



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 5JY7 / pdb\_00005jy7  
Title : Complex of Mycobacterium smegmatis trehalose synthase with maltokinase  
Authors : Futterer, K.; Kermani, A.A.; Besra, G.S.  
Deposited on : 2016-05-13  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

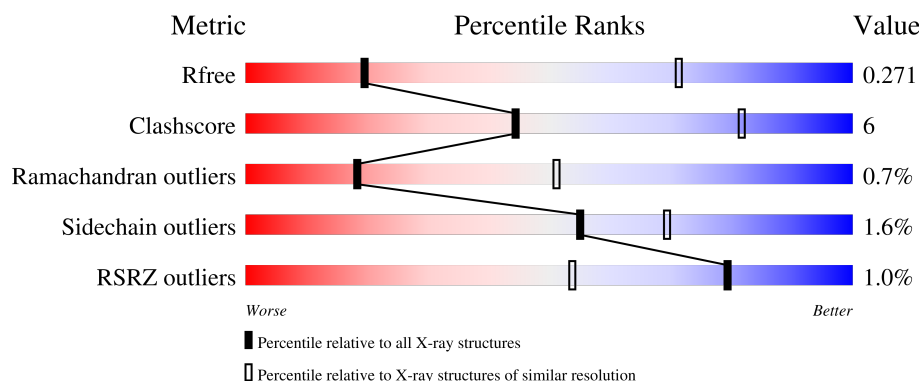
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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                      | 1747 (3.70-3.50)                                      |
| Clashscore            | 190562                      | 1827 (3.70-3.50)                                      |
| Ramachandran outliers | 187476                      | 1773 (3.70-3.50)                                      |
| Sidechain outliers    | 187428                      | 1772 (3.70-3.50)                                      |
| RSRZ outliers         | 180081                      | 1745 (3.70-3.50)                                      |

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     | 593    | <br>86% 9% 5%  |
| 1   | B     | 593    | <br>85% 10% .  |
| 1   | C     | 593    | <br>87% 8% .   |
| 1   | D     | 593    | <br>86% 10% .  |
| 1   | E     | 593    | <br>83% 10% 7% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 593    |                  |
| 1   | G     | 593    |                  |
| 1   | H     | 593    |                  |
| 2   | I     | 441    |                  |
| 2   | J     | 441    |                  |
| 2   | K     | 441    |                  |
| 2   | L     | 441    |                  |
| 2   | M     | 441    |                  |
| 2   | N     | 441    |                  |
| 2   | O     | 441    |                  |
| 2   | P     | 441    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | CA   | F     | 601 | -         | -        | -       | X                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 56343 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 Trehalose synthase/amylase TreS.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 565      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4610  | 2952 | 788 | 853 | 17 |         |         |       |
| 1   | B     | 571      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4661  | 2981 | 800 | 863 | 17 |         |         |       |
| 1   | C     | 569      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4630  | 2964 | 792 | 857 | 17 |         |         |       |
| 1   | D     | 571      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4661  | 2981 | 800 | 863 | 17 |         |         |       |
| 1   | E     | 549      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4496  | 2884 | 764 | 831 | 17 |         |         |       |
| 1   | F     | 571      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4661  | 2981 | 800 | 863 | 17 |         |         |       |
| 1   | G     | 571      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4661  | 2981 | 800 | 863 | 17 |         |         |       |
| 1   | H     | 544      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4452  | 2858 | 756 | 821 | 17 |         |         |       |

- Molecule 2 is a protein called Maltokinase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | I     | 435      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2909  | 1811 | 523 | 569 | 6 |         |         |       |
| 2   | J     | 435      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2899  | 1807 | 523 | 563 | 6 |         |         |       |
| 2   | K     | 353      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2380  | 1481 | 432 | 462 | 5 |         |         |       |
| 2   | L     | 436      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2913  | 1816 | 524 | 566 | 7 |         |         |       |
| 2   | M     | 431      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2887  | 1799 | 519 | 563 | 6 |         |         |       |
| 2   | N     | 349      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2347  | 1459 | 428 | 455 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | O     | 239      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1584  | 974 | 291 | 315 | 4 |         |         |       |
| 2   | P     | 239      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1584  | 974 | 291 | 315 | 4 |         |         |       |

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

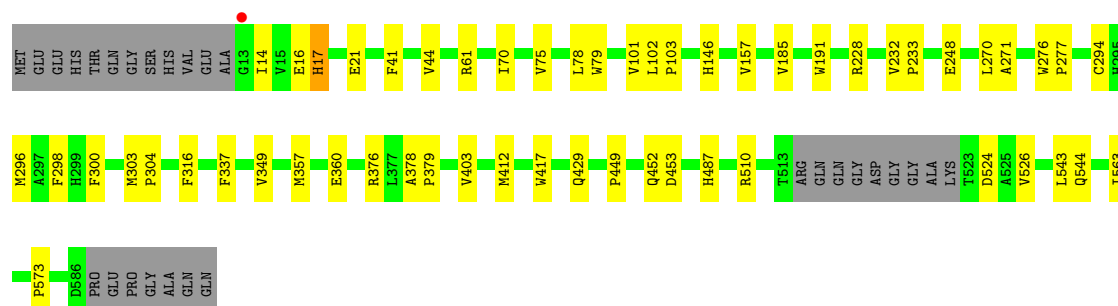
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | F     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | H     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

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.

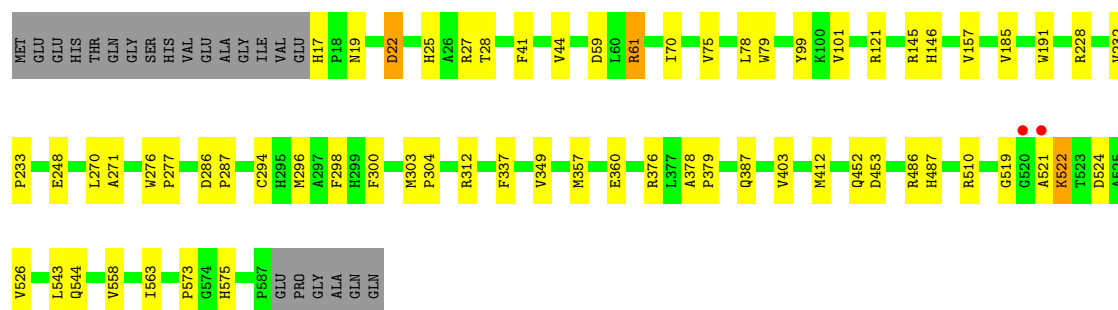
- Molecule 1: Trehalose synthase/amylase TreS

Chain A: 



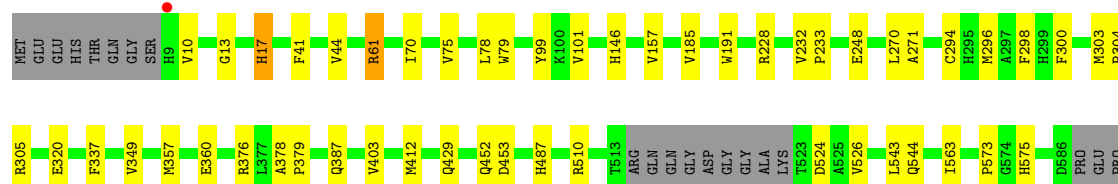
- Molecule 1: Trehalose synthase/amylase TreS

Chain B: 



- Molecule 1: Trehalose synthase/amylase TreS

Chain C: 



GLY  
ALA  
GLN

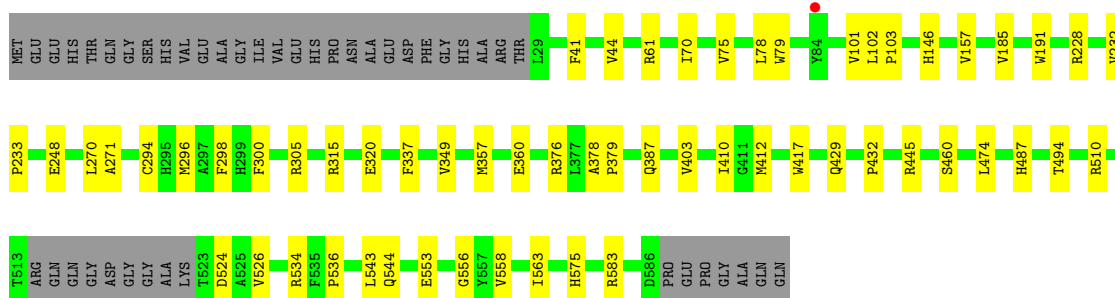
• Molecule 1: Trehalose synthase/amilase TreS

Chain D:  86% 10%



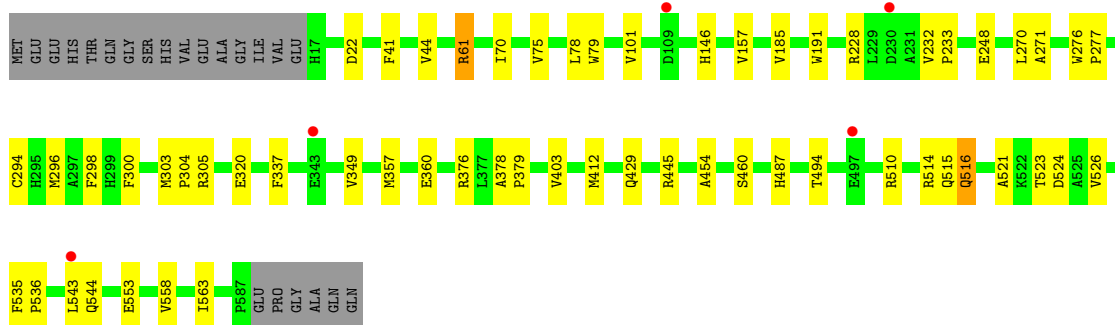
• Molecule 1: Trehalose synthase/amilase TreS

Chain E:  83% 10% 7%



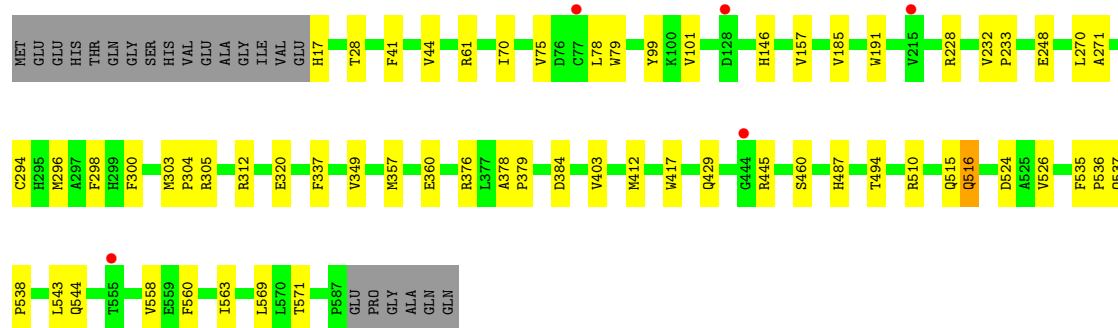
• Molecule 1: Trehalose synthase/amilase TreS

Chain F:  86% 10%

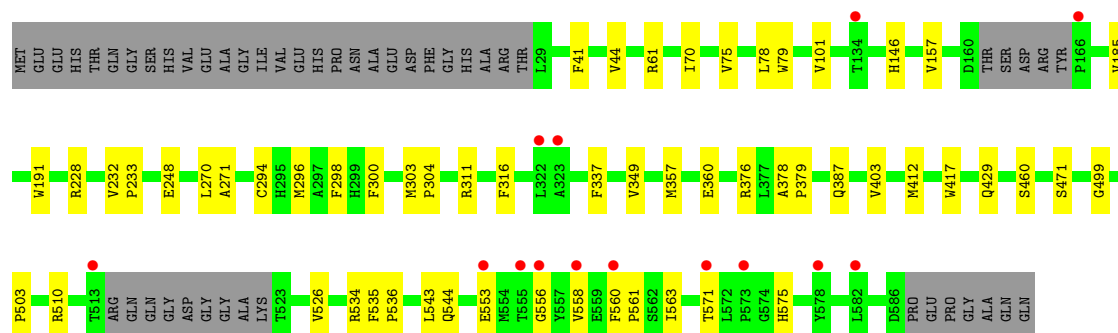
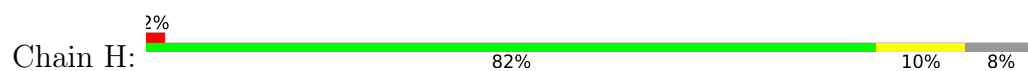


• Molecule 1: Trehalose synthase/amilase TreS

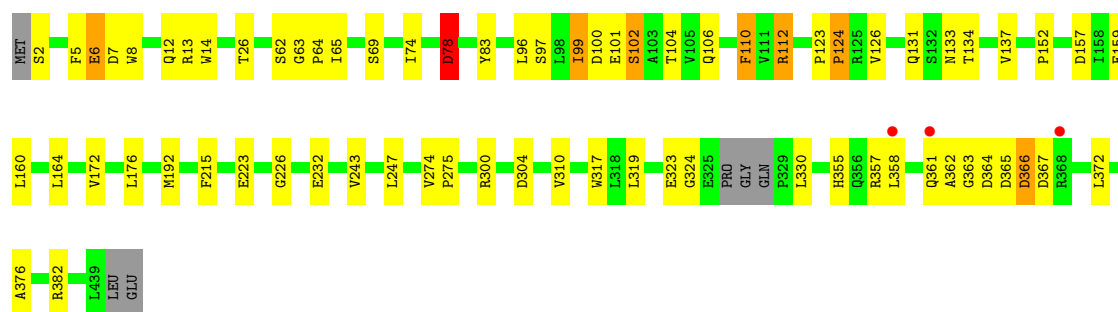
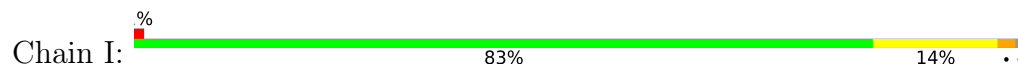
Chain G:  86% 10%



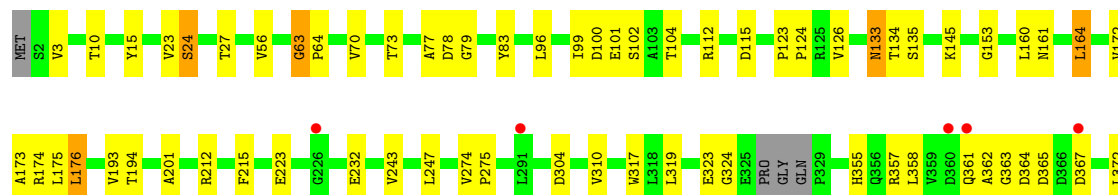
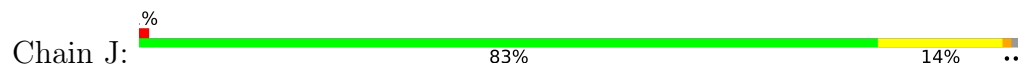
• Molecule 1: Trehalose synthase/amylase TreS

