



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:16 AM UTC

PDB ID : 1HI8 / pdb\_00001hi8  
Title : RNA dependent RNA polymerase from dsRNA bacteriophage phi6  
Authors : Grimes, J.M.; Butcher, S.J.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.  
Deposited on : 2001-01-03  
Resolution : 2.50 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| 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                                                             |

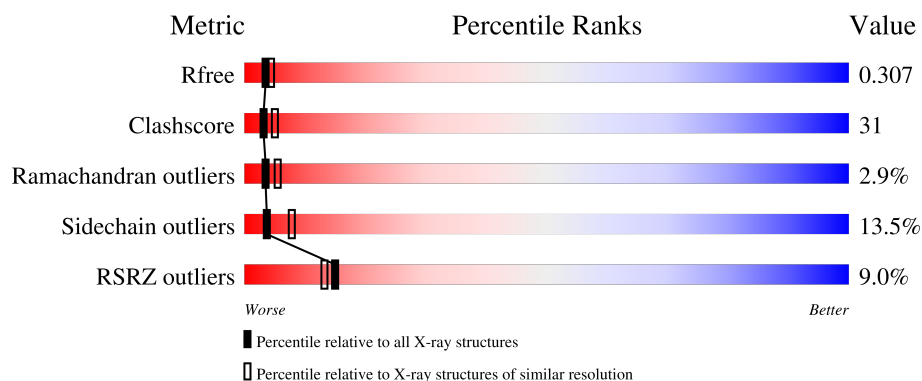
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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     | 664    | <div> <div>8%</div> <div>49%</div> <div>38%</div> <div>12%</div> </div> |
| 1   | B     | 664    | <div> <div>9%</div> <div>48%</div> <div>38%</div> <div>12%</div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10532 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 P2 PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 664      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 5265  | 3342 | 914 | 977 | 7 | 25 |         |         |       |
| 1   | B     | 664      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 5265  | 3342 | 914 | 977 | 7 | 25 |         |         |       |

There are 50 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 16      | MSE      | MET    | modified residue | UNP P11124 |
| A     | 87      | MSE      | MET    | modified residue | UNP P11124 |
| A     | 90      | MSE      | MET    | modified residue | UNP P11124 |
| A     | 95      | MSE      | MET    | modified residue | UNP P11124 |
| A     | 134     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 160     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 181     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 195     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 226     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 273     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 284     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 347     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 401     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 406     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 413     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 429     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 456     | MSE      | ILE    | SEE REMARK 999   | UNP P11124 |
| A     | 474     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 486     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 521     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 554     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 590     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 605     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 646     | MSE      | MET    | modified residue | UNP P11124 |
| A     | 662     | MSE      | MET    | modified residue | UNP P11124 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| B     | 16      | MSE      | MET    | modified residue | UNP P11124 |
| B     | 87      | MSE      | MET    | modified residue | UNP P11124 |
| B     | 90      | MSE      | MET    | modified residue | UNP P11124 |
| B     | 95      | MSE      | MET    | modified residue | UNP P11124 |
| B     | 134     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 160     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 181     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 195     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 226     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 273     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 284     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 347     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 401     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 406     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 413     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 429     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 456     | MSE      | ILE    | SEE REMARK 999   | UNP P11124 |
| B     | 474     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 486     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 521     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 554     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 590     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 605     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 646     | MSE      | MET    | modified residue | UNP P11124 |
| B     | 662     | MSE      | MET    | modified residue | UNP P11124 |

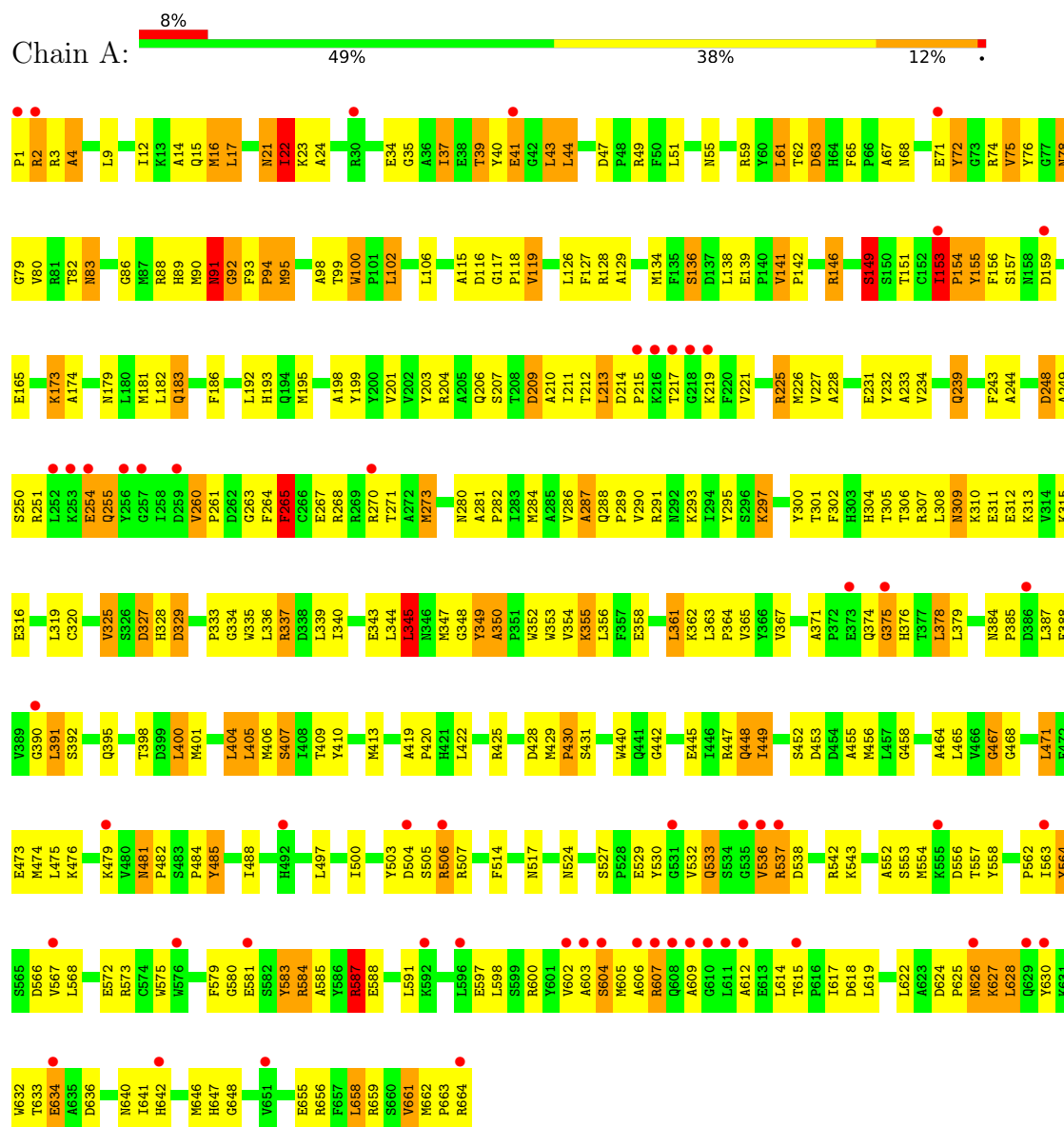
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |

### 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: P2 PROTEIN



#### • Molecule 1: P2 PROTEIN





## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 32                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 110.00Å 110.00Å 159.30Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.50<br>50.00 – 2.50                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.0 (50.00-2.50)<br>88.2 (50.00-2.50)                         | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.18 (at 2.51Å)                                                | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                        | Depositor        |
| R, $R_{free}$                                                           | 0.280 , 0.316<br>0.275 , 0.307                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3339 reflections (5.07%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.2                                                           | Xtriage          |
| Anisotropy                                                              | 0.643                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 47.2                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$    | Xtriage          |
| Estimated twinning fraction                                             | 0.006 for -h,-k,l<br>0.029 for h,-h-k,-l<br>0.016 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                           | EDS              |
| Total number of atoms                                                   | 10532                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 44.0                                                           | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: MG

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     | 0.90         | 2/5371 (0.0%)  | 1.38        | 63/7222 (0.9%)   |
| 1   | B     | 0.90         | 2/5371 (0.0%)  | 1.38        | 64/7222 (0.9%)   |
| All | All   | 0.90         | 4/10742 (0.0%) | 1.38        | 127/14444 (0.9%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 153 | ILE  | CA-C  | -5.44 | 1.47        | 1.52     |
| 1   | B     | 153 | ILE  | CA-C  | -5.39 | 1.47        | 1.52     |
| 1   | B     | 119 | VAL  | CA-CB | 5.14  | 1.60        | 1.54     |
| 1   | A     | 119 | VAL  | CA-CB | 5.10  | 1.60        | 1.54     |

All (127) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 153 | ILE  | CA-C-N | -16.08 | 99.74       | 119.84   |
| 1   | B     | 153 | ILE  | C-N-CA | -16.08 | 99.74       | 119.84   |
| 1   | A     | 153 | ILE  | CA-C-N | -16.04 | 99.79       | 119.84   |
| 1   | A     | 153 | ILE  | C-N-CA | -16.04 | 99.79       | 119.84   |
| 1   | A     | 626 | ASN  | N-CA-C | -13.87 | 92.23       | 110.53   |
| 1   | B     | 626 | ASN  | N-CA-C | -13.86 | 92.23       | 110.53   |
| 1   | B     | 467 | GLY  | N-CA-C | -13.40 | 93.61       | 112.37   |
| 1   | A     | 467 | GLY  | N-CA-C | -13.38 | 93.64       | 112.37   |
| 1   | B     | 585 | ALA  | N-CA-C | -10.18 | 99.87       | 110.97   |
| 1   | A     | 585 | ALA  | N-CA-C | -10.16 | 99.90       | 110.97   |
| 1   | A     | 333 | PRO  | N-CA-C | 9.82   | 126.56      | 110.55   |
| 1   | B     | 333 | PRO  | N-CA-C | 9.81   | 126.54      | 110.55   |
| 1   | A     | 136 | SER  | N-CA-C | 9.64   | 123.16      | 111.40   |
| 1   | B     | 136 | SER  | N-CA-C | 9.62   | 123.14      | 111.40   |
| 1   | B     | 628 | LEU  | N-CA-C | -9.52  | 101.68      | 113.20   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 628 | LEU  | N-CA-C  | -9.45 | 101.76      | 113.20   |
| 1   | A     | 583 | TYR  | N-CA-C  | -9.17 | 96.71       | 110.28   |
| 1   | B     | 583 | TYR  | N-CA-C  | -9.16 | 96.72       | 110.28   |
| 1   | A     | 376 | HIS  | N-CA-C  | -8.88 | 88.93       | 107.67   |
| 1   | B     | 376 | HIS  | N-CA-C  | -8.88 | 88.93       | 107.67   |
| 1   | A     | 405 | LEU  | N-CA-C  | -8.57 | 99.28       | 110.33   |
| 1   | B     | 405 | LEU  | N-CA-C  | -8.54 | 99.31       | 110.33   |
| 1   | B     | 153 | ILE  | N-CA-C  | 8.20  | 126.60      | 108.88   |
| 1   | A     | 153 | ILE  | N-CA-C  | 8.20  | 126.59      | 108.88   |
| 1   | B     | 115 | ALA  | CA-C-N  | 7.88  | 132.30      | 120.31   |
| 1   | B     | 115 | ALA  | C-N-CA  | 7.88  | 132.30      | 120.31   |
| 1   | A     | 115 | ALA  | CA-C-N  | 7.88  | 132.29      | 120.31   |
| 1   | A     | 115 | ALA  | C-N-CA  | 7.88  | 132.29      | 120.31   |
| 1   | B     | 149 | SER  | N-CA-C  | 7.82  | 127.47      | 110.80   |
| 1   | A     | 149 | SER  | N-CA-C  | 7.81  | 127.43      | 110.80   |
| 1   | B     | 100 | TRP  | N-CA-C  | -7.31 | 100.86      | 110.07   |
| 1   | A     | 100 | TRP  | N-CA-C  | -7.29 | 100.88      | 110.07   |
| 1   | B     | 452 | SER  | CB-CA-C | -7.16 | 108.31      | 116.54   |
| 1   | A     | 452 | SER  | CB-CA-C | -7.14 | 108.33      | 116.54   |
| 1   | A     | 115 | ALA  | N-CA-C  | 7.02  | 120.02      | 110.55   |
| 1   | B     | 115 | ALA  | N-CA-C  | 7.00  | 120.00      | 110.55   |
| 1   | B     | 468 | GLY  | N-CA-C  | -6.91 | 96.80       | 113.18   |
| 1   | A     | 468 | GLY  | N-CA-C  | -6.91 | 96.80       | 113.18   |
| 1   | A     | 98  | ALA  | N-CA-C  | -6.83 | 102.01      | 110.41   |
| 1   | B     | 98  | ALA  | N-CA-C  | -6.81 | 102.03      | 110.41   |
| 1   | B     | 485 | TYR  | N-CA-C  | 6.81  | 121.72      | 113.41   |
| 1   | A     | 485 | TYR  | N-CA-C  | 6.81  | 121.72      | 113.41   |
| 1   | B     | 533 | GLN  | N-CA-C  | 6.67  | 120.44      | 111.24   |
| 1   | A     | 533 | GLN  | N-CA-C  | 6.67  | 120.44      | 111.24   |
| 1   | B     | 136 | SER  | CA-C-N  | -6.56 | 114.14      | 123.20   |
| 1   | B     | 136 | SER  | C-N-CA  | -6.56 | 114.14      | 123.20   |
| 1   | A     | 136 | SER  | CA-C-N  | -6.55 | 114.15      | 123.20   |
| 1   | A     | 136 | SER  | C-N-CA  | -6.55 | 114.15      | 123.20   |
| 1   | B     | 91  | ASN  | N-CA-C  | 6.54  | 124.73      | 110.80   |
| 1   | A     | 91  | ASN  | N-CA-C  | 6.52  | 124.69      | 110.80   |
