



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:35 PM UTC

PDB ID : 2IQH / pdb\_00002iqh  
Title : Influenza A virus nucleoprotein NP at 3.2Å resolution  
Authors : Ye, Q.; Tao, Y.J.  
Deposited on : 2006-10-13  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

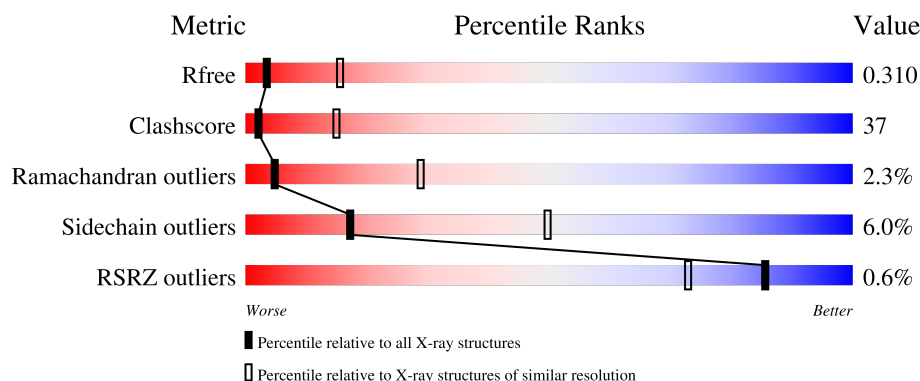
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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     | 499    | <div> <div>%</div> <div> <div></div> <div>38%</div> <div>42%</div> <div>5%</div> <div>15%</div> </div> </div> |
| 1   | B     | 499    | <div> <div>%</div> <div> <div></div> <div>42%</div> <div>39%</div> <div>•</div> <div>15%</div> </div> </div>  |
| 1   | C     | 499    | <div> <div></div> <div> <div>34%</div> <div>47%</div> <div>6%</div> <div>13%</div> </div> </div>              |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10162 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 Nucleocapsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 426      | Total | C    | N   | O   | S  | 8       | 0       | 0     |
|     |       |          | 3358  | 2084 | 623 | 625 | 26 |         |         |       |
| 1   | B     | 426      | Total | C    | N   | O   | S  | 8       | 0       | 0     |
|     |       |          | 3358  | 2084 | 623 | 625 | 26 |         |         |       |
| 1   | C     | 436      | Total | C    | N   | O   | S  | 8       | 0       | 0     |
|     |       |          | 3446  | 2137 | 642 | 641 | 26 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

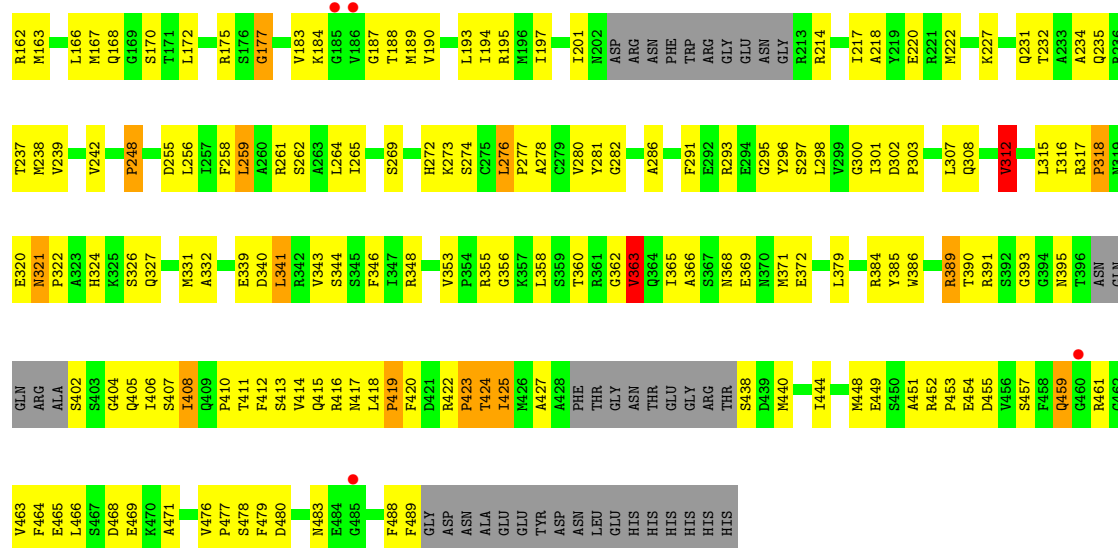
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 499     | LEU      | -      | expression tag | UNP Q1I2B5 |
| A     | 500     | GLU      | -      | expression tag | UNP Q1I2B5 |
| A     | 501     | HIS      | -      | expression tag | UNP Q1I2B5 |
| A     | 502     | HIS      | -      | expression tag | UNP Q1I2B5 |
| A     | 503     | HIS      | -      | expression tag | UNP Q1I2B5 |
| A     | 504     | HIS      | -      | expression tag | UNP Q1I2B5 |
| A     | 505     | HIS      | -      | expression tag | UNP Q1I2B5 |
| A     | 506     | HIS      | -      | expression tag | UNP Q1I2B5 |
| B     | 499     | LEU      | -      | expression tag | UNP Q1I2B5 |
| B     | 500     | GLU      | -      | expression tag | UNP Q1I2B5 |
| B     | 501     | HIS      | -      | expression tag | UNP Q1I2B5 |
| B     | 502     | HIS      | -      | expression tag | UNP Q1I2B5 |
| B     | 503     | HIS      | -      | expression tag | UNP Q1I2B5 |
| B     | 504     | HIS      | -      | expression tag | UNP Q1I2B5 |
| B     | 505     | HIS      | -      | expression tag | UNP Q1I2B5 |
| B     | 506     | HIS      | -      | expression tag | UNP Q1I2B5 |
| C     | 499     | LEU      | -      | expression tag | UNP Q1I2B5 |
| C     | 500     | GLU      | -      | expression tag | UNP Q1I2B5 |
| C     | 501     | HIS      | -      | expression tag | UNP Q1I2B5 |
| C     | 502     | HIS      | -      | expression tag | UNP Q1I2B5 |
| C     | 503     | HIS      | -      | expression tag | UNP Q1I2B5 |
| C     | 504     | HIS      | -      | expression tag | UNP Q1I2B5 |
| C     | 505     | HIS      | -      | expression tag | UNP Q1I2B5 |