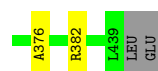


• Molecule 2: Maltokinase

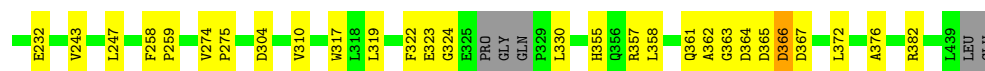
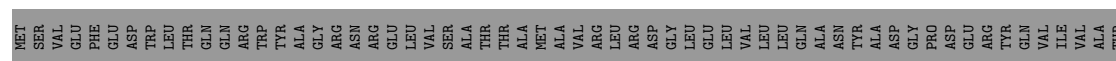


• Molecule 2: Maltokinase

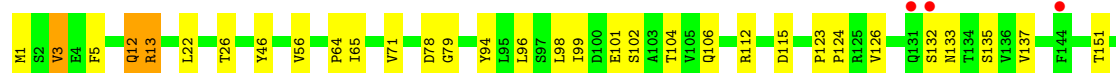
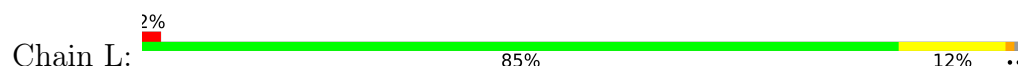




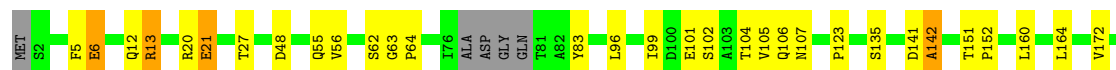
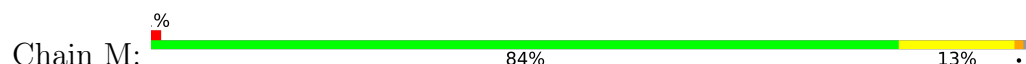
• Molecule 2: Maltokinase



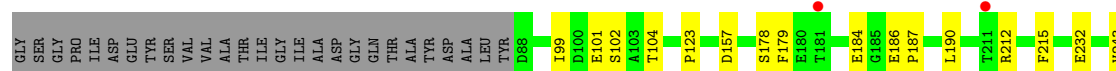
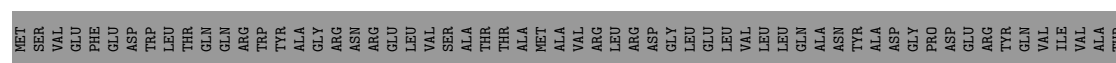
• Molecule 2: Maltokinase

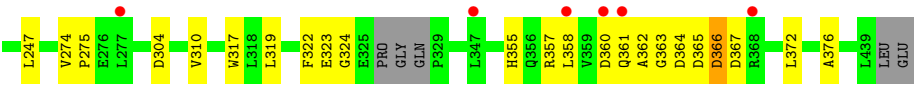


• Molecule 2: Maltokinase

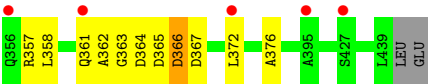
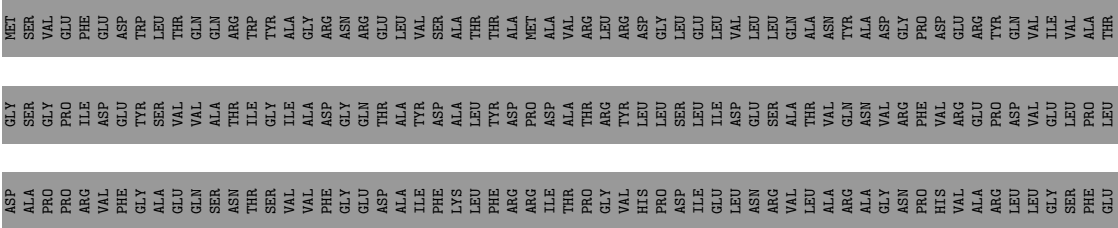


• Molecule 2: Maltokinase

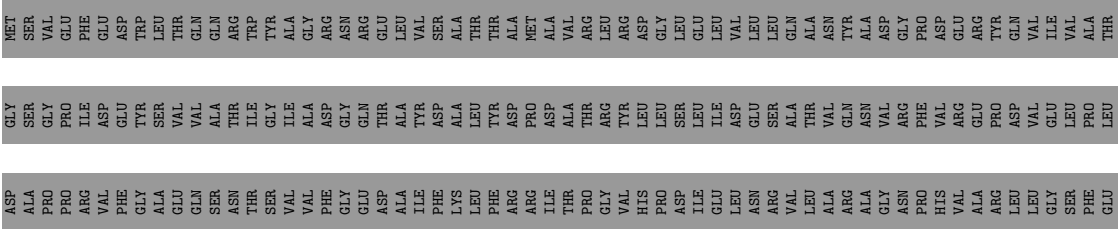




● Molecule 2: Maltokinase



● Molecule 2: Maltokinase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 315.68Å 315.68Å 124.95Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.90 – 3.60<br>49.90 – 3.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (49.90-3.60)<br>99.8 (49.90-3.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.17                                                        | Depositor        |
| $R_{sym}$                                                               | 0.17                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.30 (at 3.57Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0073                                             | Depositor        |
| R, $R_{free}$                                                           | 0.261 , 0.281<br>0.254 , 0.271                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7119 reflections (4.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 125.2                                                       | Xtriage          |
| Anisotropy                                                              | 0.002                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 79.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction                                             | 0.036 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 56343                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 111.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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     | 0.50         | 0/4754         | 0.70        | 1/6485 (0.0%)   |
| 1   | B     | 0.54         | 0/4807         | 0.71        | 1/6556 (0.0%)   |
| 1   | C     | 0.50         | 0/4774         | 0.71        | 1/6513 (0.0%)   |
| 1   | D     | 0.45         | 0/4807         | 0.68        | 1/6556 (0.0%)   |
| 1   | E     | 0.41         | 0/4636         | 0.68        | 1/6324 (0.0%)   |
| 1   | F     | 0.46         | 2/4807 (0.0%)  | 0.68        | 1/6556 (0.0%)   |
| 1   | G     | 0.40         | 0/4807         | 0.67        | 1/6556 (0.0%)   |
| 1   | H     | 0.38         | 0/4590         | 0.67        | 1/6259 (0.0%)   |
| 2   | I     | 0.63         | 0/2973         | 0.94        | 5/4091 (0.1%)   |
| 2   | J     | 0.58         | 0/2963         | 0.89        | 6/4078 (0.1%)   |
| 2   | K     | 0.49         | 0/2432         | 0.86        | 4/3343 (0.1%)   |
| 2   | L     | 0.64         | 2/2977 (0.1%)  | 0.88        | 6/4095 (0.1%)   |
| 2   | M     | 0.52         | 0/2950         | 0.86        | 4/4058 (0.1%)   |
| 2   | N     | 0.50         | 0/2398         | 0.88        | 4/3296 (0.1%)   |
| 2   | O     | 0.47         | 0/1615         | 0.91        | 4/2219 (0.2%)   |
| 2   | P     | 0.48         | 0/1615         | 0.92        | 4/2219 (0.2%)   |
| All | All   | 0.49         | 4/57905 (0.0%) | 0.76        | 45/79204 (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 |
|-----|-------|---------------------|---------------------|
| 2   | L     | 0                   | 2                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | L     | 352 | TYR  | C-N   | 14.87 | 1.53        | 1.33     |
| 2   | L     | 366 | ASP  | C-N   | 13.30 | 1.51        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 61  | ARG  | CZ-NH1 | 10.59 | 1.47        | 1.32     |
| 1   | F     | 61  | ARG  | CD-NE  | 10.57 | 1.61        | 1.46     |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 61  | ARG  | CG-CD-NE | 8.27  | 130.19      | 112.00   |
| 1   | A     | 61  | ARG  | CG-CD-NE | 7.46  | 128.42      | 112.00   |
| 1   | G     | 61  | ARG  | CG-CD-NE | 7.40  | 128.28      | 112.00   |
| 1   | E     | 61  | ARG  | CG-CD-NE | 7.38  | 128.23      | 112.00   |
| 1   | H     | 61  | ARG  | CG-CD-NE | 7.38  | 128.23      | 112.00   |
| 1   | B     | 61  | ARG  | CG-CD-NE | 7.36  | 128.19      | 112.00   |
| 1   | D     | 61  | ARG  | CG-CD-NE | 7.34  | 128.15      | 112.00   |
| 2   | J     | 133 | ASN  | N-CA-C   | 7.33  | 119.88      | 108.96   |
| 2   | J     | 367 | ASP  | N-CA-C   | 7.27  | 118.85      | 111.07   |
| 2   | P     | 274 | VAL  | CA-C-N   | 7.19  | 128.83      | 119.84   |
| 2   | P     | 274 | VAL  | C-N-CA   | 7.19  | 128.83      | 119.84   |
| 2   | I     | 133 | ASN  | N-CA-C   | 7.14  | 119.37      | 108.52   |
| 2   | O     | 274 | VAL  | CA-C-N   | 7.11  | 128.73      | 119.84   |
| 2   | O     | 274 | VAL  | C-N-CA   | 7.11  | 128.73      | 119.84   |
| 2   | N     | 274 | VAL  | CA-C-N   | 7.09  | 128.71      | 119.84   |
| 2   | N     | 274 | VAL  | C-N-CA   | 7.09  | 128.71      | 119.84   |
| 1   | C     | 61  | ARG  | CG-CD-NE | 7.04  | 127.48      | 112.00   |
| 2   | K     | 274 | VAL  | CA-C-N   | 7.00  | 128.59      | 119.84   |
| 2   | K     | 274 | VAL  | C-N-CA   | 7.00  | 128.59      | 119.84   |
| 2   | J     | 274 | VAL  | CA-C-N   | 6.92  | 128.49      | 119.84   |
| 2   | J     | 274 | VAL  | C-N-CA   | 6.92  | 128.49      | 119.84   |
| 2   | O     | 367 | ASP  | N-CA-C   | 6.92  | 118.47      | 111.07   |
| 2   | P     | 367 | ASP  | N-CA-C   | 6.90  | 118.45      | 111.07   |
| 2   | N     | 367 | ASP  | N-CA-C   | 6.88  | 118.43      | 111.07   |
| 2   | K     | 367 | ASP  | N-CA-C   | 6.87  | 118.42      | 111.07   |
| 2   | M     | 274 | VAL  | CA-C-N   | 6.83  | 128.37      | 119.84   |
| 2   | M     | 274 | VAL  | C-N-CA   | 6.83  | 128.37      | 119.84   |
| 2   | L     | 274 | VAL  | CA-C-N   | 6.81  | 128.35      | 119.84   |
| 2   | L     | 274 | VAL  | C-N-CA   | 6.81  | 128.35      | 119.84   |
| 2   | M     | 367 | ASP  | N-CA-C   | 6.68  | 118.22      | 111.07   |
| 2   | L     | 366 | ASP  | N-CA-C   | 6.52  | 121.43      | 112.04   |
| 2   | I     | 367 | ASP  | N-CA-C   | 6.47  | 118.00      | 111.07   |
| 2   | I     | 274 | VAL  | CA-C-N   | 6.23  | 127.62      | 119.84   |
| 2   | I     | 274 | VAL  | C-N-CA   | 6.23  | 127.62      | 119.84   |
| 2   | J     | 362 | ALA  | N-CA-C   | -6.02 | 105.98      | 113.15   |
| 2   | L     | 12  | GLN  | N-CA-C   | 5.93  | 117.62      | 111.03   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | K     | 362 | ALA  | N-CA-C | -5.70 | 106.18      | 113.02   |
| 2   | M     | 362 | ALA  | N-CA-C | -5.60 | 106.30      | 113.02   |
| 2   | O     | 362 | ALA  | N-CA-C | -5.50 | 106.42      | 113.02   |
| 2   | L     | 362 | ALA  | N-CA-C | -5.46 | 106.47      | 113.02   |
| 2   | I     | 362 | ALA  | N-CA-C | -5.45 | 106.47      | 113.02   |
| 2   | N     | 362 | ALA  | N-CA-C | -5.43 | 106.51      | 113.02   |
| 2   | L     | 133 | ASN  | N-CA-C | 5.31  | 116.35      | 108.60   |
| 2   | P     | 362 | ALA  | N-CA-C | -5.26 | 106.70      | 113.02   |
| 2   | J     | 63  | GLY  | N-CA-C | 5.14  | 122.84      | 112.34   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | L     | 365 | ASP  | Peptide,Mainchain |

## 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     | 4610  | 0        | 4348     | 34      | 0            |
| 1   | B     | 4661  | 0        | 4407     | 40      | 0            |
| 1   | C     | 4630  | 0        | 4359     | 33      | 0            |
| 1   | D     | 4661  | 0        | 4407     | 38      | 0            |
| 1   | E     | 4496  | 0        | 4260     | 60      | 0            |
| 1   | F     | 4661  | 0        | 4407     | 49      | 0            |
| 1   | G     | 4661  | 0        | 4407     | 77      | 0            |
| 1   | H     | 4452  | 0        | 4222     | 73      | 0            |
| 2   | I     | 2909  | 0        | 2344     | 54      | 0            |
| 2   | J     | 2899  | 0        | 2336     | 53      | 0            |
| 2   | K     | 2380  | 0        | 1950     | 40      | 0            |
| 2   | L     | 2913  | 0        | 2356     | 40      | 0            |
| 2   | M     | 2887  | 0        | 2329     | 53      | 0            |
| 2   | N     | 2347  | 0        | 1921     | 37      | 0            |
| 2   | O     | 1584  | 0        | 1255     | 43      | 0            |
| 2   | P     | 1584  | 0        | 1255     | 30      | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 56343 | 0        | 50563    | 646     | 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 6.