| 1   | A     | 309 | ASN  | N-CA-C  | -6.41 | 104.72      | 112.54   |
| 1   | B     | 309 | ASN  | N-CA-C  | -6.39 | 104.74      | 112.54   |
| 1   | A     | 63  | ASP  | N-CA-C  | 6.34  | 118.19      | 111.28   |
| 1   | A     | 458 | GLY  | N-CA-C  | 6.25  | 121.56      | 111.38   |
| 1   | B     | 458 | GLY  | N-CA-C  | 6.24  | 121.55      | 111.38   |
| 1   | B     | 63  | ASP  | N-CA-C  | 6.24  | 118.16      | 111.36   |
| 1   | B     | 141 | VAL  | CA-C-N  | -6.22 | 113.36      | 119.76   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 141 | VAL  | C-N-CA | -6.22 | 113.36      | 119.76   |
| 1   | A     | 141 | VAL  | CA-C-N | -6.21 | 113.37      | 119.76   |
| 1   | A     | 141 | VAL  | C-N-CA | -6.21 | 113.37      | 119.76   |
| 1   | A     | 350 | ALA  | CA-C-N | -6.18 | 113.26      | 119.56   |
| 1   | A     | 350 | ALA  | C-N-CA | -6.18 | 113.26      | 119.56   |
| 1   | B     | 350 | ALA  | CA-C-N | -6.16 | 113.27      | 119.56   |
| 1   | B     | 350 | ALA  | C-N-CA | -6.16 | 113.27      | 119.56   |
| 1   | A     | 345 | LEU  | N-CA-C | -5.99 | 104.44      | 110.97   |
| 1   | B     | 345 | LEU  | N-CA-C | -5.98 | 104.46      | 110.97   |
| 1   | B     | 329 | ASP  | N-CA-C | 5.97  | 117.78      | 111.28   |
| 1   | B     | 465 | LEU  | N-CA-C | 5.96  | 118.54      | 111.33   |
| 1   | A     | 465 | LEU  | N-CA-C | 5.96  | 118.54      | 111.33   |
| 1   | A     | 302 | PHE  | N-CA-C | 5.95  | 121.59      | 113.97   |
| 1   | B     | 302 | PHE  | N-CA-C | 5.95  | 121.58      | 113.97   |
| 1   | A     | 329 | ASP  | N-CA-C | 5.95  | 117.76      | 111.28   |
| 1   | A     | 22  | ILE  | N-CA-C | 5.93  | 116.11      | 110.42   |
| 1   | B     | 22  | ILE  | N-CA-C | 5.90  | 116.08      | 110.42   |
| 1   | B     | 39  | THR  | N-CA-C | 5.88  | 119.28      | 111.75   |
| 1   | A     | 39  | THR  | N-CA-C | 5.86  | 119.26      | 111.75   |
| 1   | B     | 371 | ALA  | N-CA-C | 5.84  | 113.38      | 108.13   |
| 1   | A     | 371 | ALA  | N-CA-C | 5.83  | 113.37      | 108.13   |
| 1   | B     | 374 | GLN  | N-CA-C | 5.79  | 118.84      | 109.40   |
| 1   | A     | 374 | GLN  | N-CA-C | 5.79  | 118.83      | 109.40   |
| 1   | B     | 199 | TYR  | N-CA-C | -5.77 | 101.94      | 110.48   |
| 1   | B     | 455 | ALA  | N-CA-C | 5.77  | 117.56      | 108.96   |
| 1   | A     | 455 | ALA  | N-CA-C | 5.77  | 117.55      | 108.96   |
| 1   | A     | 199 | TYR  | N-CA-C | -5.75 | 101.97      | 110.48   |
| 1   | A     | 155 | TYR  | N-CA-C | 5.72  | 120.54      | 113.50   |
| 1   | B     | 155 | TYR  | N-CA-C | 5.72  | 120.53      | 113.50   |
| 1   | A     | 287 | ALA  | N-CA-C | 5.70  | 118.26      | 111.71   |
| 1   | B     | 407 | SER  | N-CA-C | -5.70 | 104.27      | 111.11   |
| 1   | B     | 287 | ALA  | N-CA-C | 5.69  | 118.25      | 111.71   |
| 1   | A     | 407 | SER  | N-CA-C | -5.68 | 104.29      | 111.11   |
| 1   | A     | 255 | GLN  | N-CA-C | 5.58  | 117.16      | 111.14   |
| 1   | B     | 255 | GLN  | N-CA-C | 5.56  | 117.14      | 111.14   |
| 1   | A     | 449 | ILE  | N-CA-C | -5.55 | 99.55       | 107.77   |
| 1   | B     | 449 | ILE  | N-CA-C | -5.55 | 99.56       | 107.77   |
| 1   | B     | 375 | GLY  | N-CA-C | 5.49  | 126.18      | 113.18   |
| 1   | A     | 375 | GLY  | N-CA-C | 5.48  | 126.17      | 113.18   |
| 1   | B     | 95  | MSE  | N-CA-C | -5.46 | 103.28      | 110.43   |
| 1   | A     | 67  | ALA  | N-CA-C | 5.44  | 118.12      | 110.23   |
| 1   | A     | 95  | MSE  | N-CA-C | -5.44 | 103.30      | 110.43   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 265 | PHE  | N-CA-C | 5.44  | 117.24      | 109.14   |
| 1   | A     | 265 | PHE  | N-CA-C | 5.42  | 117.22      | 109.14   |
| 1   | B     | 67  | ALA  | N-CA-C | 5.40  | 118.07      | 110.23   |
| 1   | B     | 72  | TYR  | N-CA-C | -5.38 | 106.58      | 112.72   |
| 1   | A     | 94  | PRO  | N-CA-C | 5.37  | 120.74      | 111.77   |
| 1   | B     | 94  | PRO  | N-CA-C | 5.37  | 120.73      | 111.77   |
| 1   | A     | 72  | TYR  | N-CA-C | -5.36 | 106.61      | 112.72   |
| 1   | B     | 363 | LEU  | N-CA-C | 5.30  | 117.70      | 110.01   |
| 1   | A     | 363 | LEU  | N-CA-C | 5.28  | 117.66      | 110.01   |
| 1   | B     | 656 | ARG  | N-CA-C | -5.27 | 105.53      | 111.28   |
| 1   | B     | 391 | LEU  | N-CA-C | 5.25  | 121.99      | 110.80   |
| 1   | A     | 656 | ARG  | N-CA-C | -5.25 | 105.56      | 111.28   |
| 1   | A     | 391 | LEU  | N-CA-C | 5.24  | 121.96      | 110.80   |
| 1   | B     | 337 | ARG  | N-CA-C | -5.22 | 105.59      | 111.28   |
| 1   | A     | 587 | ARG  | N-CA-C | 5.21  | 116.96      | 111.28   |
| 1   | B     | 587 | ARG  | N-CA-C | 5.21  | 116.95      | 111.28   |
| 1   | A     | 337 | ARG  | N-CA-C | -5.19 | 105.63      | 111.28   |
| 1   | A     | 209 | ASP  | N-CA-C | 5.18  | 120.06      | 113.18   |
| 1   | A     | 481 | ASN  | CA-C-N | 5.16  | 125.84      | 120.12   |
| 1   | A     | 481 | ASN  | C-N-CA | 5.16  | 125.84      | 120.12   |
| 1   | B     | 481 | ASN  | CA-C-N | 5.15  | 125.84      | 120.12   |
| 1   | B     | 481 | ASN  | C-N-CA | 5.15  | 125.84      | 120.12   |
| 1   | B     | 209 | ASP  | N-CA-C | 5.14  | 120.02      | 113.18   |
| 1   | A     | 388 | GLU  | N-CA-C | -5.04 | 100.17      | 108.49   |
| 1   | B     | 388 | GLU  | N-CA-C | -5.04 | 100.17      | 108.49   |
| 1   | A     | 248 | ASP  | N-CA-C | 5.03  | 121.51      | 110.80   |
| 1   | B     | 248 | ASP  | N-CA-C | 5.01  | 121.47      | 110.80   |
| 1   | B     | 557 | THR  | N-CA-C | 5.00  | 117.84      | 111.69   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5265  | 0        | 5165     | 323     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 5265  | 0        | 5165     | 326     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 10532 | 0        | 10330    | 649     | 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 31.

All (649) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:55:ASN:HD21  | 1:B:59:ARG:HD2   | 0.98                     | 1.14              |
| 1:A:55:ASN:HD21  | 1:A:59:ARG:HD2   | 0.98                     | 1.14              |
| 1:A:22:ILE:HD12  | 1:A:22:ILE:H     | 1.15                     | 1.12              |
| 1:B:537:ARG:H    | 1:B:537:ARG:HD2  | 1.11                     | 1.12              |
| 1:A:537:ARG:H    | 1:A:537:ARG:HD2  | 1.11                     | 1.10              |
| 1:B:22:ILE:HD12  | 1:B:22:ILE:H     | 1.15                     | 1.09              |
| 1:A:55:ASN:ND2   | 1:A:59:ARG:HD2   | 1.68                     | 1.08              |
| 1:B:55:ASN:ND2   | 1:B:59:ARG:HD2   | 1.68                     | 1.06              |
| 1:A:471:LEU:HD23 | 1:A:474:MSE:HE3  | 1.42                     | 1.02              |
| 1:B:615:THR:HG22 | 1:B:617:ILE:H    | 1.22                     | 1.01              |
| 1:A:615:THR:HG22 | 1:A:617:ILE:H    | 1.22                     | 1.00              |
| 1:B:471:LEU:HD23 | 1:B:474:MSE:HE3  | 1.42                     | 0.99              |
| 1:B:563:ILE:HG22 | 1:B:567:VAL:HG23 | 1.46                     | 0.98              |
| 1:A:533:GLN:HE22 | 1:A:543:LYS:H    | 1.11                     | 0.97              |
| 1:A:563:ILE:HG22 | 1:A:567:VAL:HG23 | 1.46                     | 0.97              |
| 1:A:533:GLN:NE2  | 1:A:543:LYS:H    | 1.63                     | 0.96              |
| 1:A:68:ASN:HD22  | 1:A:78:ASN:H     | 1.12                     | 0.96              |
| 1:B:533:GLN:NE2  | 1:B:543:LYS:H    | 1.63                     | 0.95              |
| 1:B:68:ASN:HD22  | 1:B:78:ASN:H     | 1.12                     | 0.95              |
| 1:B:634:GLU:HG3  | 1:B:642:HIS:NE2  | 1.82                     | 0.95              |
| 1:A:68:ASN:ND2   | 1:A:78:ASN:H     | 1.65                     | 0.94              |
| 1:B:68:ASN:ND2   | 1:B:78:ASN:H     | 1.65                     | 0.94              |
| 1:A:537:ARG:H    | 1:A:537:ARG:CD   | 1.81                     | 0.94              |
| 1:B:537:ARG:H    | 1:B:537:ARG:CD   | 1.81                     | 0.94              |
| 1:B:626:ASN:O    | 1:B:627:LYS:HB2  | 1.68                     | 0.93              |
| 1:A:364:PRO:HA   | 1:A:387:LEU:HD22 | 1.50                     | 0.93              |
| 1:A:634:GLU:HG3  | 1:A:642:HIS:NE2  | 1.82                     | 0.93              |
| 1:A:78:ASN:HD22  | 1:A:79:GLY:N     | 1.67                     | 0.93              |
| 1:A:626:ASN:O    | 1:A:627:LYS:HB2  | 1.68                     | 0.93              |
| 1:B:364:PRO:HA   | 1:B:387:LEU:HD22 | 1.50                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:ASN:HD22  | 1:B:79:GLY:N     | 1.67                     | 0.91              |
| 1:B:533:GLN:HE22 | 1:B:543:LYS:H    | 1.11                     | 0.91              |
| 1:A:83:ASN:C     | 1:A:83:ASN:HD22  | 1.78                     | 0.91              |
| 1:B:22:ILE:H     | 1:B:22:ILE:CD1   | 1.80                     | 0.90              |
| 1:B:83:ASN:C     | 1:B:83:ASN:HD22  | 1.78                     | 0.90              |
| 1:A:22:ILE:H     | 1:A:22:ILE:CD1   | 1.80                     | 0.89              |
| 1:B:537:ARG:HD2  | 1:B:537:ARG:N    | 1.90                     | 0.87              |
| 1:A:537:ARG:HD2  | 1:A:537:ARG:N    | 1.90                     | 0.87              |
| 1:A:17:LEU:HG    | 1:A:153:ILE:HD13 | 1.60                     | 0.84              |
| 1:B:17:LEU:HG    | 1:B:153:ILE:HD13 | 1.60                     | 0.83              |
| 1:B:21:ASN:HD21  | 1:B:24:ALA:H     | 1.28                     | 0.82              |
| 1:A:405:LEU:HG   | 1:A:406:MSE:N    | 1.95                     | 0.82              |
| 1:B:602:VAL:HB   | 1:B:605:MSE:HG3  | 1.62                     | 0.81              |
| 1:A:21:ASN:HD21  | 1:A:24:ALA:H     | 1.28                     | 0.81              |
| 1:A:21:ASN:ND2   | 1:A:24:ALA:H     | 1.79                     | 0.81              |
| 1:A:602:VAL:HB   | 1:A:605:MSE:HG3  | 1.62                     | 0.80              |
| 1:B:153:ILE:HA   | 1:B:156:PHE:CE2  | 2.17                     | 0.80              |
| 1:B:173:LYS:HG3  | 1:B:193:HIS:CE1  | 2.17                     | 0.80              |
| 1:B:615:THR:HG22 | 1:B:617:ILE:N    | 1.96                     | 0.80              |
| 1:B:405:LEU:HG   | 1:B:406:MSE:N    | 1.95                     | 0.80              |
| 1:A:153:ILE:HA   | 1:A:156:PHE:CE2  | 2.17                     | 0.80              |
| 1:A:173:LYS:HG3  | 1:A:193:HIS:CE1  | 2.17                     | 0.80              |
| 1:B:21:ASN:ND2   | 1:B:24:ALA:H     | 1.79                     | 0.80              |
| 1:B:51:LEU:HD22  | 1:B:90:MSE:HE1   | 1.64                     | 0.80              |
| 1:A:51:LEU:HD22  | 1:A:90:MSE:HE1   | 1.64                     | 0.79              |
