1:A:36:MET:HE3   | 1:A:270:GLN:HE22 | 1.55                     | 0.72              |
| 1:N:219:THR:CG2  | 1:N:222:PHE:HE1  | 2.03                     | 0.72              |
| 1:G:242:TYR:HA   | 1:G:245:MET:HG2  | 1.70                     | 0.72              |
| 1:J:67:MET:HE3   | 1:J:102:THR:HA   | 1.71                     | 0.72              |
| 1:K:262:GLN:H    | 1:K:262:GLN:HE21 | 1.37                     | 0.72              |
| 1:I:242:TYR:HA   | 1:I:245:MET:HG2  | 1.72                     | 0.71              |
| 1:N:273:ALA:O    | 1:N:277:ASP:OD1  | 2.09                     | 0.71              |
| 1:M:242:TYR:HA   | 1:M:245:MET:CG   | 2.21                     | 0.71              |
| 1:P:213:LEU:HD12 | 1:P:237:TYR:CE2  | 2.26                     | 0.71              |
| 1:B:98:ASN:H     | 1:B:98:ASN:HD22  | 1.39                     | 0.70              |
| 1:M:22:PRO:HG2   | 1:M:224:LEU:CD2  | 2.21                     | 0.70              |
| 1:O:251:ASN:O    | 1:O:255:THR:HG23 | 1.91                     | 0.70              |
| 1:J:60:PRO:HG2   | 1:J:62:LEU:HD22  | 1.73                     | 0.70              |
| 1:N:67:MET:HE3   | 1:N:102:THR:CA   | 2.17                     | 0.70              |
| 1:B:242:TYR:HA   | 1:B:245:MET:HG2  | 1.73                     | 0.70              |
| 1:E:67:MET:HE3   | 1:E:102:THR:CA   | 2.14                     | 0.70              |
| 1:I:36:MET:HE1   | 1:I:270:GLN:HE22 | 1.56                     | 0.70              |
| 1:J:262:GLN:H    | 1:J:262:GLN:HE21 | 1.40                     | 0.70              |
| 1:G:251:ASN:O    | 1:G:255:THR:CG2  | 2.40                     | 0.70              |
| 1:O:150:ARG:HD3  | 1:O:153:GLU:HA   | 1.73                     | 0.69              |
| 1:E:140:VAL:HG13 | 1:E:182:ALA:HB2  | 1.73                     | 0.69              |
| 1:O:193:LYS:H    | 1:O:193:LYS:HD2  | 1.58                     | 0.69              |
| 1:H:262:GLN:HE21 | 1:H:262:GLN:N    | 1.82                     | 0.69              |
| 1:K:287:LYS:HE3  | 1:K:290:GLN:NE2  | 2.06                     | 0.69              |
| 1:B:271:THR:OG1  | 1:B:274:GLN:HG3  | 1.91                     | 0.69              |
| 1:H:199:ARG:HB2  | 1:H:199:ARG:NH1  | 2.05                     | 0.69              |
| 1:J:290:GLN:O    | 1:J:290:GLN:HG2  | 1.93                     | 0.69              |
| 1:L:262:GLN:H    | 1:L:262:GLN:NE2  | 1.86                     | 0.69              |
| 1:M:262:GLN:H    | 1:M:262:GLN:HE21 | 1.38                     | 0.69              |
| 1:A:123:LYS:H    | 1:A:123:LYS:HD3  | 1.58                     | 0.69              |
| 1:D:36:MET:HE1   | 1:D:270:GLN:HE22 | 1.56                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:67:MET:HE2   | 1:H:102:THR:HA   | 1.74                     | 0.69              |
| 1:H:98:ASN:HD21  | 1:I:64:ILE:HA    | 1.57                     | 0.69              |
| 1:I:230:ALA:O    | 1:I:231:ASN:HB2  | 1.91                     | 0.69              |
| 1:J:140:VAL:HG13 | 1:J:182:ALA:HB2  | 1.75                     | 0.69              |
| 1:F:215:GLU:HG2  | 1:F:243:ARG:NH2  | 2.07                     | 0.69              |
| 1:J:7:ILE:H      | 1:J:7:ILE:HD12   | 1.56                     | 0.69              |
| 1:A:281:TYR:C    | 1:A:281:TYR:CD2  | 2.71                     | 0.68              |
| 1:O:152:ASP:OD1  | 1:O:152:ASP:C    | 2.36                     | 0.68              |
| 1:P:192:MET:HE1  | 1:P:201:PHE:CD1  | 2.28                     | 0.68              |
| 1:D:281:TYR:C    | 1:D:281:TYR:CD2  | 2.71                     | 0.68              |
| 1:E:242:TYR:HA   | 1:E:245:MET:CG   | 2.23                     | 0.68              |
| 1:I:128:ARG:HD2  | 1:I:128:ARG:N    | 2.05                     | 0.68              |
| 1:J:118:ASP:OD1  | 1:J:161:THR:HA   | 1.93                     | 0.68              |
| 1:N:46:TYR:CD1   | 1:N:86:LEU:HD23  | 2.28                     | 0.67              |
| 1:M:32:TYR:HE2   | 1:M:36:MET:CE    | 2.07                     | 0.67              |
| 1:M:195:LEU:HD11 | 1:M:226:GLU:HB3  | 1.75                     | 0.67              |
| 1:B:251:ASN:O    | 1:B:255:THR:CG2  | 2.42                     | 0.67              |
| 1:B:251:ASN:O    | 1:B:255:THR:HG23 | 1.93                     | 0.67              |
| 1:K:199:ARG:HH11 | 1:K:199:ARG:CG   | 2.08                     | 0.67              |
| 1:E:60:PRO:HB2   | 1:E:62:LEU:HD22  | 1.76                     | 0.67              |
| 1:L:147:VAL:HG13 | 1:L:150:ARG:HH12 | 1.58                     | 0.67              |
| 1:O:67:MET:HE3   | 1:O:102:THR:CA   | 2.25                     | 0.67              |
| 1:L:98:ASN:HD22  | 1:L:98:ASN:N     | 1.92                     | 0.67              |
| 1:M:14:ARG:NH1   | 1:M:156:VAL:HG22 | 2.10                     | 0.67              |
| 1:M:281:TYR:O    | 1:M:281:TYR:CD2  | 2.48                     | 0.67              |
| 1:D:251:ASN:O    | 1:D:255:THR:HG23 | 1.95                     | 0.66              |
| 1:G:60:PRO:HB3   | 1:H:281:TYR:CE1  | 2.30                     | 0.66              |
| 1:I:216:PHE:CE1  | 1:J:271:THR:HG22 | 2.29                     | 0.66              |
| 1:M:249:ALA:O    | 1:M:253:TYR:CD2  | 2.48                     | 0.66              |
| 1:E:293:ASN:HB2  | 1:H:272:ARG:HH21 | 1.59                     | 0.66              |
| 1:I:123:LYS:HD2  | 1:I:124:ARG:N    | 1.97                     | 0.66              |
| 1:K:13:PHE:O     | 1:K:17:VAL:HG23  | 1.96                     | 0.66              |
| 1:P:29:ILE:HD13  | 1:P:55:ASN:OD1   | 1.96                     | 0.66              |
| 1:O:210:LEU:HD11 | 1:O:236:LEU:HD22 | 1.78                     | 0.66              |
| 1:E:38:GLU:OE2   | 1:E:82:ASN:ND2   | 2.28                     | 0.66              |
| 1:H:67:MET:HE3   | 1:H:102:THR:CA   | 2.26                     | 0.65              |
| 1:A:240:GLY:HA3  | 1:B:252:PHE:CE1  | 2.30                     | 0.65              |
| 1:B:199:ARG:HH11 | 1:B:199:ARG:HB2  | 1.61                     | 0.65              |
| 1:H:22:PRO:HG2   | 1:H:224:LEU:HD23 | 1.76                     | 0.65              |
| 1:O:202:LYS:HG3  | 1:O:231:ASN:HB3  | 1.77                     | 0.65              |
| 1:D:178:ALA:O    | 1:D:181:GLU:HB2  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:199:ARG:HH11 | 1:M:199:ARG:HB2  | 1.60                     | 0.65              |
| 1:O:82:ASN:ND2   | 1:O:82:ASN:H     | 1.94                     | 0.65              |
| 1:O:192:MET:HE1  | 1:O:201:PHE:HD1  | 1.59                     | 0.65              |
| 1:O:195:LEU:HD21 | 1:O:226:GLU:HB3  | 1.79                     | 0.65              |
| 1:B:36:MET:CE    | 1:B:270:GLN:HE22 | 2.08                     | 0.65              |
| 1:N:60:PRO:HB2   | 1:N:62:LEU:HD22  | 1.79                     | 0.65              |
| 1:C:22:PRO:HG2   | 1:C:224:LEU:HD22 | 1.77                     | 0.65              |
| 1:M:36:MET:HE2   | 1:M:270:GLN:HE22 | 1.62                     | 0.65              |
| 1:N:192:MET:HE1  | 1:N:201:PHE:CD1  | 2.31                     | 0.65              |
| 1:P:199:ARG:HG2  | 1:P:199:ARG:HH11 | 1.62                     | 0.65              |
| 1:E:119:GLN:HE22 | 1:E:131:LYS:HA   | 1.63                     | 0.64              |
| 1:M:195:LEU:HD12 | 1:M:222:PHE:CD2  | 2.32                     | 0.64              |
| 1:O:22:PRO:HG2   | 1:O:224:LEU:CD2  | 2.27                     | 0.64              |
| 1:O:242:TYR:HA   | 1:O:245:MET:HG2  | 1.79                     | 0.64              |
| 1:C:128:ARG:HH21 | 1:D:285:GLU:HG3  | 1.62                     | 0.64              |
| 1:E:252:PHE:CZ   | 1:F:240:GLY:HA3  | 2.32                     | 0.64              |
| 1:O:247:LYS:HE2  | 1:P:268:THR:HA   | 1.80                     | 0.64              |
| 1:M:140:VAL:HG13 | 1:M:182:ALA:HB2  | 1.78                     | 0.64              |
| 1:D:123:LYS:O    | 1:D:124:ARG:O    | 2.15                     | 0.64              |
| 1:O:266:VAL:N    | 1:O:267:PRO:HD2  | 2.13                     | 0.64              |
| 1:B:140:VAL:HG13 | 1:B:182:ALA:HB2  | 1.81                     | 0.63              |
| 1:G:60:PRO:HB2   | 1:G:62:LEU:HD22  | 1.80                     | 0.63              |
| 1:N:199:ARG:HB2  | 1:N:199:ARG:NH1  | 2.12                     | 0.63              |
| 1:F:270:GLN:HG3  | 1:F:274:GLN:HE21 | 1.63                     | 0.63              |
| 1:M:36:MET:CE    | 1:M:270:GLN:HE22 | 2.10                     | 0.63              |
| 1:P:71:LEU:HD11  | 1:P:105:SER:HB3  | 1.81                     | 0.63              |
| 1:C:140:VAL:HG13 | 1:C:182:ALA:HB2  | 1.80                     | 0.63              |
| 1:K:195:LEU:HD21 | 1:K:226:GLU:HB3  | 1.80                     | 0.63              |
| 1:I:89:ILE:HG12  | 1:I:114:VAL:HG13 | 1.81                     | 0.63              |
| 1:D:262:GLN:HE21 | 1:D:262:GLN:H    | 1.46                     | 0.63              |
| 1:H:62:LEU:HD23  | 1:I:97:PHE:CE2   | 2.34                     | 0.62              |
| 1:F:261:THR:HG23 | 1:F:263:LYS:H    | 1.63                     | 0.62              |
| 1:C:26:VAL:HG12  | 1:C:237:TYR:HB2  | 1.81                     | 0.62              |
| 1:O:14:ARG:NH1   | 1:O:156:VAL:HG22 | 2.15                     | 0.62              |
| 1:K:178:ALA:O    | 1:K:181:GLU:HB2  | 2.00                     | 0.62              |
| 1:L:138:GLU:OE1  | 1:L:138:GLU:HA   | 2.00                     | 0.62              |
| 1:F:29:ILE:HD11  | 1:F:245:MET:HE2  | 1.81                     | 0.62              |
| 1:F:98:ASN:N     | 1:F:98:ASN:ND2   | 2.48                     | 0.62              |
| 1:O:82:ASN:H     | 1:O:82:ASN:HD22  | 1.46                     | 0.62              |
| 1:B:64:ILE:HA    | 1:C:98:ASN:HD21  | 1.64                     | 0.61              |
| 1:D:49:GLY:HA3   | 1:D:88:ASP:OD2   | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:205:VAL:CG2  | 1:O:209:ILE:HD11 | 2.29                     | 0.61              |
| 1:C:199:ARG:HG2  | 1:C:199:ARG:HH11 | 1.64                     | 0.61              |
| 1:F:230:ALA:O    | 1:F:231:ASN:HB2  | 1.98                     | 0.61              |
| 1:G:38:GLU:HG3   | 1:G:83:LEU:HG    | 1.83                     | 0.61              |
| 1:H:36:MET:CE    | 1:H:270:GLN:HE22 | 2.14                     | 0.61              |
| 1:I:199:ARG:NH1  | 1:I:230:ALA:HA   | 2.15                     | 0.61              |
| 1:P:38:GLU:HG3   | 1:P:83:LEU:HG    | 1.83                     | 0.61              |
| 1:D:242:TYR:HA   | 1:D:245:MET:HG2  | 1.82                     | 0.61              |
| 1:I:140:VAL:HG13 | 1:I:182:ALA:HB2  | 1.82                     | 0.61              |
| 1:J:201:PHE:O    | 1:J:205:VAL:HG22 | 2.01                     | 0.61              |
| 1:N:199:ARG:HH11 | 1:N:199:ARG:CG   | 2.13                     | 0.61              |
| 1:O:265:ALA:C    | 1:O:267:PRO:HD2  | 2.26                     | 0.61              |
| 1:E:272:ARG:HD2  | 1:F:216:PHE:HB2  | 1.82                     | 0.61              |
| 1:H:192:MET:HE1  | 1:H:201:PHE:CD1  | 2.35                     | 0.61              |
| 1:B:140:VAL:HG12 | 1:B:144:LYS:HE3  | 1.83                     | 0.61              |
| 1:A:178:ALA:HA   | 1:A:181:GLU:HG3  | 1.84                     | 0.60              |
| 1:G:32:TYR:CE2   | 1:G:36:MET:HE3   | 2.36                     | 0.60              |
| 1:M:38:GLU:HG3   | 1:M:83:LEU:HG    | 1.82                     | 0.60              |
| 1:J:275:LEU:CD2  | 1:J:279:LEU:HD22 | 2.30                     | 0.60              |
| 1:B:262:GLN:HE21 | 1:B:262:GLN:N    | 1.98                     | 0.60              |
| 1:A:120:VAL:HA   | 1:A:134:VAL:HG13 | 1.84                     | 0.60              |
| 1:M:210:LEU:HD21 | 1:M:236:LEU:HD23 | 1.83                     | 0.60              |
| 1:D:89:ILE:HD13  | 1:D:114:VAL:HG11 | 1.84                     | 0.60              |
| 1:I:128:ARG:H    | 1:I:128:ARG:CD   | 2.08                     | 0.60              |
| 1:J:36:MET:CE    | 1:J:270:GLN:HE22 | 2.14                     | 0.60              |
| 1:O:245:MET:HB2  | 1:P:245:MET:HB3  | 1.84                     | 0.60              |
| 1:E:169:ILE:O    | 1:E:173:ILE:HG13 | 2.02                     | 0.60              |
| 1:M:245:MET:CE   | 1:N:245:MET:HE2  | 2.32                     | 0.60              |
| 1:F:121:GLY:O    | 1:F:122:GLN:O    | 2.18                     | 0.59              |
| 1:G:117:GLU:HB3  | 1:G:160:ARG:HD3  | 1.83                     | 0.59              |
| 1:K:108:LYS:NZ   | 1:P:79:ASN:OD1   | 2.35                     | 0.59              |
| 1:L:26:VAL:HG12  | 1:L:237:TYR:HB2  | 1.83                     | 0.59              |
| 1:I:240:GLY:HA3  | 1:J:252:PHE:CE1  | 2.37                     | 0.59              |
| 1:J:138:GLU:OE1  | 1:J:138:GLU:HA   | 2.02                     | 0.59              |
| 1:M:249:ALA:O    | 1:M:253:TYR:HD2  | 1.85                     | 0.59              |
| 1:G:140:VAL:HG13 | 1:G:182:ALA:HB2  | 1.84                     | 0.59              |
| 1:K:252:PHE:CE1  | 1:L:240:GLY:HA3  | 2.37                     | 0.59              |