All (646) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:I:215:PHE:CB  | 2:I:361:GLN:HE22 | 1.62                     | 1.11              |
| 2:O:215:PHE:CB  | 2:O:361:GLN:HE22 | 1.64                     | 1.11              |
| 2:L:215:PHE:CB  | 2:L:361:GLN:HE22 | 1.64                     | 1.10              |
| 2:N:215:PHE:CB  | 2:N:361:GLN:HE22 | 1.64                     | 1.10              |
| 2:K:215:PHE:CB  | 2:K:361:GLN:HE22 | 1.64                     | 1.10              |
| 2:P:215:PHE:CB  | 2:P:361:GLN:HE22 | 1.63                     | 1.10              |
| 2:J:215:PHE:CB  | 2:J:361:GLN:HE22 | 1.65                     | 1.09              |
| 2:M:215:PHE:CB  | 2:M:361:GLN:HE22 | 1.64                     | 1.09              |
| 2:K:215:PHE:HB3 | 2:K:361:GLN:HE22 | 1.16                     | 1.09              |
| 2:I:215:PHE:HB3 | 2:I:361:GLN:HE22 | 1.17                     | 1.09              |
| 2:L:215:PHE:HB3 | 2:L:361:GLN:HE22 | 1.16                     | 1.07              |
| 2:J:215:PHE:HB3 | 2:J:361:GLN:HE22 | 1.19                     | 1.06              |
| 2:N:215:PHE:HB3 | 2:N:361:GLN:HE22 | 1.17                     | 1.05              |
| 2:M:215:PHE:HB3 | 2:M:361:GLN:HE22 | 1.17                     | 1.04              |
| 2:O:215:PHE:HB3 | 2:O:361:GLN:HE22 | 1.17                     | 1.04              |
| 2:P:215:PHE:HB3 | 2:P:361:GLN:NE2  | 1.73                     | 1.04              |
| 2:P:215:PHE:HB3 | 2:P:361:GLN:HE22 | 1.16                     | 1.03              |
| 2:K:215:PHE:HB3 | 2:K:361:GLN:NE2  | 1.73                     | 1.03              |
| 2:M:215:PHE:HB3 | 2:M:361:GLN:NE2  | 1.73                     | 1.03              |
| 2:L:215:PHE:HB3 | 2:L:361:GLN:NE2  | 1.72                     | 1.02              |
| 2:O:215:PHE:HB3 | 2:O:361:GLN:NE2  | 1.73                     | 1.02              |
| 2:I:215:PHE:HB3 | 2:I:361:GLN:NE2  | 1.72                     | 1.01              |
| 2:J:215:PHE:HB3 | 2:J:361:GLN:NE2  | 1.74                     | 1.01              |
| 2:N:215:PHE:HB3 | 2:N:361:GLN:NE2  | 1.74                     | 1.00              |
| 1:E:417:TRP:CZ2 | 1:G:445:ARG:HG2  | 1.96                     | 1.00              |
| 1:G:535:PHE:HD1 | 1:H:556:GLY:HA2  | 1.27                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:535:PHE:CD1  | 1:H:556:GLY:HA2  | 1.97                     | 0.98              |
| 1:G:536:PRO:HG2  | 1:H:553:GLU:CD   | 1.92                     | 0.95              |
| 1:E:315:ARG:NH1  | 2:M:199:ASN:OD1  | 2.03                     | 0.92              |
| 2:M:358:LEU:HD11 | 2:M:376:ALA:CB   | 2.01                     | 0.91              |
| 2:O:358:LEU:HD11 | 2:O:376:ALA:CB   | 2.01                     | 0.91              |
| 1:G:536:PRO:HG2  | 1:H:553:GLU:CG   | 2.01                     | 0.90              |
| 2:L:358:LEU:HD11 | 2:L:376:ALA:CB   | 2.01                     | 0.90              |
| 2:I:215:PHE:CD2  | 2:I:361:GLN:NE2  | 2.39                     | 0.90              |
| 2:K:358:LEU:HD11 | 2:K:376:ALA:CB   | 2.01                     | 0.89              |
| 2:L:215:PHE:CD2  | 2:L:361:GLN:NE2  | 2.41                     | 0.89              |
| 2:J:215:PHE:CD2  | 2:J:361:GLN:NE2  | 2.40                     | 0.89              |
| 2:M:215:PHE:CD2  | 2:M:361:GLN:NE2  | 2.41                     | 0.89              |
| 2:O:215:PHE:CD2  | 2:O:361:GLN:NE2  | 2.41                     | 0.88              |
| 2:P:358:LEU:HD11 | 2:P:376:ALA:CB   | 2.02                     | 0.88              |
| 1:H:503:PRO:HG3  | 2:O:206:MET:HA   | 1.52                     | 0.88              |
| 2:I:358:LEU:HD11 | 2:I:376:ALA:CB   | 2.02                     | 0.88              |
| 2:N:358:LEU:HD11 | 2:N:376:ALA:CB   | 2.02                     | 0.88              |
| 2:K:215:PHE:CD2  | 2:K:361:GLN:NE2  | 2.42                     | 0.88              |
| 2:P:215:PHE:CD2  | 2:P:361:GLN:NE2  | 2.42                     | 0.88              |
| 2:J:358:LEU:HD11 | 2:J:376:ALA:CB   | 2.03                     | 0.87              |
| 1:G:558:VAL:HG21 | 1:H:536:PRO:O    | 1.73                     | 0.87              |
| 2:N:215:PHE:CD2  | 2:N:361:GLN:NE2  | 2.42                     | 0.86              |
| 1:G:538:PRO:HG3  | 1:H:560:PHE:HA   | 1.55                     | 0.86              |
| 1:C:573:PRO:HG3  | 1:D:573:PRO:HG3  | 1.59                     | 0.84              |
| 1:E:460:SER:HB3  | 1:F:460:SER:HB3  | 1.59                     | 0.84              |
| 1:G:535:PHE:CD1  | 1:H:556:GLY:CA   | 2.62                     | 0.82              |
| 1:H:503:PRO:CB   | 2:O:206:MET:HG3  | 2.08                     | 0.82              |
| 1:G:536:PRO:O    | 1:H:558:VAL:HG11 | 1.81                     | 0.81              |
| 1:E:417:TRP:CH2  | 1:G:445:ARG:HG2  | 2.17                     | 0.80              |
| 2:M:215:PHE:CB   | 2:M:361:GLN:NE2  | 2.40                     | 0.80              |
| 1:G:535:PHE:HB3  | 1:H:556:GLY:HA3  | 1.63                     | 0.79              |
| 1:E:445:ARG:HG2  | 1:G:417:TRP:CZ2  | 2.17                     | 0.78              |
| 2:J:215:PHE:HD2  | 2:J:361:GLN:NE2  | 1.81                     | 0.78              |
| 1:G:536:PRO:HG2  | 1:H:553:GLU:HG3  | 1.66                     | 0.78              |
| 1:G:536:PRO:O    | 1:H:558:VAL:HG21 | 1.83                     | 0.78              |
| 1:G:571:THR:HB   | 1:H:560:PHE:HE2  | 1.48                     | 0.77              |
| 2:I:215:PHE:HD2  | 2:I:361:GLN:NE2  | 1.81                     | 0.77              |
| 1:G:536:PRO:O    | 1:H:558:VAL:CB   | 2.33                     | 0.77              |
| 2:M:215:PHE:HD2  | 2:M:361:GLN:NE2  | 1.83                     | 0.76              |
| 2:K:215:PHE:HD2  | 2:K:361:GLN:NE2  | 1.84                     | 0.76              |
| 2:O:215:PHE:HD2  | 2:O:361:GLN:NE2  | 1.83                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:215:PHE:HD2  | 2:N:361:GLN:NE2  | 1.83                     | 0.76              |
| 2:O:215:PHE:CB   | 2:O:361:GLN:NE2  | 2.39                     | 0.76              |
| 1:E:417:TRP:CE2  | 1:G:445:ARG:HG2  | 2.20                     | 0.75              |
| 1:A:573:PRO:HG3  | 1:B:573:PRO:HG3  | 1.69                     | 0.74              |
| 1:G:535:PHE:HD1  | 1:H:556:GLY:CA   | 2.00                     | 0.74              |
| 2:P:215:PHE:HD2  | 2:P:361:GLN:NE2  | 1.84                     | 0.74              |
| 1:H:535:PHE:CE2  | 2:O:213:ASP:HA   | 2.23                     | 0.74              |
| 1:B:376:ARG:HH12 | 1:B:412:MET:HE2  | 1.53                     | 0.73              |
| 2:P:355:HIS:CD2  | 2:P:358:LEU:HD12 | 2.23                     | 0.73              |
| 2:I:355:HIS:CD2  | 2:I:358:LEU:HD12 | 2.24                     | 0.73              |
| 1:G:376:ARG:HH12 | 1:G:412:MET:HE2  | 1.53                     | 0.73              |
| 2:L:215:PHE:CB   | 2:L:361:GLN:NE2  | 2.39                     | 0.73              |
| 2:L:215:PHE:HD2  | 2:L:361:GLN:NE2  | 1.83                     | 0.73              |
| 2:K:355:HIS:CD2  | 2:K:358:LEU:HD12 | 2.23                     | 0.73              |
| 2:I:215:PHE:CB   | 2:I:361:GLN:NE2  | 2.38                     | 0.73              |
| 2:M:164:LEU:HD23 | 2:M:172:VAL:HG21 | 1.70                     | 0.73              |
| 2:M:358:LEU:HD11 | 2:M:376:ALA:HB2  | 1.70                     | 0.73              |
| 2:N:355:HIS:CD2  | 2:N:358:LEU:HD12 | 2.24                     | 0.72              |
| 2:J:361:GLN:HB3  | 2:J:372:LEU:HD13 | 1.72                     | 0.72              |
| 2:K:358:LEU:HD11 | 2:K:376:ALA:HB2  | 1.71                     | 0.72              |
| 2:O:358:LEU:HD11 | 2:O:376:ALA:HB2  | 1.71                     | 0.72              |
| 2:L:355:HIS:CD2  | 2:L:358:LEU:HD12 | 2.25                     | 0.72              |
| 2:O:355:HIS:CD2  | 2:O:358:LEU:HD12 | 2.24                     | 0.72              |
| 2:P:358:LEU:HD11 | 2:P:376:ALA:HB2  | 1.72                     | 0.72              |
| 1:E:553:GLU:HG3  | 1:F:536:PRO:HG2  | 1.71                     | 0.72              |
| 2:M:355:HIS:CD2  | 2:M:358:LEU:HD12 | 2.25                     | 0.72              |
| 2:O:361:GLN:HB3  | 2:O:372:LEU:HD13 | 1.71                     | 0.72              |
| 2:J:215:PHE:CB   | 2:J:361:GLN:NE2  | 2.41                     | 0.72              |
| 2:J:358:LEU:HD23 | 2:J:361:GLN:OE1  | 1.89                     | 0.72              |
| 2:M:361:GLN:HB3  | 2:M:372:LEU:HD13 | 1.71                     | 0.72              |
| 1:E:556:GLY:HA2  | 1:F:535:PHE:CD1  | 2.24                     | 0.71              |
| 2:N:361:GLN:HB3  | 2:N:372:LEU:HD13 | 1.72                     | 0.71              |
| 2:M:164:LEU:HD21 | 2:M:243:VAL:HG23 | 1.72                     | 0.71              |
| 2:J:355:HIS:CD2  | 2:J:358:LEU:HD12 | 2.25                     | 0.71              |
| 2:L:361:GLN:HB3  | 2:L:372:LEU:HD13 | 1.71                     | 0.71              |
| 1:G:571:THR:HB   | 1:H:560:PHE:CE2  | 2.26                     | 0.71              |
| 2:K:361:GLN:HB3  | 2:K:372:LEU:HD13 | 1.71                     | 0.71              |
| 2:I:361:GLN:HB3  | 2:I:372:LEU:HD13 | 1.70                     | 0.71              |
| 2:J:358:LEU:HD11 | 2:J:376:ALA:HB2  | 1.72                     | 0.71              |
| 2:P:361:GLN:HB3  | 2:P:372:LEU:HD13 | 1.71                     | 0.71              |
| 2:I:358:LEU:HD11 | 2:I:376:ALA:HB2  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:358:LEU:HD11 | 2:N:376:ALA:HB2  | 1.71                     | 0.71              |
| 1:C:376:ARG:HH12 | 1:C:412:MET:HE2  | 1.55                     | 0.71              |
| 2:L:358:LEU:HD11 | 2:L:376:ALA:HB2  | 1.71                     | 0.70              |
| 2:K:215:PHE:CB   | 2:K:361:GLN:NE2  | 2.40                     | 0.70              |
| 1:E:376:ARG:HH12 | 1:E:412:MET:HE2  | 1.57                     | 0.70              |
| 1:E:417:TRP:CZ2  | 1:G:445:ARG:CG   | 2.73                     | 0.70              |
| 1:H:503:PRO:CG   | 2:O:206:MET:HG3  | 2.22                     | 0.70              |
| 2:I:164:LEU:HD21 | 2:I:243:VAL:HG23 | 1.71                     | 0.70              |
| 2:P:215:PHE:CB   | 2:P:361:GLN:NE2  | 2.40                     | 0.70              |
| 1:C:17:HIS:CD2   | 1:C:99:TYR:CE2   | 2.79                     | 0.70              |
| 1:G:535:PHE:HB3  | 1:H:558:VAL:HG23 | 1.73                     | 0.69              |
| 1:H:376:ARG:HH12 | 1:H:412:MET:HE2  | 1.56                     | 0.69              |
| 2:I:358:LEU:HD23 | 2:I:361:GLN:OE1  | 1.91                     | 0.69              |
| 2:M:358:LEU:HD23 | 2:M:361:GLN:OE1  | 1.92                     | 0.69              |
| 1:E:556:GLY:CA   | 1:F:535:PHE:CD1  | 2.74                     | 0.69              |
| 2:O:358:LEU:HD23 | 2:O:361:GLN:OE1  | 1.91                     | 0.69              |
| 2:L:358:LEU:HD23 | 2:L:361:GLN:OE1  | 1.92                     | 0.69              |
| 2:K:358:LEU:HD23 | 2:K:361:GLN:OE1  | 1.92                     | 0.69              |
| 2:N:215:PHE:CB   | 2:N:361:GLN:NE2  | 2.40                     | 0.69              |
| 1:A:376:ARG:HH12 | 1:A:412:MET:HE2  | 1.56                     | 0.69              |
| 1:E:460:SER:HB3  | 1:F:460:SER:CB   | 2.23                     | 0.69              |
| 1:E:460:SER:CB   | 1:F:460:SER:HB3  | 2.22                     | 0.69              |
| 1:F:376:ARG:HH12 | 1:F:412:MET:HE2  | 1.57                     | 0.68              |
| 2:N:358:LEU:HD23 | 2:N:361:GLN:OE1  | 1.93                     | 0.68              |
| 1:G:536:PRO:O    | 1:H:558:VAL:CG1  | 2.41                     | 0.68              |
| 2:P:358:LEU:HD23 | 2:P:361:GLN:OE1  | 1.94                     | 0.68              |
| 1:D:376:ARG:HH12 | 1:D:412:MET:HE2  | 1.59                     | 0.67              |
| 1:G:536:PRO:O    | 1:H:558:VAL:CG2  | 2.43                     | 0.67              |
| 1:H:535:PHE:HE2  | 2:O:213:ASP:HA   | 1.58                     | 0.67              |
| 1:E:558:VAL:HG22 | 2:N:212:ARG:HD3  | 1.76                     | 0.67              |
| 1:H:503:PRO:HG3  | 2:O:206:MET:HG3  | 1.77                     | 0.66              |
| 1:B:121:ARG:HA   | 2:M:48:ASP:CB    | 2.26                     | 0.65              |
| 1:F:515:GLN:O    | 1:F:516:GLN:HB2  | 1.95                     | 0.65              |
| 1:G:538:PRO:CB   | 1:H:561:PRO:HD3  | 2.26                     | 0.65              |
| 2:N:357:ARG:O    | 2:N:361:GLN:HG3  | 1.97                     | 0.65              |
| 1:D:146:HIS:CD2  | 1:D:185:VAL:HG11 | 2.32                     | 0.64              |
| 2:L:94:TYR:CE2   | 2:L:98:LEU:HD11  | 2.32                     | 0.64              |
| 1:G:535:PHE:CB   | 1:H:558:VAL:CG2  | 2.76                     | 0.64              |
| 2:L:12:GLN:O     | 2:L:13:ARG:CB    | 2.46                     | 0.64              |
| 2:M:12:GLN:O     | 2:M:13:ARG:CB    | 2.46                     | 0.64              |
| 1:B:146:HIS:CD2  | 1:B:185:VAL:HG11 | 2.33                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:146:HIS:CD2  | 1:C:185:VAL:HG11 | 2.32                     | 0.64              |
| 1:G:146:HIS:CD2  | 1:G:185:VAL:HG11 | 2.34                     | 0.63              |
| 1:H:503:PRO:HG3  | 2:O:206:MET:CA   | 2.27                     | 0.63              |
| 2:I:365:ASP:HB3  | 2:I:366:ASP:CG   | 2.24                     | 0.63              |
| 2:L:151:THR:CB   | 2:L:330:LEU:HD11 | 2.29                     | 0.63              |
| 2:M:357:ARG:O    | 2:M:361:GLN:HG3  | 1.98                     | 0.63              |
| 1:E:445:ARG:HG2  | 1:G:417:TRP:CH2  | 2.33                     | 0.63              |
| 2:K:357:ARG:O    | 2:K:361:GLN:HG3  | 1.99                     | 0.63              |
| 1:H:146:HIS:CD2  | 1:H:185:VAL:HG11 | 2.33                     | 0.63              |
| 2:J:112:ARG:NH2  | 2:J:115:ASP:O    | 2.33                     | 0.62              |
| 2:I:152:PRO:O    | 2:I:330:LEU:HD13 | 1.99                     | 0.62              |
| 1:G:535:PHE:HB2  | 1:H:558:VAL:CG2  | 2.30                     | 0.62              |
| 2:P:357:ARG:O    | 2:P:361:GLN:HG3  | 1.99                     | 0.62              |
| 1:F:146:HIS:CD2  | 1:F:185:VAL:HG11 | 2.34                     | 0.62              |
| 2:L:357:ARG:O    | 2:L:361:GLN:HG3  | 1.99                     | 0.62              |
| 2:O:357:ARG:O    | 2:O:361:GLN:HG3  | 1.98                     | 0.62              |
| 1:A:146:HIS:CD2  | 1:A:185:VAL:HG11 | 2.34                     | 0.62              |
| 1:E:146:HIS:CD2  | 1:E:185:VAL:HG11 | 2.34                     | 0.62              |
| 2:I:357:ARG:O    | 2:I:361:GLN:HG3  | 2.01                     | 0.61              |
| 2:K:164:LEU:HD21 | 2:K:243:VAL:HG23 | 1.82                     | 0.61              |
| 1:E:534:ARG:HH22 | 2:M:213:ASP:CG   | 2.09                     | 0.60              |
| 1:A:453:ASP:HA   | 1:D:452:GLN:HE22 | 1.65                     | 0.60              |
| 1:G:535:PHE:CB   | 1:H:556:GLY:HA3  | 2.32                     | 0.60              |
| 1:G:460:SER:HB3  | 1:H:460:SER:HB3  | 1.84                     | 0.60              |
| 1:G:460:SER:HB3  | 1:H:460:SER:CB   | 2.32                     | 0.60              |
| 2:I:78:ASP:CG    | 2:I:78:ASP:O     | 2.45                     | 0.59              |
| 2:J:96:LEU:O     | 2:J:99:ILE:HG22  | 2.02                     | 0.59              |
| 2:J:357:ARG:O    | 2:J:361:GLN:HG3  | 2.02                     | 0.59              |
| 1:E:271:ALA:HB2  | 1:E:294:CYS:SG   | 2.43                     | 0.58              |
| 1:C:17:HIS:CD2   | 1:C:99:TYR:CZ    | 2.91                     | 0.57              |
| 1:B:519:GLY:HA2  | 1:B:522:LYS:HB2  | 1.86                     | 0.57              |
| 2:I:358:LEU:HA   | 2:I:361:GLN:HB2  | 1.87                     | 0.57              |
| 2:I:361:GLN:HB3  | 2:I:372:LEU:CD1  | 2.35                     | 0.57              |
| 2:K:160:LEU:O    | 2:K:164:LEU:HB2  | 2.05                     | 0.56              |
| 1:B:17:HIS:HD2   | 1:B:99:TYR:CE2   | 2.24                     | 0.56              |
| 1:E:553:GLU:CG   | 1:F:536:PRO:HG2  | 2.35                     | 0.56              |
| 1:F:271:ALA:HB2  | 1:F:294:CYS:SG   | 2.45                     | 0.56              |
| 1:G:536:PRO:CG   | 1:H:553:GLU:HG3  | 2.35                     | 0.56              |
| 1:G:558:VAL:HG22 | 2:O:212:ARG:HD3  | 1.88                     | 0.56              |
| 2:I:358:LEU:CD2  | 2:I:372:LEU:HB3  | 2.35                     | 0.56              |
| 1:H:499:GLY:HA3  | 2:O:199:ASN:HA   | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:14:TRP:HA    | 2:I:131:GLN:HA   | 1.87                     | 0.56              |
| 2:K:358:LEU:HA   | 2:K:361:GLN:HB2  | 1.88                     | 0.56              |
| 2:J:358:LEU:CD2  | 2:J:372:LEU:HB3  | 2.36                     | 0.56              |
| 2:N:358:LEU:HA   | 2:N:361:GLN:HB2  | 1.88                     | 0.56              |
| 1:D:27:ARG:NH1   | 1:D:120:ARG:HG2  | 2.21                     | 0.56              |
| 2:I:63:GLY:HA2   | 2:I:83:TYR:CZ    | 2.40                     | 0.56              |
| 2:I:357:ARG:O    | 2:I:361:GLN:N    | 2.39                     | 0.56              |
| 2:O:358:LEU:HA   | 2:O:361:GLN:HB2  | 1.88                     | 0.56              |
| 1:E:556:GLY:HA3  | 1:F:535:PHE:CD1  | 2.41                     | 0.55              |
| 1:G:535:PHE:HB3  | 1:H:558:VAL:CG2  | 2.35                     | 0.55              |
| 1:E:417:TRP:CH2  | 1:G:445:ARG:CG   | 2.89                     | 0.55              |
| 2:O:361:GLN:HB3  | 2:O:372:LEU:CD1  | 2.37                     | 0.55              |
| 1:B:521:ALA:HB3  | 2:J:363:GLY:O    | 2.07                     | 0.55              |
| 2:P:357:ARG:O    | 2:P:361:GLN:N    | 2.40                     | 0.55              |
| 2:M:357:ARG:O    | 2:M:361:GLN:N    | 2.39                     | 0.55              |
| 1:G:537:GLN:HA   | 1:H:558:VAL:HG11 | 1.88                     | 0.55              |
| 2:K:361:GLN:HB3  | 2:K:372:LEU:CD1  | 2.37                     | 0.55              |
| 2:L:358:LEU:HA   | 2:L:361:GLN:HB2  | 1.88                     | 0.55              |
| 1:G:536:PRO:HG2  | 1:H:553:GLU:OE1  | 2.07                     | 0.55              |
| 2:P:361:GLN:HB3  | 2:P:372:LEU:CD1  | 2.37                     | 0.55              |
| 1:E:378:ALA:HB3  | 1:E:379:PRO:HD3  | 1.89                     | 0.55              |
| 1:F:378:ALA:HB3  | 1:F:379:PRO:HD3  | 1.89                     | 0.55              |
| 2:J:63:GLY:N     | 2:J:64:PRO:HD3   | 2.21                     | 0.55              |
| 1:G:536:PRO:O    | 1:H:558:VAL:HB   | 2.06                     | 0.55              |
| 1:A:452:GLN:HE22 | 1:D:453:ASP:HA   | 1.72                     | 0.54              |
| 1:B:378:ALA:HB3  | 1:B:379:PRO:HD3  | 1.89                     | 0.54              |
| 2:M:358:LEU:CD2  | 2:M:372:LEU:HB3  | 2.37                     | 0.54              |
| 2:J:358:LEU:HA   | 2:J:361:GLN:HB2  | 1.88                     | 0.54              |
| 2:J:361:GLN:HB3  | 2:J:372:LEU:CD1  | 2.36                     | 0.54              |
| 2:P:358:LEU:HA   | 2:P:361:GLN:HB2  | 1.88                     | 0.54              |