| 1:A:615:THR:HG22 | 1:A:617:ILE:N    | 1.96                     | 0.79              |
| 1:A:51:LEU:CD2   | 1:A:90:MSE:HE1   | 2.13                     | 0.78              |
| 1:A:203:TYR:HE1  | 1:A:271:THR:HG22 | 1.48                     | 0.78              |
| 1:B:51:LEU:CD2   | 1:B:90:MSE:HE1   | 2.13                     | 0.78              |
| 1:B:206:GLN:HE21 | 1:B:270:ARG:HD2  | 1.49                     | 0.77              |
| 1:B:203:TYR:HE1  | 1:B:271:THR:HG22 | 1.48                     | 0.77              |
| 1:A:206:GLN:HE21 | 1:A:270:ARG:HD2  | 1.49                     | 0.76              |
| 1:A:563:ILE:HG22 | 1:A:563:ILE:O    | 1.86                     | 0.75              |
| 1:B:55:ASN:C     | 1:B:55:ASN:HD22  | 1.95                     | 0.75              |
| 1:B:343:GLU:HG3  | 1:B:347:MSE:CE   | 2.17                     | 0.75              |
| 1:A:55:ASN:HD22  | 1:A:55:ASN:C     | 1.95                     | 0.75              |
| 1:A:78:ASN:ND2   | 1:A:80:VAL:H     | 1.84                     | 0.75              |
| 1:B:563:ILE:HG22 | 1:B:563:ILE:O    | 1.86                     | 0.75              |
| 1:B:78:ASN:HD22  | 1:B:78:ASN:C     | 1.95                     | 0.75              |
| 1:A:343:GLU:HG3  | 1:A:347:MSE:CE   | 2.17                     | 0.74              |
| 1:A:78:ASN:HD22  | 1:A:78:ASN:C     | 1.95                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:ASN:ND2   | 1:B:80:VAL:H     | 1.84                     | 0.74              |
| 1:A:281:ALA:HB3  | 1:A:282:PRO:HD3  | 1.70                     | 0.73              |
| 1:B:47:ASP:OD2   | 1:B:49:ARG:HD3   | 1.88                     | 0.73              |
| 1:B:425:ARG:O    | 1:B:431:SER:HB2  | 1.88                     | 0.73              |
| 1:B:301:THR:HG23 | 1:B:440:TRP:O    | 1.88                     | 0.73              |
| 1:A:425:ARG:O    | 1:A:431:SER:HB2  | 1.88                     | 0.73              |
| 1:A:47:ASP:OD2   | 1:A:49:ARG:HD3   | 1.88                     | 0.73              |
| 1:A:301:THR:HG23 | 1:A:440:TRP:O    | 1.88                     | 0.73              |
| 1:A:410:TYR:HA   | 1:A:413:MSE:HE3  | 1.71                     | 0.73              |
| 1:B:410:TYR:HA   | 1:B:413:MSE:HE3  | 1.71                     | 0.73              |
| 1:A:37:ILE:HD13  | 1:A:92:GLY:HA3   | 1.70                     | 0.73              |
| 1:B:281:ALA:HB3  | 1:B:282:PRO:HD3  | 1.70                     | 0.73              |
| 1:B:22:ILE:HD12  | 1:B:22:ILE:N     | 1.99                     | 0.72              |
| 1:B:153:ILE:HG22 | 1:B:154:PRO:CD   | 2.20                     | 0.72              |
| 1:B:37:ILE:HD13  | 1:B:92:GLY:HA3   | 1.70                     | 0.72              |
| 1:A:68:ASN:HD22  | 1:A:78:ASN:N     | 1.87                     | 0.71              |
| 1:A:153:ILE:HG22 | 1:A:154:PRO:CD   | 2.20                     | 0.71              |
| 1:A:345:LEU:HD13 | 1:A:354:VAL:HG21 | 1.73                     | 0.71              |
| 1:B:583:TYR:O    | 1:B:584:ARG:CB   | 2.39                     | 0.71              |
| 1:B:626:ASN:O    | 1:B:627:LYS:CB   | 2.39                     | 0.71              |
| 1:A:226:MSE:HE1  | 1:A:244:ALA:HB2  | 1.73                     | 0.70              |
| 1:A:583:TYR:O    | 1:A:584:ARG:CB   | 2.39                     | 0.70              |
| 1:B:310:LYS:HB3  | 1:B:514:PHE:CE1  | 2.27                     | 0.70              |
| 1:B:226:MSE:HE1  | 1:B:244:ALA:HB2  | 1.73                     | 0.70              |
| 1:A:209:ASP:O    | 1:A:210:ALA:CB   | 2.40                     | 0.70              |
| 1:B:345:LEU:HD13 | 1:B:354:VAL:HG21 | 1.73                     | 0.69              |
| 1:A:310:LYS:HB3  | 1:A:514:PHE:CE1  | 2.27                     | 0.69              |
| 1:B:407:SER:HA   | 1:B:448:GLN:HE22 | 1.58                     | 0.69              |
| 1:B:68:ASN:HD22  | 1:B:78:ASN:N     | 1.87                     | 0.68              |
| 1:B:405:LEU:O    | 1:B:406:MSE:HB2  | 1.94                     | 0.68              |
| 1:A:407:SER:HA   | 1:A:448:GLN:HE22 | 1.58                     | 0.68              |
| 1:A:583:TYR:O    | 1:A:584:ARG:HB3  | 1.92                     | 0.68              |
| 1:B:209:ASP:O    | 1:B:210:ALA:HB2  | 1.94                     | 0.68              |
| 1:A:22:ILE:HD12  | 1:A:22:ILE:N     | 1.99                     | 0.68              |
| 1:A:209:ASP:O    | 1:A:210:ALA:HB2  | 1.94                     | 0.68              |
| 1:A:88:ARG:HD3   | 1:A:263:GLY:O    | 1.93                     | 0.68              |
| 1:B:209:ASP:O    | 1:B:210:ALA:CB   | 2.40                     | 0.68              |
| 1:A:405:LEU:O    | 1:A:406:MSE:HB2  | 1.93                     | 0.68              |
| 1:A:100:TRP:CZ3  | 1:A:367:VAL:HG21 | 2.29                     | 0.68              |
| 1:B:90:MSE:HE3   | 1:B:264:PHE:CD2  | 2.29                     | 0.67              |
| 1:A:37:ILE:HD13  | 1:A:92:GLY:CA    | 2.24                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:100:TRP:CZ3  | 1:B:367:VAL:HG21 | 2.29                     | 0.67              |
| 1:A:532:VAL:HG22 | 1:A:532:VAL:O    | 1.95                     | 0.67              |
| 1:B:583:TYR:O    | 1:B:584:ARG:HB3  | 1.92                     | 0.67              |
| 1:B:88:ARG:HD3   | 1:B:263:GLY:O    | 1.93                     | 0.67              |
| 1:B:37:ILE:HD13  | 1:B:92:GLY:CA    | 2.24                     | 0.67              |
| 1:B:329:ASP:O    | 1:B:390:GLY:O    | 2.13                     | 0.67              |
| 1:A:329:ASP:O    | 1:A:390:GLY:O    | 2.13                     | 0.67              |
| 1:A:471:LEU:HD23 | 1:A:474:MSE:CE   | 2.22                     | 0.67              |
| 1:A:90:MSE:HE3   | 1:A:264:PHE:CD2  | 2.29                     | 0.67              |
| 1:A:17:LEU:HG    | 1:A:153:ILE:CD1  | 2.26                     | 0.66              |
| 1:B:248:ASP:O    | 1:B:249:ALA:HB3  | 1.95                     | 0.66              |
| 1:B:251:ARG:HH11 | 1:B:255:GLN:HE22 | 1.43                     | 0.66              |
| 1:A:55:ASN:HD21  | 1:A:59:ARG:HH11  | 1.43                     | 0.66              |
| 1:B:17:LEU:HG    | 1:B:153:ILE:CD1  | 2.26                     | 0.66              |
| 1:B:153:ILE:HA   | 1:B:156:PHE:CZ   | 2.31                     | 0.66              |
| 1:B:532:VAL:O    | 1:B:532:VAL:HG22 | 1.95                     | 0.66              |
| 1:A:153:ILE:HA   | 1:A:156:PHE:CZ   | 2.31                     | 0.66              |
| 1:A:248:ASP:O    | 1:A:249:ALA:HB3  | 1.95                     | 0.66              |
| 1:A:308:LEU:N    | 1:A:308:LEU:HD12 | 2.11                     | 0.65              |
| 1:B:471:LEU:HD23 | 1:B:474:MSE:CE   | 2.22                     | 0.65              |
| 1:B:308:LEU:N    | 1:B:308:LEU:HD12 | 2.11                     | 0.65              |
| 1:A:626:ASN:O    | 1:A:627:LYS:CB   | 2.39                     | 0.65              |
| 1:A:358:GLU:O    | 1:A:362:LYS:HG3  | 1.96                     | 0.65              |
| 1:B:2:ARG:HH11   | 1:B:4:ALA:HB2    | 1.62                     | 0.65              |
| 1:A:21:ASN:C     | 1:A:21:ASN:HD22  | 2.05                     | 0.65              |
| 1:B:203:TYR:CE1  | 1:B:271:THR:HG22 | 2.32                     | 0.64              |
| 1:A:129:ALA:HA   | 1:A:429:MSE:HE1  | 1.79                     | 0.64              |
| 1:B:21:ASN:C     | 1:B:21:ASN:HD22  | 2.05                     | 0.64              |
| 1:B:358:GLU:O    | 1:B:362:LYS:HG3  | 1.97                     | 0.64              |
| 1:A:72:TYR:CE1   | 1:A:476:LYS:HD3  | 2.32                     | 0.64              |
| 1:B:3:ARG:O      | 1:B:234:VAL:O    | 2.15                     | 0.64              |
| 1:B:55:ASN:HD21  | 1:B:59:ARG:HH11  | 1.43                     | 0.64              |
| 1:A:203:TYR:CE1  | 1:A:271:THR:HG22 | 2.32                     | 0.64              |
| 1:B:405:LEU:HG   | 1:B:406:MSE:H    | 1.60                     | 0.64              |
| 1:B:641:ILE:HD12 | 1:B:641:ILE:N    | 2.12                     | 0.64              |
| 1:A:251:ARG:HH11 | 1:A:255:GLN:HE22 | 1.43                     | 0.64              |
| 1:A:533:GLN:NE2  | 1:A:543:LYS:N    | 2.42                     | 0.63              |
| 1:B:55:ASN:O     | 1:B:59:ARG:HG3   | 1.98                     | 0.63              |
| 1:B:129:ALA:HA   | 1:B:429:MSE:HE1  | 1.79                     | 0.63              |
| 1:A:405:LEU:HG   | 1:A:406:MSE:H    | 1.60                     | 0.63              |
| 1:A:3:ARG:O      | 1:A:234:VAL:O    | 2.15                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:55:ASN:O     | 1:A:59:ARG:HG3   | 1.98                     | 0.63              |
| 1:B:72:TYR:CE1   | 1:B:476:LYS:HD3  | 2.32                     | 0.63              |
| 1:B:352:TRP:CH2  | 1:B:661:VAL:HG12 | 2.34                     | 0.63              |
| 1:A:206:GLN:HB2  | 1:A:268:ARG:HG2  | 1.81                     | 0.62              |
| 1:B:21:ASN:ND2   | 1:B:21:ASN:C     | 2.57                     | 0.62              |
| 1:A:2:ARG:HH11   | 1:A:4:ALA:HB2    | 1.62                     | 0.62              |
| 1:A:614:LEU:CD2  | 1:A:641:ILE:HD11 | 2.29                     | 0.62              |
| 1:B:533:GLN:NE2  | 1:B:543:LYS:N    | 2.42                     | 0.62              |
| 1:B:563:ILE:O    | 1:B:563:ILE:CG2  | 2.47                     | 0.62              |
| 1:A:641:ILE:N    | 1:A:641:ILE:HD12 | 2.12                     | 0.62              |
| 1:A:91:ASN:O     | 1:A:93:PHE:N     | 2.31                     | 0.62              |
| 1:B:91:ASN:O     | 1:B:93:PHE:N     | 2.31                     | 0.62              |
| 1:A:447:ARG:HG3  | 1:A:447:ARG:HH11 | 1.65                     | 0.62              |
| 1:B:153:ILE:HG22 | 1:B:154:PRO:HD3  | 1.81                     | 0.62              |
| 1:A:153:ILE:HG22 | 1:A:154:PRO:HD3  | 1.81                     | 0.62              |
| 1:B:404:LEU:C    | 1:B:404:LEU:HD12 | 2.24                     | 0.62              |
| 1:A:404:LEU:HD12 | 1:A:404:LEU:C    | 2.24                     | 0.61              |
| 1:B:464:ALA:O    | 1:B:467:GLY:O    | 2.18                     | 0.61              |
| 1:B:343:GLU:HG3  | 1:B:347:MSE:HE1  | 1.82                     | 0.61              |
| 1:B:614:LEU:CD2  | 1:B:641:ILE:HD11 | 2.29                     | 0.61              |
| 1:A:563:ILE:O    | 1:A:563:ILE:CG2  | 2.47                     | 0.61              |
| 1:B:206:GLN:HB2  | 1:B:268:ARG:HG2  | 1.81                     | 0.61              |
| 1:B:55:ASN:ND2   | 1:B:88:ARG:NH2   | 2.49                     | 0.61              |
| 1:B:447:ARG:HG3  | 1:B:447:ARG:HH11 | 1.65                     | 0.61              |
| 1:A:74:ARG:HD2   | 1:A:507:ARG:HD2  | 1.83                     | 0.61              |