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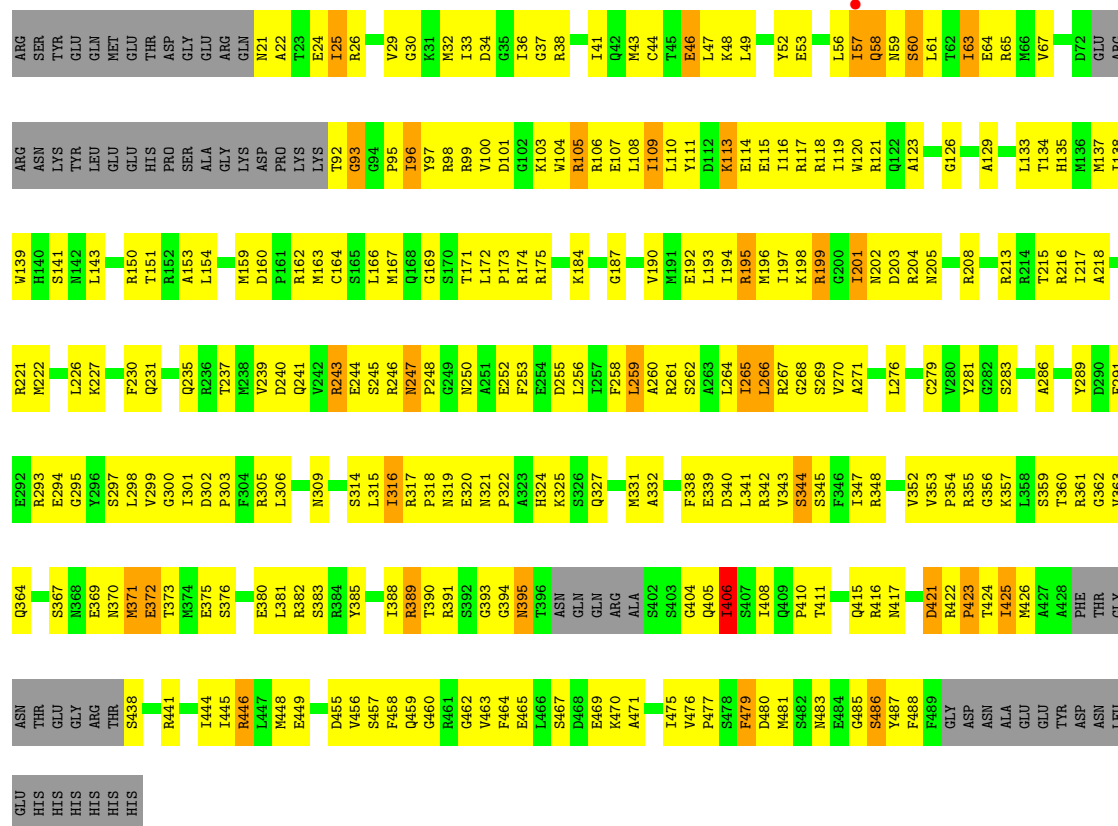
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 506     | HIS      | -      | expression tag | UNP Q1I2B5 |





### • Molecule 1: Nucleocapsid protein

Chain C: 34% 47% 6% 13%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 122.10Å 135.10Å 195.18Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 30.00 – 3.20<br>30.00 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (30.00-3.20)<br>99.1 (30.00-3.20)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.19 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.271 , 0.318<br>0.254 , 0.310                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1360 reflections (4.84%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 84.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.113                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 52.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 10162                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 75.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 1.13         | 3/3411 (0.1%)   | 1.26        | 26/4585 (0.6%)  |
| 1   | B     | 1.20         | 5/3411 (0.1%)   | 1.23        | 7/4585 (0.2%)   |
| 1   | C     | 1.07         | 3/3503 (0.1%)   | 1.20        | 16/4710 (0.3%)  |
| All | All   | 1.13         | 11/10325 (0.1%) | 1.23        | 49/13880 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 201 | ILE  | C-N   | -21.67 | 1.03        | 1.33     |
| 1   | C     | 201 | ILE  | C-N   | -13.13 | 1.15        | 1.33     |
| 1   | C     | 202 | ASN  | C-N   | -12.72 | 1.15        | 1.33     |
| 1   | A     | 201 | ILE  | C-N   | -8.12  | 1.22        | 1.33     |
| 1   | B     | 312 | VAL  | CA-CB | -5.70  | 1.47        | 1.54     |
| 1   | C     | 445 | ILE  | CA-CB | -5.51  | 1.48        | 1.54     |
| 1   | A     | 289 | TYR  | CA-C  | -5.34  | 1.45        | 1.52     |
| 1   | A     | 146 | ALA  | CA-CB | -5.32  | 1.46        | 1.53     |
| 1   | B     | 146 | ALA  | CA-CB | -5.18  | 1.45        | 1.53     |
| 1   | B     | 148 | TYR  | CA-C  | -5.12  | 1.46        | 1.52     |
| 1   | B     | 332 | ALA  | C-O   | 5.10   | 1.30        | 1.24     |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 201 | ILE  | O-C-N | -8.11 | 112.82      | 122.06   |
| 1   | C     | 201 | ILE  | O-C-N | -7.90 | 112.86      | 122.18   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 202 | ASN  | N-CA-C  | -7.57 | 103.30      | 112.54   |
| 1   | A     | 179 | ALA  | N-CA-C  | -7.14 | 104.18      | 113.17   |
| 1   | C     | 184 | LYS  | CA-C-N  | -7.04 | 116.21      | 122.47   |
| 1   | C     | 184 | LYS  | C-N-CA  | -7.04 | 116.21      | 122.47   |
| 1   | A     | 136 | MET  | N-CA-C  | -6.83 | 104.42      | 112.89   |
| 1   | C     | 201 | ILE  | N-CA-C  | -6.80 | 103.02      | 113.16   |
| 1   | A     | 317 | ARG  | CA-C-N  | 6.74  | 126.25      | 119.24   |
| 1   | A     | 317 | ARG  | C-N-CA  | 6.74  | 126.25      | 119.24   |
| 1   | A     | 137 | MET  | N-CA-C  | -6.74 | 104.01      | 111.82   |
| 1   | C     | 476 | VAL  | CA-C-N  | 6.66  | 126.57      | 119.85   |