| 1:L:122:GLN:HG2  | 1:P:122:GLN:HB2  | 1.84                     | 0.59              |
| 1:D:98:ASN:N     | 1:D:98:ASN:ND2   | 2.49                     | 0.59              |
| 1:G:147:VAL:HG13 | 1:G:150:ARG:HH12 | 1.67                     | 0.59              |
| 1:E:293:ASN:CB   | 1:H:272:ARG:HH21 | 2.16                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:120:VAL:CG2  | 1:J:132:GLU:HB3  | 2.33                     | 0.59              |
| 1:K:200:ARG:O    | 1:K:203:GLU:HB3  | 2.03                     | 0.59              |
| 1:B:136:ALA:O    | 1:B:140:VAL:HG23 | 2.02                     | 0.59              |
| 1:G:158:MET:HG3  | 1:G:186:MET:HB2  | 1.84                     | 0.59              |
| 1:N:38:GLU:OE2   | 1:N:82:ASN:ND2   | 2.35                     | 0.59              |
| 1:L:262:GLN:HE21 | 1:L:262:GLN:N    | 1.87                     | 0.59              |
| 1:F:242:TYR:HA   | 1:F:245:MET:CG   | 2.29                     | 0.59              |
| 1:M:253:TYR:CD1  | 1:N:26:VAL:HG21  | 2.38                     | 0.59              |
| 1:C:252:PHE:CE1  | 1:D:240:GLY:HA3  | 2.38                     | 0.58              |
| 1:E:24:GLN:HG2   | 1:E:237:TYR:HE1  | 1.68                     | 0.58              |
| 1:B:98:ASN:HD22  | 1:B:98:ASN:N     | 2.00                     | 0.58              |
| 1:J:202:LYS:HE2  | 1:J:231:ASN:O    | 2.02                     | 0.58              |
| 1:J:120:VAL:HG23 | 1:J:132:GLU:HB3  | 1.84                     | 0.58              |
| 1:K:22:PRO:HG2   | 1:K:224:LEU:HD22 | 1.85                     | 0.58              |
| 1:A:242:TYR:HA   | 1:A:245:MET:CG   | 2.30                     | 0.58              |
| 1:D:281:TYR:C    | 1:D:281:TYR:HD2  | 2.12                     | 0.58              |
| 1:O:282:TYR:CZ   | 1:O:286:GLU:HG2  | 2.39                     | 0.58              |
| 1:K:192:MET:HE1  | 1:K:201:PHE:HD1  | 1.67                     | 0.58              |
| 1:M:242:TYR:HA   | 1:M:245:MET:HG3  | 1.85                     | 0.58              |
| 1:N:203:GLU:O    | 1:N:206:LYS:HE2  | 2.04                     | 0.58              |
| 1:G:242:TYR:HA   | 1:G:245:MET:CG   | 2.34                     | 0.58              |
| 1:H:123:LYS:O    | 1:H:124:ARG:C    | 2.47                     | 0.58              |
| 1:L:220:PRO:HB2  | 1:L:222:PHE:CE2  | 2.39                     | 0.58              |
| 1:O:38:GLU:OE2   | 1:O:82:ASN:ND2   | 2.36                     | 0.58              |
| 1:K:192:MET:HE1  | 1:K:201:PHE:CD1  | 2.39                     | 0.58              |
| 1:B:276:TYR:N    | 1:B:276:TYR:HD1  | 2.01                     | 0.58              |
| 1:P:266:VAL:N    | 1:P:267:PRO:HD2  | 2.19                     | 0.58              |
| 1:M:266:VAL:HA   | 1:M:269:MET:HG3  | 1.87                     | 0.57              |
| 1:A:36:MET:CE    | 1:B:250:LEU:HB2  | 2.33                     | 0.57              |
| 1:H:263:LYS:O    | 1:H:266:VAL:HG22 | 2.04                     | 0.57              |
| 1:D:150:ARG:HD3  | 1:D:152:ASP:O    | 2.04                     | 0.57              |
| 1:M:216:PHE:CE2  | 1:N:271:THR:HA   | 2.39                     | 0.57              |
| 1:D:123:LYS:O    | 1:D:124:ARG:C    | 2.47                     | 0.57              |
| 1:G:216:PHE:O    | 1:H:272:ARG:NH1  | 2.37                     | 0.57              |
| 1:D:60:PRO:HG2   | 1:D:62:LEU:HD22  | 1.86                     | 0.57              |
| 1:F:143:ILE:O    | 1:F:147:VAL:HG23 | 2.03                     | 0.57              |
| 1:K:251:ASN:O    | 1:K:255:THR:HG23 | 2.05                     | 0.57              |
| 1:O:70:VAL:HG12  | 1:O:106:PHE:HZ   | 1.69                     | 0.57              |
| 1:D:29:ILE:HD11  | 1:D:245:MET:HE2  | 1.85                     | 0.57              |
| 1:M:253:TYR:CE1  | 1:N:26:VAL:HG21  | 2.40                     | 0.57              |
| 1:B:7:ILE:HD13   | 1:B:7:ILE:N      | 2.20                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:87:VAL:HG23  | 1:M:111:VAL:HG11 | 1.87                     | 0.57              |
| 1:M:178:ALA:O    | 1:M:181:GLU:HB2  | 2.04                     | 0.57              |
| 1:O:120:VAL:HB   | 1:O:123:LYS:HE3  | 1.86                     | 0.56              |
| 1:E:36:MET:HE3   | 1:E:270:GLN:HE22 | 1.66                     | 0.56              |
| 1:C:25:VAL:HG22  | 1:C:236:LEU:HD12 | 1.87                     | 0.56              |
| 1:J:199:ARG:HB2  | 1:J:199:ARG:NH1  | 2.20                     | 0.56              |
| 1:B:263:LYS:HB2  | 1:B:263:LYS:NZ   | 2.21                     | 0.56              |
| 1:I:189:PRO:HB2  | 1:I:192:MET:HE2  | 1.87                     | 0.56              |
| 1:C:47:LEU:HB2   | 1:C:85:LEU:HD11  | 1.88                     | 0.56              |
| 1:P:18:ALA:O     | 1:P:21:GLN:NE2   | 2.39                     | 0.56              |
| 1:E:170:ASP:OD2  | 1:E:200:ARG:NH2  | 2.39                     | 0.56              |
| 1:A:252:PHE:CE1  | 1:B:240:GLY:HA3  | 2.41                     | 0.56              |
| 1:J:199:ARG:HH12 | 1:J:230:ALA:HA   | 1.71                     | 0.56              |
| 1:K:266:VAL:HA   | 1:K:269:MET:HE3  | 1.88                     | 0.56              |
| 1:J:111:VAL:O    | 1:J:155:PHE:HE1  | 1.89                     | 0.56              |
| 1:F:67:MET:HE1   | 1:F:105:SER:OG   | 2.06                     | 0.55              |
| 1:N:119:GLN:OE1  | 1:N:131:LYS:HA   | 2.06                     | 0.55              |
| 1:O:160:ARG:NH2  | 1:O:190:GLU:HG3  | 2.18                     | 0.55              |
| 1:A:150:ARG:HD3  | 1:A:153:GLU:HA   | 1.87                     | 0.55              |
| 1:D:29:ILE:HG13  | 1:D:30:THR:HG23  | 1.88                     | 0.55              |
| 1:I:215:GLU:HG2  | 1:I:243:ARG:HE   | 1.71                     | 0.55              |
| 1:J:282:TYR:O    | 1:J:285:GLU:N    | 2.39                     | 0.55              |
| 1:P:265:ALA:C    | 1:P:267:PRO:HD2  | 2.31                     | 0.55              |
| 1:I:71:LEU:HD23  | 1:I:106:PHE:CE1  | 2.42                     | 0.55              |
| 1:K:140:VAL:HG22 | 1:K:182:ALA:HB2  | 1.88                     | 0.55              |
| 1:K:240:GLY:HA3  | 1:L:252:PHE:CE1  | 2.41                     | 0.55              |
| 1:O:240:GLY:HA3  | 1:P:252:PHE:CE1  | 2.41                     | 0.55              |
| 1:H:223:THR:OG1  | 1:H:226:GLU:HG3  | 2.07                     | 0.55              |
| 1:N:192:MET:SD   | 1:N:197:ASP:HB3  | 2.46                     | 0.55              |
| 1:L:242:TYR:HA   | 1:L:245:MET:HG2  | 1.88                     | 0.55              |
| 1:M:36:MET:CE    | 1:M:270:GLN:NE2  | 2.70                     | 0.55              |
| 1:B:36:MET:HE1   | 1:B:270:GLN:HE22 | 1.71                     | 0.55              |
| 1:B:117:GLU:HG3  | 1:B:119:GLN:HG2  | 1.87                     | 0.55              |
| 1:B:150:ARG:HD3  | 1:B:152:ASP:O    | 2.06                     | 0.55              |
| 1:K:89:ILE:HD13  | 1:K:114:VAL:CG2  | 2.35                     | 0.55              |
| 1:O:82:ASN:ND2   | 1:O:82:ASN:N     | 2.55                     | 0.55              |
| 1:A:118:ASP:OD1  | 1:A:161:THR:HA   | 2.06                     | 0.55              |
| 1:C:123:LYS:HD3  | 1:C:124:ARG:H    | 1.71                     | 0.55              |
| 1:I:266:VAL:HA   | 1:I:269:MET:HG3  | 1.88                     | 0.55              |
| 1:C:252:PHE:CZ   | 1:D:240:GLY:HA3  | 2.41                     | 0.55              |
| 1:N:192:MET:HE1  | 1:N:201:PHE:HD1  | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:215:GLU:HG2  | 1:P:243:ARG:HH21 | 1.71                     | 0.55              |
| 1:B:276:TYR:N    | 1:B:276:TYR:CD1  | 2.73                     | 0.55              |
| 1:I:32:TYR:CZ    | 1:I:36:MET:HE3   | 2.42                     | 0.55              |
| 1:K:287:LYS:HE3  | 1:K:290:GLN:HE22 | 1.69                     | 0.55              |
| 1:M:46:TYR:HD1   | 1:M:86:LEU:HG    | 1.70                     | 0.55              |
| 1:I:7:ILE:HG23   | 1:I:11:ALA:HB3   | 1.89                     | 0.54              |
| 1:O:32:TYR:CE2   | 1:O:36:MET:HE3   | 2.42                     | 0.54              |
| 1:A:119:GLN:HE22 | 1:A:132:GLU:H    | 1.56                     | 0.54              |
| 1:B:128:ARG:HG2  | 1:B:129:PRO:CD   | 2.35                     | 0.54              |
| 1:H:113:ALA:HB2  | 1:H:156:VAL:HB   | 1.89                     | 0.54              |
| 1:H:117:GLU:HB3  | 1:H:160:ARG:HD3  | 1.89                     | 0.54              |
| 1:N:219:THR:HG23 | 1:N:222:PHE:CE1  | 2.37                     | 0.54              |
| 1:P:249:ALA:O    | 1:P:253:TYR:CD2  | 2.61                     | 0.54              |
| 1:E:245:MET:CB   | 1:F:245:MET:HB2  | 2.36                     | 0.54              |
| 1:G:192:MET:HG3  | 1:G:198:TYR:CE1  | 2.43                     | 0.54              |
| 1:N:265:ALA:O    | 1:N:268:THR:HG23 | 2.08                     | 0.54              |
| 1:A:275:LEU:O    | 1:A:279:LEU:HB2  | 2.07                     | 0.54              |
| 1:B:127:HIS:ND1  | 1:B:128:ARG:O    | 2.35                     | 0.54              |
| 1:H:271:THR:HG23 | 1:H:274:GLN:OE1  | 2.07                     | 0.54              |
| 1:K:287:LYS:CE   | 1:K:290:GLN:HE22 | 2.21                     | 0.54              |
| 1:E:243:ARG:HB2  | 1:F:269:MET:HG2  | 1.90                     | 0.54              |
| 1:K:36:MET:HE1   | 1:K:270:GLN:HE22 | 1.73                     | 0.54              |
| 1:L:117:GLU:HB3  | 1:L:160:ARG:HD3  | 1.90                     | 0.54              |
| 1:O:29:ILE:HD13  | 1:O:242:TYR:HB2  | 1.89                     | 0.54              |
| 1:P:85:LEU:HD23  | 1:P:111:VAL:HG22 | 1.88                     | 0.54              |
| 1:F:121:GLY:O    | 1:F:122:GLN:C    | 2.50                     | 0.54              |
| 1:M:170:ASP:HA   | 1:M:173:ILE:HD12 | 1.90                     | 0.54              |
| 1:B:98:ASN:N     | 1:B:98:ASN:ND2   | 2.55                     | 0.54              |
| 1:L:266:VAL:HA   | 1:L:269:MET:HG3  | 1.90                     | 0.54              |
| 1:N:203:GLU:O    | 1:N:206:LYS:CE   | 2.56                     | 0.54              |
| 1:B:223:THR:OG1  | 1:B:226:GLU:HG3  | 2.08                     | 0.54              |
| 1:F:36:MET:HE3   | 1:F:270:GLN:NE2  | 2.22                     | 0.54              |
| 1:G:98:ASN:HD21  | 1:J:64:ILE:HA    | 1.73                     | 0.54              |
| 1:G:143:ILE:O    | 1:G:147:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:281:TYR:C    | 1:A:281:TYR:HD2  | 2.13                     | 0.54              |
| 1:N:86:LEU:HA    | 1:N:113:ALA:O    | 2.08                     | 0.54              |
| 1:C:230:ALA:O    | 1:C:231:ASN:HB2  | 2.08                     | 0.53              |
| 1:J:199:ARG:HB2  | 1:J:199:ARG:HH11 | 1.73                     | 0.53              |
| 1:A:128:ARG:HH22 | 1:B:289:ASP:CG   | 2.16                     | 0.53              |
| 1:J:170:ASP:HA   | 1:J:173:ILE:HD12 | 1.89                     | 0.53              |
| 1:J:195:LEU:HD12 | 1:J:222:PHE:CE2  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:202:LYS:HG2  | 1:K:209:ILE:HG12 | 1.90                     | 0.53              |
| 1:L:147:VAL:HG13 | 1:L:150:ARG:NH1  | 2.22                     | 0.53              |
| 1:B:40:VAL:HG12  | 1:B:40:VAL:O     | 2.07                     | 0.53              |
| 1:I:139:MET:HG3  | 1:I:143:ILE:HD11 | 1.89                     | 0.53              |
| 1:J:98:ASN:N     | 1:J:98:ASN:ND2   | 2.47                     | 0.53              |
| 1:J:120:VAL:HG11 | 1:J:123:LYS:HD3  | 1.89                     | 0.53              |
| 1:P:188:PHE:C    | 1:P:188:PHE:CD2  | 2.86                     | 0.53              |
| 1:B:124:ARG:O    | 1:B:125:CYS:C    | 2.51                     | 0.53              |
| 1:D:36:MET:CE    | 1:D:270:GLN:HE22 | 2.20                     | 0.53              |
| 1:D:193:LYS:HD2  | 1:D:193:LYS:N    | 2.23                     | 0.53              |
| 1:K:86:LEU:HA    | 1:K:113:ALA:O    | 2.08                     | 0.53              |
| 1:L:67:MET:CE    | 1:L:102:THR:HA   | 2.27                     | 0.53              |
| 1:N:233:ASP:N    | 1:N:233:ASP:OD2  | 2.38                     | 0.53              |
| 1:N:237:TYR:N    | 1:N:237:TYR:CD1  | 2.77                     | 0.53              |
| 1:P:67:MET:HE2   | 1:P:102:THR:OG1  | 2.09                     | 0.53              |
| 1:P:291:LEU:HB3  | 1:P:292:PHE:CE2  | 2.44                     | 0.53              |
| 1:E:36:MET:CE    | 1:E:270:GLN:NE2  | 2.67                     | 0.53              |
| 1:E:192:MET:HE1  | 1:E:201:PHE:CD1  | 2.44                     | 0.53              |
| 1:K:205:VAL:HG21 | 1:K:209:ILE:HD11 | 1.90                     | 0.53              |
| 1:M:205:VAL:HG21 | 1:M:209:ILE:HD11 | 1.90                     | 0.53              |
| 1:N:150:ARG:HD3  | 1:N:152:ASP:O    | 2.07                     | 0.53              |
| 1:O:245:MET:HB2  | 1:P:245:MET:CB   | 2.38                     | 0.53              |
| 1:P:188:PHE:C    | 1:P:188:PHE:HD2  | 2.17                     | 0.53              |