| 1:A:352:TRP:CH2  | 1:A:661:VAL:HG12 | 2.34                     | 0.61              |
| 1:A:464:ALA:O    | 1:A:467:GLY:O    | 2.18                     | 0.61              |
| 1:A:14:ALA:O     | 1:A:17:LEU:HB2   | 2.01                     | 0.61              |
| 1:A:21:ASN:ND2   | 1:A:21:ASN:C     | 2.57                     | 0.61              |
| 1:B:273:MSE:HE2  | 1:B:392:SER:CB   | 2.31                     | 0.61              |
| 1:A:55:ASN:ND2   | 1:A:88:ARG:NH2   | 2.49                     | 0.61              |
| 1:B:225:ARG:HG3  | 1:B:225:ARG:HH11 | 1.66                     | 0.60              |
| 1:A:361:LEU:O    | 1:A:362:LYS:HG2  | 2.01                     | 0.60              |
| 1:A:273:MSE:HE2  | 1:A:392:SER:CB   | 2.31                     | 0.60              |
| 1:B:14:ALA:O     | 1:B:17:LEU:HB2   | 2.01                     | 0.60              |
| 1:A:225:ARG:HG3  | 1:A:225:ARG:HH11 | 1.67                     | 0.60              |
| 1:B:361:LEU:O    | 1:B:362:LYS:HG2  | 2.01                     | 0.60              |
| 1:B:182:LEU:HG   | 1:B:355:LYS:HG3  | 1.84                     | 0.60              |
| 1:B:361:LEU:C    | 1:B:362:LYS:HG2  | 2.27                     | 0.60              |
| 1:A:602:VAL:CB   | 1:A:605:MSE:HG3  | 2.32                     | 0.60              |
| 1:B:74:ARG:HD2   | 1:B:507:ARG:HD2  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:17:LEU:O     | 1:B:153:ILE:O    | 2.20                     | 0.60              |
| 1:A:447:ARG:HG3  | 1:A:447:ARG:NH1  | 2.17                     | 0.60              |
| 1:B:447:ARG:HG3  | 1:B:447:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:320:CYS:SG   | 1:A:456:MSE:HG3  | 2.42                     | 0.59              |
| 1:A:343:GLU:HG3  | 1:A:347:MSE:HE1  | 1.82                     | 0.59              |
| 1:A:17:LEU:O     | 1:A:153:ILE:O    | 2.20                     | 0.59              |
| 1:A:182:LEU:HG   | 1:A:355:LYS:HG3  | 1.84                     | 0.59              |
| 1:A:361:LEU:C    | 1:A:362:LYS:HG2  | 2.27                     | 0.59              |
| 1:B:71:GLU:H     | 1:B:71:GLU:CD    | 2.11                     | 0.59              |
| 1:B:320:CYS:SG   | 1:B:456:MSE:HG3  | 2.42                     | 0.59              |
| 1:A:71:GLU:CD    | 1:A:71:GLU:H     | 2.11                     | 0.59              |
| 1:A:297:LYS:HG3  | 1:A:297:LYS:O    | 2.02                     | 0.59              |
| 1:A:552:ALA:HB3  | 1:A:619:LEU:HD13 | 1.83                     | 0.59              |
| 1:B:204:ARG:HD2  | 1:B:529:GLU:OE1  | 2.03                     | 0.59              |
| 1:B:552:ALA:HB3  | 1:B:619:LEU:HD13 | 1.83                     | 0.59              |
| 1:B:207:SER:HB2  | 1:B:527:SER:HB3  | 1.85                     | 0.59              |
| 1:A:204:ARG:HD2  | 1:A:529:GLU:OE1  | 2.03                     | 0.59              |
| 1:B:305:THR:OG1  | 1:B:306:THR:N    | 2.32                     | 0.59              |
| 1:B:287:ALA:O    | 1:B:291:ARG:HG3  | 2.03                     | 0.58              |
| 1:A:181:MSE:HG2  | 1:A:186:PHE:CD2  | 2.38                     | 0.58              |
| 1:A:207:SER:HB2  | 1:A:527:SER:HB3  | 1.85                     | 0.58              |
| 1:B:138:LEU:HB2  | 1:B:662:MSE:HE2  | 1.85                     | 0.58              |
| 1:A:563:ILE:HG23 | 1:A:566:ASP:HB2  | 1.86                     | 0.58              |
| 1:B:663:PRO:HG2  | 1:B:664:ARG:H    | 1.69                     | 0.58              |
| 1:B:297:LYS:O    | 1:B:297:LYS:HG3  | 2.02                     | 0.58              |
| 1:A:138:LEU:HB2  | 1:A:662:MSE:HE2  | 1.85                     | 0.58              |
| 1:A:217:THR:OG1  | 1:A:219:LYS:HG2  | 2.03                     | 0.58              |
| 1:A:88:ARG:HB2   | 1:A:211:ILE:HD13 | 1.86                     | 0.58              |
| 1:A:55:ASN:CG    | 1:A:88:ARG:HH22  | 2.12                     | 0.57              |
| 1:A:286:VAL:O    | 1:A:289:PRO:HD2  | 2.04                     | 0.57              |
| 1:A:287:ALA:O    | 1:A:291:ARG:HG3  | 2.03                     | 0.57              |
| 1:B:217:THR:OG1  | 1:B:219:LYS:HG2  | 2.03                     | 0.57              |
| 1:B:181:MSE:HG2  | 1:B:186:PHE:CD2  | 2.38                     | 0.57              |
| 1:B:300:TYR:HD1  | 1:B:301:THR:HG22 | 1.70                     | 0.57              |
| 1:B:563:ILE:HG23 | 1:B:566:ASP:HB2  | 1.86                     | 0.57              |
| 1:B:174:ALA:HA   | 1:B:195:MSE:HE1  | 1.87                     | 0.57              |
| 1:B:55:ASN:CG    | 1:B:88:ARG:HH22  | 2.12                     | 0.57              |
| 1:A:174:ALA:HA   | 1:A:195:MSE:HE1  | 1.87                     | 0.57              |
| 1:A:572:GLU:OE1  | 1:A:583:TYR:O    | 2.22                     | 0.57              |
| 1:B:336:LEU:O    | 1:B:340:ILE:HG13 | 2.05                     | 0.57              |
| 1:A:2:ARG:NH1    | 1:A:4:ALA:HB2    | 2.20                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:572:GLU:OE1  | 1:B:583:TYR:O    | 2.22                     | 0.57              |
| 1:B:286:VAL:O    | 1:B:289:PRO:HD2  | 2.04                     | 0.56              |
| 1:B:633:THR:HG22 | 1:B:636:ASP:OD2  | 2.05                     | 0.56              |
| 1:A:506:ARG:O    | 1:A:507:ARG:HB2  | 2.05                     | 0.56              |
| 1:B:2:ARG:NH1    | 1:B:4:ALA:HB2    | 2.20                     | 0.56              |
| 1:B:88:ARG:HB2   | 1:B:211:ILE:HD13 | 1.86                     | 0.56              |
| 1:B:91:ASN:O     | 1:B:267:GLU:CD   | 2.48                     | 0.56              |
| 1:A:91:ASN:O     | 1:A:267:GLU:CD   | 2.48                     | 0.56              |
| 1:A:563:ILE:CG2  | 1:A:567:VAL:HG23 | 2.28                     | 0.56              |
| 1:B:311:GLU:O    | 1:B:315:LYS:HB2  | 2.06                     | 0.56              |
| 1:B:506:ARG:O    | 1:B:507:ARG:HB2  | 2.05                     | 0.56              |
| 1:B:602:VAL:CB   | 1:B:605:MSE:HG3  | 2.32                     | 0.56              |
| 1:B:384:ASN:O    | 1:B:385:PRO:C    | 2.49                     | 0.56              |
| 1:A:633:THR:HG22 | 1:A:636:ASP:OD2  | 2.05                     | 0.56              |
| 1:B:615:THR:CG2  | 1:B:617:ILE:HB   | 2.36                     | 0.56              |
| 1:A:311:GLU:O    | 1:A:315:LYS:HB2  | 2.06                     | 0.56              |
| 1:A:336:LEU:O    | 1:A:340:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:615:THR:CG2  | 1:A:617:ILE:HB   | 2.36                     | 0.56              |
| 1:A:663:PRO:HG2  | 1:A:664:ARG:H    | 1.69                     | 0.56              |
| 1:B:339:LEU:HD23 | 1:B:339:LEU:C    | 2.31                     | 0.56              |
| 1:B:641:ILE:N    | 1:B:641:ILE:CD1  | 2.69                     | 0.56              |
| 1:A:339:LEU:C    | 1:A:339:LEU:HD23 | 2.31                     | 0.55              |
| 1:B:55:ASN:CG    | 1:B:88:ARG:NH2   | 2.65                     | 0.55              |
| 1:B:226:MSE:CE   | 1:B:244:ALA:HB2  | 2.36                     | 0.55              |
| 1:A:55:ASN:CG    | 1:A:88:ARG:NH2   | 2.65                     | 0.55              |
| 1:A:481:ASN:OD1  | 1:A:482:PRO:HD2  | 2.07                     | 0.55              |
| 1:A:55:ASN:ND2   | 1:A:59:ARG:CD    | 2.57                     | 0.55              |
| 1:A:226:MSE:CE   | 1:A:244:ALA:HB2  | 2.36                     | 0.55              |
| 1:A:573:ARG:HG2  | 1:A:573:ARG:HH11 | 1.72                     | 0.55              |
| 1:A:579:PHE:O    | 1:A:580:GLY:C    | 2.49                     | 0.55              |
| 1:A:633:THR:N    | 1:A:636:ASP:OD2  | 2.39                     | 0.55              |
| 1:A:300:TYR:HD1  | 1:A:301:THR:HG22 | 1.70                     | 0.55              |
| 1:A:325:VAL:HG13 | 1:A:453:ASP:HB2  | 1.88                     | 0.55              |
| 1:B:173:LYS:HG3  | 1:B:193:HIS:HE1  | 1.69                     | 0.55              |
| 1:B:348:GLY:O    | 1:B:349:TYR:O    | 2.25                     | 0.55              |
| 1:B:579:PHE:O    | 1:B:580:GLY:C    | 2.49                     | 0.55              |
| 1:A:641:ILE:N    | 1:A:641:ILE:CD1  | 2.69                     | 0.55              |
| 1:B:181:MSE:HG2  | 1:B:186:PHE:CE2  | 2.42                     | 0.55              |
| 1:A:83:ASN:C     | 1:A:83:ASN:ND2   | 2.53                     | 0.55              |
| 1:B:325:VAL:HG13 | 1:B:453:ASP:HB2  | 1.88                     | 0.55              |
| 1:B:481:ASN:OD1  | 1:B:482:PRO:HD2  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:301:THR:HB   | 1:B:448:GLN:O    | 2.08                     | 0.54              |
| 1:A:173:LYS:HG3  | 1:A:193:HIS:HE1  | 1.69                     | 0.54              |
| 1:A:251:ARG:HH11 | 1:A:255:GLN:NE2  | 2.05                     | 0.54              |
| 1:B:573:ARG:HG2  | 1:B:573:ARG:HH11 | 1.72                     | 0.54              |
| 1:A:181:MSE:HG2  | 1:A:186:PHE:CE2  | 2.42                     | 0.54              |
| 1:A:384:ASN:O    | 1:A:385:PRO:C    | 2.49                     | 0.54              |
| 1:A:406:MSE:O    | 1:A:407:SER:C    | 2.51                     | 0.54              |
| 1:B:55:ASN:ND2   | 1:B:59:ARG:CD    | 2.57                     | 0.54              |
| 1:B:537:ARG:CD   | 1:B:537:ARG:N    | 2.59                     | 0.54              |
| 1:B:606:ALA:O    | 1:B:609:ALA:N    | 2.40                     | 0.54              |
| 1:A:348:GLY:O    | 1:A:349:TYR:O    | 2.25                     | 0.54              |
| 1:A:606:ALA:HB3  | 1:A:609:ALA:HB2  | 1.89                     | 0.53              |
| 1:B:251:ARG:HH11 | 1:B:255:GLN:NE2  | 2.05                     | 0.53              |
| 1:B:291:ARG:HB3  | 1:B:295:TYR:CE2  | 2.44                     | 0.53              |
| 1:B:606:ALA:HB3  | 1:B:609:ALA:HB2  | 1.89                     | 0.53              |
| 1:A:301:THR:HB   | 1:A:448:GLN:O    | 2.08                     | 0.53              |
| 1:A:291:ARG:HB3  | 1:A:295:TYR:CE2  | 2.44                     | 0.53              |
| 1:B:563:ILE:O    | 1:B:564:TYR:C    | 2.51                     | 0.53              |
| 1:B:153:ILE:CD1  | 1:B:198:ALA:HB3  | 2.39                     | 0.53              |
| 1:B:615:THR:HG21 | 1:B:617:ILE:HB   | 1.91                     | 0.53              |
| 1:A:35:GLY:O     | 1:A:92:GLY:HA3   | 2.09                     | 0.53              |
| 1:A:413:MSE:HE1  | 1:A:488:ILE:HD13 | 1.91                     | 0.53              |
| 1:A:615:THR:HG21 | 1:A:617:ILE:HB   | 1.91                     | 0.53              |
| 1:B:206:GLN:HB2  | 1:B:268:ARG:CG   | 2.39                     | 0.53              |
| 1:A:153:ILE:CD1  | 1:A:198:ALA:HB3  | 2.39                     | 0.53              |