| 1:H:271:ALA:HB2  | 1:H:294:CYS:SG   | 2.47                     | 0.54              |
| 1:G:378:ALA:HB3  | 1:G:379:PRO:HD3  | 1.88                     | 0.54              |
| 1:H:316:PHE:CE1  | 2:O:312:ARG:HG2  | 2.42                     | 0.54              |
| 1:H:378:ALA:HB3  | 1:H:379:PRO:HD3  | 1.89                     | 0.54              |
| 2:M:358:LEU:HA   | 2:M:361:GLN:HB2  | 1.88                     | 0.54              |
| 1:B:19:ASN:O     | 1:B:22:ASP:HB3   | 2.07                     | 0.54              |
| 2:L:3:VAL:O      | 2:L:5:PHE:N      | 2.41                     | 0.54              |
| 2:O:358:LEU:CD2  | 2:O:372:LEU:HB3  | 2.38                     | 0.54              |
| 2:K:357:ARG:O    | 2:K:361:GLN:N    | 2.41                     | 0.54              |
| 2:M:361:GLN:HB3  | 2:M:372:LEU:CD1  | 2.37                     | 0.53              |
| 2:N:365:ASP:HB3  | 2:N:366:ASP:CG   | 2.33                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:160:LEU:HD12 | 2:J:247:LEU:HD21 | 1.90                     | 0.53              |
| 2:J:164:LEU:HD21 | 2:J:243:VAL:HG23 | 1.91                     | 0.53              |
| 2:L:358:LEU:CD2  | 2:L:372:LEU:HB3  | 2.37                     | 0.53              |
| 1:D:378:ALA:HB3  | 1:D:379:PRO:HD3  | 1.89                     | 0.53              |
| 2:I:5:PHE:O      | 2:I:6:GLU:C      | 2.51                     | 0.53              |
| 1:A:449:PRO:HD3  | 1:D:417:TRP:CG   | 2.44                     | 0.53              |
| 1:C:378:ALA:HB3  | 1:C:379:PRO:HD3  | 1.89                     | 0.53              |
| 1:E:417:TRP:CZ2  | 1:G:445:ARG:CD   | 2.92                     | 0.53              |
| 1:H:534:ARG:NH1  | 2:O:213:ASP:OD1  | 2.41                     | 0.53              |
| 2:J:357:ARG:O    | 2:J:361:GLN:N    | 2.41                     | 0.53              |
| 1:A:378:ALA:HB3  | 1:A:379:PRO:HD3  | 1.90                     | 0.53              |
| 2:J:23:VAL:O     | 2:J:24:SER:C     | 2.51                     | 0.53              |
| 2:O:357:ARG:O    | 2:O:361:GLN:N    | 2.41                     | 0.53              |
| 2:P:358:LEU:CD2  | 2:P:372:LEU:HB3  | 2.39                     | 0.53              |
| 1:D:228:ARG:HD2  | 1:D:298:PHE:HE2  | 1.73                     | 0.53              |
| 2:I:164:LEU:HD21 | 2:I:243:VAL:CG2  | 2.35                     | 0.53              |
| 2:L:357:ARG:O    | 2:L:361:GLN:N    | 2.41                     | 0.53              |
| 2:N:179:PHE:CZ   | 2:N:190:LEU:HB3  | 2.44                     | 0.53              |
| 2:N:357:ARG:O    | 2:N:361:GLN:N    | 2.42                     | 0.53              |
| 2:L:361:GLN:HB3  | 2:L:372:LEU:CD1  | 2.37                     | 0.53              |
| 2:O:365:ASP:HB3  | 2:O:366:ASP:CG   | 2.34                     | 0.53              |
| 1:G:384:ASP:HA   | 1:H:471:SER:CB   | 2.39                     | 0.53              |
| 2:K:358:LEU:CD2  | 2:K:372:LEU:HB3  | 2.38                     | 0.53              |
| 1:B:486:ARG:CD   | 2:J:365:ASP:O    | 2.58                     | 0.52              |
| 2:M:164:LEU:HD21 | 2:M:243:VAL:CG2  | 2.40                     | 0.52              |
| 2:I:215:PHE:CD2  | 2:I:361:GLN:CD   | 2.88                     | 0.52              |
| 2:I:8:TRP:HE3    | 2:I:12:GLN:OE1   | 1.93                     | 0.52              |
| 1:E:460:SER:CB   | 1:F:460:SER:CB   | 2.86                     | 0.52              |
| 2:I:62:SER:C     | 2:I:64:PRO:HD3   | 2.35                     | 0.52              |
| 2:P:365:ASP:HB3  | 2:P:366:ASP:CG   | 2.34                     | 0.52              |
| 1:B:270:LEU:HG   | 1:B:296:MET:HB2  | 1.92                     | 0.52              |
| 1:D:271:ALA:HB2  | 1:D:294:CYS:SG   | 2.50                     | 0.52              |
| 1:E:558:VAL:HA   | 2:N:212:ARG:HE   | 1.74                     | 0.52              |
| 2:L:22:LEU:HA    | 2:L:46:TYR:HA    | 1.92                     | 0.52              |
| 1:A:228:ARG:HD2  | 1:A:298:PHE:HE2  | 1.75                     | 0.52              |
| 2:N:358:LEU:CD2  | 2:N:372:LEU:HB3  | 2.39                     | 0.52              |
| 2:O:215:PHE:CD2  | 2:O:361:GLN:CD   | 2.88                     | 0.52              |
| 1:D:270:LEU:HG   | 1:D:296:MET:HB2  | 1.92                     | 0.52              |
| 2:N:215:PHE:CD2  | 2:N:361:GLN:CD   | 2.88                     | 0.52              |
| 1:C:270:LEU:HG   | 1:C:296:MET:HB2  | 1.91                     | 0.52              |
| 1:C:228:ARG:HD2  | 1:C:298:PHE:HE2  | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:270:LEU:HG   | 1:E:296:MET:HB2  | 1.92                     | 0.51              |
| 1:G:271:ALA:HB2  | 1:G:294:CYS:SG   | 2.49                     | 0.51              |
| 1:G:360:GLU:OE2  | 2:P:231:GLY:HA3  | 2.10                     | 0.51              |
| 1:D:514:ARG:HA   | 1:D:523:THR:HG21 | 1.93                     | 0.51              |
| 1:H:270:LEU:HG   | 1:H:296:MET:HB2  | 1.91                     | 0.51              |
| 2:M:160:LEU:HD12 | 2:M:247:LEU:HD11 | 1.93                     | 0.51              |
| 2:N:361:GLN:HB3  | 2:N:372:LEU:CD1  | 2.38                     | 0.51              |
| 1:F:270:LEU:HG   | 1:F:296:MET:HB2  | 1.92                     | 0.51              |
| 2:J:215:PHE:CD2  | 2:J:361:GLN:CD   | 2.88                     | 0.51              |
| 2:M:215:PHE:CD2  | 2:M:361:GLN:CD   | 2.89                     | 0.51              |
| 2:P:215:PHE:CD2  | 2:P:361:GLN:CD   | 2.89                     | 0.51              |
| 1:G:270:LEU:HG   | 1:G:296:MET:HB2  | 1.92                     | 0.50              |
| 2:L:215:PHE:CD2  | 2:L:361:GLN:CD   | 2.89                     | 0.50              |
| 2:N:101:GLU:N    | 2:N:102:SER:HA   | 2.26                     | 0.50              |
| 1:H:228:ARG:HD2  | 1:H:298:PHE:HE2  | 1.75                     | 0.50              |
| 2:I:8:TRP:CD1    | 2:I:74:ILE:HA    | 2.46                     | 0.50              |
| 2:L:96:LEU:O     | 2:L:99:ILE:HG22  | 2.10                     | 0.50              |
| 1:B:271:ALA:HB2  | 1:B:294:CYS:SG   | 2.51                     | 0.50              |
| 2:K:215:PHE:CD2  | 2:K:361:GLN:CD   | 2.90                     | 0.50              |
| 1:F:228:ARG:HD2  | 1:F:298:PHE:HE2  | 1.77                     | 0.50              |
| 2:I:12:GLN:O     | 2:I:13:ARG:CB    | 2.59                     | 0.50              |
| 2:I:124:PRO:HD2  | 2:I:137:VAL:O    | 2.12                     | 0.50              |
| 1:E:228:ARG:HD2  | 1:E:298:PHE:HE2  | 1.76                     | 0.49              |
| 2:J:363:GLY:N    | 2:J:364:ASP:CB   | 2.75                     | 0.49              |
| 1:E:553:GLU:CD   | 1:F:536:PRO:HG2  | 2.37                     | 0.49              |
| 1:A:270:LEU:HG   | 1:A:296:MET:HB2  | 1.93                     | 0.49              |
| 2:P:304:ASP:HB2  | 2:P:324:GLY:O    | 2.12                     | 0.49              |
| 1:E:412:MET:HE3  | 1:E:429:GLN:OE1  | 2.13                     | 0.49              |
| 2:L:101:GLU:N    | 2:L:102:SER:HA   | 2.26                     | 0.49              |
| 2:L:304:ASP:HB2  | 2:L:324:GLY:O    | 2.13                     | 0.49              |
| 2:O:363:GLY:N    | 2:O:364:ASP:CB   | 2.76                     | 0.49              |
| 2:I:160:LEU:HD12 | 2:I:247:LEU:HD11 | 1.95                     | 0.49              |
| 2:L:1:MET:HE2    | 2:L:26:THR:HB    | 1.95                     | 0.49              |
| 1:B:312:ARG:HD3  | 2:I:226:GLY:O    | 2.13                     | 0.49              |
| 1:E:534:ARG:NH1  | 2:M:213:ASP:OD1  | 2.44                     | 0.49              |
| 2:M:304:ASP:HB2  | 2:M:324:GLY:O    | 2.12                     | 0.49              |
| 1:E:445:ARG:HG2  | 1:G:417:TRP:CE2  | 2.47                     | 0.48              |
| 2:M:105:VAL:O    | 2:M:107:ASN:N    | 2.47                     | 0.48              |
| 2:N:157:ASP:HA   | 2:N:322:PHE:HB2  | 1.96                     | 0.48              |
| 2:O:304:ASP:HB2  | 2:O:324:GLY:O    | 2.12                     | 0.48              |
| 1:E:536:PRO:HG2  | 1:F:553:GLU:HG3  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:228:ARG:HD2  | 1:G:298:PHE:HE2  | 1.78                     | 0.48              |
| 1:A:271:ALA:HB2  | 1:A:294:CYS:SG   | 2.53                     | 0.48              |
| 2:O:243:VAL:HG11 | 2:O:319:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:271:ALA:HB2  | 1:C:294:CYS:SG   | 2.53                     | 0.48              |
| 1:F:514:ARG:HA   | 1:F:523:THR:HG21 | 1.96                     | 0.48              |
| 2:M:96:LEU:O     | 2:M:99:ILE:HG22  | 2.13                     | 0.48              |
| 2:N:304:ASP:HB2  | 2:N:324:GLY:O    | 2.13                     | 0.48              |
| 1:F:79:TRP:CD1   | 1:F:79:TRP:C     | 2.92                     | 0.48              |
| 2:I:8:TRP:O      | 2:I:12:GLN:HG2   | 2.13                     | 0.48              |
| 2:M:20:ARG:O     | 2:M:21:GLU:CB    | 2.60                     | 0.48              |
| 2:M:243:VAL:HG11 | 2:M:319:LEU:HD22 | 1.96                     | 0.48              |
| 1:E:41:PHE:HB2   | 1:E:403:VAL:HG22 | 1.95                     | 0.48              |
| 2:K:243:VAL:HG11 | 2:K:319:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:41:PHE:HB2   | 1:C:403:VAL:HG22 | 1.96                     | 0.47              |
| 2:I:243:VAL:HG11 | 2:I:319:LEU:HD22 | 1.96                     | 0.47              |
| 2:M:152:PRO:HG2  | 2:M:330:LEU:HD12 | 1.96                     | 0.47              |
| 2:J:101:GLU:N    | 2:J:102:SER:HA   | 2.28                     | 0.47              |
| 1:B:357:MET:HA   | 1:B:360:GLU:HG3  | 1.96                     | 0.47              |
| 1:E:79:TRP:CD1   | 1:E:79:TRP:C     | 2.92                     | 0.47              |
| 1:G:312:ARG:NH1  | 2:P:228:ASP:O    | 2.46                     | 0.47              |
| 1:G:515:GLN:O    | 1:G:516:GLN:HB2  | 2.14                     | 0.47              |
| 2:J:164:LEU:HD21 | 2:J:243:VAL:CG2  | 2.44                     | 0.47              |
| 1:F:376:ARG:HH12 | 1:F:412:MET:CE   | 2.27                     | 0.47              |
| 2:J:63:GLY:HA2   | 2:J:83:TYR:CZ    | 2.50                     | 0.47              |
| 2:L:164:LEU:HD11 | 2:L:243:VAL:HG23 | 1.96                     | 0.47              |
| 2:L:243:VAL:HG11 | 2:L:319:LEU:HD22 | 1.95                     | 0.47              |
| 2:M:358:LEU:HD11 | 2:M:376:ALA:HB3  | 1.93                     | 0.47              |
| 2:N:243:VAL:HG11 | 2:N:319:LEU:HD22 | 1.96                     | 0.47              |
| 2:P:363:GLY:N    | 2:P:364:ASP:CB   | 2.78                     | 0.47              |
| 1:H:79:TRP:CD1   | 1:H:79:TRP:C     | 2.93                     | 0.47              |
| 2:K:164:LEU:HD13 | 2:K:247:LEU:CD1  | 2.45                     | 0.47              |
| 2:K:363:GLY:N    | 2:K:364:ASP:CB   | 2.77                     | 0.47              |
| 1:A:70:ILE:HG21  | 1:A:78:LEU:HD11  | 1.97                     | 0.47              |
| 2:K:304:ASP:HB2  | 2:K:324:GLY:O    | 2.13                     | 0.47              |
| 2:M:141:ASP:O    | 2:M:142:ALA:HB2  | 2.14                     | 0.47              |
| 1:F:544:GLN:OE1  | 1:F:544:GLN:N    | 2.47                     | 0.47              |
| 2:J:323:GLU:N    | 2:J:324:GLY:HA2  | 2.30                     | 0.47              |
| 2:N:323:GLU:N    | 2:N:324:GLY:HA2  | 2.30                     | 0.47              |
| 2:N:363:GLY:N    | 2:N:364:ASP:CB   | 2.78                     | 0.47              |
| 1:B:228:ARG:HD2  | 1:B:298:PHE:HE2  | 1.79                     | 0.46              |
| 1:B:558:VAL:HG22 | 2:J:212:ARG:NE   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:79:TRP:CD1   | 1:D:79:TRP:C     | 2.92                     | 0.46              |
| 1:H:311:ARG:O    | 2:O:226:GLY:C    | 2.58                     | 0.46              |
| 2:J:173:ALA:O    | 2:J:174:ARG:C    | 2.58                     | 0.46              |
| 2:N:186:GLU:CB   | 2:N:187:PRO:HD2  | 2.44                     | 0.46              |
| 2:P:243:VAL:HG11 | 2:P:319:LEU:HD22 | 1.96                     | 0.46              |
| 2:J:304:ASP:HB2  | 2:J:324:GLY:O    | 2.16                     | 0.46              |
| 2:M:363:GLY:N    | 2:M:364:ASP:CB   | 2.78                     | 0.46              |
| 1:F:445:ARG:HG2  | 1:H:417:TRP:CE2  | 2.50                     | 0.46              |
| 1:G:544:GLN:OE1  | 1:G:544:GLN:N    | 2.48                     | 0.46              |
| 2:I:363:GLY:N    | 2:I:364:ASP:CB   | 2.78                     | 0.46              |
| 2:J:361:GLN:CB   | 2:J:372:LEU:HD13 | 2.45                     | 0.46              |
| 2:M:63:GLY:HA2   | 2:M:83:TYR:CZ    | 2.50                     | 0.46              |
| 2:L:323:GLU:N    | 2:L:324:GLY:HA2  | 2.31                     | 0.46              |
| 1:B:337:PHE:HB3  | 1:B:403:VAL:HB   | 1.98                     | 0.46              |
| 1:G:41:PHE:HB2   | 1:G:403:VAL:HG22 | 1.98                     | 0.46              |
| 2:I:304:ASP:HB2  | 2:I:324:GLY:O    | 2.16                     | 0.46              |
| 1:C:544:GLN:OE1  | 1:C:544:GLN:N    | 2.47                     | 0.46              |
| 1:D:514:ARG:HD2  | 1:D:523:THR:HB   | 1.97                     | 0.46              |
| 1:F:157:VAL:HB   | 1:F:191:TRP:HB3  | 1.98                     | 0.46              |
| 2:I:101:GLU:N    | 2:I:102:SER:HA   | 2.31                     | 0.46              |
| 2:I:361:GLN:CB   | 2:I:372:LEU:HD13 | 2.43                     | 0.46              |
| 1:C:510:ARG:HB2  | 1:C:526:VAL:HG22 | 1.98                     | 0.46              |
| 1:G:70:ILE:HG21  | 1:G:78:LEU:HD11  | 1.98                     | 0.46              |
| 1:G:412:MET:HE3  | 1:G:429:GLN:OE1  | 2.16                     | 0.46              |
| 1:G:569:LEU:CD1  | 1:H:561:PRO:HG2  | 2.44                     | 0.46              |
| 2:M:323:GLU:N    | 2:M:324:GLY:HA2  | 2.31                     | 0.46              |
| 1:D:27:ARG:NH2   | 1:D:120:ARG:HD3  | 2.30                     | 0.46              |
| 1:F:558:VAL:HG22 | 2:M:212:ARG:HD3  | 1.98                     | 0.46              |
| 1:G:510:ARG:HB2  | 1:G:526:VAL:HG22 | 1.98                     | 0.46              |
| 2:J:243:VAL:HG11 | 2:J:319:LEU:HD22 | 1.97                     | 0.46              |
| 1:E:487:HIS:ND1  | 1:E:524:ASP:OD2  | 2.49                     | 0.46              |
| 1:H:41:PHE:HB2   | 1:H:403:VAL:HG22 | 1.98                     | 0.46              |
| 2:K:323:GLU:N    | 2:K:324:GLY:HA2  | 2.31                     | 0.46              |
| 1:C:79:TRP:CD1   | 1:C:79:TRP:C     | 2.95                     | 0.45              |
| 2:K:157:ASP:HA   | 2:K:322:PHE:HB2  | 1.98                     | 0.45              |
| 2:L:64:PRO:CB    | 2:L:65:ILE:HA    | 2.46                     | 0.45              |
| 2:L:112:ARG:NH2  | 2:L:115:ASP:O    | 2.48                     | 0.45              |
| 2:N:358:LEU:HD11 | 2:N:376:ALA:HB3  | 1.94                     | 0.45              |
| 2:K:361:GLN:CB   | 2:K:372:LEU:HD13 | 2.45                     | 0.45              |
| 1:E:157:VAL:HB   | 1:E:191:TRP:HB3  | 1.98                     | 0.45              |
| 1:H:157:VAL:HB   | 1:H:191:TRP:HB3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:164:LEU:HG   | 2:I:172:VAL:HG21 | 1.98                     | 0.45              |
| 2:O:323:GLU:N    | 2:O:324:GLY:HA2  | 2.31                     | 0.45              |
| 1:E:300:PHE:HB3  | 1:E:349:VAL:HG11 | 1.98                     | 0.45              |
| 1:F:412:MET:HE3  | 1:F:429:GLN:OE1  | 2.17                     | 0.45              |
| 1:H:544:GLN:OE1  | 1:H:544:GLN:N    | 2.48                     | 0.45              |
| 2:L:363:GLY:N    | 2:L:364:ASP:CB   | 2.79                     | 0.45              |
| 1:A:79:TRP:CD1   | 1:A:79:TRP:C     | 2.94                     | 0.45              |
| 1:A:357:MET:HA   | 1:A:360:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:544:GLN:OE1  | 1:A:544:GLN:N    | 2.48                     | 0.45              |
| 1:C:543:LEU:HB2  | 1:C:563:ILE:HG21 | 1.99                     | 0.45              |
| 1:E:558:VAL:CG2  | 1:F:535:PHE:HB3  | 2.46                     | 0.45              |
| 1:H:70:ILE:HG21  | 1:H:78:LEU:HD11  | 1.99                     | 0.45              |
| 1:H:510:ARG:HB2  | 1:H:526:VAL:HG22 | 1.99                     | 0.45              |
| 1:B:70:ILE:HG21  | 1:B:78:LEU:HD11  | 1.98                     | 0.45              |
| 1:D:157:VAL:HB   | 1:D:191:TRP:HB3  | 1.98                     | 0.45              |
| 2:M:232:GLU:HG3  | 2:M:317:TRP:HZ2  | 1.81                     | 0.45              |
| 1:B:453:ASP:HA   | 1:C:452:GLN:HE22 | 1.81                     | 0.45              |
| 1:D:510:ARG:HB2  | 1:D:526:VAL:HG22 | 1.99                     | 0.45              |
| 2:J:361:GLN:O    | 2:J:364:ASP:O    | 2.34                     | 0.45              |
| 1:B:543:LEU:HB2  | 1:B:563:ILE:HG21 | 1.99                     | 0.45              |
| 1:F:337:PHE:HB3  | 1:F:403:VAL:HB   | 1.98                     | 0.45              |
| 1:G:300:PHE:HB3  | 1:G:349:VAL:HG11 | 1.99                     | 0.45              |
| 1:A:300:PHE:HB3  | 1:A:349:VAL:HG11 | 1.98                     | 0.45              |
| 1:B:487:HIS:ND1  | 1:B:524:ASP:OD2  | 2.50                     | 0.45              |
| 1:E:510:ARG:HB2  | 1:E:526:VAL:HG22 | 1.99                     | 0.45              |
| 1:H:300:PHE:HB3  | 1:H:349:VAL:HG11 | 1.99                     | 0.45              |
| 2:M:164:LEU:CD2  | 2:M:172:VAL:HG21 | 2.41                     | 0.45              |
| 1:D:70:ILE:HG21  | 1:D:78:LEU:HD11  | 1.99                     | 0.45              |
| 1:F:521:ALA:HB3  | 2:M:364:ASP:H    | 1.82                     | 0.45              |
| 2:J:232:GLU:HG3  | 2:J:317:TRP:HZ2  | 1.81                     | 0.45              |
| 1:A:157:VAL:HB   | 1:A:191:TRP:HB3  | 1.99                     | 0.44              |
| 1:A:412:MET:HE3  | 1:A:429:GLN:OE1  | 2.17                     | 0.44              |
| 1:D:41:PHE:HB2   | 1:D:403:VAL:HG22 | 1.98                     | 0.44              |
| 1:G:157:VAL:HB   | 1:G:191:TRP:HB3  | 1.98                     | 0.44              |
| 1:G:535:PHE:HB3  | 1:H:556:GLY:CA   | 2.41                     | 0.44              |
| 2:J:358:LEU:HD11 | 2:J:376:ALA:HB3  | 1.95                     | 0.44              |
| 2:O:363:GLY:H    | 2:O:364:ASP:CB   | 2.30                     | 0.44              |
| 1:B:79:TRP:CD1   | 1:B:79:TRP:C     | 2.95                     | 0.44              |
| 1:C:357:MET:HA   | 1:C:360:GLU:HG3  | 1.98                     | 0.44              |
| 1:D:300:PHE:HB3  | 1:D:349:VAL:HG11 | 1.99                     | 0.44              |
| 1:E:544:GLN:N    | 1:E:544:GLN:OE1  | 2.49                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:538:PRO:HB2  | 1:H:561:PRO:HD3  | 1.99                     | 0.44              |
| 1:G:357:MET:HA   | 1:G:360:GLU:HG3  | 1.99                     | 0.44              |
| 1:E:558:VAL:CG2  | 1:F:535:PHE:CB   | 2.96                     | 0.44              |
| 1:B:41:PHE:HB2   | 1:B:403:VAL:HG22 | 1.99                     | 0.44              |
| 1:B:157:VAL:HB   | 1:B:191:TRP:HB3  | 1.99                     | 0.44              |
| 1:B:510:ARG:HB2  | 1:B:526:VAL:HG22 | 1.99                     | 0.44              |