| 1   | C     | 476 | VAL  | C-N-CA  | 6.66  | 126.57      | 119.85   |
| 1   | A     | 276 | LEU  | CA-C-N  | 6.55  | 126.53      | 119.78   |
| 1   | A     | 276 | LEU  | C-N-CA  | 6.55  | 126.53      | 119.78   |
| 1   | B     | 321 | ASN  | N-CA-C  | 6.31  | 118.02      | 109.24   |
| 1   | A     | 139 | TRP  | N-CA-C  | -6.18 | 104.54      | 111.28   |
| 1   | C     | 195 | ARG  | N-CA-C  | -6.15 | 104.50      | 111.14   |
| 1   | C     | 479 | PHE  | N-CA-C  | 6.13  | 122.45      | 110.56   |
| 1   | B     | 363 | VAL  | CB-CA-C | -5.80 | 105.93      | 111.44   |
| 1   | C     | 344 | SER  | N-CA-C  | -5.77 | 103.73      | 112.04   |
| 1   | A     | 353 | VAL  | CA-C-N  | 5.76  | 126.08      | 119.92   |
| 1   | A     | 353 | VAL  | C-N-CA  | 5.76  | 126.08      | 119.92   |
| 1   | A     | 418 | LEU  | CA-C-N  | 5.73  | 125.68      | 119.78   |
| 1   | A     | 418 | LEU  | C-N-CA  | 5.73  | 125.68      | 119.78   |
| 1   | B     | 480 | ASP  | N-CA-C  | -5.70 | 106.12      | 112.57   |
| 1   | B     | 419 | PRO  | N-CA-C  | 5.62  | 119.29      | 110.80   |
| 1   | A     | 372 | GLU  | N-CA-C  | -5.60 | 105.08      | 111.07   |
| 1   | A     | 312 | VAL  | CB-CA-C | -5.53 | 103.33      | 110.84   |
| 1   | A     | 216 | ARG  | N-CA-C  | 5.40  | 116.97      | 111.14   |
| 1   | A     | 409 | GLN  | CA-C-N  | 5.34  | 126.18      | 119.98   |
| 1   | A     | 409 | GLN  | C-N-CA  | 5.34  | 126.18      | 119.98   |
| 1   | C     | 268 | GLY  | N-CA-C  | -5.30 | 104.52      | 112.89   |
| 1   | C     | 425 | ILE  | CB-CA-C | -5.25 | 104.97      | 112.22   |
| 1   | B     | 276 | LEU  | N-CA-C  | 5.22  | 117.57      | 110.01   |
| 1   | C     | 93  | GLY  | N-CA-C  | 5.17  | 118.65      | 111.10   |
| 1   | A     | 184 | LYS  | N-CA-C  | 5.17  | 117.72      | 110.23   |
| 1   | A     | 338 | PHE  | N-CA-C  | -5.17 | 104.74      | 112.54   |
| 1   | A     | 392 | SER  | N-CA-C  | 5.15  | 117.50      | 110.24   |
| 1   | A     | 473 | SER  | N-CA-C  | 5.15  | 116.86      | 109.04   |
| 1   | C     | 63  | ILE  | CB-CA-C | -5.14 | 105.39      | 111.81   |
| 1   | B     | 276 | LEU  | CA-C-N  | 5.09  | 125.06      | 120.03   |
| 1   | B     | 276 | LEU  | C-N-CA  | 5.09  | 125.06      | 120.03   |
| 1   | C     | 425 | ILE  | N-CA-C  | 5.08  | 115.85      | 110.72   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 148 | TYR  | N-CA-C | 5.08  | 117.87      | 109.85   |
| 1   | A     | 29  | VAL  | N-CA-C | -5.03 | 105.66      | 113.16   |
| 1   | A     | 346 | PHE  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 1   | C     | 153 | ALA  | N-CA-C | 5.01  | 116.82      | 111.36   |
| 1   | A     | 196 | MET  | N-CA-C | -5.00 | 105.72      | 111.07   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 201 | ILE  | Mainchain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3358  | 0        | 3355     | 272     | 0            |
| 1   | B     | 3358  | 0        | 3354     | 232     | 0            |
| 1   | C     | 3446  | 0        | 3427     | 312     | 0            |
| All | All   | 10162 | 0        | 10136    | 755     | 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 37.

All (755) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:TYR:HB3  | 1:A:116:ILE:HD11 | 1.46                     | 0.95              |