| 1:A:206:GLN:HB2  | 1:A:268:ARG:CG   | 2.39                     | 0.53              |
| 1:A:74:ARG:HB3   | 1:A:503:TYR:CD2  | 2.44                     | 0.52              |
| 1:A:3:ARG:O      | 1:A:4:ALA:HB3    | 2.09                     | 0.52              |
| 1:B:3:ARG:O      | 1:B:4:ALA:HB3    | 2.09                     | 0.52              |
| 1:B:300:TYR:CE2  | 1:B:313:LYS:HG2  | 2.45                     | 0.52              |
| 1:A:300:TYR:CE2  | 1:A:313:LYS:HG2  | 2.45                     | 0.52              |
| 1:B:406:MSE:O    | 1:B:407:SER:C    | 2.51                     | 0.52              |
| 1:B:563:ILE:CG2  | 1:B:567:VAL:HG23 | 2.28                     | 0.52              |
| 1:A:410:TYR:HA   | 1:A:413:MSE:CE   | 2.40                     | 0.52              |
| 1:B:100:TRP:CH2  | 1:B:367:VAL:HG21 | 2.44                     | 0.52              |
| 1:B:232:TYR:HA   | 1:B:239:GLN:O    | 2.10                     | 0.52              |
| 1:B:413:MSE:HE1  | 1:B:488:ILE:HD13 | 1.91                     | 0.52              |
| 1:B:1:PRO:O      | 1:B:2:ARG:HB3    | 2.09                     | 0.52              |
| 1:B:35:GLY:O     | 1:B:92:GLY:HA3   | 2.09                     | 0.52              |
| 1:A:1:PRO:O      | 1:A:2:ARG:HB3    | 2.09                     | 0.52              |
| 1:B:153:ILE:HG22 | 1:B:154:PRO:N    | 2.23                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:407:SER:CA   | 1:A:448:GLN:HE22 | 2.23                     | 0.52              |
| 1:B:74:ARG:HB3   | 1:B:503:TYR:CD2  | 2.44                     | 0.52              |
| 1:A:90:MSE:HE3   | 1:A:264:PHE:HD2  | 1.74                     | 0.51              |
| 1:A:232:TYR:HA   | 1:A:239:GLN:O    | 2.09                     | 0.51              |
| 1:A:153:ILE:HG22 | 1:A:154:PRO:N    | 2.23                     | 0.51              |
| 1:A:214:ASP:OD2  | 1:A:215:PRO:HD2  | 2.11                     | 0.51              |
| 1:A:614:LEU:HD21 | 1:A:641:ILE:HD11 | 1.93                     | 0.51              |
| 1:B:179:ASN:O    | 1:B:183:GLN:HG2  | 2.11                     | 0.51              |
| 1:B:286:VAL:C    | 1:B:289:PRO:HD2  | 2.36                     | 0.51              |
| 1:A:286:VAL:C    | 1:A:289:PRO:HD2  | 2.36                     | 0.51              |
| 1:B:410:TYR:HA   | 1:B:413:MSE:CE   | 2.40                     | 0.51              |
| 1:B:214:ASP:OD2  | 1:B:215:PRO:HD2  | 2.11                     | 0.51              |
| 1:B:209:ASP:O    | 1:B:209:ASP:OD1  | 2.29                     | 0.51              |
| 1:A:100:TRP:CH2  | 1:A:367:VAL:HG21 | 2.44                     | 0.51              |
| 1:A:404:LEU:C    | 1:A:404:LEU:CD1  | 2.84                     | 0.51              |
| 1:A:209:ASP:O    | 1:A:209:ASP:OD1  | 2.29                     | 0.50              |
| 1:A:563:ILE:O    | 1:A:564:TYR:C    | 2.51                     | 0.50              |
| 1:B:633:THR:N    | 1:B:636:ASP:OD2  | 2.39                     | 0.50              |
| 1:A:361:LEU:HD13 | 1:A:395:GLN:HG3  | 1.94                     | 0.50              |
| 1:B:83:ASN:C     | 1:B:83:ASN:ND2   | 2.53                     | 0.50              |
| 1:B:614:LEU:HD21 | 1:B:641:ILE:HD11 | 1.92                     | 0.50              |
| 1:A:304:HIS:HA   | 1:A:309:ASN:ND2  | 2.27                     | 0.50              |
| 1:B:449:ILE:O    | 1:B:449:ILE:HG13 | 2.12                     | 0.50              |
| 1:A:179:ASN:O    | 1:A:183:GLN:HG2  | 2.11                     | 0.50              |
| 1:B:126:LEU:O    | 1:B:127:PHE:C    | 2.54                     | 0.50              |
| 1:A:254:GLU:H    | 1:A:254:GLU:CD   | 2.20                     | 0.50              |
| 1:B:404:LEU:C    | 1:B:404:LEU:CD1  | 2.84                     | 0.50              |
| 1:A:126:LEU:O    | 1:A:127:PHE:C    | 2.54                     | 0.50              |
| 1:A:305:THR:OG1  | 1:A:306:THR:N    | 2.32                     | 0.50              |
| 1:B:361:LEU:HD13 | 1:B:395:GLN:HG3  | 1.94                     | 0.50              |
| 1:A:141:VAL:HB   | 1:A:142:PRO:HD2  | 1.94                     | 0.50              |
| 1:A:71:GLU:CD    | 1:A:71:GLU:N     | 2.70                     | 0.49              |
| 1:B:350:ALA:HB1  | 1:B:352:TRP:NE1  | 2.27                     | 0.49              |
| 1:A:12:ILE:O     | 1:A:16:MSE:HG2   | 2.13                     | 0.49              |
| 1:A:21:ASN:HD22  | 1:A:23:LYS:N     | 2.10                     | 0.49              |
| 1:A:251:ARG:HB2  | 1:A:255:GLN:HE21 | 1.77                     | 0.49              |
| 1:A:401:MSE:HE2  | 1:A:401:MSE:HA   | 1.94                     | 0.49              |
| 1:A:442:GLY:O    | 1:A:447:ARG:NE   | 2.46                     | 0.49              |
| 1:B:12:ILE:O     | 1:B:16:MSE:HG2   | 2.13                     | 0.49              |
| 1:B:21:ASN:HD21  | 1:B:24:ALA:N     | 2.04                     | 0.49              |
| 1:B:21:ASN:HD22  | 1:B:23:LYS:N     | 2.10                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:251:ARG:HB2  | 1:B:255:GLN:HE21 | 1.77                     | 0.49              |
| 1:B:404:LEU:C    | 1:B:405:LEU:O    | 2.52                     | 0.49              |
| 1:A:40:TYR:O     | 1:A:41:GLU:C     | 2.56                     | 0.49              |
| 1:B:401:MSE:HE2  | 1:B:401:MSE:HA   | 1.94                     | 0.49              |
| 1:B:407:SER:CA   | 1:B:448:GLN:HE22 | 2.23                     | 0.49              |
| 1:B:442:GLY:O    | 1:B:447:ARG:NE   | 2.46                     | 0.49              |
| 1:A:288:GLN:HB3  | 1:A:289:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:305:THR:HG1  | 1:A:306:THR:H    | 1.56                     | 0.49              |
| 1:B:304:HIS:HA   | 1:B:309:ASN:ND2  | 2.27                     | 0.49              |
| 1:A:304:HIS:HA   | 1:A:309:ASN:HD21 | 1.77                     | 0.49              |
| 1:A:21:ASN:HD21  | 1:A:24:ALA:N     | 2.04                     | 0.49              |
| 1:A:75:VAL:HG21  | 1:A:500:ILE:HG21 | 1.94                     | 0.49              |
| 1:A:350:ALA:HB1  | 1:A:352:TRP:NE1  | 2.27                     | 0.49              |
| 1:A:201:VAL:HG23 | 1:A:365:VAL:HG13 | 1.93                     | 0.49              |
| 1:A:449:ILE:HG13 | 1:A:449:ILE:O    | 2.12                     | 0.49              |
| 1:A:506:ARG:HG3  | 1:A:506:ARG:HH11 | 1.78                     | 0.49              |
| 1:B:71:GLU:CD    | 1:B:71:GLU:N     | 2.70                     | 0.49              |
| 1:B:622:LEU:HD21 | 1:B:641:ILE:HG23 | 1.95                     | 0.49              |
| 1:A:173:LYS:CG   | 1:A:193:HIS:CE1  | 2.94                     | 0.49              |
| 1:A:405:LEU:O    | 1:A:406:MSE:CB   | 2.56                     | 0.49              |
| 1:B:182:LEU:HD21 | 1:B:355:LYS:HG2  | 1.94                     | 0.49              |
| 1:A:95:MSE:SE    | 1:A:268:ARG:HA   | 2.63                     | 0.48              |
| 1:A:248:ASP:O    | 1:A:249:ALA:CB   | 2.61                     | 0.48              |
| 1:B:254:GLU:CD   | 1:B:254:GLU:H    | 2.20                     | 0.48              |
| 1:B:201:VAL:HG23 | 1:B:365:VAL:HG13 | 1.93                     | 0.48              |
| 1:B:288:GLN:HB3  | 1:B:289:PRO:HD3  | 1.94                     | 0.48              |
| 1:B:40:TYR:O     | 1:B:41:GLU:C     | 2.56                     | 0.48              |
| 1:A:182:LEU:HD21 | 1:A:355:LYS:HG2  | 1.94                     | 0.48              |
| 1:A:622:LEU:HD21 | 1:A:641:ILE:HG23 | 1.95                     | 0.48              |
| 1:B:78:ASN:C     | 1:B:78:ASN:ND2   | 2.65                     | 0.48              |
| 1:B:304:HIS:HA   | 1:B:309:ASN:HD21 | 1.77                     | 0.48              |
| 1:A:78:ASN:ND2   | 1:A:78:ASN:C     | 2.65                     | 0.48              |
| 1:B:327:ASP:O    | 1:B:328:HIS:C    | 2.57                     | 0.48              |
| 1:B:506:ARG:HG3  | 1:B:506:ARG:HH11 | 1.77                     | 0.48              |
| 1:A:606:ALA:O    | 1:A:609:ALA:N    | 2.40                     | 0.48              |
| 1:B:504:ASP:OD2  | 1:B:506:ARG:HB2  | 2.14                     | 0.48              |
| 1:B:532:VAL:O    | 1:B:532:VAL:CG2  | 2.61                     | 0.48              |
| 1:A:504:ASP:OD2  | 1:A:506:ARG:HB2  | 2.14                     | 0.48              |
| 1:B:75:VAL:HG21  | 1:B:500:ILE:HG21 | 1.94                     | 0.48              |
| 1:B:117:GLY:HA2  | 1:B:335:TRP:CD2  | 2.49                     | 0.48              |
| 1:B:141:VAL:HB   | 1:B:142:PRO:HD2  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:532:VAL:O    | 1:A:532:VAL:CG2  | 2.61                     | 0.48              |
| 1:A:603:ALA:O    | 1:A:604:SER:HB3  | 2.14                     | 0.48              |
| 1:B:579:PHE:C    | 1:B:581:GLU:N    | 2.68                     | 0.48              |
| 1:B:260:VAL:CG2  | 1:B:260:VAL:O    | 2.62                     | 0.47              |
| 1:B:281:ALA:HB3  | 1:B:282:PRO:CD   | 2.44                     | 0.47              |
| 1:B:603:ALA:O    | 1:B:604:SER:HB3  | 2.14                     | 0.47              |
| 1:A:260:VAL:O    | 1:A:260:VAL:CG2  | 2.62                     | 0.47              |
| 1:B:95:MSE:SE    | 1:B:268:ARG:HA   | 2.63                     | 0.47              |
| 1:A:117:GLY:HA2  | 1:A:335:TRP:CD2  | 2.49                     | 0.47              |
| 1:A:288:GLN:N    | 1:A:289:PRO:CD   | 2.78                     | 0.47              |
| 1:B:405:LEU:O    | 1:B:406:MSE:CB   | 2.56                     | 0.47              |
| 1:A:91:ASN:O     | 1:A:267:GLU:OE2  | 2.32                     | 0.47              |
| 1:A:225:ARG:HD2  | 1:A:225:ARG:HA   | 1.66                     | 0.47              |
| 1:A:228:ALA:HB1  | 1:A:232:TYR:HB3  | 1.97                     | 0.47              |
| 1:A:327:ASP:O    | 1:A:328:HIS:C    | 2.57                     | 0.47              |
| 1:A:602:VAL:O    | 1:A:604:SER:N    | 2.48                     | 0.47              |
| 1:B:21:ASN:HD22  | 1:B:22:ILE:N     | 2.13                     | 0.47              |
| 1:B:91:ASN:O     | 1:B:267:GLU:OE2  | 2.32                     | 0.47              |
| 1:B:347:MSE:HB3  | 1:B:347:MSE:HE2  | 1.75                     | 0.47              |
| 1:B:602:VAL:O    | 1:B:604:SER:N    | 2.48                     | 0.47              |
| 1:A:647:HIS:ND1  | 1:A:648:GLY:N    | 2.63                     | 0.47              |
| 1:B:286:VAL:HG21 | 1:B:353:TRP:CZ2  | 2.50                     | 0.47              |
| 1:B:361:LEU:C    | 1:B:362:LYS:CG   | 2.88                     | 0.47              |
| 1:B:406:MSE:HA   | 1:B:409:THR:HB   | 1.97                     | 0.47              |
| 1:A:21:ASN:HD22  | 1:A:22:ILE:N     | 2.13                     | 0.46              |