| 1:F:106:PHE:HD1  | 1:F:111:VAL:HG21 | 1.74                     | 0.53              |
| 1:C:207:VAL:HB   | 1:C:208:PRO:HD2  | 1.91                     | 0.53              |
| 1:A:152:ASP:OD1  | 1:A:152:ASP:C    | 2.51                     | 0.53              |
| 1:I:251:ASN:O    | 1:I:255:THR:HG23 | 2.08                     | 0.53              |
| 1:K:94:GLY:HA2   | 1:O:122:GLN:NE2  | 2.24                     | 0.53              |
| 1:L:20:GLU:HG2   | 1:L:23:LEU:HA    | 1.91                     | 0.53              |
| 1:M:60:PRO:HG2   | 1:M:62:LEU:HD22  | 1.91                     | 0.53              |
| 1:K:114:VAL:HG13 | 1:K:155:PHE:CZ   | 2.44                     | 0.52              |
| 1:M:255:THR:HG22 | 1:M:258:ARG:HH22 | 1.74                     | 0.52              |
| 1:P:158:MET:HE2  | 1:P:186:MET:CB   | 2.39                     | 0.52              |
| 1:B:120:VAL:HG11 | 1:B:123:LYS:HD2  | 1.91                     | 0.52              |
| 1:O:16:ALA:C     | 1:O:23:LEU:HD22  | 2.34                     | 0.52              |
| 1:O:271:THR:HG22 | 1:P:216:PHE:CE1  | 2.44                     | 0.52              |
| 1:E:262:GLN:H    | 1:E:262:GLN:HE21 | 1.56                     | 0.52              |
| 1:A:22:PRO:HD2   | 1:A:224:LEU:HD22 | 1.91                     | 0.52              |
| 1:N:8:SER:O      | 1:N:11:ALA:N     | 2.41                     | 0.52              |
| 1:O:194:THR:N    | 1:O:197:ASP:OD2  | 2.34                     | 0.52              |
| 1:O:246:ASN:HB3  | 1:P:36:MET:HE1   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:281:TYR:CD2  | 1:A:281:TYR:O    | 2.62                     | 0.52              |
| 1:B:223:THR:H    | 1:B:226:GLU:HG3  | 1.75                     | 0.52              |
| 1:C:271:THR:H    | 1:C:274:GLN:NE2  | 2.07                     | 0.52              |
| 1:D:177:ILE:O    | 1:D:181:GLU:HG2  | 2.09                     | 0.52              |
| 1:F:158:MET:HE2  | 1:F:186:MET:HB2  | 1.90                     | 0.52              |
| 1:I:36:MET:HE2   | 1:I:270:GLN:HE22 | 1.74                     | 0.52              |
| 1:J:210:LEU:HD12 | 1:J:234:ILE:HG21 | 1.90                     | 0.52              |
| 1:L:251:ASN:O    | 1:L:255:THR:CG2  | 2.56                     | 0.52              |
| 1:N:123:LYS:O    | 1:N:124:ARG:C    | 2.52                     | 0.52              |
| 1:L:283:ALA:HA   | 1:L:286:GLU:HG2  | 1.92                     | 0.52              |
| 1:M:36:MET:HE2   | 1:M:270:GLN:NE2  | 2.24                     | 0.52              |
| 1:N:262:GLN:H    | 1:N:262:GLN:HE21 | 1.56                     | 0.52              |
| 1:O:70:VAL:HG12  | 1:O:106:PHE:CZ   | 2.44                     | 0.52              |
| 1:K:215:GLU:HG3  | 1:K:243:ARG:HE   | 1.75                     | 0.52              |
| 1:N:195:LEU:HD21 | 1:N:226:GLU:HB3  | 1.91                     | 0.52              |
| 1:P:47:LEU:HB2   | 1:P:85:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:269:MET:HB3  | 1:B:243:ARG:HB3  | 1.92                     | 0.52              |
| 1:D:68:ASP:O     | 1:D:72:VAL:HG13  | 2.10                     | 0.52              |
| 1:F:282:TYR:CE2  | 1:F:286:GLU:OE2  | 2.62                     | 0.52              |
| 1:C:99:ILE:HD11  | 1:C:142:ARG:HG2  | 1.91                     | 0.52              |
| 1:C:269:MET:HE1  | 1:D:215:GLU:OE2  | 2.10                     | 0.52              |
| 1:E:262:GLN:H    | 1:E:262:GLN:NE2  | 2.08                     | 0.52              |
| 1:L:140:VAL:HG13 | 1:L:182:ALA:HB2  | 1.92                     | 0.52              |
| 1:M:195:LEU:HD12 | 1:M:222:PHE:CE2  | 2.46                     | 0.52              |
| 1:M:39:ALA:CB    | 1:M:278:TYR:HE1  | 2.23                     | 0.51              |
| 1:P:241:ALA:O    | 1:P:245:MET:HG2  | 2.10                     | 0.51              |
| 1:A:98:ASN:HD21  | 1:D:64:ILE:HA    | 1.75                     | 0.51              |
| 1:H:150:ARG:HD3  | 1:H:152:ASP:O    | 2.10                     | 0.51              |
| 1:K:243:ARG:HB3  | 1:L:269:MET:HB3  | 1.92                     | 0.51              |
| 1:J:150:ARG:HD3  | 1:J:152:ASP:O    | 2.09                     | 0.51              |
| 1:J:152:ASP:OD1  | 1:J:152:ASP:C    | 2.51                     | 0.51              |
| 1:P:209:ILE:N    | 1:P:233:ASP:OD2  | 2.31                     | 0.51              |
| 1:I:32:TYR:OH    | 1:I:36:MET:HE3   | 2.10                     | 0.51              |
| 1:A:177:ILE:O    | 1:A:181:GLU:HG3  | 2.10                     | 0.51              |
| 1:G:188:PHE:C    | 1:G:188:PHE:CD2  | 2.87                     | 0.51              |
| 1:K:71:LEU:HD11  | 1:K:105:SER:HB3  | 1.91                     | 0.51              |
| 1:O:188:PHE:HD2  | 1:O:188:PHE:C    | 2.18                     | 0.51              |
| 1:B:94:GLY:HA2   | 1:C:122:GLN:NE2  | 2.25                     | 0.51              |
| 1:L:205:VAL:HG21 | 1:L:209:ILE:HD11 | 1.91                     | 0.51              |
| 1:M:255:THR:HG22 | 1:M:258:ARG:NH2  | 2.26                     | 0.51              |
| 1:D:46:TYR:HE2   | 1:D:48:SER:HB2   | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:245:MET:HB3  | 1:F:245:MET:HB2  | 1.91                     | 0.51              |
| 1:I:128:ARG:N    | 1:I:128:ARG:CD   | 2.70                     | 0.51              |
| 1:J:192:MET:HG3  | 1:J:198:TYR:CE1  | 2.46                     | 0.51              |
| 1:M:199:ARG:HB2  | 1:M:199:ARG:NH1  | 2.25                     | 0.51              |
| 1:F:60:PRO:CB    | 1:F:62:LEU:HD22  | 2.39                     | 0.51              |
| 1:H:94:GLY:HA2   | 1:I:122:GLN:NE2  | 2.25                     | 0.51              |
| 1:F:150:ARG:HD3  | 1:F:152:ASP:O    | 2.11                     | 0.51              |
| 1:G:188:PHE:C    | 1:G:188:PHE:HD2  | 2.19                     | 0.51              |
| 1:J:290:GLN:O    | 1:J:290:GLN:CG   | 2.58                     | 0.51              |
| 1:N:271:THR:OG1  | 1:N:273:ALA:HB3  | 2.10                     | 0.51              |
| 1:B:266:VAL:N    | 1:B:267:PRO:CD   | 2.74                     | 0.51              |
| 1:C:281:TYR:C    | 1:C:281:TYR:CD2  | 2.89                     | 0.51              |
| 1:P:258:ARG:HA   | 1:P:258:ARG:HE   | 1.74                     | 0.51              |
| 1:G:46:TYR:CE2   | 1:G:238:CYS:HB2  | 2.45                     | 0.50              |
| 1:O:67:MET:HE3   | 1:O:102:THR:OG1  | 2.11                     | 0.50              |
| 1:K:113:ALA:HB2  | 1:K:156:VAL:HB   | 1.94                     | 0.50              |
| 1:F:73:ASP:O     | 1:F:77:ILE:HG13  | 2.11                     | 0.50              |
| 1:G:22:PRO:HG2   | 1:G:224:LEU:HD22 | 1.93                     | 0.50              |
| 1:K:199:ARG:HG2  | 1:K:199:ARG:NH1  | 2.22                     | 0.50              |
| 1:L:125:CYS:HB3  | 1:P:138:GLU:OE2  | 2.11                     | 0.50              |
| 1:E:24:GLN:HG2   | 1:E:237:TYR:CE1  | 2.46                     | 0.50              |
| 1:I:219:THR:HG22 | 1:I:220:PRO:O    | 2.11                     | 0.50              |
| 1:M:202:LYS:HE3  | 1:M:233:ASP:OD2  | 2.11                     | 0.50              |
| 1:O:67:MET:HE2   | 1:O:102:THR:HA   | 1.87                     | 0.50              |
| 1:A:85:LEU:O     | 1:A:111:VAL:HG13 | 2.11                     | 0.50              |
| 1:C:99:ILE:CD1   | 1:C:142:ARG:HG2  | 2.41                     | 0.50              |
| 1:N:175:ARG:O    | 1:N:178:ALA:HB3  | 2.11                     | 0.50              |
| 1:B:120:VAL:HG11 | 1:B:123:LYS:CD   | 2.42                     | 0.50              |
| 1:F:67:MET:CE    | 1:F:105:SER:CB   | 2.89                     | 0.50              |
| 1:I:36:MET:HE1   | 1:I:270:GLN:NE2  | 2.24                     | 0.50              |
| 1:L:169:ILE:HG12 | 1:L:173:ILE:HD11 | 1.93                     | 0.50              |
| 1:N:89:ILE:HG12  | 1:N:114:VAL:HG22 | 1.93                     | 0.50              |
| 1:C:188:PHE:C    | 1:C:188:PHE:CD2  | 2.90                     | 0.50              |
| 1:C:215:GLU:CD   | 1:C:215:GLU:H    | 2.20                     | 0.50              |
| 1:F:140:VAL:HG13 | 1:F:182:ALA:HB2  | 1.92                     | 0.50              |
| 1:K:188:PHE:C    | 1:K:188:PHE:CD2  | 2.88                     | 0.50              |
| 1:O:188:PHE:C    | 1:O:188:PHE:CD2  | 2.88                     | 0.50              |
| 1:C:13:PHE:O     | 1:C:17:VAL:HG23  | 2.12                     | 0.50              |
| 1:K:188:PHE:C    | 1:K:188:PHE:HD2  | 2.19                     | 0.50              |
| 1:M:216:PHE:HB2  | 1:N:272:ARG:HG3  | 1.93                     | 0.50              |
| 1:O:262:GLN:NE2  | 1:P:221:LEU:HB3  | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:47:LEU:HD23  | 1:N:87:VAL:HG13  | 1.93                     | 0.50              |
| 1:N:236:LEU:HD21 | 1:N:238:CYS:HB3  | 1.94                     | 0.50              |
| 1:A:49:GLY:HA3   | 1:A:88:ASP:OD2   | 2.12                     | 0.49              |
| 1:G:36:MET:HE2   | 1:G:270:GLN:HE22 | 1.77                     | 0.49              |
| 1:J:263:LYS:O    | 1:J:266:VAL:HG13 | 2.12                     | 0.49              |
| 1:L:192:MET:HB2  | 1:L:198:TYR:CE2  | 2.47                     | 0.49              |
| 1:M:123:LYS:O    | 1:M:124:ARG:C    | 2.55                     | 0.49              |
| 1:M:150:ARG:HD3  | 1:M:152:ASP:O    | 2.12                     | 0.49              |
| 1:E:284:TYR:CD1  | 1:F:60:PRO:HG3   | 2.47                     | 0.49              |
| 1:G:210:LEU:HD23 | 1:G:210:LEU:C    | 2.37                     | 0.49              |
| 1:N:220:PRO:HD2  | 1:N:222:PHE:CZ   | 2.47                     | 0.49              |
| 1:P:192:MET:HE1  | 1:P:201:PHE:HD1  | 1.72                     | 0.49              |
| 1:P:192:MET:HG3  | 1:P:198:TYR:CE1  | 2.47                     | 0.49              |
| 1:F:270:GLN:HG3  | 1:F:274:GLN:NE2  | 2.27                     | 0.49              |
| 1:D:20:GLU:OE1   | 1:D:43:LYS:HE2   | 2.11                     | 0.49              |
| 1:E:59:ILE:CD1   | 1:E:64:ILE:HB    | 2.42                     | 0.49              |
| 1:L:290:GLN:O    | 1:L:290:GLN:HG2  | 2.12                     | 0.49              |
| 1:N:71:LEU:HD11  | 1:N:105:SER:HB3  | 1.93                     | 0.49              |
| 1:O:223:THR:OG1  | 1:O:226:GLU:HG3  | 2.13                     | 0.49              |
| 1:J:95:GLY:O     | 1:J:99:ILE:HG13  | 2.12                     | 0.49              |
| 1:M:213:LEU:HD11 | 1:M:227:LEU:HD11 | 1.94                     | 0.49              |
| 1:O:284:TYR:CE1  | 1:P:60:PRO:CD    | 2.95                     | 0.49              |
| 1:F:64:ILE:HA    | 1:M:98:ASN:HD21  | 1.77                     | 0.49              |
| 1:J:136:ALA:HB2  | 1:J:175:ARG:HG2  | 1.93                     | 0.49              |
| 1:J:171:ALA:O    | 1:J:174:GLU:HB3  | 2.12                     | 0.49              |
| 1:P:139:MET:HE3  | 1:P:143:ILE:HD11 | 1.94                     | 0.49              |
| 1:P:258:ARG:HB3  | 1:P:259:ASP:OD1  | 2.12                     | 0.49              |
| 1:G:90:ASP:HA    | 1:G:117:GLU:OE1  | 2.13                     | 0.49              |
| 1:M:49:GLY:HA3   | 1:M:88:ASP:OD2   | 2.12                     | 0.49              |
| 1:F:10:GLY:HA2   | 1:F:112:GLY:O    | 2.12                     | 0.49              |
| 1:H:136:ALA:O    | 1:H:140:VAL:HG23 | 2.12                     | 0.49              |
| 1:J:199:ARG:NH1  | 1:J:230:ALA:HA   | 2.28                     | 0.49              |
| 1:B:13:PHE:O     | 1:B:17:VAL:HG23  | 2.13                     | 0.49              |
| 1:O:22:PRO:HG2   | 1:O:224:LEU:HD23 | 1.94                     | 0.49              |
| 1:P:89:ILE:HG12  | 1:P:114:VAL:HG22 | 1.94                     | 0.49              |
| 1:A:22:PRO:HD3   | 1:A:228:LYS:HB2  | 1.95                     | 0.49              |
| 1:E:188:PHE:C    | 1:E:188:PHE:CD2  | 2.91                     | 0.49              |
| 1:L:71:LEU:HD21  | 1:L:105:SER:HB3  | 1.95                     | 0.49              |
| 1:H:64:ILE:HA    | 1:I:98:ASN:HD21  | 1.78                     | 0.48              |
| 1:I:176:ALA:O    | 1:I:180:VAL:HG23 | 2.13                     | 0.48              |
| 1:J:160:ARG:CZ   | 1:J:190:GLU:HG3  | 2.41                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:169:ILE:HG12 | 1:J:173:ILE:HD11 | 1.95                     | 0.48              |
| 1:P:220:PRO:HD2  | 1:P:222:PHE:CZ   | 2.48                     | 0.48              |
| 1:A:103:ILE:O    | 1:A:107:ILE:HG13 | 2.13                     | 0.48              |
| 1:A:266:VAL:N    | 1:A:267:PRO:CD   | 2.75                     | 0.48              |
| 1:G:290:GLN:O    | 1:G:290:GLN:HG2  | 2.13                     | 0.48              |
| 1:H:275:LEU:HD22 | 1:H:279:LEU:HD11 | 1.95                     | 0.48              |
| 1:L:13:PHE:O     | 1:L:17:VAL:HG23  | 2.13                     | 0.48              |
| 1:I:205:VAL:HG21 | 1:I:209:ILE:HD11 | 1.94                     | 0.48              |
| 1:L:59:ILE:HD12  | 1:L:64:ILE:HB    | 1.94                     | 0.48              |
| 1:M:188:PHE:C    | 1:M:188:PHE:CD2  | 2.91                     | 0.48              |