| 1:B:100:VAL:CG2  | 1:B:105:ARG:HD3  | 1.98                     | 0.94              |
| 1:A:58:GLN:HG3   | 1:A:315:LEU:HG   | 1.50                     | 0.93              |
| 1:C:465:GLU:HG3  | 1:C:467:SER:H    | 1.32                     | 0.92              |
| 1:C:353:VAL:HG22 | 1:C:354:PRO:HD2  | 1.52                     | 0.92              |
| 1:A:483:ASN:H    | 1:A:483:ASN:HD22 | 1.09                     | 0.92              |
| 1:A:226:LEU:HD13 | 1:A:230:PHE:HE1  | 1.31                     | 0.91              |
| 1:C:154:LEU:HD21 | 1:C:167:MET:HE3  | 1.51                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:341:LEU:HB2  | 1:C:486:SER:HA   | 1.53                     | 0.90              |
| 1:A:238:MET:HE3  | 1:A:255:ASP:OD1  | 1.73                     | 0.89              |
| 1:A:163:MET:HE3  | 1:A:261:ARG:HG2  | 1.56                     | 0.87              |
| 1:C:134:THR:HA   | 1:C:137:MET:HE3  | 1.56                     | 0.86              |
| 1:B:21:ASN:CB    | 1:B:24:GLU:HG3   | 2.04                     | 0.86              |
| 1:B:42:GLN:HG2   | 1:B:119:ILE:HD11 | 1.59                     | 0.84              |
| 1:B:360:THR:HG22 | 1:B:362:GLY:H    | 1.43                     | 0.84              |
| 1:A:250:ASN:HA   | 1:A:253:PHE:HB3  | 1.58                     | 0.83              |
| 1:C:262:SER:HA   | 1:C:448:MET:HE3  | 1.59                     | 0.83              |
| 1:A:308:GLN:HE22 | 1:A:383:SER:H    | 1.24                     | 0.83              |
| 1:C:106:ARG:HH12 | 1:C:367:SER:HA   | 1.45                     | 0.82              |
| 1:A:189:MET:HE2  | 1:A:192:GLU:OE1  | 1.79                     | 0.82              |
| 1:C:276:LEU:HB2  | 1:C:281:TYR:HE1  | 1.42                     | 0.82              |
| 1:A:238:MET:HE1  | 1:A:258:PHE:HD2  | 1.43                     | 0.82              |
| 1:B:265:ILE:HD11 | 1:B:448:MET:HG2  | 1.63                     | 0.81              |
| 1:A:196:MET:HE1  | 1:A:219:TYR:HB2  | 1.61                     | 0.81              |
| 1:A:114:GLU:HB3  | 1:A:117:ARG:HH21 | 1.46                     | 0.81              |
| 1:A:461:ARG:HG3  | 1:B:413:SER:OG   | 1.82                     | 0.80              |
| 1:B:324:HIS:CD2  | 1:B:358:LEU:HD12 | 2.17                     | 0.80              |
| 1:A:71:PHE:HE1   | 1:A:117:ARG:HA   | 1.48                     | 0.79              |
| 1:B:96:ILE:HG13  | 1:B:109:ILE:HD12 | 1.62                     | 0.79              |
| 1:B:231:GLN:NE2  | 1:B:269:SER:HB3  | 1.97                     | 0.79              |
| 1:A:324:HIS:HD2  | 1:A:359:SER:H    | 1.30                     | 0.79              |
| 1:C:231:GLN:NE2  | 1:C:269:SER:HB2  | 1.96                     | 0.79              |
| 1:A:121:ARG:HG2  | 1:A:121:ARG:HH11 | 1.47                     | 0.78              |
| 1:A:227:LYS:HE3  | 1:A:236:ARG:HB3  | 1.65                     | 0.78              |
| 1:A:114:GLU:HA   | 1:A:117:ARG:HE   | 1.47                     | 0.78              |
| 1:C:33:ILE:HD12  | 1:C:281:TYR:HE2  | 1.49                     | 0.78              |
| 1:A:114:GLU:CB   | 1:A:117:ARG:HH21 | 1.97                     | 0.77              |