| 1:A:281:ALA:HB3  | 1:A:282:PRO:CD   | 2.44                     | 0.46              |
| 1:B:597:GLU:O    | 1:B:598:LEU:C    | 2.57                     | 0.46              |
| 1:A:406:MSE:HA   | 1:A:409:THR:HB   | 1.97                     | 0.46              |
| 1:A:286:VAL:HG21 | 1:A:353:TRP:CZ2  | 2.50                     | 0.46              |
| 1:A:410:TYR:HD1  | 1:A:413:MSE:CE   | 2.28                     | 0.46              |
| 1:B:173:LYS:CG   | 1:B:193:HIS:CE1  | 2.94                     | 0.46              |
| 1:A:334:GLY:O    | 1:A:337:ARG:HB3  | 2.16                     | 0.46              |
| 1:A:579:PHE:C    | 1:A:581:GLU:N    | 2.68                     | 0.46              |
| 1:B:288:GLN:N    | 1:B:289:PRO:CD   | 2.78                     | 0.46              |
| 1:B:401:MSE:HE2  | 1:B:401:MSE:N    | 2.31                     | 0.46              |
| 1:B:407:SER:CB   | 1:B:448:GLN:HE22 | 2.29                     | 0.46              |
| 1:A:153:ILE:HD12 | 1:A:198:ALA:HB3  | 1.98                     | 0.46              |
| 1:A:624:ASP:O    | 1:A:626:ASN:O    | 2.34                     | 0.46              |
| 1:B:228:ALA:HB1  | 1:B:232:TYR:HB3  | 1.97                     | 0.46              |
| 1:A:17:LEU:HD12  | 1:A:17:LEU:HA    | 1.69                     | 0.46              |
| 1:A:128:ARG:HG3  | 1:A:339:LEU:HD21 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:361:LEU:C    | 1:A:362:LYS:CG   | 2.88                     | 0.46              |
| 1:B:647:HIS:ND1  | 1:B:648:GLY:N    | 2.63                     | 0.46              |
| 1:B:334:GLY:O    | 1:B:337:ARG:HB3  | 2.16                     | 0.46              |
| 1:B:410:TYR:HD1  | 1:B:413:MSE:CE   | 2.28                     | 0.46              |
| 1:A:34:GLU:OE1   | 1:A:251:ARG:NH2  | 2.42                     | 0.46              |
| 1:A:136:SER:OG   | 1:A:293:LYS:NZ   | 2.49                     | 0.46              |
| 1:A:347:MSE:HE2  | 1:A:347:MSE:HB3  | 1.75                     | 0.46              |
| 1:B:90:MSE:HE3   | 1:B:264:PHE:HD2  | 1.74                     | 0.46              |
| 1:B:128:ARG:HG3  | 1:B:339:LEU:HD21 | 1.98                     | 0.46              |
| 1:A:44:LEU:HD12  | 1:A:44:LEU:HA    | 1.64                     | 0.46              |
| 1:A:407:SER:CB   | 1:A:448:GLN:HE22 | 2.29                     | 0.46              |
| 1:A:3:ARG:HH22   | 1:A:231:GLU:CD   | 2.24                     | 0.45              |
| 1:A:343:GLU:OE1  | 1:A:343:GLU:HA   | 2.15                     | 0.45              |
| 1:A:401:MSE:HE2  | 1:A:401:MSE:N    | 2.31                     | 0.45              |
| 1:A:606:ALA:O    | 1:A:607:ARG:C    | 2.59                     | 0.45              |
| 1:B:343:GLU:OE1  | 1:B:343:GLU:HA   | 2.15                     | 0.45              |
| 1:B:606:ALA:O    | 1:B:607:ARG:C    | 2.59                     | 0.45              |
| 1:A:400:LEU:HA   | 1:A:400:LEU:HD12 | 1.67                     | 0.45              |
| 1:B:602:VAL:CG1  | 1:B:605:MSE:HG3  | 2.47                     | 0.45              |
| 1:A:78:ASN:HD21  | 1:A:80:VAL:H     | 1.62                     | 0.45              |
| 1:A:99:THR:HA    | 1:A:227:VAL:HB   | 1.99                     | 0.45              |
| 1:A:475:LEU:HD21 | 1:A:482:PRO:HG3  | 1.98                     | 0.45              |
| 1:B:343:GLU:HG3  | 1:B:347:MSE:HE2  | 1.98                     | 0.45              |
| 1:A:55:ASN:ND2   | 1:A:55:ASN:C     | 2.68                     | 0.45              |
| 1:B:99:THR:HA    | 1:B:227:VAL:HB   | 1.99                     | 0.45              |
| 1:B:248:ASP:O    | 1:B:249:ALA:CB   | 2.61                     | 0.45              |
| 1:B:400:LEU:HD12 | 1:B:400:LEU:HA   | 1.67                     | 0.45              |
| 1:A:21:ASN:ND2   | 1:A:23:LYS:N     | 2.64                     | 0.45              |
| 1:A:597:GLU:O    | 1:A:598:LEU:C    | 2.57                     | 0.45              |
| 1:B:136:SER:OG   | 1:B:293:LYS:NZ   | 2.49                     | 0.45              |
| 1:A:182:LEU:CD2  | 1:A:355:LYS:HG2  | 2.47                     | 0.45              |
| 1:A:404:LEU:C    | 1:A:405:LEU:O    | 2.52                     | 0.45              |
| 1:A:536:VAL:HG22 | 1:A:542:ARG:HG3  | 1.98                     | 0.45              |
| 1:A:664:ARG:HA   | 1:A:664:ARG:NE   | 2.32                     | 0.45              |
| 1:B:21:ASN:ND2   | 1:B:23:LYS:N     | 2.64                     | 0.45              |
| 1:B:475:LEU:HD21 | 1:B:482:PRO:HG3  | 1.98                     | 0.45              |
| 1:B:536:VAL:HG22 | 1:B:542:ARG:HG3  | 1.98                     | 0.45              |
| 1:A:533:GLN:HB3  | 1:A:536:VAL:CG1  | 2.47                     | 0.45              |
| 1:B:117:GLY:O    | 1:B:118:PRO:C    | 2.59                     | 0.45              |
| 1:B:182:LEU:CD2  | 1:B:355:LYS:HG2  | 2.47                     | 0.45              |
| 1:B:624:ASP:O    | 1:B:626:ASN:O    | 2.34                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:664:ARG:HA   | 1:B:664:ARG:NE   | 2.32                     | 0.45              |
| 1:A:102:LEU:HD12 | 1:A:233:ALA:HA   | 1.99                     | 0.45              |
| 1:A:529:GLU:HG2  | 1:A:530:TYR:CD1  | 2.52                     | 0.45              |
| 1:B:153:ILE:HD12 | 1:B:198:ALA:HB3  | 1.98                     | 0.45              |
| 1:B:658:LEU:HD23 | 1:B:658:LEU:HA   | 1.66                     | 0.45              |
| 1:A:182:LEU:CD2  | 1:A:355:LYS:CG   | 2.95                     | 0.45              |
| 1:A:225:ARG:NH2  | 1:A:268:ARG:NH1  | 2.65                     | 0.45              |
| 1:A:602:VAL:CG1  | 1:A:605:MSE:HG3  | 2.47                     | 0.45              |
| 1:A:422:LEU:HA   | 1:A:422:LEU:HD23 | 1.82                     | 0.45              |
| 1:B:34:GLU:OE1   | 1:B:251:ARG:NH2  | 2.42                     | 0.45              |
| 1:B:51:LEU:HD21  | 1:B:90:MSE:HE1   | 1.97                     | 0.45              |
| 1:B:225:ARG:NH2  | 1:B:268:ARG:NH1  | 2.65                     | 0.45              |
| 1:B:529:GLU:HG2  | 1:B:530:TYR:CD1  | 2.52                     | 0.45              |
| 1:A:273:MSE:HE2  | 1:A:392:SER:OG   | 2.18                     | 0.44              |
| 1:B:182:LEU:CD2  | 1:B:355:LYS:CG   | 2.95                     | 0.44              |
| 1:B:226:MSE:HA   | 1:B:243:PHE:O    | 2.17                     | 0.44              |
| 1:B:273:MSE:HE2  | 1:B:392:SER:OG   | 2.18                     | 0.44              |
| 1:B:428:ASP:OD1  | 1:B:430:PRO:HD2  | 2.17                     | 0.44              |
| 1:A:225:ARG:HG3  | 1:A:225:ARG:NH1  | 2.32                     | 0.44              |
| 1:A:226:MSE:HA   | 1:A:243:PHE:O    | 2.17                     | 0.44              |
| 1:A:138:LEU:HG   | 1:A:662:MSE:CE   | 2.48                     | 0.44              |
| 1:A:568:LEU:HD23 | 1:A:568:LEU:HA   | 1.87                     | 0.44              |
| 1:B:78:ASN:HD21  | 1:B:80:VAL:H     | 1.62                     | 0.44              |
| 1:B:587:ARG:HD2  | 1:B:587:ARG:HA   | 1.72                     | 0.44              |
| 1:B:134:MSE:SE   | 1:B:404:LEU:HD22 | 2.68                     | 0.44              |
| 1:B:1:PRO:O      | 1:B:2:ARG:CB     | 2.66                     | 0.44              |
| 1:B:533:GLN:HB3  | 1:B:536:VAL:CG1  | 2.47                     | 0.44              |
| 1:A:428:ASP:OD1  | 1:A:430:PRO:HD2  | 2.18                     | 0.44              |
| 1:B:3:ARG:HH22   | 1:B:231:GLU:CD   | 2.24                     | 0.44              |
| 1:B:138:LEU:HG   | 1:B:662:MSE:CE   | 2.48                     | 0.44              |
| 1:B:355:LYS:HE2  | 1:B:358:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:1:PRO:O      | 1:A:2:ARG:CB     | 2.66                     | 0.44              |
| 1:A:615:THR:O    | 1:A:618:ASP:HB2  | 2.18                     | 0.44              |
| 1:B:225:ARG:HG3  | 1:B:225:ARG:NH1  | 2.32                     | 0.43              |
| 1:A:355:LYS:HE2  | 1:A:358:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:554:MSE:HE3  | 1:A:554:MSE:HB3  | 1.80                     | 0.43              |
| 1:B:225:ARG:NH1  | 1:B:268:ARG:NH2  | 2.66                     | 0.43              |
| 1:B:268:ARG:NH2  | 1:B:270:ARG:HE   | 2.16                     | 0.43              |
| 1:B:305:THR:HG1  | 1:B:306:THR:H    | 1.60                     | 0.43              |
| 1:B:484:PRO:HG2  | 1:B:485:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:173:LYS:O    | 1:A:174:ALA:C    | 2.61                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:268:ARG:NH2  | 1:A:270:ARG:HE   | 2.16                     | 0.43              |
| 1:A:628:LEU:HA   | 1:A:628:LEU:HD12 | 1.54                     | 0.43              |
| 1:B:225:ARG:HH12 | 1:B:268:ARG:NH2  | 2.16                     | 0.43              |
| 1:B:265:PHE:CD1  | 1:B:265:PHE:N    | 2.86                     | 0.43              |
| 1:B:280:ASN:O    | 1:B:284:MSE:HG3  | 2.18                     | 0.43              |
| 1:A:407:SER:HA   | 1:A:448:GLN:NE2  | 2.30                     | 0.43              |
| 1:B:39:THR:HG22  | 1:B:40:TYR:CD2   | 2.53                     | 0.43              |
| 1:B:102:LEU:HD12 | 1:B:233:ALA:HA   | 1.99                     | 0.43              |
| 1:A:86:GLY:O     | 1:A:89:HIS:CD2   | 2.72                     | 0.43              |
| 1:A:484:PRO:HG2  | 1:A:485:TYR:CE2  | 2.53                     | 0.43              |
| 1:B:44:LEU:HA    | 1:B:44:LEU:HD12  | 1.64                     | 0.43              |
| 1:B:268:ARG:HH22 | 1:B:270:ARG:HH21 | 1.67                     | 0.43              |
| 1:B:524:ASN:HD21 | 1:B:627:LYS:NZ   | 2.16                     | 0.43              |
| 1:A:268:ARG:HH22 | 1:A:270:ARG:HH21 | 1.67                     | 0.43              |
| 1:A:280:ASN:O    | 1:A:284:MSE:HG3  | 2.18                     | 0.43              |
| 1:B:51:LEU:HD13  | 1:B:261:PRO:HD2  | 2.01                     | 0.43              |
| 1:B:146:ARG:O    | 1:B:149:SER:HB3  | 2.19                     | 0.43              |
| 1:B:155:TYR:O    | 1:B:156:PHE:C    | 2.61                     | 0.43              |
| 1:A:65:PHE:CD1   | 1:A:563:ILE:HD13 | 2.54                     | 0.43              |
| 1:A:117:GLY:O    | 1:A:118:PRO:C    | 2.59                     | 0.43              |
| 1:A:401:MSE:HE2  | 1:A:401:MSE:CA   | 2.49                     | 0.43              |
| 1:A:65:PHE:CD1   | 1:A:563:ILE:CD1  | 3.02                     | 0.43              |
| 1:A:524:ASN:HD21 | 1:A:627:LYS:NZ   | 2.16                     | 0.43              |
| 1:B:471:LEU:O    | 1:B:474:MSE:HB3  | 2.19                     | 0.43              |
| 1:B:615:THR:O    | 1:B:618:ASP:HB2  | 2.18                     | 0.43              |