| 1:O:72:VAL:HG22  | 1:P:76:ARG:HH22  | 1.79                     | 0.48              |
| 1:O:119:GLN:HE22 | 1:O:162:ASP:HB2  | 1.78                     | 0.48              |
| 1:P:178:ALA:O    | 1:P:181:GLU:HB2  | 2.12                     | 0.48              |
| 1:I:22:PRO:HG2   | 1:I:224:LEU:CD2  | 2.42                     | 0.48              |
| 1:K:208:PRO:O    | 1:K:209:ILE:HD13 | 2.14                     | 0.48              |
| 1:O:263:LYS:O    | 1:O:266:VAL:HG13 | 2.14                     | 0.48              |
| 1:P:135:PRO:O    | 1:P:136:ALA:C    | 2.56                     | 0.48              |
| 1:P:276:TYR:N    | 1:P:276:TYR:HD1  | 2.11                     | 0.48              |
| 1:H:242:TYR:HA   | 1:H:245:MET:CG   | 2.40                     | 0.48              |
| 1:M:233:ASP:C    | 1:M:234:ILE:HG13 | 2.38                     | 0.48              |
| 1:N:203:GLU:O    | 1:N:206:LYS:NZ   | 2.45                     | 0.48              |
| 1:A:89:ILE:HG12  | 1:A:114:VAL:HG22 | 1.95                     | 0.48              |
| 1:E:178:ALA:O    | 1:E:181:GLU:HB2  | 2.13                     | 0.48              |
| 1:F:52:VAL:O     | 1:F:56:SER:HB2   | 2.13                     | 0.48              |
| 1:C:266:VAL:N    | 1:C:267:PRO:CD   | 2.76                     | 0.48              |
| 1:E:68:ASP:O     | 1:E:72:VAL:HG13  | 2.14                     | 0.48              |
| 1:E:251:ASN:O    | 1:E:255:THR:HG23 | 2.13                     | 0.48              |
| 1:G:115:HIS:HA   | 1:G:158:MET:O    | 2.14                     | 0.48              |
| 1:J:89:ILE:HG12  | 1:J:114:VAL:HG13 | 1.94                     | 0.48              |
| 1:M:222:PHE:HA   | 1:M:226:GLU:OE1  | 2.14                     | 0.48              |
| 1:M:240:GLY:HA3  | 1:N:252:PHE:CE1  | 2.49                     | 0.48              |
| 1:O:216:PHE:CE1  | 1:P:271:THR:HG22 | 2.48                     | 0.48              |
| 1:P:199:ARG:HH11 | 1:P:199:ARG:CG   | 2.27                     | 0.48              |
| 1:B:148:ASP:OD2  | 1:D:287:LYS:CE   | 2.53                     | 0.48              |
| 1:G:38:GLU:HG3   | 1:G:83:LEU:CG    | 2.43                     | 0.48              |
| 1:L:88:ASP:OD1   | 1:L:115:HIS:CE1  | 2.67                     | 0.48              |
| 1:N:131:LYS:O    | 1:N:132:GLU:CB   | 2.61                     | 0.48              |
| 1:P:140:VAL:HG13 | 1:P:182:ALA:HB2  | 1.95                     | 0.48              |
| 1:A:71:LEU:HD23  | 1:A:106:PHE:CE1  | 2.49                     | 0.48              |
| 1:A:140:VAL:HG13 | 1:A:182:ALA:HB2  | 1.95                     | 0.48              |
| 1:C:215:GLU:HG3  | 1:D:269:MET:SD   | 2.54                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:195:LEU:HD21 | 1:D:226:GLU:HB3  | 1.96                     | 0.48              |
| 1:F:38:GLU:HA    | 1:F:83:LEU:HD11  | 1.95                     | 0.48              |
| 1:L:188:PHE:C    | 1:L:188:PHE:HD2  | 2.22                     | 0.48              |
| 1:M:262:GLN:NE2  | 1:N:237:TYR:CD2  | 2.81                     | 0.48              |
| 1:P:249:ALA:O    | 1:P:253:TYR:HD2  | 1.97                     | 0.48              |
| 1:H:266:VAL:N    | 1:H:267:PRO:CD   | 2.76                     | 0.48              |
| 1:D:230:ALA:O    | 1:D:231:ASN:HB2  | 2.14                     | 0.47              |
| 1:H:156:VAL:HG11 | 1:H:186:MET:HE3  | 1.96                     | 0.47              |
| 1:L:43:LYS:O     | 1:L:84:PRO:HD2   | 2.14                     | 0.47              |
| 1:L:188:PHE:C    | 1:L:188:PHE:CD2  | 2.92                     | 0.47              |
| 1:M:29:ILE:HG21  | 1:M:55:ASN:ND2   | 2.28                     | 0.47              |
| 1:O:72:VAL:HG22  | 1:P:76:ARG:NH2   | 2.29                     | 0.47              |
| 1:P:158:MET:HE2  | 1:P:186:MET:HB2  | 1.96                     | 0.47              |
| 1:F:205:VAL:HG21 | 1:F:209:ILE:HD11 | 1.95                     | 0.47              |
| 1:K:114:VAL:CG1  | 1:K:155:PHE:HZ   | 2.27                     | 0.47              |
| 1:L:150:ARG:HD3  | 1:L:153:GLU:HA   | 1.94                     | 0.47              |
| 1:O:188:PHE:HZ   | 1:O:212:ASN:ND2  | 2.02                     | 0.47              |
| 1:P:276:TYR:N    | 1:P:276:TYR:CD1  | 2.82                     | 0.47              |
| 1:G:279:LEU:HA   | 1:G:279:LEU:HD12 | 1.50                     | 0.47              |
| 1:I:124:ARG:HH12 | 1:I:128:ARG:HH21 | 1.63                     | 0.47              |
| 1:J:188:PHE:C    | 1:J:188:PHE:CD2  | 2.92                     | 0.47              |
| 1:M:238:CYS:SG   | 1:M:239:CYS:N    | 2.87                     | 0.47              |
| 1:O:17:VAL:HG23  | 1:O:23:LEU:HD23  | 1.97                     | 0.47              |
| 1:F:169:ILE:O    | 1:F:169:ILE:HG13 | 2.13                     | 0.47              |
| 1:G:36:MET:CE    | 1:G:270:GLN:HE22 | 2.27                     | 0.47              |
| 1:O:86:LEU:HA    | 1:O:113:ALA:O    | 2.14                     | 0.47              |
| 1:G:176:ALA:O    | 1:G:180:VAL:HG23 | 2.14                     | 0.47              |
| 1:K:114:VAL:CG1  | 1:K:155:PHE:CZ   | 2.97                     | 0.47              |
| 1:A:98:ASN:ND2   | 1:D:64:ILE:HA    | 2.29                     | 0.47              |
| 1:A:177:ILE:O    | 1:A:181:GLU:CG   | 2.62                     | 0.47              |
| 1:D:98:ASN:HD22  | 1:D:98:ASN:H     | 1.58                     | 0.47              |
| 1:G:118:ASP:HB3  | 1:G:139:MET:HG2  | 1.97                     | 0.47              |
| 1:K:150:ARG:HD3  | 1:K:152:ASP:O    | 2.15                     | 0.47              |
| 1:L:64:ILE:HA    | 1:P:98:ASN:ND2   | 2.27                     | 0.47              |
| 1:M:242:TYR:HA   | 1:M:245:MET:HG2  | 1.95                     | 0.47              |
| 1:N:71:LEU:HA    | 1:N:71:LEU:HD23  | 1.13                     | 0.47              |
| 1:N:262:GLN:HG3  | 1:N:269:MET:HE1  | 1.96                     | 0.47              |
| 1:N:263:LYS:O    | 1:N:266:VAL:HG22 | 2.14                     | 0.47              |
| 1:D:266:VAL:HG22 | 1:D:267:PRO:HD3  | 1.97                     | 0.47              |
| 1:H:115:HIS:HA   | 1:H:158:MET:O    | 2.15                     | 0.47              |
| 1:L:266:VAL:N    | 1:L:267:PRO:HD2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:262:GLN:HE21 | 1:M:262:GLN:N    | 2.09                     | 0.47              |
| 1:D:89:ILE:HD13  | 1:D:114:VAL:CG1  | 2.44                     | 0.47              |
| 1:E:122:GLN:HB2  | 1:N:122:GLN:HB2  | 1.97                     | 0.47              |
| 1:F:36:MET:CE    | 1:F:270:GLN:HE22 | 2.24                     | 0.47              |
| 1:H:20:GLU:OE1   | 1:H:43:LYS:CE    | 2.53                     | 0.47              |
| 1:L:276:TYR:HA   | 1:L:281:TYR:HD1  | 1.79                     | 0.47              |
| 1:A:200:ARG:O    | 1:A:203:GLU:HB3  | 2.14                     | 0.47              |
| 1:E:188:PHE:C    | 1:E:188:PHE:HD2  | 2.22                     | 0.47              |
| 1:F:67:MET:HE1   | 1:F:105:SER:CB   | 2.45                     | 0.47              |
| 1:J:71:LEU:HD11  | 1:J:105:SER:HB3  | 1.96                     | 0.47              |
| 1:M:138:GLU:OE1  | 1:M:138:GLU:HA   | 2.15                     | 0.47              |
| 1:A:122:GLN:HB2  | 1:D:122:GLN:OE1  | 2.14                     | 0.46              |
| 1:F:159:ALA:HB3  | 1:F:187:ILE:CD1  | 2.45                     | 0.46              |
| 1:L:38:GLU:HA    | 1:L:83:LEU:HD11  | 1.96                     | 0.46              |
| 1:N:178:ALA:O    | 1:N:181:GLU:HB2  | 2.15                     | 0.46              |
| 1:A:279:LEU:HD23 | 1:A:279:LEU:HA   | 1.73                     | 0.46              |
| 1:H:213:LEU:HD11 | 1:H:227:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:251:ASN:O    | 1:B:255:THR:HG22 | 2.14                     | 0.46              |
| 1:P:241:ALA:O    | 1:P:245:MET:CG   | 2.64                     | 0.46              |
| 1:N:85:LEU:O     | 1:N:111:VAL:HG13 | 2.15                     | 0.46              |
| 1:B:68:ASP:HA    | 1:B:71:LEU:HB2   | 1.97                     | 0.46              |
| 1:H:188:PHE:C    | 1:H:188:PHE:CD2  | 2.93                     | 0.46              |
| 1:J:160:ARG:NH2  | 1:J:190:GLU:CG   | 2.66                     | 0.46              |
| 1:O:239:CYS:O    | 1:O:243:ARG:HG3  | 2.15                     | 0.46              |
| 1:C:122:GLN:CG   | 1:C:123:LYS:H    | 2.19                     | 0.46              |
| 1:H:67:MET:CE    | 1:H:102:THR:CA   | 2.80                     | 0.46              |
| 1:H:225:ASP:OD1  | 1:H:225:ASP:N    | 2.49                     | 0.46              |
| 1:H:237:TYR:N    | 1:H:237:TYR:CD1  | 2.84                     | 0.46              |
| 1:J:106:PHE:HD1  | 1:J:111:VAL:HG21 | 1.80                     | 0.46              |
| 1:N:160:ARG:HA   | 1:N:188:PHE:HB3  | 1.98                     | 0.46              |
| 1:P:38:GLU:HG3   | 1:P:83:LEU:CG    | 2.44                     | 0.46              |
| 1:M:20:GLU:HG2   | 1:M:23:LEU:HA    | 1.96                     | 0.46              |
| 1:B:202:LYS:HD2  | 1:B:202:LYS:O    | 2.15                     | 0.46              |
| 1:D:251:ASN:O    | 1:D:255:THR:CG2  | 2.63                     | 0.46              |
| 1:F:103:ILE:O    | 1:F:107:ILE:HG13 | 2.15                     | 0.46              |
| 1:J:188:PHE:C    | 1:J:188:PHE:HD2  | 2.24                     | 0.46              |
| 1:O:213:LEU:HD11 | 1:O:235:ALA:HB1  | 1.98                     | 0.46              |
| 1:A:288:LEU:HD23 | 1:A:292:PHE:HE1  | 1.81                     | 0.46              |
| 1:C:281:TYR:O    | 1:C:282:TYR:C    | 2.59                     | 0.46              |
| 1:D:285:GLU:N    | 1:D:285:GLU:OE1  | 2.49                     | 0.46              |
| 1:G:263:LYS:O    | 1:G:266:VAL:HG13 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:7:ILE:HG22   | 1:J:11:ALA:HB3   | 1.98                     | 0.46              |
| 1:K:27:GLY:HA2   | 1:K:46:TYR:HB3   | 1.98                     | 0.46              |
| 1:M:46:TYR:HE2   | 1:M:48:SER:HB3   | 1.80                     | 0.46              |
| 1:M:87:VAL:HG23  | 1:M:111:VAL:CG1  | 2.45                     | 0.46              |
| 1:M:220:PRO:HB2  | 1:M:222:PHE:CE1  | 2.50                     | 0.46              |
| 1:A:176:ALA:O    | 1:A:180:VAL:HG23 | 2.15                     | 0.45              |
| 1:C:242:TYR:C    | 1:C:242:TYR:CD2  | 2.93                     | 0.45              |
| 1:D:266:VAL:N    | 1:D:267:PRO:CD   | 2.79                     | 0.45              |
| 1:F:192:MET:HE3  | 1:F:197:ASP:HB3  | 1.98                     | 0.45              |
| 1:J:32:TYR:CZ    | 1:J:36:MET:HE3   | 2.51                     | 0.45              |
| 1:P:289:ASP:C    | 1:P:291:LEU:H    | 2.25                     | 0.45              |
| 1:B:188:PHE:C    | 1:B:188:PHE:CD2  | 2.93                     | 0.45              |
| 1:G:178:ALA:O    | 1:G:181:GLU:HB2  | 2.16                     | 0.45              |
| 1:H:140:VAL:HG13 | 1:H:182:ALA:HB2  | 1.98                     | 0.45              |
| 1:L:89:ILE:HG12  | 1:L:114:VAL:HG13 | 1.98                     | 0.45              |
| 1:O:242:TYR:HA   | 1:O:245:MET:CG   | 2.45                     | 0.45              |
| 1:G:181:GLU:HA   | 1:G:181:GLU:OE1  | 2.16                     | 0.45              |
| 1:I:68:ASP:O     | 1:I:72:VAL:HG12  | 2.16                     | 0.45              |
| 1:K:122:GLN:CD   | 1:O:94:GLY:HA2   | 2.41                     | 0.45              |
| 1:O:266:VAL:N    | 1:O:267:PRO:CD   | 2.78                     | 0.45              |
| 1:G:32:TYR:CZ    | 1:G:36:MET:HE3   | 2.51                     | 0.45              |
| 1:G:46:TYR:HE2   | 1:G:238:CYS:HB2  | 1.80                     | 0.45              |
| 1:M:128:ARG:NH2  | 1:N:289:ASP:OD1  | 2.49                     | 0.45              |
| 1:N:241:ALA:O    | 1:N:245:MET:HG3  | 2.15                     | 0.45              |
| 1:O:36:MET:HE2   | 1:O:270:GLN:HE22 | 1.81                     | 0.45              |
| 1:O:227:LEU:HD22 | 1:O:232:VAL:HG11 | 1.98                     | 0.45              |
| 1:B:118:ASP:OD1  | 1:B:161:THR:HA   | 2.17                     | 0.45              |
| 1:C:205:VAL:HG21 | 1:C:209:ILE:HD11 | 1.99                     | 0.45              |
| 1:E:216:PHE:CB   | 1:F:272:ARG:HG3  | 2.36                     | 0.45              |
| 1:F:176:ALA:O    | 1:F:180:VAL:HG23 | 2.16                     | 0.45              |
| 1:H:275:LEU:HD22 | 1:H:279:LEU:CD1  | 2.47                     | 0.45              |
| 1:I:220:PRO:HG2  | 1:I:222:PHE:CZ   | 2.52                     | 0.45              |
| 1:K:21:GLN:HA    | 1:K:22:PRO:HA    | 1.81                     | 0.45              |
| 1:K:90:ASP:HB3   | 1:K:91:THR:H     | 1.55                     | 0.45              |
| 1:K:125:CYS:HB3  | 1:O:138:GLU:OE2  | 2.17                     | 0.45              |
| 1:M:220:PRO:O    | 1:M:222:PHE:HD1  | 1.99                     | 0.45              |
| 1:A:266:VAL:HG22 | 1:A:267:PRO:HD3  | 1.99                     | 0.45              |