| 1:A:238:MET:HE1  | 1:A:258:PHE:CD2  | 2.19                     | 0.77              |
| 1:A:272:HIS:CD2  | 1:B:411:THR:HA   | 2.19                     | 0.77              |
| 1:A:340:ASP:O    | 1:A:343:VAL:HG12 | 1.85                     | 0.77              |
| 1:C:154:LEU:HD21 | 1:C:167:MET:CE   | 2.15                     | 0.77              |
| 1:A:483:ASN:HD22 | 1:A:483:ASN:N    | 1.82                     | 0.77              |
| 1:A:317:ARG:HD3  | 1:A:369:GLU:OE1  | 1.84                     | 0.76              |
| 1:B:317:ARG:HG2  | 1:B:320:GLU:OE2  | 1.85                     | 0.76              |
| 1:A:390:THR:HG22 | 1:A:391:ARG:H    | 1.50                     | 0.76              |
| 1:A:111:TYR:HB3  | 1:A:116:ILE:CD1  | 2.15                     | 0.76              |
| 1:B:489:PHE:HB2  | 1:C:405:GLN:HG3  | 1.68                     | 0.75              |
| 1:A:242:VAL:HG11 | 1:A:256:LEU:HD21 | 1.68                     | 0.75              |
| 1:C:327:GLN:O    | 1:C:331:MET:HG3  | 1.84                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:43:MET:HA    | 1:B:43:MET:HE2   | 1.67                     | 0.75              |
| 1:B:21:ASN:HB3   | 1:B:24:GLU:HG3   | 1.67                     | 0.75              |
| 1:B:217:ILE:HG13 | 1:B:218:ALA:N    | 2.02                     | 0.75              |
| 1:B:217:ILE:HG13 | 1:B:218:ALA:H    | 1.49                     | 0.75              |
| 1:C:422:ARG:HB3  | 1:C:423:PRO:HD3  | 1.68                     | 0.75              |
| 1:C:276:LEU:HB2  | 1:C:281:TYR:CE1  | 2.21                     | 0.74              |
| 1:A:174:ARG:HD3  | 1:A:174:ARG:N    | 2.03                     | 0.74              |
| 1:C:353:VAL:CG2  | 1:C:354:PRO:HD2  | 2.17                     | 0.74              |
| 1:A:232:THR:OG1  | 1:A:235:GLN:HG3  | 1.87                     | 0.74              |
| 1:A:483:ASN:H    | 1:A:483:ASN:ND2  | 1.86                     | 0.73              |
| 1:C:243:ARG:HG2  | 1:C:243:ARG:HH11 | 1.53                     | 0.73              |
| 1:C:267:ARG:O    | 1:C:395:ASN:ND2  | 2.21                     | 0.73              |
| 1:B:100:VAL:HG21 | 1:B:105:ARG:HD3  | 1.70                     | 0.73              |
| 1:A:71:PHE:CE1   | 1:A:117:ARG:HA   | 2.24                     | 0.73              |
| 1:C:299:VAL:O    | 1:C:388:ILE:HG23 | 1.89                     | 0.73              |
| 1:B:160:ASP:HB3  | 1:B:163:MET:HG3  | 1.69                     | 0.73              |
| 1:A:226:LEU:HD13 | 1:A:230:PHE:CE1  | 2.22                     | 0.72              |
| 1:A:342:ARG:HB3  | 1:A:479:PHE:CE2  | 2.23                     | 0.72              |
| 1:A:407:SER:OG   | 1:C:267:ARG:NH1  | 2.22                     | 0.72              |
| 1:B:324:HIS:HD2  | 1:B:358:LEU:HD12 | 1.53                     | 0.72              |
| 1:A:486:SER:HB3  | 1:B:408:ILE:HD11 | 1.70                     | 0.72              |
| 1:C:270:VAL:HG12 | 1:C:271:ALA:N    | 2.05                     | 0.72              |
| 1:C:104:TRP:CZ2  | 1:C:376:SER:HB3  | 2.25                     | 0.71              |
| 1:C:199:ARG:HG2  | 1:C:199:ARG:HH11 | 1.56                     | 0.71              |