| 1:A:225:ARG:NH1  | 1:A:268:ARG:NH2  | 2.66                     | 0.42              |
| 1:A:39:THR:HG22  | 1:A:40:TYR:CD2   | 2.53                     | 0.42              |
| 1:A:517:ASN:C    | 1:A:517:ASN:OD1  | 2.61                     | 0.42              |
| 1:A:533:GLN:O    | 1:A:536:VAL:HG13 | 2.19                     | 0.42              |
| 1:B:61:LEU:O     | 1:B:62:THR:C     | 2.62                     | 0.42              |
| 1:A:146:ARG:O    | 1:A:149:SER:HB3  | 2.19                     | 0.42              |
| 1:A:265:PHE:N    | 1:A:265:PHE:CD1  | 2.86                     | 0.42              |
| 1:B:86:GLY:O     | 1:B:89:HIS:CD2   | 2.72                     | 0.42              |
| 1:B:336:LEU:CD2  | 1:B:405:LEU:HB2  | 2.50                     | 0.42              |
| 1:A:51:LEU:HD13  | 1:A:261:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:134:MSE:SE   | 1:A:404:LEU:HD22 | 2.68                     | 0.42              |
| 1:A:225:ARG:HH12 | 1:A:268:ARG:NH2  | 2.16                     | 0.42              |
| 1:B:116:ASP:O    | 1:B:335:TRP:CD1  | 2.73                     | 0.42              |
| 1:B:407:SER:HA   | 1:B:448:GLN:NE2  | 2.30                     | 0.42              |
| 1:B:533:GLN:O    | 1:B:536:VAL:HG13 | 2.19                     | 0.42              |
| 1:B:573:ARG:HG2  | 1:B:573:ARG:NH1  | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:61:LEU:O     | 1:A:62:THR:C     | 2.62                     | 0.42              |
| 1:A:138:LEU:CB   | 1:A:662:MSE:HE2  | 2.49                     | 0.42              |
| 1:A:336:LEU:CD2  | 1:A:405:LEU:HB2  | 2.50                     | 0.42              |
| 1:B:65:PHE:CD1   | 1:B:563:ILE:HD13 | 2.54                     | 0.42              |
| 1:A:311:GLU:O    | 1:A:312:GLU:C    | 2.63                     | 0.42              |
| 1:A:419:ALA:O    | 1:A:420:PRO:C    | 2.63                     | 0.42              |
| 1:A:553:SER:O    | 1:A:554:MSE:C    | 2.63                     | 0.42              |
| 1:B:364:PRO:HA   | 1:B:387:LEU:CD2  | 2.36                     | 0.42              |
| 1:A:116:ASP:O    | 1:A:335:TRP:CD1  | 2.73                     | 0.42              |
| 1:A:308:LEU:N    | 1:A:308:LEU:CD1  | 2.82                     | 0.42              |
| 1:B:91:ASN:C     | 1:B:93:PHE:H     | 2.27                     | 0.42              |
| 1:A:15:GLN:C     | 1:A:17:LEU:N     | 2.78                     | 0.42              |
| 1:B:419:ALA:O    | 1:B:420:PRO:C    | 2.63                     | 0.42              |
| 1:B:615:THR:HG22 | 1:B:617:ILE:HB   | 2.02                     | 0.42              |
| 1:A:445:GLU:OE2  | 1:A:464:ALA:N    | 2.34                     | 0.42              |
| 1:B:55:ASN:ND2   | 1:B:88:ARG:HH22  | 2.18                     | 0.42              |
| 1:B:82:THR:OG1   | 1:B:83:ASN:N     | 2.53                     | 0.42              |
| 1:B:173:LYS:O    | 1:B:174:ALA:C    | 2.61                     | 0.42              |
| 1:A:155:TYR:O    | 1:A:156:PHE:C    | 2.61                     | 0.41              |
| 1:A:471:LEU:O    | 1:A:474:MSE:HB3  | 2.19                     | 0.41              |
| 1:A:553:SER:HB3  | 1:A:619:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:597:GLU:O    | 1:A:600:ARG:HG3  | 2.20                     | 0.41              |
| 1:B:65:PHE:CD1   | 1:B:563:ILE:CD1  | 3.02                     | 0.41              |
| 1:B:311:GLU:O    | 1:B:312:GLU:C    | 2.63                     | 0.41              |
| 1:A:91:ASN:C     | 1:A:93:PHE:H     | 2.27                     | 0.41              |
| 1:B:72:TYR:CZ    | 1:B:476:LYS:HD3  | 2.55                     | 0.41              |
| 1:B:138:LEU:CB   | 1:B:662:MSE:HE2  | 2.49                     | 0.41              |
| 1:B:517:ASN:OD1  | 1:B:517:ASN:C    | 2.61                     | 0.41              |
| 1:B:628:LEU:HD12 | 1:B:628:LEU:HA   | 1.54                     | 0.41              |
| 1:A:51:LEU:HD22  | 1:A:90:MSE:CE    | 2.43                     | 0.41              |
| 1:A:82:THR:OG1   | 1:A:83:ASN:N     | 2.53                     | 0.41              |
| 1:A:557:THR:HG22 | 1:A:558:TYR:CD2  | 2.56                     | 0.41              |
| 1:B:597:GLU:O    | 1:B:600:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:213:LEU:C    | 1:A:213:LEU:CD2  | 2.94                     | 0.41              |
| 1:A:268:ARG:CZ   | 1:A:270:ARG:HE   | 2.34                     | 0.41              |
| 1:A:573:ARG:HG2  | 1:A:573:ARG:NH1  | 2.34                     | 0.41              |
| 1:A:617:ILE:HG23 | 1:A:632:TRP:CE3  | 2.56                     | 0.41              |
| 1:B:15:GLN:C     | 1:B:17:LEU:N     | 2.78                     | 0.41              |
| 1:B:401:MSE:HE2  | 1:B:401:MSE:CA   | 2.49                     | 0.41              |
| 1:B:410:TYR:HD1  | 1:B:413:MSE:HE1  | 1.86                     | 0.41              |
| 1:B:617:ILE:HG23 | 1:B:632:TRP:CE3  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:658:LEU:HD23 | 1:A:658:LEU:HA   | 1.66                     | 0.41              |
| 1:B:90:MSE:HA    | 1:B:90:MSE:HE2   | 2.03                     | 0.41              |
| 1:B:445:GLU:OE2  | 1:B:464:ALA:N    | 2.34                     | 0.41              |
| 1:A:90:MSE:HE2   | 1:A:90:MSE:HA    | 2.03                     | 0.41              |
| 1:A:273:MSE:HE2  | 1:A:392:SER:HB3  | 2.03                     | 0.41              |
| 1:A:344:LEU:HA   | 1:A:347:MSE:HE3  | 2.02                     | 0.41              |
| 1:B:350:ALA:HB1  | 1:B:352:TRP:CE2  | 2.56                     | 0.41              |
| 1:B:553:SER:HB3  | 1:B:619:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:65:PHE:CG    | 1:A:563:ILE:HD13 | 2.56                     | 0.41              |
| 1:A:213:LEU:C    | 1:A:213:LEU:HD23 | 2.46                     | 0.41              |
| 1:A:289:PRO:O    | 1:A:290:VAL:C    | 2.61                     | 0.41              |
| 1:A:337:ARG:CZ   | 1:A:362:LYS:HD2  | 2.51                     | 0.41              |
| 1:B:94:PRO:HB2   | 1:B:269:ARG:HG3  | 2.02                     | 0.41              |
| 1:B:268:ARG:CZ   | 1:B:270:ARG:HE   | 2.34                     | 0.41              |
| 1:B:289:PRO:O    | 1:B:290:VAL:C    | 2.61                     | 0.41              |
| 1:B:337:ARG:CZ   | 1:B:362:LYS:HD2  | 2.51                     | 0.41              |
| 1:B:554:MSE:HE3  | 1:B:554:MSE:HB3  | 1.80                     | 0.41              |
| 1:B:557:THR:HG22 | 1:B:558:TYR:CD2  | 2.56                     | 0.41              |
| 1:A:3:ARG:HH11   | 1:A:3:ARG:HD3    | 1.72                     | 0.41              |
| 1:A:655:GLU:HG2  | 1:A:659:ARG:NH1  | 2.36                     | 0.41              |
| 1:B:3:ARG:O      | 1:B:3:ARG:CG     | 2.66                     | 0.41              |
| 1:B:213:LEU:C    | 1:B:213:LEU:HD23 | 2.45                     | 0.41              |
| 1:B:254:GLU:CD   | 1:B:254:GLU:N    | 2.79                     | 0.41              |
| 1:B:344:LEU:HA   | 1:B:347:MSE:HE3  | 2.02                     | 0.41              |
| 1:B:449:ILE:HD12 | 1:B:496:PHE:CD2  | 2.56                     | 0.41              |
| 1:B:598:LEU:O    | 1:B:598:LEU:HD12 | 2.21                     | 0.41              |
| 1:A:587:ARG:HA   | 1:A:587:ARG:HD2  | 1.72                     | 0.40              |
| 1:B:17:LEU:HA    | 1:B:17:LEU:HD12  | 1.69                     | 0.40              |
| 1:B:369:ALA:HA   | 1:B:370:PRO:HD2  | 1.87                     | 0.40              |
| 1:B:655:GLU:HG2  | 1:B:659:ARG:NH1  | 2.36                     | 0.40              |
| 1:B:655:GLU:O    | 1:B:656:ARG:C    | 2.64                     | 0.40              |
| 1:A:72:TYR:CZ    | 1:A:476:LYS:HD3  | 2.55                     | 0.40              |
| 1:A:350:ALA:HB1  | 1:A:352:TRP:CE2  | 2.56                     | 0.40              |
| 1:A:410:TYR:HD1  | 1:A:413:MSE:HE1  | 1.86                     | 0.40              |
| 1:B:96:ILE:HA    | 1:B:97:PRO:HA    | 1.80                     | 0.40              |
| 1:B:281:ALA:O    | 1:B:282:PRO:C    | 2.64                     | 0.40              |
| 1:B:286:VAL:HG21 | 1:B:353:TRP:CE2  | 2.56                     | 0.40              |
| 1:B:568:LEU:HD23 | 1:B:568:LEU:HA   | 1.87                     | 0.40              |
| 1:B:630:TYR:CD1  | 1:B:630:TYR:C    | 2.99                     | 0.40              |
| 1:B:579:PHE:CB   | 1:B:581:GLU:HB2  | 2.51                     | 0.40              |
| 1:A:3:ARG:O      | 1:A:3:ARG:CG     | 2.66                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:43:LEU:HD22 | 1:A:44:LEU:N    | 2.36                     | 0.40              |
| 1:A:68:ASN:HB3  | 1:A:76:TYR:CE1  | 2.57                     | 0.40              |
| 1:A:378:LEU:C   | 1:A:378:LEU:CD2 | 2.94                     | 0.40              |
| 1:A:575:TRP:CG  | 1:A:583:TYR:HB2 | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 1   | A     | 561/664 (84%)   | 490 (87%)  | 54 (10%) | 17 (3%)  | 3           | 5 |
| 1   | B     | 662/664 (100%)  | 586 (88%)  | 58 (9%)  | 18 (3%)  | 4           | 6 |
| All | All   | 1223/1328 (92%) | 1076 (88%) | 112 (9%) | 35 (3%)  | 3           | 5 |

All (35) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 91  | ASN  |
| 1   | A     | 149 | SER  |
| 1   | A     | 349 | TYR  |
| 1   | A     | 375 | GLY  |
| 1   | A     | 584 | ARG  |
| 1   | A     | 604 | SER  |
| 1   | A     | 607 | ARG  |
| 1   | B     | 91  | ASN  |
| 1   | B     | 149 | SER  |
| 1   | B     | 210 | ALA  |
| 1   | B     | 349 | TYR  |
| 1   | B     | 375 | GLY  |
| 1   | B     | 584 | ARG  |
| 1   | B     | 604 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 607 | ARG  |
| 1   | A     | 92  | GLY  |
| 1   | A     | 153 | ILE  |
| 1   | A     | 627 | LYS  |
| 1   | B     | 92  | GLY  |
| 1   | B     | 153 | ILE  |
| 1   | B     | 627 | LYS  |
| 1   | A     | 2   | ARG  |
| 1   | A     | 538 | ASP  |
| 1   | A     | 564 | TYR  |
| 1   | A     | 612 | ALA  |
| 1   | A     | 630 | TYR  |
| 1   | B     | 2   | ARG  |
| 1   | B     | 538 | ASP  |
| 1   | B     | 564 | TYR  |
| 1   | B     | 612 | ALA  |
| 1   | B     | 630 | TYR  |
| 1   | A     | 4   | ALA  |
| 1   | A     | 154 | PRO  |
| 1   | B     | 4   | ALA  |
| 1   | B     | 154 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric | Outliers  | Percentiles |   |
|-----|-------|------------------|-----------|-----------|-------------|---|
| 1   | A     | 557/532 (105%)   | 482 (86%) | 75 (14%)  | 4           | 8 |
| 1   | B     | 557/532 (105%)   | 482 (86%) | 75 (14%)  | 4           | 8 |
| All | All   | 1114/1064 (105%) | 964 (86%) | 150 (14%) | 4           | 8 |

All (150) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | LEU  |
| 1   | A     | 16  | MSE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | LEU  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 22  | ILE  |