| 1:H:91:THR:HG22  | 1:H:142:ARG:NH1  | 2.32                     | 0.45              |
| 1:E:89:ILE:HG23  | 1:E:114:VAL:HG22 | 1.98                     | 0.45              |
| 1:E:250:LEU:HD22 | 1:F:36:MET:CE    | 2.39                     | 0.45              |
| 1:I:188:PHE:C    | 1:I:188:PHE:CD2  | 2.93                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:200:ARG:HE   | 1:L:200:ARG:HB3  | 1.60                     | 0.45              |
| 1:C:251:ASN:O    | 1:C:255:THR:HG23 | 2.16                     | 0.45              |
| 1:F:138:GLU:O    | 1:F:141:ASP:HB2  | 2.16                     | 0.45              |
| 1:I:178:ALA:O    | 1:I:181:GLU:HB2  | 2.16                     | 0.45              |
| 1:M:199:ARG:HD3  | 1:M:230:ALA:HA   | 1.98                     | 0.45              |
| 1:O:81:THR:OG1   | 1:O:82:ASN:N     | 2.50                     | 0.45              |
| 1:P:261:THR:HG23 | 1:P:263:LYS:H    | 1.82                     | 0.45              |
| 1:A:48:SER:O     | 1:A:52:VAL:HG23  | 2.16                     | 0.45              |
| 1:B:178:ALA:O    | 1:B:181:GLU:HB2  | 2.16                     | 0.45              |
| 1:E:284:TYR:CE1  | 1:F:60:PRO:CG    | 3.00                     | 0.45              |
| 1:G:271:THR:HG22 | 1:H:216:PHE:CE1  | 2.52                     | 0.45              |
| 1:K:122:GLN:NE2  | 1:O:94:GLY:HA2   | 2.32                     | 0.45              |
| 1:N:46:TYR:CE2   | 1:N:48:SER:HA    | 2.52                     | 0.45              |
| 1:N:194:THR:O    | 1:N:197:ASP:HB2  | 2.17                     | 0.45              |
| 1:N:219:THR:CG2  | 1:N:222:PHE:CE1  | 2.92                     | 0.45              |
| 1:O:230:ALA:O    | 1:O:231:ASN:HB2  | 2.16                     | 0.45              |
| 1:O:284:TYR:HE1  | 1:P:60:PRO:CD    | 2.30                     | 0.45              |
| 1:E:52:VAL:O     | 1:E:56:SER:HB2   | 2.17                     | 0.45              |
| 1:E:138:GLU:O    | 1:E:141:ASP:HB2  | 2.18                     | 0.44              |
| 1:L:230:ALA:O    | 1:L:231:ASN:HB2  | 2.16                     | 0.44              |
| 1:P:46:TYR:CE2   | 1:P:48:SER:HA    | 2.52                     | 0.44              |
| 1:G:281:TYR:CD2  | 1:G:281:TYR:C    | 2.95                     | 0.44              |
| 1:H:89:ILE:HG23  | 1:H:114:VAL:CG2  | 2.46                     | 0.44              |
| 1:M:192:MET:HB2  | 1:M:198:TYR:CE2  | 2.52                     | 0.44              |
| 1:N:201:PHE:O    | 1:N:205:VAL:HG22 | 2.17                     | 0.44              |
| 1:O:72:VAL:CG2   | 1:P:76:ARG:NH2   | 2.80                     | 0.44              |
| 1:E:150:ARG:HD3  | 1:E:153:GLU:HA   | 2.00                     | 0.44              |
| 1:F:271:THR:OG1  | 1:F:274:GLN:HG3  | 2.17                     | 0.44              |
| 1:I:188:PHE:CD2  | 1:I:210:LEU:HD22 | 2.52                     | 0.44              |
| 1:E:94:GLY:HA3   | 1:E:98:ASN:OD1   | 2.17                     | 0.44              |
| 1:E:266:VAL:N    | 1:E:267:PRO:CD   | 2.80                     | 0.44              |
| 1:F:64:ILE:HA    | 1:M:98:ASN:ND2   | 2.32                     | 0.44              |
| 1:F:67:MET:CE    | 1:F:105:SER:HB2  | 2.48                     | 0.44              |
| 1:H:67:MET:HE3   | 1:H:102:THR:OG1  | 2.17                     | 0.44              |
| 1:H:119:GLN:HE22 | 1:H:131:LYS:HG3  | 1.82                     | 0.44              |
| 1:L:86:LEU:HD12  | 1:L:87:VAL:H     | 1.82                     | 0.44              |
| 1:N:115:HIS:ND1  | 1:N:115:HIS:O    | 2.49                     | 0.44              |
| 1:O:60:PRO:HB2   | 1:O:62:LEU:HD13  | 2.00                     | 0.44              |
| 1:P:231:ASN:HD22 | 1:P:231:ASN:HA   | 1.65                     | 0.44              |
| 1:J:7:ILE:HD12   | 1:J:7:ILE:N      | 2.29                     | 0.44              |
| 1:N:281:TYR:CD2  | 1:N:281:TYR:C    | 2.95                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:136:ALA:HA   | 1:O:175:ARG:NH1  | 2.32                     | 0.44              |
| 1:A:274:GLN:HE21 | 1:A:274:GLN:HB3  | 1.58                     | 0.44              |
| 1:D:199:ARG:HH11 | 1:D:199:ARG:HB2  | 1.82                     | 0.44              |
| 1:G:287:LYS:HE3  | 1:G:290:GLN:HE22 | 1.82                     | 0.44              |
| 1:H:291:LEU:HD23 | 1:H:291:LEU:HA   | 1.76                     | 0.44              |
| 1:K:262:GLN:H    | 1:K:262:GLN:NE2  | 2.10                     | 0.44              |
| 1:M:239:CYS:SG   | 1:M:242:TYR:CE1  | 3.11                     | 0.44              |
| 1:O:52:VAL:HG21  | 1:O:70:VAL:HG22  | 1.99                     | 0.44              |
| 1:B:288:LEU:HG   | 1:D:97:PHE:CZ    | 2.53                     | 0.44              |
| 1:M:274:GLN:HA   | 1:M:277:ASP:HB2  | 2.00                     | 0.44              |
| 1:M:285:GLU:C    | 1:M:287:LYS:H    | 2.26                     | 0.44              |
| 1:C:46:TYR:HE2   | 1:C:48:SER:HB2   | 1.82                     | 0.44              |
| 1:C:270:GLN:HG3  | 1:C:274:GLN:HE21 | 1.83                     | 0.44              |
| 1:F:119:GLN:HE22 | 1:F:162:ASP:HB2  | 1.83                     | 0.44              |
| 1:G:192:MET:HE3  | 1:G:198:TYR:HA   | 1.99                     | 0.44              |
| 1:I:71:LEU:HD23  | 1:I:71:LEU:HA    | 1.80                     | 0.44              |
| 1:K:46:TYR:HE2   | 1:K:238:CYS:HB2  | 1.83                     | 0.44              |
| 1:M:202:LYS:HG2  | 1:M:209:ILE:CG1  | 2.48                     | 0.44              |
| 1:N:138:GLU:HA   | 1:N:138:GLU:OE1  | 2.18                     | 0.44              |
| 1:O:284:TYR:CE1  | 1:P:60:PRO:CG    | 3.01                     | 0.44              |
| 1:G:38:GLU:HA    | 1:G:83:LEU:HD11  | 2.00                     | 0.44              |
| 1:M:46:TYR:CE2   | 1:M:48:SER:HB3   | 2.53                     | 0.44              |
| 1:C:76:ARG:HH22  | 1:D:72:VAL:HG22  | 1.84                     | 0.43              |
| 1:D:193:LYS:HD2  | 1:D:193:LYS:H    | 1.83                     | 0.43              |
| 1:K:46:TYR:CE2   | 1:K:238:CYS:HB2  | 2.52                     | 0.43              |
| 1:O:124:ARG:O    | 1:O:126:GLY:N    | 2.50                     | 0.43              |
| 1:P:152:ASP:C    | 1:P:152:ASP:OD1  | 2.61                     | 0.43              |
| 1:C:115:HIS:O    | 1:C:115:HIS:ND1  | 2.51                     | 0.43              |
| 1:J:282:TYR:O    | 1:J:283:ALA:C    | 2.61                     | 0.43              |
| 1:L:40:VAL:O     | 1:L:40:VAL:HG12  | 2.18                     | 0.43              |
| 1:M:68:ASP:HA    | 1:M:71:LEU:HB2   | 2.00                     | 0.43              |
| 1:M:262:GLN:NE2  | 1:N:237:TYR:HD2  | 2.16                     | 0.43              |
| 1:A:59:ILE:CD1   | 1:A:64:ILE:HB    | 2.49                     | 0.43              |
| 1:E:279:LEU:HD23 | 1:E:279:LEU:HA   | 1.84                     | 0.43              |
| 1:H:57:LEU:HD11  | 1:H:69:ASP:HB3   | 2.01                     | 0.43              |
| 1:H:89:ILE:CG2   | 1:H:114:VAL:CG2  | 2.96                     | 0.43              |
| 1:K:287:LYS:HE2  | 1:P:148:ASP:OD2  | 2.18                     | 0.43              |
| 1:M:253:TYR:HE1  | 1:N:26:VAL:CG2   | 2.32                     | 0.43              |
| 1:P:210:LEU:HD12 | 1:P:234:ILE:HG21 | 2.00                     | 0.43              |
| 1:B:60:PRO:HG2   | 1:B:62:LEU:HD22  | 2.00                     | 0.43              |
| 1:B:106:PHE:HD1  | 1:B:111:VAL:HG21 | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:ARG:O    | 1:C:126:GLY:N    | 2.52                     | 0.43              |
| 1:D:118:ASP:HB3  | 1:D:139:MET:HE2  | 2.00                     | 0.43              |
| 1:F:128:ARG:HD3  | 1:H:282:TYR:CZ   | 2.53                     | 0.43              |
| 1:F:274:GLN:O    | 1:F:275:LEU:C    | 2.61                     | 0.43              |
| 1:G:150:ARG:HD3  | 1:G:153:GLU:HA   | 2.00                     | 0.43              |
| 1:H:89:ILE:HG12  | 1:H:114:VAL:HG22 | 1.99                     | 0.43              |
| 1:K:203:GLU:O    | 1:K:206:LYS:HE2  | 2.18                     | 0.43              |
| 1:L:276:TYR:HA   | 1:L:281:TYR:CD1  | 2.53                     | 0.43              |
| 1:E:230:ALA:O    | 1:E:231:ASN:HB2  | 2.17                     | 0.43              |
| 1:H:289:ASP:O    | 1:H:293:ASN:HB3  | 2.18                     | 0.43              |
| 1:L:152:ASP:OD2  | 1:L:154:THR:OG1  | 2.33                     | 0.43              |
| 1:N:131:LYS:O    | 1:N:132:GLU:HB2  | 2.19                     | 0.43              |
| 1:O:118:ASP:HB3  | 1:O:139:MET:HG2  | 2.01                     | 0.43              |
| 1:P:21:GLN:HA    | 1:P:22:PRO:HA    | 1.86                     | 0.43              |
| 1:L:99:ILE:HD11  | 1:L:142:ARG:HG2  | 2.00                     | 0.43              |
| 1:N:139:MET:HA   | 1:N:142:ARG:HD2  | 2.00                     | 0.43              |
| 1:E:119:GLN:HE22 | 1:E:131:LYS:CA   | 2.31                     | 0.43              |
| 1:G:38:GLU:HG3   | 1:G:83:LEU:CD1   | 2.49                     | 0.43              |
| 1:G:269:MET:HE2  | 1:H:240:GLY:CA   | 2.49                     | 0.43              |
| 1:J:67:MET:HE2   | 1:J:102:THR:HA   | 1.96                     | 0.43              |
| 1:K:64:ILE:HA    | 1:O:98:ASN:HD21  | 1.84                     | 0.43              |
| 1:L:20:GLU:OE1   | 1:L:43:LYS:HE2   | 2.19                     | 0.43              |
| 1:M:246:ASN:HB3  | 1:N:36:MET:HE1   | 2.01                     | 0.43              |
| 1:N:12:LYS:HB3   | 1:N:84:PRO:HG3   | 2.01                     | 0.43              |
| 1:C:32:TYR:OH    | 1:C:36:MET:HE3   | 2.19                     | 0.43              |
| 1:C:186:MET:HG2  | 1:C:208:PRO:HB2  | 2.00                     | 0.43              |
| 1:D:21:GLN:HA    | 1:D:22:PRO:C     | 2.41                     | 0.43              |
| 1:E:147:VAL:HG13 | 1:E:150:ARG:NH1  | 2.33                     | 0.43              |
| 1:H:135:PRO:O    | 1:H:138:GLU:HB3  | 2.19                     | 0.43              |
| 1:I:196:ASP:O    | 1:I:200:ARG:HG3  | 2.19                     | 0.43              |
| 1:M:275:LEU:HD23 | 1:M:275:LEU:HA   | 1.93                     | 0.43              |
| 1:G:241:ALA:O    | 1:G:245:MET:HG2  | 2.18                     | 0.43              |
| 1:O:43:LYS:O     | 1:O:84:PRO:HD2   | 2.19                     | 0.43              |
| 1:B:188:PHE:C    | 1:B:188:PHE:HD2  | 2.27                     | 0.43              |
| 1:C:188:PHE:C    | 1:C:188:PHE:HD2  | 2.27                     | 0.43              |
| 1:E:122:GLN:NE2  | 1:N:94:GLY:CA    | 2.75                     | 0.43              |
| 1:F:188:PHE:C    | 1:F:188:PHE:CD2  | 2.97                     | 0.43              |
| 1:H:202:LYS:HE2  | 1:H:231:ASN:O    | 2.19                     | 0.43              |
| 1:L:177:ILE:O    | 1:L:181:GLU:HG2  | 2.19                     | 0.43              |
| 1:M:195:LEU:HD12 | 1:M:222:PHE:HD2  | 1.80                     | 0.43              |
| 1:N:60:PRO:CB    | 1:N:62:LEU:HD22  | 2.45                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:199:ARG:HH11 | 1:C:199:ARG:CG   | 2.29                     | 0.42              |
| 1:G:202:LYS:HE2  | 1:G:233:ASP:OD2  | 2.19                     | 0.42              |
| 1:G:263:LYS:HB2  | 1:G:263:LYS:NZ   | 2.34                     | 0.42              |
| 1:K:250:LEU:HB2  | 1:L:36:MET:CE    | 2.44                     | 0.42              |
| 1:N:22:PRO:HG2   | 1:N:224:LEU:CD2  | 2.49                     | 0.42              |
| 1:N:207:VAL:HB   | 1:N:208:PRO:HD2  | 2.01                     | 0.42              |
| 1:O:98:ASN:N     | 1:O:98:ASN:HD22  | 2.17                     | 0.42              |
| 1:O:252:PHE:CZ   | 1:P:240:GLY:HA3  | 2.51                     | 0.42              |
| 1:A:20:GLU:HG2   | 1:A:23:LEU:HA    | 2.00                     | 0.42              |
| 1:A:188:PHE:CD2  | 1:A:210:LEU:HD22 | 2.54                     | 0.42              |
| 1:D:188:PHE:C    | 1:D:188:PHE:CD2  | 2.97                     | 0.42              |
| 1:C:68:ASP:HA    | 1:C:71:LEU:HB2   | 2.01                     | 0.42              |
| 1:F:272:ARG:HB3  | 1:F:272:ARG:NH2  | 2.34                     | 0.42              |
| 1:I:150:ARG:HD3  | 1:I:152:ASP:O    | 2.18                     | 0.42              |
| 1:M:32:TYR:HB2   | 1:N:55:ASN:HA    | 2.01                     | 0.42              |
| 1:M:285:GLU:OE2  | 1:M:285:GLU:HA   | 2.19                     | 0.42              |
| 1:N:24:GLN:HG2   | 1:N:224:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:21:GLN:HA    | 1:A:22:PRO:HA    | 1.92                     | 0.42              |
| 1:E:40:VAL:O     | 1:E:40:VAL:HG12  | 2.18                     | 0.42              |
| 1:H:36:MET:HE2   | 1:H:270:GLN:HE22 | 1.83                     | 0.42              |
| 1:H:143:ILE:HD13 | 1:H:184:ALA:HB2  | 2.02                     | 0.42              |
| 1:N:208:PRO:O    | 1:N:209:ILE:HD13 | 2.19                     | 0.42              |
| 1:O:36:MET:HE2   | 1:O:270:GLN:NE2  | 2.35                     | 0.42              |