| 1:C:33:ILE:HG23  | 1:C:281:TYR:CD2  | 2.25                     | 0.71              |
| 1:C:221:ARG:HH11 | 1:C:221:ARG:HG2  | 1.55                     | 0.71              |
| 1:A:235:GLN:O    | 1:A:239:VAL:HG23 | 1.91                     | 0.71              |
| 1:B:262:SER:HA   | 1:B:448:MET:HE3  | 1.72                     | 0.71              |
| 1:A:296:TYR:CD1  | 1:A:302:ASP:HB3  | 2.26                     | 0.71              |
| 1:C:198:LYS:HD3  | 1:C:201:ILE:HD12 | 1.71                     | 0.71              |
| 1:B:321:ASN:HD22 | 1:B:322:PRO:CD   | 2.03                     | 0.71              |
| 1:A:324:HIS:CD2  | 1:A:359:SER:H    | 2.09                     | 0.70              |
| 1:A:267:ARG:HG3  | 1:A:393:GLY:O    | 1.92                     | 0.70              |
| 1:C:192:GLU:O    | 1:C:195:ARG:HG2  | 1.92                     | 0.70              |
| 1:A:426:MET:HE2  | 1:A:426:MET:HA   | 1.73                     | 0.70              |
| 1:C:246:ARG:HH11 | 1:C:246:ARG:HG2  | 1.56                     | 0.70              |
| 1:B:92:THR:HG22  | 1:B:93:GLY:N     | 2.07                     | 0.70              |
| 1:B:227:LYS:HB2  | 1:B:239:VAL:HG11 | 1.73                     | 0.70              |
| 1:B:21:ASN:HB2   | 1:B:24:GLU:HG3   | 1.73                     | 0.69              |
| 1:A:489:PHE:HB2  | 1:B:405:GLN:HG3  | 1.74                     | 0.69              |
| 1:B:155:VAL:HG23 | 1:B:156:ARG:N    | 2.06                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:63:ILE:O     | 1:C:67:VAL:HG23  | 1.92                     | 0.69              |
| 1:C:289:TYR:CE1  | 1:C:294:GLU:HG2  | 2.27                     | 0.69              |
| 1:A:453:PRO:HG3  | 1:B:420:PHE:CE1  | 2.28                     | 0.69              |
| 1:A:460:GLY:H    | 1:B:415:GLN:HE21 | 1.40                     | 0.69              |
| 1:B:321:ASN:HD22 | 1:B:322:PRO:HD2  | 1.58                     | 0.69              |
| 1:B:412:PHE:H    | 1:B:416:ARG:NH2  | 1.90                     | 0.69              |
| 1:C:198:LYS:HA   | 1:C:201:ILE:HD12 | 1.74                     | 0.69              |
| 1:A:37:GLY:HA3   | 1:A:285:VAL:HG21 | 1.75                     | 0.69              |
| 1:A:340:ASP:HB2  | 1:B:408:ILE:HD13 | 1.74                     | 0.69              |
| 1:B:138:ILE:HD12 | 1:B:183:VAL:HG21 | 1.76                     | 0.69              |
| 1:C:93:GLY:HA3   | 1:C:110:LEU:HD23 | 1.75                     | 0.68              |
| 1:C:44:CYS:HA    | 1:C:49:LEU:HD12  | 1.75                     | 0.68              |
| 1:A:92:THR:N     | 1:A:113:LYS:HG2  | 2.09                     | 0.68              |
| 1:A:406:ILE:HD11 | 1:C:162:ARG:HD2  | 1.76                     | 0.68              |
| 1:C:172:LEU:HD12 | 1:C:173:PRO:HD2  | 1.76                     | 0.68              |
| 1:B:156:ARG:HH12 | 1:B:195:ARG:NH1  | 1.92                     | 0.67              |
| 1:C:340:ASP:HB3  | 1:C:343:VAL:HG22 | 1.75                     | 0.67              |
| 1:C:29:VAL:O     | 1:C:33:ILE:HG12  | 1.93                     | 0.67              |
| 1:C:113:LYS:H    | 1:C:113:LYS:HD2  | 1.59                     | 0.67              |
| 1:B:422:ARG:HB3  | 1:B:423:PRO:HD3  | 1.77                     | 0.67              |