| 1:B:544:GLN:N    | 1:B:544:GLN:OE1  | 2.47                     | 0.44              |
| 1:C:300:PHE:HB3  | 1:C:349:VAL:HG11 | 2.00                     | 0.44              |
| 1:D:357:MET:HA   | 1:D:360:GLU:HG3  | 2.00                     | 0.44              |
| 1:G:337:PHE:HB3  | 1:G:403:VAL:HB   | 1.99                     | 0.44              |
| 2:N:99:ILE:HD11  | 2:N:178:SER:N    | 2.33                     | 0.44              |
| 1:B:300:PHE:HB3  | 1:B:349:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:544:GLN:N    | 1:D:544:GLN:OE1  | 2.47                     | 0.44              |
| 1:F:70:ILE:HG21  | 1:F:78:LEU:HD11  | 1.99                     | 0.44              |
| 2:I:110:PHE:N    | 2:I:110:PHE:CD1  | 2.85                     | 0.44              |
| 2:J:100:ASP:HA   | 2:J:112:ARG:HD2  | 1.99                     | 0.44              |
| 2:P:323:GLU:N    | 2:P:324:GLY:HA2  | 2.31                     | 0.44              |
| 1:D:337:PHE:HB3  | 1:D:403:VAL:HB   | 2.00                     | 0.44              |
| 1:E:70:ILE:HG21  | 1:E:78:LEU:HD11  | 1.98                     | 0.44              |
| 2:I:323:GLU:N    | 2:I:324:GLY:HA2  | 2.32                     | 0.44              |
| 2:M:361:GLN:CB   | 2:M:372:LEU:HD13 | 2.45                     | 0.44              |
| 1:A:41:PHE:HB2   | 1:A:403:VAL:HG22 | 1.98                     | 0.44              |
| 1:C:70:ILE:HG21  | 1:C:78:LEU:HD11  | 1.99                     | 0.44              |
| 1:C:412:MET:HE3  | 1:C:429:GLN:OE1  | 2.18                     | 0.44              |
| 1:D:376:ARG:HH12 | 1:D:412:MET:CE   | 2.28                     | 0.44              |
| 1:D:543:LEU:HB2  | 1:D:563:ILE:HG21 | 2.00                     | 0.44              |
| 1:H:412:MET:HE3  | 1:H:429:GLN:OE1  | 2.18                     | 0.44              |
| 1:B:17:HIS:CD2   | 1:B:99:TYR:CE2   | 3.04                     | 0.43              |
| 1:E:556:GLY:CA   | 1:F:535:PHE:HD1  | 2.27                     | 0.43              |
| 1:A:510:ARG:HB2  | 1:A:526:VAL:HG22 | 1.99                     | 0.43              |
| 1:A:337:PHE:HB3  | 1:A:403:VAL:HB   | 1.99                     | 0.43              |
| 1:A:543:LEU:HB2  | 1:A:563:ILE:HG21 | 2.00                     | 0.43              |
| 1:C:157:VAL:HB   | 1:C:191:TRP:HB3  | 1.99                     | 0.43              |
| 1:C:337:PHE:HB3  | 1:C:403:VAL:HB   | 1.99                     | 0.43              |
| 1:E:357:MET:HA   | 1:E:360:GLU:HG3  | 1.99                     | 0.43              |
| 1:F:357:MET:HA   | 1:F:360:GLU:HG3  | 1.99                     | 0.43              |
| 1:F:510:ARG:HB2  | 1:F:526:VAL:HG22 | 2.00                     | 0.43              |
| 2:I:232:GLU:HG3  | 2:I:317:TRP:HZ2  | 1.82                     | 0.43              |
| 1:F:41:PHE:HB2   | 1:F:403:VAL:HG22 | 1.99                     | 0.43              |
| 1:H:503:PRO:HB3  | 2:O:206:MET:HG3  | 1.94                     | 0.43              |
| 2:I:159:GLU:OE1  | 2:I:300:ARG:NH2  | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:363:GLY:H    | 2:K:364:ASP:CB   | 2.32                     | 0.43              |
| 2:M:361:GLN:O    | 2:M:364:ASP:O    | 2.36                     | 0.43              |
| 2:P:358:LEU:HD11 | 2:P:376:ALA:HB3  | 1.94                     | 0.43              |
| 2:P:363:GLY:H    | 2:P:364:ASP:CB   | 2.32                     | 0.43              |
| 1:C:376:ARG:HH12 | 1:C:412:MET:CE   | 2.28                     | 0.43              |
| 1:E:432:PRO:HG3  | 1:F:454:ALA:HB2  | 2.01                     | 0.43              |
| 1:E:583:ARG:NH1  | 2:N:360:ASP:HB3  | 2.34                     | 0.43              |
| 2:P:232:GLU:HG3  | 2:P:317:TRP:HZ2  | 1.82                     | 0.43              |
| 1:E:337:PHE:HB3  | 1:E:403:VAL:HB   | 2.01                     | 0.43              |
| 2:L:361:GLN:CB   | 2:L:372:LEU:HD13 | 2.44                     | 0.43              |
| 1:F:487:HIS:ND1  | 1:F:524:ASP:OD2  | 2.50                     | 0.43              |
| 1:G:460:SER:CB   | 1:H:460:SER:HB3  | 2.49                     | 0.43              |
| 1:G:487:HIS:ND1  | 1:G:524:ASP:OD2  | 2.52                     | 0.43              |
| 2:K:232:GLU:HG3  | 2:K:317:TRP:HZ2  | 1.83                     | 0.43              |
| 2:M:101:GLU:N    | 2:M:102:SER:HA   | 2.33                     | 0.43              |
| 2:O:232:GLU:HG3  | 2:O:317:TRP:HZ2  | 1.82                     | 0.43              |
| 1:H:337:PHE:HB3  | 1:H:403:VAL:HB   | 1.99                     | 0.43              |
| 2:L:232:GLU:HG3  | 2:L:317:TRP:HZ2  | 1.83                     | 0.43              |
| 2:M:363:GLY:H    | 2:M:364:ASP:CB   | 2.32                     | 0.43              |
| 2:N:365:ASP:HB3  | 2:N:366:ASP:CA   | 2.48                     | 0.43              |
| 2:O:365:ASP:HB3  | 2:O:366:ASP:CA   | 2.49                     | 0.43              |
| 1:G:79:TRP:CD1   | 1:G:79:TRP:C     | 2.94                     | 0.43              |
| 2:I:157:ASP:OD2  | 2:I:192:MET:HE1  | 2.18                     | 0.43              |
| 2:J:363:GLY:H    | 2:J:364:ASP:CB   | 2.31                     | 0.43              |
| 2:O:358:LEU:HD11 | 2:O:376:ALA:HB3  | 1.93                     | 0.43              |
| 2:O:361:GLN:O    | 2:O:364:ASP:O    | 2.37                     | 0.43              |
| 1:A:70:ILE:HD13  | 1:A:78:LEU:HD11  | 2.01                     | 0.43              |
| 1:E:556:GLY:HA3  | 1:F:535:PHE:HB3  | 2.01                     | 0.43              |
| 1:F:300:PHE:HB3  | 1:F:349:VAL:HG11 | 1.99                     | 0.43              |
| 2:N:232:GLU:HG3  | 2:N:317:TRP:HZ2  | 1.83                     | 0.43              |
| 1:A:303:MET:HB3  | 1:A:304:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:453:ASP:HA   | 1:D:452:GLN:NE2  | 2.31                     | 0.42              |
| 1:E:543:LEU:HB2  | 1:E:563:ILE:HG21 | 2.00                     | 0.42              |
| 1:H:357:MET:HA   | 1:H:360:GLU:HG3  | 2.00                     | 0.42              |
| 2:L:78:ASP:HA    | 2:L:79:GLY:HA2   | 1.75                     | 0.42              |
| 2:N:363:GLY:H    | 2:N:364:ASP:CB   | 2.32                     | 0.42              |
| 2:J:175:LEU:HD23 | 2:J:176:LEU:N    | 2.33                     | 0.42              |
| 2:L:164:LEU:HD21 | 2:L:243:VAL:HG23 | 1.99                     | 0.42              |
| 1:B:376:ARG:HH12 | 1:B:412:MET:CE   | 2.27                     | 0.42              |
| 1:D:20:ALA:C     | 1:D:22:ASP:H     | 2.27                     | 0.42              |
| 1:G:70:ILE:HG23  | 1:G:75:VAL:CG2   | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:358:LEU:HD11 | 2:K:376:ALA:HB3  | 1.94                     | 0.42              |
| 1:A:16:GLU:O     | 1:A:17:HIS:ND1   | 2.52                     | 0.42              |
| 1:A:417:TRP:CG   | 1:D:449:PRO:HD3  | 2.54                     | 0.42              |
| 1:D:303:MET:HB3  | 1:D:304:PRO:HD3  | 2.01                     | 0.42              |
| 1:D:515:GLN:O    | 1:D:515:GLN:HG2  | 2.20                     | 0.42              |
| 1:G:543:LEU:HB2  | 1:G:563:ILE:HG21 | 2.00                     | 0.42              |
| 2:K:258:PHE:HA   | 2:K:259:PRO:HD3  | 1.95                     | 0.42              |
| 2:M:365:ASP:HB3  | 2:M:366:ASP:CA   | 2.49                     | 0.42              |
| 2:P:365:ASP:HB3  | 2:P:366:ASP:CA   | 2.49                     | 0.42              |
| 1:A:232:VAL:N    | 1:A:233:PRO:CD   | 2.83                     | 0.42              |
| 1:E:558:VAL:HG21 | 1:F:535:PHE:HB2  | 2.01                     | 0.42              |
| 1:F:70:ILE:HG23  | 1:F:75:VAL:CG2   | 2.50                     | 0.42              |
| 1:F:303:MET:HB3  | 1:F:304:PRO:HD3  | 2.01                     | 0.42              |
| 1:H:232:VAL:N    | 1:H:233:PRO:CD   | 2.83                     | 0.42              |
| 1:H:543:LEU:HB2  | 1:H:563:ILE:HG21 | 2.00                     | 0.42              |
| 2:I:358:LEU:HD11 | 2:I:376:ALA:HB3  | 1.94                     | 0.42              |
| 2:K:126:VAL:CG2  | 2:K:137:VAL:HG23 | 2.50                     | 0.42              |
| 2:N:361:GLN:O    | 2:N:364:ASP:O    | 2.37                     | 0.42              |
| 2:O:243:VAL:O    | 2:O:247:LEU:HB2  | 2.19                     | 0.42              |
| 2:K:365:ASP:HB3  | 2:K:366:ASP:CA   | 2.50                     | 0.42              |
| 1:G:569:LEU:HD13 | 1:H:561:PRO:HG2  | 2.01                     | 0.42              |
| 1:B:70:ILE:HD13  | 1:B:78:LEU:HD11  | 2.02                     | 0.42              |
| 1:E:102:LEU:HA   | 1:E:103:PRO:HD2  | 1.87                     | 0.42              |
| 1:G:376:ARG:HH12 | 1:G:412:MET:CE   | 2.29                     | 0.42              |
| 2:I:63:GLY:N     | 2:I:64:PRO:HD3   | 2.35                     | 0.42              |
| 2:J:361:GLN:HA   | 2:J:364:ASP:CB   | 2.50                     | 0.42              |
| 1:F:543:LEU:HB2  | 1:F:563:ILE:HG21 | 2.00                     | 0.42              |
| 2:J:133:ASN:HD22 | 2:J:145:LYS:HG3  | 1.85                     | 0.42              |
| 2:K:243:VAL:O    | 2:K:247:LEU:HB2  | 2.19                     | 0.42              |
| 2:M:365:ASP:HB3  | 2:M:366:ASP:HA   | 2.02                     | 0.42              |
| 1:C:17:HIS:HD2   | 1:C:99:TYR:CE2   | 2.35                     | 0.42              |
| 1:C:70:ILE:HD13  | 1:C:78:LEU:HD11  | 2.01                     | 0.42              |
| 1:D:232:VAL:N    | 1:D:233:PRO:CD   | 2.83                     | 0.42              |
| 1:G:560:PHE:CE2  | 1:H:571:THR:HB   | 2.55                     | 0.42              |
| 2:I:96:LEU:O     | 2:I:99:ILE:HG22  | 2.20                     | 0.42              |
| 2:J:77:ALA:O     | 2:J:78:ASP:C     | 2.63                     | 0.42              |
| 2:N:243:VAL:O    | 2:N:247:LEU:HB2  | 2.20                     | 0.42              |
| 1:A:276:TRP:CD2  | 1:A:277:PRO:HD2  | 2.55                     | 0.41              |
| 1:A:487:HIS:ND1  | 1:A:524:ASP:OD2  | 2.52                     | 0.41              |
| 1:B:70:ILE:HG23  | 1:B:75:VAL:CG2   | 2.50                     | 0.41              |
| 1:B:486:ARG:HD3  | 2:J:365:ASP:O    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:303:MET:HB3  | 1:C:304:PRO:HD3  | 2.01                     | 0.41              |
| 1:G:305:ARG:HH12 | 1:G:320:GLU:HB3  | 1.85                     | 0.41              |
| 1:H:503:PRO:HB2  | 2:O:206:MET:HG3  | 1.98                     | 0.41              |
| 2:I:5:PHE:O      | 2:I:7:ASP:N      | 2.53                     | 0.41              |
| 2:I:99:ILE:O     | 2:I:112:ARG:HB3  | 2.20                     | 0.41              |
| 2:K:143:ILE:HG23 | 2:K:194:THR:HG23 | 2.02                     | 0.41              |
| 2:L:243:VAL:O    | 2:L:247:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:145:ARG:HG3  | 1:B:146:HIS:HD2  | 1.85                     | 0.41              |
| 1:B:303:MET:HB3  | 1:B:304:PRO:HD3  | 2.01                     | 0.41              |
| 1:F:514:ARG:NE   | 1:F:523:THR:OG1  | 2.52                     | 0.41              |
| 2:J:363:GLY:CA   | 2:J:364:ASP:CB   | 2.98                     | 0.41              |
| 2:K:361:GLN:O    | 2:K:364:ASP:O    | 2.38                     | 0.41              |
| 2:L:126:VAL:HG23 | 2:L:137:VAL:HG23 | 2.03                     | 0.41              |
| 2:M:5:PHE:O      | 2:M:6:GLU:C      | 2.63                     | 0.41              |
| 2:M:62:SER:C     | 2:M:64:PRO:HD3   | 2.45                     | 0.41              |
| 1:A:70:ILE:HG23  | 1:A:75:VAL:CG2   | 2.50                     | 0.41              |
| 1:D:276:TRP:CD2  | 1:D:277:PRO:HD2  | 2.55                     | 0.41              |
| 1:D:387:GLN:HG2  | 1:D:575:HIS:ND1  | 2.36                     | 0.41              |
| 1:E:305:ARG:HH12 | 1:E:320:GLU:HB3  | 1.85                     | 0.41              |
| 1:H:303:MET:HB3  | 1:H:304:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:376:ARG:HH12 | 1:A:412:MET:CE   | 2.30                     | 0.41              |
| 1:B:519:GLY:CA   | 1:B:522:LYS:HB2  | 2.50                     | 0.41              |
| 1:C:70:ILE:HG23  | 1:C:75:VAL:CG2   | 2.50                     | 0.41              |
| 1:H:387:GLN:HG2  | 1:H:575:HIS:ND1  | 2.36                     | 0.41              |
| 1:B:232:VAL:N    | 1:B:233:PRO:CD   | 2.83                     | 0.41              |
| 1:D:70:ILE:HD13  | 1:D:78:LEU:HD11  | 2.03                     | 0.41              |
| 1:F:232:VAL:N    | 1:F:233:PRO:CD   | 2.84                     | 0.41              |
| 2:J:78:ASP:HA    | 2:J:79:GLY:HA2   | 1.71                     | 0.41              |
| 1:D:305:ARG:HH12 | 1:D:320:GLU:HB3  | 1.86                     | 0.41              |
| 2:I:164:LEU:HD13 | 2:I:247:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:102:LEU:HA   | 1:A:103:PRO:HD2  | 1.87                     | 0.41              |
| 1:C:487:HIS:ND1  | 1:C:524:ASP:OD2  | 2.52                     | 0.41              |
| 1:D:70:ILE:HG23  | 1:D:75:VAL:CG2   | 2.51                     | 0.41              |
| 2:I:223:GLU:HA   | 2:I:382:ARG:NH1  | 2.36                     | 0.41              |
| 2:M:258:PHE:HA   | 2:M:259:PRO:HD3  | 1.94                     | 0.41              |
| 1:C:232:VAL:N    | 1:C:233:PRO:CD   | 2.84                     | 0.41              |
| 1:E:70:ILE:HG23  | 1:E:75:VAL:CG2   | 2.50                     | 0.41              |
| 1:E:494:THR:O    | 1:E:510:ARG:HA   | 2.21                     | 0.41              |
| 1:A:316:PHE:CZ   | 2:J:201:ALA:HB3  | 2.56                     | 0.41              |
| 1:B:276:TRP:CD2  | 1:B:277:PRO:HD2  | 2.56                     | 0.41              |
| 1:E:232:VAL:N    | 1:E:233:PRO:CD   | 2.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:558:VAL:HG23 | 1:F:535:PHE:HB3  | 2.03                     | 0.41              |
| 1:G:232:VAL:N    | 1:G:233:PRO:CD   | 2.83                     | 0.41              |
| 1:G:515:GLN:O    | 1:G:516:GLN:CB   | 2.69                     | 0.41              |
| 2:I:363:GLY:H    | 2:I:364:ASP:CB   | 2.34                     | 0.41              |
| 2:J:10:THR:HA    | 2:J:15:TYR:CD2   | 2.56                     | 0.41              |
| 2:J:63:GLY:N     | 2:J:64:PRO:CD    | 2.84                     | 0.41              |
| 2:K:127:PHE:O    | 2:K:129:ALA:N    | 2.54                     | 0.41              |
| 2:K:164:LEU:HD21 | 2:K:243:VAL:CG2  | 2.48                     | 0.41              |
| 2:L:363:GLY:H    | 2:L:364:ASP:CB   | 2.34                     | 0.41              |
| 2:M:151:THR:CB   | 2:M:330:LEU:HD11 | 2.51                     | 0.41              |
| 2:O:363:GLY:CA   | 2:O:364:ASP:CB   | 2.99                     | 0.41              |
| 1:A:452:GLN:NE2  | 1:D:453:ASP:HA   | 2.35                     | 0.41              |
| 1:C:17:HIS:NE2   | 1:C:99:TYR:CE2   | 2.89                     | 0.41              |
| 1:E:376:ARG:HH12 | 1:E:412:MET:CE   | 2.28                     | 0.41              |
| 1:F:305:ARG:HH12 | 1:F:320:GLU:HB3  | 1.85                     | 0.41              |
| 1:F:494:THR:O    | 1:F:510:ARG:HA   | 2.20                     | 0.41              |
| 1:G:303:MET:HB3  | 1:G:304:PRO:HD3  | 2.03                     | 0.41              |
| 1:G:494:THR:O    | 1:G:510:ARG:HA   | 2.21                     | 0.41              |
| 1:G:535:PHE:CG   | 1:H:556:GLY:O    | 2.74                     | 0.41              |
| 1:H:70:ILE:HG23  | 1:H:75:VAL:CG2   | 2.52                     | 0.41              |
| 2:K:365:ASP:HB3  | 2:K:366:ASP:CG   | 2.46                     | 0.41              |
| 2:M:361:GLN:HA   | 2:M:364:ASP:CB   | 2.51                     | 0.41              |
| 1:B:387:GLN:HG2  | 1:B:575:HIS:ND1  | 2.36                     | 0.40              |
| 2:K:152:PRO:O    | 2:K:330:LEU:HD13 | 2.20                     | 0.40              |
| 1:B:452:GLN:HE22 | 1:C:453:ASP:HA   | 1.86                     | 0.40              |
| 1:C:305:ARG:HH12 | 1:C:320:GLU:HB3  | 1.87                     | 0.40              |
| 1:F:276:TRP:CD2  | 1:F:277:PRO:HD2  | 2.55                     | 0.40              |
| 1:G:70:ILE:HD13  | 1:G:78:LEU:HD11  | 2.03                     | 0.40              |
| 1:B:286:ASP:HA   | 1:B:287:PRO:HD3  | 1.93                     | 0.40              |
| 2:I:64:PRO:HA    | 2:I:65:ILE:O     | 2.21                     | 0.40              |
| 2:K:223:GLU:HA   | 2:K:382:ARG:NH1  | 2.37                     | 0.40              |
| 2:P:361:GLN:O    | 2:P:364:ASP:O    | 2.39                     | 0.40              |
| 1:C:573:PRO:HD3  | 1:D:573:PRO:HD3  | 2.03                     | 0.40              |
| 1:E:387:GLN:HG2  | 1:E:575:HIS:ND1  | 2.37                     | 0.40              |
| 1:H:70:ILE:HD13  | 1:H:78:LEU:HD11  | 2.03                     | 0.40              |
| 2:I:160:LEU:HD13 | 2:I:160:LEU:HA   | 1.94                     | 0.40              |
| 2:J:223:GLU:HA   | 2:J:382:ARG:NH1  | 2.35                     | 0.40              |
| 2:L:361:GLN:O    | 2:L:364:ASP:O    | 2.39                     | 0.40              |
| 1:C:387:GLN:HG2  | 1:C:575:HIS:ND1  | 2.37                     | 0.40              |
| 1:E:410:ILE:HG22 | 1:E:474:LEU:HB2  | 2.03                     | 0.40              |
| 1:E:558:VAL:HA   | 2:N:212:ARG:NE   | 2.35                     | 0.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:G:17:HIS:CD2 | 1:G:99:TYR:CD1  | 3.09                     | 0.40              |
| 2:J:243:VAL:O  | 2:J:247:LEU:HB2 | 2.22                     | 0.40              |
| 2:J:361:GLN:C  | 2:J:363:GLY:H   | 2.30                     | 0.40              |
| 2:M:243:VAL:O  | 2:M:247:LEU:HB2 | 2.21                     | 0.40              |
| 2:P:243:VAL:O  | 2:P:247:LEU:HB2 | 2.20                     | 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     | 561/593 (95%) | 546 (97%) | 13 (2%)  | 2 (0%)   | 30          | 61  |
| 1   | B     | 569/593 (96%) | 551 (97%) | 16 (3%)  | 2 (0%)   | 30          | 61  |
| 1   | C     | 565/593 (95%) | 549 (97%) | 14 (2%)  | 2 (0%)   | 30          | 61  |
| 1   | D     | 569/593 (96%) | 550 (97%) | 16 (3%)  | 3 (0%)   | 24          | 57  |
| 1   | E     | 545/593 (92%) | 533 (98%) | 12 (2%)  | 0        | 100         | 100 |
| 1   | F     | 569/593 (96%) | 553 (97%) | 14 (2%)  | 2 (0%)   | 30          | 61  |
| 1   | G     | 569/593 (96%) | 548 (96%) | 20 (4%)  | 1 (0%)   | 43          | 72  |
| 1   | H     | 538/593 (91%) | 528 (98%) | 10 (2%)  | 0        | 100         | 100 |
| 2   | I     | 431/441 (98%) | 382 (89%) | 43 (10%) | 6 (1%)   | 9           | 38  |
| 2   | J     | 431/441 (98%) | 382 (89%) | 41 (10%) | 8 (2%)   | 6           | 33  |
| 2   | K     | 349/441 (79%) | 318 (91%) | 25 (7%)  | 6 (2%)   | 7           | 35  |
| 2   | L     | 432/441 (98%) | 388 (90%) | 35 (8%)  | 9 (2%)   | 5           | 31  |
| 2   | M     | 425/441 (96%) | 381 (90%) | 35 (8%)  | 9 (2%)   | 5           | 31  |
| 2   | N     | 345/441 (78%) | 318 (92%) | 24 (7%)  | 3 (1%)   | 14          | 46  |
| 2   | O     | 235/441 (53%) | 221 (94%) | 13 (6%)  | 1 (0%)   | 30          | 61  |
| 2   | P     | 235/441 (53%) | 220 (94%) | 14 (6%)  | 1 (0%)   | 30          | 61  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------|
| All | All   | 7368/8272 (89%) | 6968 (95%) | 345 (5%) | 55 (1%)  | 18 51       |