| 1:A:207:VAL:HB   | 1:A:208:PRO:HD2  | 2.01                     | 0.42              |
| 1:B:208:PRO:HA   | 1:B:233:ASP:OD2  | 2.20                     | 0.42              |
| 1:J:128:ARG:O    | 1:J:129:PRO:C    | 2.62                     | 0.42              |
| 1:N:130:GLY:O    | 1:N:131:LYS:CB   | 2.63                     | 0.42              |
| 1:O:29:ILE:HG13  | 1:O:30:THR:HG23  | 2.02                     | 0.42              |
| 1:P:201:PHE:O    | 1:P:205:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:47:LEU:HB2   | 1:A:85:LEU:HD11  | 2.01                     | 0.42              |
| 1:J:67:MET:HE3   | 1:J:102:THR:CA   | 2.45                     | 0.42              |
| 1:K:94:GLY:HA3   | 1:K:98:ASN:OD1   | 2.20                     | 0.42              |
| 1:L:181:GLU:HA   | 1:L:181:GLU:OE1  | 2.20                     | 0.42              |
| 1:L:252:PHE:O    | 1:L:256:VAL:HG23 | 2.19                     | 0.42              |
| 1:M:48:SER:O     | 1:M:52:VAL:HG23  | 2.19                     | 0.42              |
| 1:M:210:LEU:HD21 | 1:M:236:LEU:CD2  | 2.48                     | 0.42              |
| 1:M:216:PHE:HB2  | 1:N:272:ARG:HD2  | 2.01                     | 0.42              |
| 1:N:71:LEU:CD2   | 1:N:106:PHE:CE1  | 3.02                     | 0.42              |
| 1:N:251:ASN:C    | 1:N:251:ASN:HD22 | 2.27                     | 0.42              |
| 1:O:247:LYS:HB2  | 1:P:270:GLN:HB2  | 2.02                     | 0.42              |
| 1:P:266:VAL:N    | 1:P:267:PRO:CD   | 2.81                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:ARG:O    | 1:C:125:CYS:C    | 2.62                     | 0.42              |
| 1:H:181:GLU:OE1  | 1:H:181:GLU:HA   | 2.20                     | 0.42              |
| 1:H:282:TYR:C    | 1:H:284:TYR:N    | 2.77                     | 0.42              |
| 1:J:160:ARG:HG3  | 1:J:188:PHE:CG   | 2.54                     | 0.42              |
| 1:N:207:VAL:HB   | 1:N:208:PRO:CD   | 2.49                     | 0.42              |
| 1:N:266:VAL:HG23 | 1:N:267:PRO:HD3  | 2.01                     | 0.42              |
| 1:O:193:LYS:H    | 1:O:193:LYS:CD   | 2.30                     | 0.42              |
| 1:P:215:GLU:HG2  | 1:P:243:ARG:NH2  | 2.34                     | 0.42              |
| 1:C:223:THR:HG1  | 1:C:226:GLU:HG3  | 1.78                     | 0.42              |
| 1:E:205:VAL:CG2  | 1:E:209:ILE:HD11 | 2.50                     | 0.42              |
| 1:M:29:ILE:HD11  | 1:M:245:MET:HE2  | 2.00                     | 0.42              |
| 1:P:82:ASN:H     | 1:P:82:ASN:ND2   | 2.17                     | 0.42              |
| 1:I:272:ARG:NH1  | 1:J:216:PHE:O    | 2.51                     | 0.42              |
| 1:J:21:GLN:HA    | 1:J:22:PRO:HA    | 1.80                     | 0.42              |
| 1:J:86:LEU:HD12  | 1:J:87:VAL:N     | 2.34                     | 0.42              |
| 1:M:277:ASP:O    | 1:M:279:LEU:N    | 2.52                     | 0.42              |
| 1:N:82:ASN:ND2   | 1:N:82:ASN:H     | 2.17                     | 0.42              |
| 1:B:210:LEU:C    | 1:B:210:LEU:HD23 | 2.44                     | 0.42              |
| 1:G:272:ARG:HG3  | 1:H:216:PHE:HB2  | 2.02                     | 0.42              |
| 1:N:52:VAL:O     | 1:N:56:SER:HB2   | 2.20                     | 0.42              |
| 1:N:192:MET:CE   | 1:N:201:PHE:CD1  | 3.01                     | 0.42              |
| 1:N:282:TYR:O    | 1:N:286:GLU:HG3  | 2.19                     | 0.42              |
| 1:P:131:LYS:O    | 1:P:132:GLU:HB2  | 2.20                     | 0.42              |
| 1:D:59:ILE:HB    | 1:D:60:PRO:HD2   | 2.02                     | 0.41              |
| 1:F:280:GLY:O    | 1:F:284:TYR:HD1  | 2.03                     | 0.41              |
| 1:M:216:PHE:HB2  | 1:N:272:ARG:CD   | 2.50                     | 0.41              |
| 1:M:243:ARG:HG2  | 1:M:243:ARG:HH11 | 1.85                     | 0.41              |
| 1:O:21:GLN:HA    | 1:O:22:PRO:HA    | 1.94                     | 0.41              |
| 1:P:123:LYS:HG3  | 1:P:124:ARG:H    | 1.85                     | 0.41              |
| 1:D:52:VAL:O     | 1:D:56:SER:HB2   | 2.20                     | 0.41              |
| 1:D:82:ASN:ND2   | 1:D:82:ASN:H     | 2.18                     | 0.41              |
| 1:D:285:GLU:HG2  | 1:H:128:ARG:HH22 | 1.85                     | 0.41              |
| 1:G:281:TYR:HD1  | 1:H:60:PRO:HB3   | 1.85                     | 0.41              |
| 1:H:287:LYS:HE3  | 1:H:290:GLN:NE2  | 2.35                     | 0.41              |
| 1:N:7:ILE:CG2    | 1:N:12:LYS:HG2   | 2.50                     | 0.41              |
| 1:N:236:LEU:HD11 | 1:N:238:CYS:HB3  | 2.03                     | 0.41              |
| 1:P:121:GLY:O    | 1:P:122:GLN:C    | 2.63                     | 0.41              |
| 1:D:115:HIS:HA   | 1:D:158:MET:O    | 2.20                     | 0.41              |
| 1:I:138:GLU:O    | 1:I:141:ASP:HB2  | 2.21                     | 0.41              |
| 1:M:46:TYR:CE2   | 1:M:48:SER:CB    | 3.03                     | 0.41              |
| 1:O:67:MET:CE    | 1:O:102:THR:CA   | 2.81                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:284:TYR:CD1  | 1:P:60:PRO:HG3   | 2.54                     | 0.41              |
| 1:P:22:PRO:HB3   | 1:P:232:VAL:O    | 2.21                     | 0.41              |
| 1:E:125:CYS:N    | 1:N:138:GLU:OE2  | 2.49                     | 0.41              |
| 1:E:152:ASP:OD1  | 1:E:152:ASP:C    | 2.63                     | 0.41              |
| 1:K:261:THR:HG23 | 1:K:263:LYS:H    | 1.86                     | 0.41              |
| 1:P:55:ASN:HD22  | 1:P:55:ASN:H     | 1.68                     | 0.41              |
| 1:A:186:MET:HG2  | 1:A:208:PRO:HB2  | 2.02                     | 0.41              |
| 1:F:272:ARG:HB3  | 1:F:272:ARG:CZ   | 2.50                     | 0.41              |
| 1:G:76:ARG:NH2   | 1:H:72:VAL:HG22  | 2.35                     | 0.41              |
| 1:L:34:ALA:O     | 1:L:37:ALA:HB3   | 2.21                     | 0.41              |
| 1:L:215:GLU:HG2  | 1:L:243:ARG:HE   | 1.86                     | 0.41              |
| 1:A:262:GLN:HE21 | 1:A:262:GLN:N    | 2.04                     | 0.41              |
| 1:A:288:LEU:HD23 | 1:A:292:PHE:CE1  | 2.56                     | 0.41              |
| 1:C:271:THR:OG1  | 1:C:274:GLN:HG3  | 2.21                     | 0.41              |
| 1:E:59:ILE:HD12  | 1:E:64:ILE:HB    | 2.02                     | 0.41              |
| 1:E:123:LYS:O    | 1:E:124:ARG:C    | 2.62                     | 0.41              |
| 1:E:139:MET:HG2  | 1:E:179:TYR:CZ   | 2.55                     | 0.41              |
| 1:I:123:LYS:CD   | 1:I:124:ARG:H    | 2.03                     | 0.41              |
| 1:K:152:ASP:OD1  | 1:K:154:THR:OG1  | 2.38                     | 0.41              |
| 1:P:46:TYR:CG    | 1:P:236:LEU:HD11 | 2.56                     | 0.41              |
| 1:B:219:THR:HG22 | 1:B:220:PRO:O    | 2.21                     | 0.41              |
| 1:D:71:LEU:HD23  | 1:D:106:PHE:CZ   | 2.55                     | 0.41              |
| 1:E:240:GLY:HA3  | 1:F:252:PHE:CE1  | 2.55                     | 0.41              |
| 1:I:89:ILE:HD13  | 1:I:114:VAL:HG11 | 2.03                     | 0.41              |
| 1:K:230:ALA:O    | 1:K:231:ASN:HB2  | 2.21                     | 0.41              |
| 1:N:87:VAL:HB    | 1:N:114:VAL:HG23 | 2.03                     | 0.41              |
| 1:O:22:PRO:HG2   | 1:O:224:LEU:HD22 | 2.01                     | 0.41              |
| 1:O:123:LYS:O    | 1:O:124:ARG:C    | 2.63                     | 0.41              |
| 1:P:291:LEU:HB3  | 1:P:292:PHE:CD2  | 2.55                     | 0.41              |
| 1:D:134:VAL:HB   | 1:D:138:GLU:HB3  | 2.03                     | 0.41              |
| 1:F:36:MET:CE    | 1:F:270:GLN:NE2  | 2.83                     | 0.41              |
| 1:F:96:ALA:HB2   | 1:M:125:CYS:O    | 2.21                     | 0.41              |
| 1:F:152:ASP:OD1  | 1:F:152:ASP:C    | 2.63                     | 0.41              |
| 1:G:74:ALA:O     | 1:G:78:THR:HG23  | 2.20                     | 0.41              |
| 1:G:275:LEU:HD22 | 1:G:279:LEU:HD22 | 2.02                     | 0.41              |
| 1:I:290:GLN:O    | 1:I:290:GLN:HG2  | 2.20                     | 0.41              |
| 1:J:20:GLU:HG2   | 1:J:23:LEU:HA    | 2.02                     | 0.41              |
| 1:J:36:MET:HE3   | 1:J:270:GLN:HE22 | 1.84                     | 0.41              |
| 1:K:134:VAL:HB   | 1:K:138:GLU:HG2  | 2.03                     | 0.41              |
| 1:M:287:LYS:O    | 1:M:289:ASP:N    | 2.54                     | 0.41              |
| 1:O:95:GLY:O     | 1:O:99:ILE:HD12  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:115:HIS:O    | 1:O:115:HIS:ND1  | 2.54                     | 0.41              |
| 1:P:150:ARG:HD3  | 1:P:152:ASP:O    | 2.21                     | 0.41              |
| 1:P:282:TYR:O    | 1:P:286:GLU:HG2  | 2.21                     | 0.41              |
| 1:C:199:ARG:NH2  | 1:C:229:GLY:O    | 2.49                     | 0.41              |
| 1:D:46:TYR:CE2   | 1:D:48:SER:HB2   | 2.55                     | 0.41              |
| 1:E:219:THR:HG22 | 1:E:220:PRO:O    | 2.20                     | 0.41              |
| 1:G:188:PHE:CG   | 1:G:210:LEU:HD22 | 2.56                     | 0.41              |
| 1:H:205:VAL:HG21 | 1:H:209:ILE:HD11 | 2.03                     | 0.41              |
| 1:H:220:PRO:HD2  | 1:H:222:PHE:CE1  | 2.57                     | 0.41              |
| 1:K:290:GLN:HE21 | 1:K:290:GLN:HB3  | 1.58                     | 0.41              |
| 1:M:14:ARG:NH2   | 1:M:153:GLU:O    | 2.49                     | 0.41              |
| 1:B:207:VAL:HB   | 1:B:208:PRO:HD2  | 2.03                     | 0.40              |
| 1:D:205:VAL:CG2  | 1:D:209:ILE:HD11 | 2.46                     | 0.40              |
| 1:E:54:ALA:O     | 1:F:32:TYR:HB2   | 2.21                     | 0.40              |
| 1:F:29:ILE:HG21  | 1:F:55:ASN:ND2   | 2.37                     | 0.40              |
| 1:G:98:ASN:ND2   | 1:J:64:ILE:HA    | 2.36                     | 0.40              |
| 1:G:209:ILE:HD13 | 1:G:209:ILE:HA   | 1.83                     | 0.40              |
| 1:I:150:ARG:HE   | 1:I:157:ILE:HD12 | 1.86                     | 0.40              |
| 1:N:22:PRO:HG2   | 1:N:224:LEU:HD22 | 2.02                     | 0.40              |
| 1:O:284:TYR:CE1  | 1:P:60:PRO:HD2   | 2.56                     | 0.40              |
| 1:B:64:ILE:HA    | 1:C:98:ASN:ND2   | 2.33                     | 0.40              |
| 1:G:124:ARG:O    | 1:G:125:CYS:C    | 2.65                     | 0.40              |
| 1:K:215:GLU:CG   | 1:K:243:ARG:HE   | 2.34                     | 0.40              |
| 1:L:40:VAL:O     | 1:L:40:VAL:CG1   | 2.68                     | 0.40              |
| 1:L:123:LYS:HG3  | 1:L:124:ARG:H    | 1.86                     | 0.40              |
| 1:L:292:PHE:HE2  | 1:O:141:ASP:HB3  | 1.87                     | 0.40              |
| 1:M:216:PHE:CZ   | 1:N:271:THR:HG22 | 2.56                     | 0.40              |
| 1:N:276:TYR:N    | 1:N:276:TYR:HD1  | 2.20                     | 0.40              |
| 1:O:283:ALA:O    | 1:O:287:LYS:HB2  | 2.22                     | 0.40              |
| 1:P:199:ARG:CG   | 1:P:199:ARG:NH1  | 2.84                     | 0.40              |
| 1:H:189:PRO:HD2  | 1:H:210:LEU:O    | 2.22                     | 0.40              |
| 1:I:169:ILE:O    | 1:I:169:ILE:HG13 | 2.18                     | 0.40              |
| 1:M:67:MET:CE    | 1:M:102:THR:CA   | 2.95                     | 0.40              |
| 1:B:152:ASP:OD1  | 1:B:152:ASP:C    | 2.64                     | 0.40              |
| 1:D:161:THR:O    | 1:D:190:GLU:HB2  | 2.21                     | 0.40              |
| 1:H:52:VAL:O     | 1:H:56:SER:HB2   | 2.21                     | 0.40              |
| 1:I:21:GLN:HA    | 1:I:22:PRO:HA    | 1.86                     | 0.40              |
| 1:J:202:LYS:HG3  | 1:J:231:ASN:O    | 2.22                     | 0.40              |
| 1:M:68:ASP:O     | 1:M:72:VAL:HG12  | 2.21                     | 0.40              |
| 1:N:43:LYS:C     | 1:N:83:LEU:HD22  | 2.45                     | 0.40              |
| 1:N:188:PHE:C    | 1:N:188:PHE:CD2  | 2.99                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:N:210:LEU:HD21 | 1:N:236:LEU:HB3 | 2.04                     | 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     | 288/298 (97%)   | 273 (95%)  | 13 (4%)  | 2 (1%)   | 18          | 48  |
| 1   | B     | 284/298 (95%)   | 268 (94%)  | 12 (4%)  | 4 (1%)   | 9           | 30  |
| 1   | C     | 285/298 (96%)   | 266 (93%)  | 16 (6%)  | 3 (1%)   | 11          | 36  |
| 1   | D     | 285/298 (96%)   | 274 (96%)  | 9 (3%)   | 2 (1%)   | 18          | 48  |
| 1   | E     | 286/298 (96%)   | 271 (95%)  | 13 (4%)  | 2 (1%)   | 18          | 48  |
| 1   | F     | 284/298 (95%)   | 268 (94%)  | 14 (5%)  | 2 (1%)   | 18          | 48  |
| 1   | G     | 285/298 (96%)   | 272 (95%)  | 13 (5%)  | 0        | 100         | 100 |
| 1   | H     | 286/298 (96%)   | 272 (95%)  | 12 (4%)  | 2 (1%)   | 18          | 48  |