| 1:C:96:ILE:HG12  | 1:C:109:ILE:HG21 | 1.77                     | 0.67              |
| 1:B:262:SER:HA   | 1:B:448:MET:CE   | 2.25                     | 0.67              |
| 1:C:96:ILE:HG12  | 1:C:109:ILE:CG2  | 2.25                     | 0.66              |
| 1:C:345:SER:HA   | 1:C:352:VAL:HG23 | 1.77                     | 0.66              |
| 1:B:193:LEU:HD23 | 1:B:222:MET:HE3  | 1.76                     | 0.66              |
| 1:C:195:ARG:NH2  | 1:C:222:MET:HE1  | 2.11                     | 0.66              |
| 1:C:316:ILE:HD11 | 1:C:320:GLU:HB2  | 1.77                     | 0.66              |
| 1:A:315:LEU:HD12 | 1:A:365:ILE:HD13 | 1.78                     | 0.66              |
| 1:B:274:SER:OG   | 1:B:389:ARG:HD3  | 1.95                     | 0.66              |
| 1:C:33:ILE:HG21  | 1:C:291:PHE:CD2  | 2.30                     | 0.66              |
| 1:C:25:ILE:HG13  | 1:C:26:ARG:H     | 1.60                     | 0.66              |
| 1:C:171:THR:O    | 1:C:171:THR:HG22 | 1.96                     | 0.66              |
| 1:C:243:ARG:HG2  | 1:C:243:ARG:NH1  | 2.10                     | 0.66              |
| 1:C:360:THR:HG22 | 1:C:362:GLY:H    | 1.60                     | 0.66              |
| 1:A:375:GLU:N    | 1:A:375:GLU:OE1  | 2.30                     | 0.65              |
| 1:C:98:ARG:O     | 1:C:105:ARG:N    | 2.27                     | 0.65              |
| 1:A:151:THR:HG23 | 1:A:161:PRO:HB3  | 1.77                     | 0.65              |
| 1:C:193:LEU:O    | 1:C:197:ILE:HG12 | 1.94                     | 0.65              |
| 1:A:417:ASN:O    | 1:A:419:PRO:HD3  | 1.96                     | 0.65              |
| 1:C:114:GLU:HG3  | 1:C:117:ARG:HH21 | 1.62                     | 0.65              |
| 1:A:244:GLU:OE1  | 1:A:244:GLU:HA   | 1.95                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:109:ILE:CD1  | 1:C:111:TYR:HB2  | 2.27                     | 0.65              |
| 1:A:26:ARG:HH11  | 1:A:295:GLY:HA3  | 1.62                     | 0.65              |
| 1:C:46:GLU:OE1   | 1:C:46:GLU:HA    | 1.97                     | 0.64              |
| 1:C:325:LYS:HG2  | 1:C:360:THR:HG21 | 1.79                     | 0.64              |
| 1:B:69:SER:OG    | 1:B:92:THR:HG21  | 1.97                     | 0.64              |
| 1:B:162:ARG:HG2  | 1:C:404:GLY:O    | 1.98                     | 0.64              |
| 1:A:242:VAL:HG13 | 1:A:252:GLU:HG3  | 1.78                     | 0.64              |
| 1:C:410:PRO:HA   | 1:C:416:ARG:NH2  | 2.12                     | 0.64              |
| 1:A:111:TYR:CB   | 1:A:116:ILE:HD11 | 2.26                     | 0.64              |
| 1:B:95:PRO:HA    | 1:B:108:LEU:HD23 | 1.80                     | 0.64              |
| 1:B:113:LYS:O    | 1:B:117:ARG:HB2  | 1.97                     | 0.64              |
| 1:A:227:LYS:HB2  | 1:A:239:VAL:HG11 | 1.79                     | 0.63              |
| 1:C:422:ARG:HH11 | 1:C:422:ARG:HG2  | 1.64                     | 0.63              |
| 1:A:62:THR:O     | 1:A:65:ARG:HG2   | 1.98                     | 0.63              |
| 1:A:340:ASP:CB   | 1:B:408:ILE:HD13 | 2.29                     | 0.63              |
| 1:C:194:ILE:HD12 | 1:C:253:PHE:HD1  | 1.64                     | 0.63              |