All (55) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ILE  |
| 1   | B     | 25  | HIS  |
| 1   | C     | 10  | VAL  |
| 2   | I     | 275 | PRO  |
| 2   | J     | 275 | PRO  |
| 2   | K     | 275 | PRO  |
| 2   | L     | 275 | PRO  |
| 2   | M     | 106 | GLN  |
| 2   | M     | 275 | PRO  |
| 2   | N     | 275 | PRO  |
| 2   | O     | 275 | PRO  |
| 2   | P     | 275 | PRO  |
| 1   | A     | 17  | HIS  |
| 1   | B     | 22  | ASP  |
| 1   | D     | 516 | GLN  |
| 1   | F     | 516 | GLN  |
| 1   | G     | 516 | GLN  |
| 2   | I     | 6   | GLU  |
| 2   | I     | 78  | ASP  |
| 2   | J     | 70  | VAL  |
| 2   | J     | 124 | PRO  |
| 2   | K     | 128 | GLY  |
| 2   | L     | 13  | ARG  |
| 2   | L     | 106 | GLN  |
| 2   | L     | 365 | ASP  |
| 2   | M     | 21  | GLU  |
| 2   | N     | 123 | PRO  |
| 1   | D     | 522 | LYS  |
| 1   | F     | 22  | ASP  |
| 2   | J     | 24  | SER  |
| 2   | J     | 73  | THR  |
| 2   | K     | 106 | GLN  |
| 2   | K     | 124 | PRO  |
| 2   | M     | 6   | GLU  |
| 1   | D     | 24  | GLY  |
| 2   | I     | 123 | PRO  |
| 2   | J     | 56  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 123 | PRO  |
| 2   | K     | 184 | GLU  |
| 2   | L     | 123 | PRO  |
| 2   | M     | 13  | ARG  |
| 2   | M     | 123 | PRO  |
| 2   | M     | 142 | ALA  |
| 2   | M     | 184 | GLU  |
| 2   | N     | 184 | GLU  |
| 1   | C     | 13  | GLY  |
| 2   | I     | 106 | GLN  |
| 2   | L     | 3   | VAL  |
| 2   | I     | 124 | PRO  |
| 2   | L     | 124 | PRO  |
| 2   | L     | 56  | VAL  |
| 2   | L     | 71  | VAL  |
| 2   | J     | 123 | PRO  |
| 2   | J     | 153 | GLY  |
| 2   | M     | 56  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 489/512 (96%) | 485 (99%) | 4 (1%)   | 73          | 77 |
| 1   | B     | 495/512 (97%) | 487 (98%) | 8 (2%)   | 55          | 69 |
| 1   | C     | 489/512 (96%) | 484 (99%) | 5 (1%)   | 68          | 75 |
| 1   | D     | 495/512 (97%) | 491 (99%) | 4 (1%)   | 73          | 77 |
| 1   | E     | 480/512 (94%) | 477 (99%) | 3 (1%)   | 78          | 79 |
| 1   | F     | 495/512 (97%) | 491 (99%) | 4 (1%)   | 73          | 77 |
| 1   | G     | 495/512 (97%) | 491 (99%) | 4 (1%)   | 73          | 77 |
| 1   | H     | 475/512 (93%) | 472 (99%) | 3 (1%)   | 78          | 79 |
| 2   | I     | 211/351 (60%) | 195 (92%) | 16 (8%)  | 12          | 39 |
| 2   | J     | 208/351 (59%) | 195 (94%) | 13 (6%)  | 16          | 44 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | K     | 178/351 (51%)   | 174 (98%)  | 4 (2%)   | 45          | 65 |
| 2   | L     | 210/351 (60%)   | 204 (97%)  | 6 (3%)   | 37          | 60 |
| 2   | M     | 210/351 (60%)   | 205 (98%)  | 5 (2%)   | 43          | 63 |
| 2   | N     | 175/351 (50%)   | 172 (98%)  | 3 (2%)   | 53          | 69 |
| 2   | O     | 110/351 (31%)   | 108 (98%)  | 2 (2%)   | 51          | 68 |
| 2   | P     | 110/351 (31%)   | 108 (98%)  | 2 (2%)   | 51          | 68 |
| All | All   | 5325/6904 (77%) | 5239 (98%) | 86 (2%)  | 55          | 69 |