| 1   | A     | 37  | ILE  |
| 1   | A     | 41  | GLU  |
| 1   | A     | 43  | LEU  |
| 1   | A     | 44  | LEU  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 63  | ASP  |
| 1   | A     | 75  | VAL  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 94  | PRO  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 119 | VAL  |
| 1   | A     | 139 | GLU  |
| 1   | A     | 146 | ARG  |
| 1   | A     | 151 | THR  |
| 1   | A     | 153 | ILE  |
| 1   | A     | 157 | SER  |
| 1   | A     | 159 | ASP  |
| 1   | A     | 165 | GLU  |
| 1   | A     | 173 | LYS  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 192 | LEU  |
| 1   | A     | 212 | THR  |
| 1   | A     | 213 | LEU  |
| 1   | A     | 221 | VAL  |
| 1   | A     | 225 | ARG  |
| 1   | A     | 239 | GLN  |
| 1   | A     | 250 | SER  |
| 1   | A     | 254 | GLU  |
| 1   | A     | 260 | VAL  |
| 1   | A     | 265 | PHE  |
| 1   | A     | 273 | MSE  |
| 1   | A     | 297 | LYS  |
| 1   | A     | 307 | ARG  |
| 1   | A     | 316 | GLU  |
| 1   | A     | 319 | LEU  |
| 1   | A     | 325 | VAL  |
| 1   | A     | 327 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 345 | LEU  |
| 1   | A     | 355 | LYS  |
| 1   | A     | 356 | LEU  |
| 1   | A     | 361 | LEU  |
| 1   | A     | 378 | LEU  |
| 1   | A     | 379 | LEU  |
| 1   | A     | 391 | LEU  |
| 1   | A     | 398 | THR  |
| 1   | A     | 400 | LEU  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 430 | PRO  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 471 | LEU  |
| 1   | A     | 473 | GLU  |
| 1   | A     | 479 | LYS  |
| 1   | A     | 497 | LEU  |
| 1   | A     | 505 | SER  |
| 1   | A     | 506 | ARG  |
| 1   | A     | 536 | VAL  |
| 1   | A     | 537 | ARG  |
| 1   | A     | 556 | ASP  |
| 1   | A     | 562 | PRO  |
| 1   | A     | 587 | ARG  |
| 1   | A     | 588 | GLU  |
| 1   | A     | 591 | LEU  |
| 1   | A     | 625 | PRO  |
| 1   | A     | 634 | GLU  |
| 1   | A     | 640 | ASN  |
| 1   | A     | 646 | MSE  |
| 1   | A     | 658 | LEU  |
| 1   | A     | 661 | VAL  |
| 1   | B     | 9   | LEU  |
| 1   | B     | 16  | MSE  |
| 1   | B     | 17  | LEU  |
| 1   | B     | 21  | ASN  |
| 1   | B     | 22  | ILE  |
| 1   | B     | 37  | ILE  |
| 1   | B     | 41  | GLU  |
| 1   | B     | 43  | LEU  |
| 1   | B     | 44  | LEU  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 63  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 75  | VAL  |
| 1   | B     | 78  | ASN  |
| 1   | B     | 83  | ASN  |
| 1   | B     | 94  | PRO  |
| 1   | B     | 102 | LEU  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 119 | VAL  |
| 1   | B     | 139 | GLU  |
| 1   | B     | 146 | ARG  |
| 1   | B     | 151 | THR  |
| 1   | B     | 153 | ILE  |
| 1   | B     | 157 | SER  |
| 1   | B     | 159 | ASP  |
| 1   | B     | 165 | GLU  |
| 1   | B     | 173 | LYS  |
| 1   | B     | 183 | GLN  |
| 1   | B     | 192 | LEU  |
| 1   | B     | 212 | THR  |
| 1   | B     | 213 | LEU  |
| 1   | B     | 221 | VAL  |
| 1   | B     | 225 | ARG  |
| 1   | B     | 239 | GLN  |
| 1   | B     | 250 | SER  |
| 1   | B     | 254 | GLU  |
| 1   | B     | 260 | VAL  |
| 1   | B     | 265 | PHE  |
| 1   | B     | 273 | MSE  |
| 1   | B     | 297 | LYS  |
| 1   | B     | 307 | ARG  |
| 1   | B     | 316 | GLU  |
| 1   | B     | 319 | LEU  |
| 1   | B     | 325 | VAL  |
| 1   | B     | 327 | ASP  |
| 1   | B     | 345 | LEU  |
| 1   | B     | 355 | LYS  |
| 1   | B     | 356 | LEU  |
| 1   | B     | 361 | LEU  |
| 1   | B     | 378 | LEU  |
| 1   | B     | 379 | LEU  |
| 1   | B     | 391 | LEU  |
| 1   | B     | 398 | THR  |
| 1   | B     | 400 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 404 | LEU  |
| 1   | B     | 430 | PRO  |
| 1   | B     | 448 | GLN  |
| 1   | B     | 471 | LEU  |
| 1   | B     | 473 | GLU  |
| 1   | B     | 479 | LYS  |
| 1   | B     | 497 | LEU  |
| 1   | B     | 505 | SER  |
| 1   | B     | 506 | ARG  |
| 1   | B     | 536 | VAL  |
| 1   | B     | 537 | ARG  |
| 1   | B     | 556 | ASP  |
| 1   | B     | 562 | PRO  |
| 1   | B     | 587 | ARG  |
| 1   | B     | 588 | GLU  |
| 1   | B     | 591 | LEU  |
| 1   | B     | 625 | PRO  |
| 1   | B     | 634 | GLU  |
| 1   | B     | 640 | ASN  |
| 1   | B     | 646 | MSE  |
| 1   | B     | 658 | LEU  |
| 1   | B     | 661 | VAL  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | ASN  |
| 1   | A     | 25  | GLN  |
| 1   | A     | 26  | GLN  |
| 1   | A     | 55  | ASN  |
| 1   | A     | 68  | ASN  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 89  | HIS  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 191 | GLN  |
| 1   | A     | 193 | HIS  |
| 1   | A     | 206 | GLN  |
| 1   | A     | 255 | GLN  |
| 1   | A     | 280 | ASN  |
| 1   | A     | 309 | ASN  |
| 1   | A     | 376 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 441 | GLN  |
| 1   | A     | 443 | HIS  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 469 | HIS  |
| 1   | A     | 524 | ASN  |
| 1   | A     | 525 | GLN  |
| 1   | A     | 533 | GLN  |
| 1   | A     | 629 | GLN  |
| 1   | B     | 21  | ASN  |
| 1   | B     | 25  | GLN  |
| 1   | B     | 26  | GLN  |
| 1   | B     | 55  | ASN  |
| 1   | B     | 68  | ASN  |
| 1   | B     | 78  | ASN  |
| 1   | B     | 83  | ASN  |
| 1   | B     | 89  | HIS  |
| 1   | B     | 183 | GLN  |
| 1   | B     | 191 | GLN  |
| 1   | B     | 193 | HIS  |
| 1   | B     | 206 | GLN  |
| 1   | B     | 255 | GLN  |
| 1   | B     | 280 | ASN  |
| 1   | B     | 309 | ASN  |
| 1   | B     | 376 | HIS  |
| 1   | B     | 441 | GLN  |
| 1   | B     | 443 | HIS  |
| 1   | B     | 448 | GLN  |
| 1   | B     | 469 | HIS  |
| 1   | B     | 524 | ASN  |
| 1   | B     | 525 | GLN  |
| 1   | B     | 533 | GLN  |
| 1   | B     | 629 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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     | 639/664 (96%)   | 0.62   | 56 (8%) 15 14  | 18, 40, 74, 138       | 0     |
| 1   | B     | 639/664 (96%)   | 0.68   | 59 (9%) 14 13  | 18, 40, 74, 138       | 0     |
| All | All   | 1278/1328 (96%) | 0.65   | 115 (8%) 15 13 | 18, 40, 74, 138       | 0     |

All (115) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 1   | PRO  | 7.0  |
| 1   | B     | 535 | GLY  | 6.9  |
| 1   | A     | 1   | PRO  | 6.5  |
| 1   | B     | 609 | ALA  | 6.5  |
| 1   | B     | 606 | ALA  | 6.4  |
| 1   | A     | 603 | ALA  | 6.0  |
| 1   | B     | 603 | ALA  | 5.6  |
| 1   | B     | 607 | ARG  | 5.2  |
| 1   | A     | 537 | ARG  | 5.0  |
| 1   | A     | 610 | GLY  | 4.7  |
| 1   | B     | 642 | HIS  | 4.3  |
| 1   | A     | 629 | GLN  | 4.3  |
| 1   | A     | 576 | TRP  | 4.2  |
| 1   | B     | 611 | LEU  | 4.1  |
| 1   | A     | 611 | LEU  | 4.1  |
| 1   | A     | 609 | ALA  | 3.9  |
| 1   | B     | 153 | ILE  | 3.9  |
| 1   | B     | 608 | GLN  | 3.9  |
| 1   | B     | 537 | ARG  | 3.8  |
| 1   | B     | 536 | VAL  | 3.8  |
| 1   | A     | 535 | GLY  | 3.8  |
| 1   | A     | 604 | SER  | 3.7  |
| 1   | B     | 534 | SER  | 3.7  |
| 1   | B     | 610 | GLY  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 218 | GLY  | 3.5  |
| 1   | A     | 664 | ARG  | 3.4  |
| 1   | A     | 216 | LYS  | 3.4  |
| 1   | A     | 607 | ARG  | 3.4  |
| 1   | A     | 612 | ALA  | 3.3  |
| 1   | A     | 630 | TYR  | 3.2  |
| 1   | B     | 60  | TYR  | 3.2  |
| 1   | A     | 592 | LYS  | 3.2  |
| 1   | A     | 373 | GLU  | 3.2  |
| 1   | B     | 64  | HIS  | 3.1  |
| 1   | B     | 259 | ASP  | 3.0  |
| 1   | A     | 608 | GLN  | 3.0  |
| 1   | A     | 642 | HIS  | 3.0  |
| 1   | B     | 630 | TYR  | 3.0  |
| 1   | A     | 71  | GLU  | 3.0  |
| 1   | A     | 492 | HIS  | 2.9  |
| 1   | A     | 634 | GLU  | 2.9  |
| 1   | B     | 604 | SER  | 2.9  |
| 1   | B     | 634 | GLU  | 2.9  |
| 1   | A     | 536 | VAL  | 2.8  |
| 1   | A     | 606 | ALA  | 2.8  |
| 1   | B     | 612 | ALA  | 2.8  |
| 1   | B     | 216 | LYS  | 2.8  |
| 1   | B     | 664 | ARG  | 2.8  |
| 1   | B     | 651 | VAL  | 2.8  |
| 1   | B     | 532 | VAL  | 2.7  |
| 1   | A     | 253 | LYS  | 2.7  |
| 1   | A     | 581 | GLU  | 2.7  |
| 1   | B     | 576 | TRP  | 2.7  |
| 1   | B     | 506 | ARG  | 2.6  |
| 1   | B     | 596 | LEU  | 2.6  |
| 1   | B     | 652 | GLU  | 2.6  |
| 1   | B     | 492 | HIS  | 2.6  |
| 1   | B     | 581 | GLU  | 2.6  |
| 1   | A     | 2   | ARG  | 2.5  |
| 1   | B     | 617 | ILE  | 2.5  |
| 1   | A     | 215 | PRO  | 2.5  |
| 1   | A     | 254 | GLU  | 2.4  |
| 1   | B     | 172 | GLU  | 2.4  |
| 1   | A     | 30  | ARG  | 2.4  |
| 1   | B     | 215 | PRO  | 2.4  |
| 1   | B     | 613 | GLU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 602 | VAL  | 2.4  |
| 1   | A     | 626 | ASN  | 2.4  |
| 1   | B     | 552 | ALA  | 2.4  |
| 1   | B     | 635 | ALA  | 2.4  |
| 1   | A     | 217 | THR  | 2.4  |
| 1   | A     | 615 | THR  | 2.4  |
| 1   | B     | 633 | THR  | 2.4  |
| 1   | A     | 252 | LEU  | 2.4  |
| 1   | A     | 479 | LYS  | 2.4  |
| 1   | B     | 632 | TRP  | 2.4  |
| 1   | A     | 563 | ILE  | 2.3  |
| 1   | B     | 2   | ARG  | 2.3  |
| 1   | B     | 629 | GLN  | 2.3  |
| 1   | A     | 386 | ASP  | 2.3  |
| 1   | B     | 214 | ASP  | 2.3  |
| 1   | A     | 219 | LYS  | 2.3  |
| 1   | A     | 555 | LYS  | 2.3  |
| 1   | B     | 315 | LYS  | 2.3  |
| 1   | B     | 518 | ILE  | 2.2  |
| 1   | A     | 506 | ARG  | 2.2  |
| 1   | A     | 259 | ASP  | 2.2  |
| 1   | B     | 165 | GLU  | 2.2  |
| 1   | B     | 270 | ARG  | 2.2  |
| 1   | A     | 256 | TYR  | 2.2  |
| 1   | A     | 390 | GLY  | 2.2  |
| 1   | B     | 452 | SER  | 2.2  |
| 1   | B     | 146 | ARG  | 2.2  |
| 1   | B     | 593 | ARG  | 2.2  |
| 1   | B     | 91  | ASN  | 2.2  |
| 1   | A     | 153 | ILE  | 2.2  |
| 1   | B     | 641 | ILE  | 2.2  |
| 1   | A     | 257 | GLY  | 2.1  |
| 1   | A     | 531 | GLY  | 2.1  |
| 1   | A     | 159 | ASP  | 2.1  |
| 1   | A     | 651 | VAL  | 2.1  |
| 1   | A     | 218 | GLY  | 2.1  |
| 1   | A     | 270 | ARG  | 2.1  |
| 1   | B     | 40  | TYR  | 2.1  |
| 1   | A     | 596 | LEU  | 2.1  |
| 1   | B     | 516 | GLY  | 2.1  |
| 1   | A     | 567 | VAL  | 2.1  |
| 1   | A     | 504 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 30  | ARG  | 2.0  |
| 1   | B     | 619 | LEU  | 2.0  |
| 1   | B     | 626 | ASN  | 2.0  |
| 1   | B     | 505 | SER  | 2.0  |
| 1   | A     | 41  | GLU  | 2.0  |
| 1   | B     | 622 | LEU  | 2.0  |
| 1   | A     | 375 | GLY  | 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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MG   | B     | 665 | 1/1   | 0.84 | 0.23 | 42,42,42,42                 | 0     |
| 2   | MG   | A     | 665 | 1/1   | 0.85 | 0.22 | 42,42,42,42                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.