| 1   | I     | 287/298 (96%)   | 274 (96%)  | 11 (4%)  | 2 (1%)   | 18          | 48  |
| 1   | J     | 286/298 (96%)   | 274 (96%)  | 8 (3%)   | 4 (1%)   | 9           | 30  |
| 1   | K     | 284/298 (95%)   | 272 (96%)  | 10 (4%)  | 2 (1%)   | 18          | 48  |
| 1   | L     | 284/298 (95%)   | 270 (95%)  | 10 (4%)  | 4 (1%)   | 9           | 30  |
| 1   | M     | 285/298 (96%)   | 262 (92%)  | 15 (5%)  | 8 (3%)   | 4           | 15  |
| 1   | N     | 285/298 (96%)   | 267 (94%)  | 12 (4%)  | 6 (2%)   | 5           | 21  |
| 1   | O     | 286/298 (96%)   | 269 (94%)  | 10 (4%)  | 7 (2%)   | 4           | 18  |
| 1   | P     | 284/298 (95%)   | 271 (95%)  | 9 (3%)   | 4 (1%)   | 9           | 30  |
| All | All   | 4564/4768 (96%) | 4323 (95%) | 187 (4%) | 54 (1%)  | 10          | 34  |

All (54) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 125 | CYS  |
| 1   | C     | 281 | TYR  |
| 1   | D     | 124 | ARG  |
| 1   | E     | 124 | ARG  |
| 1   | F     | 122 | GLN  |
| 1   | F     | 124 | ARG  |
| 1   | M     | 269 | MET  |
| 1   | N     | 132 | GLU  |
| 1   | O     | 7   | ILE  |
| 1   | O     | 124 | ARG  |
| 1   | O     | 125 | CYS  |
| 1   | O     | 136 | ALA  |
| 1   | B     | 124 | ARG  |
| 1   | C     | 125 | CYS  |
| 1   | H     | 124 | ARG  |
| 1   | L     | 121 | GLY  |
| 1   | M     | 278 | TYR  |
| 1   | M     | 289 | ASP  |
| 1   | N     | 131 | LYS  |
| 1   | O     | 121 | GLY  |
| 1   | P     | 132 | GLU  |
| 1   | C     | 124 | ARG  |
| 1   | H     | 283 | ALA  |
| 1   | I     | 121 | GLY  |
| 1   | I     | 124 | ARG  |
| 1   | J     | 283 | ALA  |
| 1   | K     | 124 | ARG  |
| 1   | L     | 276 | TYR  |
| 1   | L     | 282 | TYR  |
| 1   | M     | 124 | ARG  |
| 1   | M     | 277 | ASP  |
| 1   | M     | 288 | LEU  |
| 1   | N     | 121 | GLY  |
| 1   | N     | 124 | ARG  |
| 1   | N     | 290 | GLN  |
| 1   | O     | 8   | SER  |
| 1   | B     | 65  | SER  |
| 1   | E     | 129 | PRO  |
| 1   | P     | 290 | GLN  |
| 1   | A     | 118 | ASP  |
| 1   | D     | 135 | PRO  |
| 1   | J     | 124 | ARG  |
| 1   | J     | 131 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 290 | GLN  |
| 1   | K     | 121 | GLY  |
| 1   | M     | 286 | GLU  |
| 1   | P     | 281 | TYR  |
| 1   | B     | 129 | PRO  |
| 1   | L     | 129 | PRO  |
| 1   | N     | 9   | ALA  |
| 1   | O     | 135 | PRO  |
| 1   | A     | 121 | GLY  |
| 1   | M     | 121 | GLY  |
| 1   | P     | 137 | GLY  |

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

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 216/223 (97%) | 185 (86%) | 31 (14%) | 3           | 11 |
| 1   | B     | 213/223 (96%) | 183 (86%) | 30 (14%) | 3           | 11 |
| 1   | C     | 214/223 (96%) | 181 (85%) | 33 (15%) | 2           | 9  |
| 1   | D     | 214/223 (96%) | 185 (86%) | 29 (14%) | 3           | 12 |
| 1   | E     | 215/223 (96%) | 188 (87%) | 27 (13%) | 4           | 14 |
| 1   | F     | 213/223 (96%) | 182 (85%) | 31 (15%) | 3           | 10 |
| 1   | G     | 214/223 (96%) | 184 (86%) | 30 (14%) | 3           | 11 |
| 1   | H     | 215/223 (96%) | 184 (86%) | 31 (14%) | 3           | 11 |
| 1   | I     | 216/223 (97%) | 182 (84%) | 34 (16%) | 2           | 9  |
| 1   | J     | 215/223 (96%) | 182 (85%) | 33 (15%) | 3           | 9  |
| 1   | K     | 213/223 (96%) | 186 (87%) | 27 (13%) | 4           | 14 |
| 1   | L     | 213/223 (96%) | 178 (84%) | 35 (16%) | 2           | 8  |
| 1   | M     | 214/223 (96%) | 183 (86%) | 31 (14%) | 3           | 10 |
| 1   | N     | 214/223 (96%) | 176 (82%) | 38 (18%) | 2           | 6  |
| 1   | O     | 215/223 (96%) | 178 (83%) | 37 (17%) | 2           | 7  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles        |
|-----|-------|-----------------|------------|-----------|--------------------|
| 1   | P     | 213/223 (96%)   | 173 (81%)  | 40 (19%)  | <b>1</b> <b>5</b>  |
| All | All   | 3427/3568 (96%) | 2910 (85%) | 517 (15%) | <b>3</b> <b>10</b> |

All (517) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | LEU  |
| 1   | A     | 21  | GLN  |
| 1   | A     | 25  | VAL  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 72  | VAL  |
| 1   | A     | 81  | THR  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 122 | GLN  |
| 1   | A     | 123 | LYS  |
| 1   | A     | 124 | ARG  |
| 1   | A     | 128 | ARG  |
| 1   | A     | 162 | ASP  |
| 1   | A     | 177 | ILE  |
| 1   | A     | 193 | LYS  |
| 1   | A     | 199 | ARG  |
| 1   | A     | 202 | LYS  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 209 | ILE  |
| 1   | A     | 218 | SER  |
| 1   | A     | 224 | LEU  |
| 1   | A     | 247 | LYS  |
| 1   | A     | 255 | THR  |
| 1   | A     | 258 | ARG  |
| 1   | A     | 262 | GLN  |
| 1   | A     | 263 | LYS  |
| 1   | A     | 266 | VAL  |
| 1   | A     | 272 | ARG  |
| 1   | A     | 275 | LEU  |
| 1   | A     | 287 | LYS  |
| 1   | A     | 290 | GLN  |
| 1   | B     | 7   | ILE  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 25  | VAL  |
| 1   | B     | 48  | SER  |
| 1   | B     | 62  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 67  | MET  |
| 1   | B     | 72  | VAL  |
| 1   | B     | 75  | ASN  |
| 1   | B     | 82  | ASN  |
| 1   | B     | 98  | ASN  |
| 1   | B     | 114 | VAL  |
| 1   | B     | 117 | GLU  |
| 1   | B     | 122 | GLN  |
| 1   | B     | 124 | ARG  |
| 1   | B     | 128 | ARG  |
| 1   | B     | 134 | VAL  |
| 1   | B     | 169 | ILE  |
| 1   | B     | 188 | PHE  |
| 1   | B     | 195 | LEU  |
| 1   | B     | 199 | ARG  |
| 1   | B     | 202 | LYS  |
| 1   | B     | 205 | VAL  |
| 1   | B     | 215 | GLU  |
| 1   | B     | 232 | VAL  |
| 1   | B     | 255 | THR  |
| 1   | B     | 262 | GLN  |
| 1   | B     | 263 | LYS  |
| 1   | B     | 275 | LEU  |
| 1   | B     | 286 | GLU  |
| 1   | B     | 287 | LYS  |
| 1   | C     | 7   | ILE  |
| 1   | C     | 21  | GLN  |
| 1   | C     | 25  | VAL  |
| 1   | C     | 48  | SER  |
| 1   | C     | 62  | LEU  |
| 1   | C     | 65  | SER  |
| 1   | C     | 72  | VAL  |
| 1   | C     | 81  | THR  |
| 1   | C     | 82  | ASN  |
| 1   | C     | 114 | VAL  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 117 | GLU  |
| 1   | C     | 120 | VAL  |
| 1   | C     | 122 | GLN  |
| 1   | C     | 150 | ARG  |
| 1   | C     | 154 | THR  |
| 1   | C     | 181 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 188 | PHE  |
| 1   | C     | 190 | GLU  |
| 1   | C     | 193 | LYS  |
| 1   | C     | 195 | LEU  |
| 1   | C     | 199 | ARG  |
| 1   | C     | 202 | LYS  |
| 1   | C     | 206 | LYS  |
| 1   | C     | 218 | SER  |
| 1   | C     | 219 | THR  |
| 1   | C     | 224 | LEU  |
| 1   | C     | 242 | TYR  |
| 1   | C     | 262 | GLN  |
| 1   | C     | 266 | VAL  |
| 1   | C     | 275 | LEU  |
| 1   | C     | 277 | ASP  |
| 1   | C     | 286 | GLU  |
| 1   | D     | 6   | LEU  |
| 1   | D     | 21  | GLN  |
| 1   | D     | 25  | VAL  |
| 1   | D     | 48  | SER  |
| 1   | D     | 62  | LEU  |
| 1   | D     | 71  | LEU  |
| 1   | D     | 72  | VAL  |
| 1   | D     | 82  | ASN  |
| 1   | D     | 98  | ASN  |
| 1   | D     | 128 | ARG  |
| 1   | D     | 150 | ARG  |
| 1   | D     | 153 | GLU  |
| 1   | D     | 167 | GLU  |
| 1   | D     | 188 | PHE  |
| 1   | D     | 192 | MET  |
| 1   | D     | 193 | LYS  |
| 1   | D     | 199 | ARG  |
| 1   | D     | 202 | LYS  |
| 1   | D     | 215 | GLU  |
| 1   | D     | 242 | TYR  |
| 1   | D     | 255 | THR  |
| 1   | D     | 262 | GLN  |
| 1   | D     | 263 | LYS  |
| 1   | D     | 275 | LEU  |
| 1   | D     | 276 | TYR  |
| 1   | D     | 281 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 285 | GLU  |
| 1   | D     | 286 | GLU  |
| 1   | D     | 290 | GLN  |
| 1   | E     | 6   | LEU  |
| 1   | E     | 21  | GLN  |
| 1   | E     | 25  | VAL  |
| 1   | E     | 62  | LEU  |
| 1   | E     | 71  | LEU  |
| 1   | E     | 72  | VAL  |
| 1   | E     | 81  | THR  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 107 | ILE  |
| 1   | E     | 114 | VAL  |
| 1   | E     | 120 | VAL  |
| 1   | E     | 122 | GLN  |
| 1   | E     | 150 | ARG  |
| 1   | E     | 188 | PHE  |
| 1   | E     | 193 | LYS  |
| 1   | E     | 195 | LEU  |
| 1   | E     | 202 | LYS  |
| 1   | E     | 206 | LYS  |
| 1   | E     | 215 | GLU  |
| 1   | E     | 224 | LEU  |
| 1   | E     | 245 | MET  |
| 1   | E     | 262 | GLN  |
| 1   | E     | 263 | LYS  |
| 1   | E     | 266 | VAL  |
| 1   | E     | 275 | LEU  |
| 1   | E     | 285 | GLU  |
| 1   | E     | 287 | LYS  |
| 1   | F     | 21  | GLN  |
| 1   | F     | 25  | VAL  |
| 1   | F     | 43  | LYS  |
| 1   | F     | 48  | SER  |
| 1   | F     | 62  | LEU  |
| 1   | F     | 64  | ILE  |
| 1   | F     | 72  | VAL  |
| 1   | F     | 82  | ASN  |
| 1   | F     | 98  | ASN  |
| 1   | F     | 114 | VAL  |
| 1   | F     | 116 | LEU  |
| 1   | F     | 150 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 153 | GLU  |
| 1   | F     | 162 | ASP  |
| 1   | F     | 169 | ILE  |
| 1   | F     | 193 | LYS  |
| 1   | F     | 199 | ARG  |
| 1   | F     | 202 | LYS  |
| 1   | F     | 203 | GLU  |
| 1   | F     | 215 | GLU  |
| 1   | F     | 219 | THR  |
| 1   | F     | 254 | GLU  |
| 1   | F     | 255 | THR  |
| 1   | F     | 261 | THR  |
| 1   | F     | 262 | GLN  |
| 1   | F     | 266 | VAL  |
| 1   | F     | 269 | MET  |
| 1   | F     | 275 | LEU  |
| 1   | F     | 287 | LYS  |
| 1   | F     | 290 | GLN  |
| 1   | F     | 291 | LEU  |
| 1   | G     | 6   | LEU  |
| 1   | G     | 21  | GLN  |
| 1   | G     | 25  | VAL  |
| 1   | G     | 45  | VAL  |
| 1   | G     | 62  | LEU  |
| 1   | G     | 72  | VAL  |
| 1   | G     | 82  | ASN  |
| 1   | G     | 128 | ARG  |
| 1   | G     | 153 | GLU  |
| 1   | G     | 169 | ILE  |
| 1   | G     | 188 | PHE  |
| 1   | G     | 190 | GLU  |
| 1   | G     | 193 | LYS  |
| 1   | G     | 194 | THR  |
| 1   | G     | 196 | ASP  |
| 1   | G     | 199 | ARG  |
| 1   | G     | 202 | LYS  |
| 1   | G     | 206 | LYS  |
| 1   | G     | 215 | GLU  |
| 1   | G     | 231 | ASN  |
| 1   | G     | 255 | THR  |
| 1   | G     | 258 | ARG  |
| 1   | G     | 262 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 263 | LYS  |
| 1   | G     | 266 | VAL  |
| 1   | G     | 275 | LEU  |
| 1   | G     | 287 | LYS  |
| 1   | G     | 288 | LEU  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 292 | PHE  |
| 1   | H     | 7   | ILE  |
| 1   | H     | 48  | SER  |
| 1   | H     | 62  | LEU  |
| 1   | H     | 67  | MET  |
| 1   | H     | 72  | VAL  |
| 1   | H     | 82  | ASN  |
| 1   | H     | 123 | LYS  |
| 1   | H     | 124 | ARG  |
| 1   | H     | 131 | LYS  |
| 1   | H     | 135 | PRO  |
| 1   | H     | 150 | ARG  |
| 1   | H     | 188 | PHE  |
| 1   | H     | 195 | LEU  |
| 1   | H     | 196 | ASP  |
| 1   | H     | 199 | ARG  |
| 1   | H     | 202 | LYS  |
| 1   | H     | 205 | VAL  |
| 1   | H     | 206 | LYS  |
| 1   | H     | 215 | GLU  |
| 1   | H     | 218 | SER  |
| 1   | H     | 251 | ASN  |
| 1   | H     | 255 | THR  |
| 1   | H     | 258 | ARG  |
| 1   | H     | 261 | THR  |
| 1   | H     | 262 | GLN  |
| 1   | H     | 263 | LYS  |
| 1   | H     | 275 | LEU  |
| 1   | H     | 277 | ASP  |
| 1   | H     | 287 | LYS  |
| 1   | H     | 292 | PHE  |
| 1   | H     | 293 | ASN  |
| 1   | I     | 6   | LEU  |
| 1   | I     | 21  | GLN  |
| 1   | I     | 23  | LEU  |
| 1   | I     | 25  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 62  | LEU  |
| 1   | I     | 68  | ASP  |
| 1   | I     | 71  | LEU  |
| 1   | I     | 72  | VAL  |
| 1   | I     | 81  | THR  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 114 | VAL  |
| 1   | I     | 117 | GLU  |
| 1   | I     | 123 | LYS  |
| 1   | I     | 128 | ARG  |
| 1   | I     | 131 | LYS  |
| 1   | I     | 150 | ARG  |
| 1   | I     | 169 | ILE  |
| 1   | I     | 188 | PHE  |
| 1   | I     | 193 | LYS  |
| 1   | I     | 196 | ASP  |
| 1   | I     | 199 | ARG  |
| 1   | I     | 202 | LYS  |
| 1   | I     | 205 | VAL  |
| 1   | I     | 218 | SER  |
| 1   | I     | 224 | LEU  |
| 1   | I     | 233 | ASP  |
| 1   | I     | 255 | THR  |
| 1   | I     | 258 | ARG  |
| 1   | I     | 262 | GLN  |
| 1   | I     | 272 | ARG  |
| 1   | I     | 274 | GLN  |
| 1   | I     | 275 | LEU  |
| 1   | I     | 287 | LYS  |
| 1   | I     | 294 | GLN  |
| 1   | J     | 6   | LEU  |
| 1   | J     | 7   | ILE  |
| 1   | J     | 25  | VAL  |
| 1   | J     | 45  | VAL  |
| 1   | J     | 48  | SER  |
| 1   | J     | 62  | LEU  |
| 1   | J     | 67  | MET  |
| 1   | J     | 72  | VAL  |
| 1   | J     | 82  | ASN  |
| 1   | J     | 98  | ASN  |
| 1   | J     | 114 | VAL  |
| 1   | J     | 124 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 125 | CYS  |
| 1   | J     | 132 | GLU  |
| 1   | J     | 150 | ARG  |
| 1   | J     | 177 | ILE  |
| 1   | J     | 188 | PHE  |
| 1   | J     | 193 | LYS  |
| 1   | J     | 199 | ARG  |
| 1   | J     | 202 | LYS  |
| 1   | J     | 203 | GLU  |
| 1   | J     | 209 | ILE  |
| 1   | J     | 215 | GLU  |
| 1   | J     | 231 | ASN  |
| 1   | J     | 243 | ARG  |
| 1   | J     | 262 | GLN  |
| 1   | J     | 263 | LYS  |
| 1   | J     | 266 | VAL  |
| 1   | J     | 272 | ARG  |