All (86) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | GLU  |
| 1   | A     | 44  | VAL  |
| 1   | A     | 101 | VAL  |
| 1   | A     | 248 | GLU  |
| 1   | B     | 27  | ARG  |
| 1   | B     | 28  | THR  |
| 1   | B     | 44  | VAL  |
| 1   | B     | 59  | ASP  |
| 1   | B     | 61  | ARG  |
| 1   | B     | 101 | VAL  |
| 1   | B     | 248 | GLU  |
| 1   | B     | 522 | LYS  |
| 1   | C     | 17  | HIS  |
| 1   | C     | 44  | VAL  |
| 1   | C     | 61  | ARG  |
| 1   | C     | 101 | VAL  |
| 1   | C     | 248 | GLU  |
| 1   | D     | 22  | ASP  |
| 1   | D     | 44  | VAL  |
| 1   | D     | 101 | VAL  |
| 1   | D     | 248 | GLU  |
| 1   | E     | 44  | VAL  |
| 1   | E     | 101 | VAL  |
| 1   | E     | 248 | GLU  |
| 1   | F     | 44  | VAL  |
| 1   | F     | 61  | ARG  |
| 1   | F     | 101 | VAL  |
| 1   | F     | 248 | GLU  |
| 1   | G     | 28  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 44  | VAL  |
| 1   | G     | 101 | VAL  |
| 1   | G     | 248 | GLU  |
| 1   | H     | 44  | VAL  |
| 1   | H     | 101 | VAL  |
| 1   | H     | 248 | GLU  |
| 2   | I     | 2   | SER  |
| 2   | I     | 26  | THR  |
| 2   | I     | 69  | SER  |
| 2   | I     | 78  | ASP  |
| 2   | I     | 97  | SER  |
| 2   | I     | 99  | ILE  |
| 2   | I     | 100 | ASP  |
| 2   | I     | 102 | SER  |
| 2   | I     | 104 | THR  |
| 2   | I     | 110 | PHE  |
| 2   | I     | 112 | ARG  |
| 2   | I     | 126 | VAL  |
| 2   | I     | 134 | THR  |
| 2   | I     | 176 | LEU  |
| 2   | I     | 310 | VAL  |
| 2   | I     | 366 | ASP  |
| 2   | J     | 3   | VAL  |
| 2   | J     | 27  | THR  |
| 2   | J     | 104 | THR  |
| 2   | J     | 126 | VAL  |
| 2   | J     | 134 | THR  |
| 2   | J     | 135 | SER  |
| 2   | J     | 161 | ASN  |
| 2   | J     | 164 | LEU  |
| 2   | J     | 172 | VAL  |
| 2   | J     | 176 | LEU  |
| 2   | J     | 193 | VAL  |
| 2   | J     | 194 | THR  |
| 2   | J     | 310 | VAL  |
| 2   | K     | 102 | SER  |
| 2   | K     | 194 | THR  |
| 2   | K     | 310 | VAL  |
| 2   | K     | 366 | ASP  |
| 2   | L     | 104 | THR  |
| 2   | L     | 132 | SER  |
| 2   | L     | 135 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 157 | ASP  |
| 2   | L     | 164 | LEU  |
| 2   | L     | 310 | VAL  |
| 2   | M     | 27  | THR  |
| 2   | M     | 55  | GLN  |
| 2   | M     | 104 | THR  |
| 2   | M     | 135 | SER  |
| 2   | M     | 310 | VAL  |
| 2   | N     | 104 | THR  |
| 2   | N     | 310 | VAL  |
| 2   | N     | 366 | ASP  |
| 2   | O     | 310 | VAL  |
| 2   | O     | 366 | ASP  |
| 2   | P     | 310 | VAL  |
| 2   | P     | 366 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | HIS  |
| 1   | A     | 34  | ASN  |
| 1   | A     | 146 | HIS  |
| 1   | A     | 197 | HIS  |
| 1   | A     | 275 | GLN  |
| 1   | A     | 452 | GLN  |
| 1   | A     | 530 | ASN  |
| 1   | B     | 17  | HIS  |
| 1   | B     | 34  | ASN  |
| 1   | B     | 146 | HIS  |
| 1   | B     | 197 | HIS  |
| 1   | B     | 275 | GLN  |
| 1   | B     | 452 | GLN  |
| 1   | B     | 530 | ASN  |
| 1   | C     | 17  | HIS  |
| 1   | C     | 34  | ASN  |
| 1   | C     | 146 | HIS  |
| 1   | C     | 197 | HIS  |
| 1   | C     | 275 | GLN  |
| 1   | C     | 452 | GLN  |
| 1   | C     | 530 | ASN  |
| 1   | D     | 34  | ASN  |
| 1   | D     | 146 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 197 | HIS  |
| 1   | D     | 198 | GLN  |
| 1   | D     | 275 | GLN  |
| 1   | D     | 452 | GLN  |
| 1   | E     | 34  | ASN  |
| 1   | E     | 132 | ASN  |
| 1   | E     | 146 | HIS  |
| 1   | E     | 197 | HIS  |
| 1   | E     | 198 | GLN  |
| 1   | E     | 275 | GLN  |
| 1   | E     | 459 | HIS  |
| 1   | E     | 530 | ASN  |
| 1   | F     | 34  | ASN  |
| 1   | F     | 132 | ASN  |
| 1   | F     | 146 | HIS  |
| 1   | F     | 197 | HIS  |
| 1   | F     | 198 | GLN  |
| 1   | F     | 275 | GLN  |
| 1   | F     | 530 | ASN  |
| 1   | G     | 34  | ASN  |
| 1   | G     | 132 | ASN  |
| 1   | G     | 146 | HIS  |
| 1   | G     | 197 | HIS  |
| 1   | G     | 198 | GLN  |
| 1   | G     | 275 | GLN  |
| 1   | G     | 530 | ASN  |
| 1   | H     | 34  | ASN  |
| 1   | H     | 132 | ASN  |
| 1   | H     | 146 | HIS  |
| 1   | H     | 197 | HIS  |
| 1   | H     | 198 | GLN  |
| 1   | H     | 275 | GLN  |
| 1   | H     | 530 | ASN  |
| 2   | I     | 371 | GLN  |
| 2   | J     | 11  | GLN  |
| 2   | J     | 371 | GLN  |
| 2   | K     | 371 | GLN  |
| 2   | L     | 11  | GLN  |
| 2   | L     | 155 | HIS  |
| 2   | M     | 155 | HIS  |
| 2   | M     | 361 | GLN  |
| 2   | M     | 371 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 161 | ASN  |
| 2   | O     | 371 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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     | 565/593 (95%)   | -0.44  | 1 (0%) 91 80  | 34, 53, 96, 118       | 0       |
| 1   | B     | 571/593 (96%)   | -0.46  | 2 (0%) 88 70  | 28, 43, 64, 79        | 0       |
| 1   | C     | 569/593 (95%)   | -0.45  | 1 (0%) 91 80  | 35, 51, 79, 106       | 0       |
| 1   | D     | 571/593 (96%)   | -0.37  | 1 (0%) 91 80  | 44, 77, 111, 129      | 0       |
| 1   | E     | 549/593 (92%)   | -0.18  | 1 (0%) 91 80  | 67, 102, 176, 208     | 0       |
| 1   | F     | 571/593 (96%)   | -0.14  | 5 (0%) 81 56  | 68, 119, 249, 314     | 0       |
| 1   | G     | 571/593 (96%)   | -0.10  | 5 (0%) 81 56  | 80, 142, 218, 251     | 0       |
| 1   | H     | 544/593 (91%)   | 0.17   | 14 (2%) 57 33 | 89, 159, 248, 316     | 0       |
| 2   | I     | 435/441 (98%)   | -0.30  | 3 (0%) 84 61  | 38, 62, 111, 129      | 0       |
| 2   | J     | 435/441 (98%)   | -0.04  | 5 (1%) 78 52  | 55, 92, 152, 171      | 0       |
| 2   | K     | 353/441 (80%)   | 0.06   | 3 (0%) 82 58  | 106, 160, 228, 246    | 0       |
| 2   | L     | 436/441 (98%)   | 0.06   | 7 (1%) 70 43  | 88, 119, 163, 181     | 0       |
| 2   | M     | 431/441 (97%)   | -0.05  | 3 (0%) 84 61  | 99, 131, 188, 228     | 0       |
| 2   | N     | 349/441 (79%)   | 0.04   | 8 (2%) 61 35  | 116, 177, 233, 254    | 0       |
| 2   | O     | 239/441 (54%)   | 0.12   | 7 (2%) 53 30  | 168, 210, 253, 266    | 0       |
| 2   | P     | 239/441 (54%)   | 0.15   | 7 (2%) 53 30  | 150, 195, 247, 256    | 0       |
| All | All   | 7428/8272 (89%) | -0.16  | 73 (0%) 79 54 | 28, 106, 220, 316     | 0       |

All (73) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 361 | GLN  | 7.7  |
| 2   | L     | 358 | LEU  | 5.6  |
| 1   | H     | 323 | ALA  | 5.4  |
| 1   | H     | 558 | VAL  | 4.9  |
| 2   | I     | 361 | GLN  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 215 | VAL  | 4.0  |
| 2   | I     | 358 | LEU  | 3.9  |
| 2   | O     | 320 | ILE  | 3.5  |
| 2   | N     | 277 | LEU  | 3.4  |
| 2   | K     | 128 | GLY  | 3.3  |
| 2   | J     | 361 | GLN  | 3.3  |
| 1   | H     | 166 | PRO  | 3.1  |
| 1   | F     | 497 | GLU  | 3.1  |
| 2   | N     | 360 | ASP  | 3.1  |
| 1   | G     | 128 | ASP  | 3.1  |
| 2   | L     | 215 | PHE  | 3.1  |
| 2   | O     | 361 | GLN  | 3.0  |
| 2   | K     | 177 | GLY  | 3.0  |
| 2   | N     | 181 | THR  | 3.0  |
| 1   | G     | 77  | CYS  | 2.9  |
| 1   | H     | 134 | THR  | 2.9  |
| 1   | C     | 9   | HIS  | 2.8  |
| 1   | G     | 555 | THR  | 2.8  |
| 2   | K     | 132 | SER  | 2.8  |
| 1   | B     | 520 | GLY  | 2.8  |
| 2   | N     | 361 | GLN  | 2.7  |
| 2   | O     | 427 | SER  | 2.7  |
| 1   | H     | 555 | THR  | 2.6  |
| 1   | H     | 582 | LEU  | 2.5  |
| 1   | H     | 556 | GLY  | 2.5  |
| 2   | N     | 347 | LEU  | 2.5  |
| 2   | L     | 268 | ALA  | 2.5  |
| 1   | D     | 507 | ALA  | 2.5  |
| 2   | P     | 368 | ARG  | 2.4  |
| 2   | L     | 131 | GLN  | 2.4  |
| 1   | G     | 444 | GLY  | 2.4  |
| 1   | H     | 573 | PRO  | 2.4  |
| 1   | H     | 553 | GLU  | 2.4  |
| 1   | A     | 13  | GLY  | 2.4  |
| 2   | M     | 177 | GLY  | 2.4  |
| 1   | H     | 571 | THR  | 2.4  |
| 2   | J     | 291 | LEU  | 2.3  |
| 2   | L     | 144 | PHE  | 2.3  |
| 2   | L     | 132 | SER  | 2.3  |
| 2   | N     | 368 | ARG  | 2.3  |
| 2   | P     | 388 | CYS  | 2.3  |
| 2   | O     | 356 | GLN  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 521 | ALA  | 2.3  |
| 2   | I     | 368 | ARG  | 2.2  |
| 2   | N     | 358 | LEU  | 2.2  |
| 1   | H     | 578 | TYR  | 2.2  |
| 1   | H     | 322 | LEU  | 2.2  |
| 2   | J     | 367 | ASP  | 2.2  |
| 1   | H     | 513 | THR  | 2.2  |
| 2   | M     | 419 | ALA  | 2.2  |
| 2   | N     | 211 | THR  | 2.2  |
| 2   | O     | 372 | LEU  | 2.2  |
| 2   | P     | 277 | LEU  | 2.1  |
| 1   | F     | 109 | ASP  | 2.1  |
| 2   | P     | 384 | CYS  | 2.1  |
| 1   | F     | 543 | LEU  | 2.1  |
| 2   | P     | 320 | ILE  | 2.1  |
| 2   | O     | 331 | ASP  | 2.1  |
| 2   | M     | 388 | CYS  | 2.1  |
| 2   | O     | 395 | ALA  | 2.1  |
| 1   | F     | 230 | ASP  | 2.1  |
| 2   | J     | 226 | GLY  | 2.0  |
| 2   | J     | 360 | ASP  | 2.0  |
| 1   | E     | 84  | TYR  | 2.0  |
| 1   | F     | 343 | GLU  | 2.0  |
| 1   | H     | 560 | PHE  | 2.0  |
| 2   | P     | 198 | ALA  | 2.0  |
| 2   | P     | 353 | ALA  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | CA   | F     | 601 | 1/1   | 0.71 | 0.53 | 20,20,20,20                 | 0     |
| 3   | CA   | D     | 601 | 1/1   | 0.84 | 0.06 | 20,20,20,20                 | 0     |
| 3   | CA   | H     | 601 | 1/1   | 0.96 | 0.29 | 20,20,20,20                 | 0     |
| 3   | CA   | E     | 601 | 1/1   | 0.97 | 0.18 | 20,20,20,20                 | 0     |
| 3   | CA   | G     | 601 | 1/1   | 0.99 | 0.20 | 20,20,20,20                 | 0     |
| 3   | CA   | C     | 601 | 1/1   | 1.00 | 0.02 | 20,20,20,20                 | 0     |
| 3   | CA   | A     | 601 | 1/1   | 1.00 | 0.05 | 20,20,20,20                 | 0     |
| 3   | CA   | B     | 601 | 1/1   | 1.00 | 0.01 | 20,20,20,20                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.