| 1   | J     | 275 | LEU  |
| 1   | J     | 287 | LYS  |
| 1   | J     | 288 | LEU  |
| 1   | J     | 290 | GLN  |
| 1   | K     | 25  | VAL  |
| 1   | K     | 62  | LEU  |
| 1   | K     | 67  | MET  |
| 1   | K     | 72  | VAL  |
| 1   | K     | 75  | ASN  |
| 1   | K     | 82  | ASN  |
| 1   | K     | 90  | ASP  |
| 1   | K     | 114 | VAL  |
| 1   | K     | 125 | CYS  |
| 1   | K     | 140 | VAL  |
| 1   | K     | 150 | ARG  |
| 1   | K     | 188 | PHE  |
| 1   | K     | 193 | LYS  |
| 1   | K     | 196 | ASP  |
| 1   | K     | 199 | ARG  |
| 1   | K     | 202 | LYS  |
| 1   | K     | 206 | LYS  |
| 1   | K     | 214 | THR  |
| 1   | K     | 215 | GLU  |
| 1   | K     | 221 | LEU  |
| 1   | K     | 224 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 255 | THR  |
| 1   | K     | 262 | GLN  |
| 1   | K     | 266 | VAL  |
| 1   | K     | 271 | THR  |
| 1   | K     | 275 | LEU  |
| 1   | K     | 285 | GLU  |
| 1   | L     | 7   | ILE  |
| 1   | L     | 25  | VAL  |
| 1   | L     | 26  | VAL  |
| 1   | L     | 62  | LEU  |
| 1   | L     | 65  | SER  |
| 1   | L     | 81  | THR  |
| 1   | L     | 82  | ASN  |
| 1   | L     | 98  | ASN  |
| 1   | L     | 114 | VAL  |
| 1   | L     | 117 | GLU  |
| 1   | L     | 120 | VAL  |
| 1   | L     | 122 | GLN  |
| 1   | L     | 123 | LYS  |
| 1   | L     | 125 | CYS  |
| 1   | L     | 133 | CYS  |
| 1   | L     | 134 | VAL  |
| 1   | L     | 150 | ARG  |
| 1   | L     | 188 | PHE  |
| 1   | L     | 190 | GLU  |
| 1   | L     | 193 | LYS  |
| 1   | L     | 196 | ASP  |
| 1   | L     | 199 | ARG  |
| 1   | L     | 202 | LYS  |
| 1   | L     | 215 | GLU  |
| 1   | L     | 218 | SER  |
| 1   | L     | 255 | THR  |
| 1   | L     | 258 | ARG  |
| 1   | L     | 262 | GLN  |
| 1   | L     | 270 | GLN  |
| 1   | L     | 271 | THR  |
| 1   | L     | 275 | LEU  |
| 1   | L     | 277 | ASP  |
| 1   | L     | 279 | LEU  |
| 1   | L     | 287 | LYS  |
| 1   | L     | 292 | PHE  |
| 1   | M     | 17  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 21  | GLN  |
| 1   | M     | 23  | LEU  |
| 1   | M     | 25  | VAL  |
| 1   | M     | 62  | LEU  |
| 1   | M     | 67  | MET  |
| 1   | M     | 72  | VAL  |
| 1   | M     | 75  | ASN  |
| 1   | M     | 81  | THR  |
| 1   | M     | 82  | ASN  |
| 1   | M     | 128 | ARG  |
| 1   | M     | 150 | ARG  |
| 1   | M     | 161 | THR  |
| 1   | M     | 162 | ASP  |
| 1   | M     | 167 | GLU  |
| 1   | M     | 188 | PHE  |
| 1   | M     | 190 | GLU  |
| 1   | M     | 193 | LYS  |
| 1   | M     | 195 | LEU  |
| 1   | M     | 199 | ARG  |
| 1   | M     | 203 | GLU  |
| 1   | M     | 213 | LEU  |
| 1   | M     | 225 | ASP  |
| 1   | M     | 262 | GLN  |
| 1   | M     | 269 | MET  |
| 1   | M     | 271 | THR  |
| 1   | M     | 272 | ARG  |
| 1   | M     | 275 | LEU  |
| 1   | M     | 277 | ASP  |
| 1   | M     | 287 | LYS  |
| 1   | M     | 288 | LEU  |
| 1   | N     | 6   | LEU  |
| 1   | N     | 7   | ILE  |
| 1   | N     | 23  | LEU  |
| 1   | N     | 48  | SER  |
| 1   | N     | 62  | LEU  |
| 1   | N     | 65  | SER  |
| 1   | N     | 71  | LEU  |
| 1   | N     | 72  | VAL  |
| 1   | N     | 82  | ASN  |
| 1   | N     | 103 | ILE  |
| 1   | N     | 120 | VAL  |
| 1   | N     | 124 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 125 | CYS  |
| 1   | N     | 131 | LYS  |
| 1   | N     | 140 | VAL  |
| 1   | N     | 150 | ARG  |
| 1   | N     | 153 | GLU  |
| 1   | N     | 154 | THR  |
| 1   | N     | 188 | PHE  |
| 1   | N     | 193 | LYS  |
| 1   | N     | 195 | LEU  |
| 1   | N     | 199 | ARG  |
| 1   | N     | 202 | LYS  |
| 1   | N     | 203 | GLU  |
| 1   | N     | 213 | LEU  |
| 1   | N     | 214 | THR  |
| 1   | N     | 215 | GLU  |
| 1   | N     | 233 | ASP  |
| 1   | N     | 237 | TYR  |
| 1   | N     | 251 | ASN  |
| 1   | N     | 254 | GLU  |
| 1   | N     | 258 | ARG  |
| 1   | N     | 262 | GLN  |
| 1   | N     | 268 | THR  |
| 1   | N     | 275 | LEU  |
| 1   | N     | 276 | TYR  |
| 1   | N     | 277 | ASP  |
| 1   | N     | 291 | LEU  |
| 1   | O     | 7   | ILE  |
| 1   | O     | 8   | SER  |
| 1   | O     | 17  | VAL  |
| 1   | O     | 21  | GLN  |
| 1   | O     | 25  | VAL  |
| 1   | O     | 26  | VAL  |
| 1   | O     | 48  | SER  |
| 1   | O     | 72  | VAL  |
| 1   | O     | 75  | ASN  |
| 1   | O     | 81  | THR  |
| 1   | O     | 82  | ASN  |
| 1   | O     | 99  | ILE  |
| 1   | O     | 114 | VAL  |
| 1   | O     | 120 | VAL  |
| 1   | O     | 123 | LYS  |
| 1   | O     | 124 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 152 | ASP  |
| 1   | O     | 188 | PHE  |
| 1   | O     | 193 | LYS  |
| 1   | O     | 195 | LEU  |
| 1   | O     | 199 | ARG  |
| 1   | O     | 202 | LYS  |
| 1   | O     | 206 | LYS  |
| 1   | O     | 213 | LEU  |
| 1   | O     | 215 | GLU  |
| 1   | O     | 218 | SER  |
| 1   | O     | 221 | LEU  |
| 1   | O     | 231 | ASN  |
| 1   | O     | 232 | VAL  |
| 1   | O     | 247 | LYS  |
| 1   | O     | 255 | THR  |
| 1   | O     | 263 | LYS  |
| 1   | O     | 266 | VAL  |
| 1   | O     | 275 | LEU  |
| 1   | O     | 282 | TYR  |
| 1   | O     | 285 | GLU  |
| 1   | O     | 287 | LYS  |
| 1   | P     | 21  | GLN  |
| 1   | P     | 25  | VAL  |
| 1   | P     | 26  | VAL  |
| 1   | P     | 55  | ASN  |
| 1   | P     | 62  | LEU  |
| 1   | P     | 72  | VAL  |
| 1   | P     | 75  | ASN  |
| 1   | P     | 78  | THR  |
| 1   | P     | 81  | THR  |
| 1   | P     | 82  | ASN  |
| 1   | P     | 85  | LEU  |
| 1   | P     | 87  | VAL  |
| 1   | P     | 116 | LEU  |
| 1   | P     | 123 | LYS  |
| 1   | P     | 131 | LYS  |
| 1   | P     | 188 | PHE  |
| 1   | P     | 193 | LYS  |
| 1   | P     | 196 | ASP  |
| 1   | P     | 199 | ARG  |
| 1   | P     | 202 | LYS  |
| 1   | P     | 203 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 206 | LYS  |
| 1   | P     | 215 | GLU  |
| 1   | P     | 231 | ASN  |
| 1   | P     | 232 | VAL  |
| 1   | P     | 233 | ASP  |
| 1   | P     | 236 | LEU  |
| 1   | P     | 243 | ARG  |
| 1   | P     | 245 | MET  |
| 1   | P     | 254 | GLU  |
| 1   | P     | 258 | ARG  |
| 1   | P     | 259 | ASP  |
| 1   | P     | 261 | THR  |
| 1   | P     | 263 | LYS  |
| 1   | P     | 266 | VAL  |
| 1   | P     | 277 | ASP  |
| 1   | P     | 288 | LEU  |
| 1   | P     | 290 | GLN  |
| 1   | P     | 291 | LEU  |
| 1   | P     | 292 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 98  | ASN  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 246 | ASN  |
| 1   | A     | 262 | GLN  |
| 1   | A     | 270 | GLN  |
| 1   | A     | 274 | GLN  |
| 1   | B     | 98  | ASN  |
| 1   | B     | 246 | ASN  |
| 1   | B     | 262 | GLN  |
| 1   | B     | 270 | GLN  |
| 1   | B     | 290 | GLN  |
| 1   | C     | 98  | ASN  |
| 1   | C     | 122 | GLN  |
| 1   | C     | 127 | HIS  |
| 1   | C     | 246 | ASN  |
| 1   | C     | 262 | GLN  |
| 1   | C     | 274 | GLN  |
| 1   | C     | 290 | GLN  |
| 1   | D     | 82  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 98  | ASN  |
| 1   | D     | 246 | ASN  |
| 1   | D     | 262 | GLN  |
| 1   | D     | 270 | GLN  |
| 1   | E     | 75  | ASN  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 119 | GLN  |
| 1   | E     | 122 | GLN  |
| 1   | E     | 246 | ASN  |
| 1   | E     | 251 | ASN  |
| 1   | E     | 262 | GLN  |
| 1   | E     | 270 | GLN  |
| 1   | E     | 293 | ASN  |
| 1   | F     | 55  | ASN  |
| 1   | F     | 98  | ASN  |
| 1   | F     | 119 | GLN  |
| 1   | F     | 262 | GLN  |
| 1   | F     | 270 | GLN  |
| 1   | F     | 274 | GLN  |
| 1   | G     | 246 | ASN  |
| 1   | G     | 262 | GLN  |
| 1   | G     | 270 | GLN  |
| 1   | G     | 290 | GLN  |
| 1   | H     | 75  | ASN  |
| 1   | H     | 98  | ASN  |
| 1   | H     | 119 | GLN  |
| 1   | H     | 231 | ASN  |
| 1   | H     | 246 | ASN  |
| 1   | H     | 251 | ASN  |
| 1   | H     | 262 | GLN  |
| 1   | H     | 290 | GLN  |
| 1   | H     | 293 | ASN  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 98  | ASN  |
| 1   | I     | 122 | GLN  |
| 1   | I     | 246 | ASN  |
| 1   | I     | 251 | ASN  |
| 1   | I     | 270 | GLN  |
| 1   | I     | 290 | GLN  |
| 1   | J     | 98  | ASN  |
| 1   | J     | 246 | ASN  |
| 1   | J     | 251 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 262 | GLN  |
| 1   | J     | 270 | GLN  |
| 1   | K     | 122 | GLN  |
| 1   | K     | 246 | ASN  |
| 1   | K     | 262 | GLN  |
| 1   | K     | 270 | GLN  |
| 1   | K     | 290 | GLN  |
| 1   | L     | 98  | ASN  |
| 1   | L     | 246 | ASN  |
| 1   | L     | 262 | GLN  |
| 1   | L     | 274 | GLN  |
| 1   | L     | 290 | GLN  |
| 1   | M     | 24  | GLN  |
| 1   | M     | 82  | ASN  |
| 1   | M     | 127 | HIS  |
| 1   | M     | 246 | ASN  |
| 1   | M     | 262 | GLN  |
| 1   | M     | 270 | GLN  |
| 1   | N     | 82  | ASN  |
| 1   | N     | 122 | GLN  |
| 1   | N     | 246 | ASN  |
| 1   | N     | 251 | ASN  |
| 1   | N     | 262 | GLN  |
| 1   | N     | 270 | GLN  |
| 1   | O     | 82  | ASN  |
| 1   | O     | 98  | ASN  |
| 1   | O     | 119 | GLN  |
| 1   | O     | 122 | GLN  |
| 1   | O     | 231 | ASN  |
| 1   | O     | 246 | ASN  |
| 1   | O     | 251 | ASN  |
| 1   | O     | 270 | GLN  |
| 1   | O     | 274 | GLN  |
| 1   | P     | 82  | ASN  |
| 1   | P     | 98  | ASN  |
| 1   | P     | 231 | ASN  |
| 1   | P     | 246 | ASN  |
| 1   | P     | 262 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 290/298 (97%)   | 0.26   | 3 (1%) 79 73  | 26, 44, 60, 67        | 0     |
| 1   | B     | 286/298 (95%)   | 0.11   | 1 (0%) 90 87  | 28, 45, 60, 67        | 0     |
| 1   | C     | 287/298 (96%)   | 0.21   | 3 (1%) 79 73  | 29, 46, 61, 69        | 0     |
| 1   | D     | 287/298 (96%)   | 0.06   | 1 (0%) 90 87  | 32, 46, 61, 67        | 0     |
| 1   | E     | 288/298 (96%)   | 0.25   | 1 (0%) 90 87  | 32, 46, 62, 73        | 0     |
| 1   | F     | 286/298 (95%)   | 0.18   | 3 (1%) 79 73  | 32, 48, 63, 71        | 0     |
| 1   | G     | 287/298 (96%)   | 0.03   | 2 (0%) 84 79  | 30, 46, 60, 68        | 0     |
| 1   | H     | 288/298 (96%)   | 0.07   | 3 (1%) 79 73  | 34, 47, 62, 70        | 0     |
| 1   | I     | 289/298 (96%)   | 0.09   | 1 (0%) 90 87  | 33, 46, 61, 70        | 0     |
| 1   | J     | 288/298 (96%)   | 0.12   | 3 (1%) 79 73  | 33, 47, 62, 67        | 0     |
| 1   | K     | 286/298 (95%)   | 0.12   | 0 100 100     | 32, 47, 62, 76        | 0     |
| 1   | L     | 286/298 (95%)   | 0.16   | 0 100 100     | 33, 48, 64, 74        | 0     |
| 1   | M     | 287/298 (96%)   | 0.49   | 10 (3%) 47 38 | 33, 49, 65, 80        | 0     |
| 1   | N     | 287/298 (96%)   | 0.65   | 11 (3%) 44 36 | 33, 50, 65, 72        | 0     |
| 1   | O     | 288/298 (96%)   | 0.67   | 10 (3%) 47 38 | 34, 50, 71, 88        | 0     |
| 1   | P     | 286/298 (95%)   | 0.42   | 6 (2%) 63 54  | 33, 49, 69, 78        | 0     |
| All | All   | 4596/4768 (96%) | 0.24   | 58 (1%) 75 67 | 26, 47, 63, 88        | 0     |

All (58) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 282 | TYR  | 3.2  |
| 1   | N     | 217 | GLY  | 3.2  |
| 1   | N     | 219 | THR  | 2.9  |
| 1   | O     | 129 | PRO  | 2.9  |
| 1   | M     | 191 | ALA  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 220 | PRO  | 2.8  |
| 1   | M     | 281 | TYR  | 2.8  |
| 1   | P     | 292 | PHE  | 2.7  |
| 1   | C     | 282 | TYR  | 2.7  |
| 1   | F     | 162 | ASP  | 2.7  |
| 1   | J     | 219 | THR  | 2.6  |
| 1   | N     | 166 | ALA  | 2.6  |
| 1   | N     | 232 | VAL  | 2.5  |
| 1   | D     | 191 | ALA  | 2.5  |
| 1   | F     | 191 | ALA  | 2.5  |
| 1   | N     | 218 | SER  | 2.5  |
| 1   | M     | 220 | PRO  | 2.5  |
| 1   | O     | 222 | PHE  | 2.5  |
| 1   | J     | 165 | ALA  | 2.5  |
| 1   | O     | 191 | ALA  | 2.5  |
| 1   | B     | 191 | ALA  | 2.4  |
| 1   | C     | 191 | ALA  | 2.4  |
| 1   | G     | 290 | GLN  | 2.4  |
| 1   | I     | 219 | THR  | 2.4  |
| 1   | H     | 282 | TYR  | 2.4  |
| 1   | O     | 121 | GLY  | 2.4  |
| 1   | P     | 26  | VAL  | 2.4  |
| 1   | O     | 224 | LEU  | 2.3  |
| 1   | P     | 250 | LEU  | 2.3  |
| 1   | A     | 293 | ASN  | 2.3  |
| 1   | M     | 284 | TYR  | 2.3  |
| 1   | M     | 293 | ASN  | 2.3  |
| 1   | M     | 219 | THR  | 2.3  |
| 1   | J     | 130 | GLY  | 2.3  |
| 1   | A     | 166 | ALA  | 2.2  |
| 1   | C     | 251 | ASN  | 2.2  |
| 1   | O     | 123 | LYS  | 2.2  |
| 1   | G     | 191 | ALA  | 2.2  |
| 1   | O     | 230 | ALA  | 2.2  |
| 1   | A     | 219 | THR  | 2.1  |
| 1   | O     | 128 | ARG  | 2.1  |
| 1   | N     | 214 | THR  | 2.1  |
| 1   | P     | 260 | GLY  | 2.1  |
| 1   | F     | 292 | PHE  | 2.1  |
| 1   | M     | 288 | LEU  | 2.1  |
| 1   | H     | 191 | ALA  | 2.1  |
| 1   | P     | 218 | SER  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 199 | ARG  | 2.1  |
| 1   | H     | 281 | TYR  | 2.1  |
| 1   | E     | 191 | ALA  | 2.1  |
| 1   | M     | 230 | ALA  | 2.1  |
| 1   | N     | 182 | ALA  | 2.1  |
| 1   | M     | 285 | GLU  | 2.1  |
| 1   | P     | 258 | ARG  | 2.0  |
| 1   | N     | 194 | THR  | 2.0  |
| 1   | O     | 17  | VAL  | 2.0  |
| 1   | N     | 129 | PRO  | 2.0  |
| 1   | N     | 186 | MET  | 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.