| 1:A:342:ARG:HB3  | 1:A:479:PHE:CD2  | 2.34                     | 0.62              |
| 1:A:415:GLN:NE2  | 1:C:460:GLY:H    | 1.97                     | 0.62              |
| 1:C:340:ASP:OD1  | 1:C:486:SER:HB3  | 1.99                     | 0.62              |
| 1:A:97:TYR:CE2   | 1:A:106:ARG:HG3  | 2.34                     | 0.62              |
| 1:C:246:ARG:HG2  | 1:C:246:ARG:NH1  | 2.12                     | 0.62              |
| 1:B:237:THR:HB   | 1:B:440:MET:SD   | 2.39                     | 0.62              |
| 1:B:272:HIS:CD2  | 1:C:411:THR:HA   | 2.34                     | 0.62              |
| 1:A:197:ILE:HG23 | 1:A:201:ILE:HG13 | 1.80                     | 0.62              |
| 1:A:154:LEU:HD21 | 1:A:167:MET:HG2  | 1.81                     | 0.62              |
| 1:C:221:ARG:HG2  | 1:C:221:ARG:NH1  | 2.14                     | 0.62              |
| 1:A:344:SER:O    | 1:A:348:ARG:HB2  | 1.99                     | 0.62              |
| 1:B:297:SER:O    | 1:B:303:PRO:HD3  | 1.99                     | 0.62              |
| 1:C:246:ARG:C    | 1:C:248:PRO:HD3  | 2.25                     | 0.62              |
| 1:A:180:GLY:O    | 1:A:183:VAL:HG12 | 2.00                     | 0.61              |
| 1:A:32:MET:HE2   | 1:A:131:ALA:HB1  | 1.82                     | 0.61              |
| 1:A:176:SER:OG   | 1:A:180:GLY:HA3  | 1.99                     | 0.61              |
| 1:B:120:TRP:CZ2  | 1:B:129:ALA:HB3  | 2.34                     | 0.61              |
| 1:B:151:THR:O    | 1:B:155:VAL:HG13 | 2.00                     | 0.61              |
| 1:C:151:THR:HA   | 1:C:154:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:121:ARG:HB3  | 1:A:126:GLY:HA2  | 1.82                     | 0.61              |
| 1:C:265:ILE:HG13 | 1:C:266:LEU:H    | 1.65                     | 0.61              |
| 1:B:238:MET:O    | 1:B:242:VAL:HG23 | 2.00                     | 0.61              |
| 1:B:134:THR:HA   | 1:B:137:MET:HE3  | 1.82                     | 0.61              |
| 1:A:92:THR:N     | 1:A:113:LYS:HZ3  | 1.99                     | 0.61              |
| 1:C:240:ASP:HA   | 1:C:243:ARG:NH1  | 2.14                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:58:GLN:HG3   | 1:A:315:LEU:CG   | 2.26                     | 0.60              |
| 1:A:242:VAL:HG11 | 1:A:256:LEU:CD2  | 2.31                     | 0.60              |
| 1:C:231:GLN:HG3  | 1:C:395:ASN:OD1  | 2.02                     | 0.60              |
| 1:B:459:GLN:H    | 1:B:459:GLN:HE21 | 1.48                     | 0.60              |
| 1:B:348:ARG:HG2  | 1:B:348:ARG:HH11 | 1.66                     | 0.60              |
| 1:A:162:ARG:HD3  | 1:B:402:SER:HB2  | 1.83                     | 0.60              |
| 1:B:346:PHE:CZ   | 1:B:477:PRO:HB3  | 2.37                     | 0.60              |
| 1:A:255:ASP:O    | 1:A:258:PHE:HB3  | 2.02                     | 0.60              |
| 1:C:265:ILE:HD11 | 1:C:448:MET:HE2  | 1.82                     | 0.60              |
| 1:A:43:MET:O     | 1:A:47:LEU:HD23  | 2.02                     | 0.59              |
| 1:B:464:PHE:CZ   | 1:B:471:ALA:HB1  | 2.37                     | 0.59              |
| 1:C:380:GLU:OE2  | 1:C:382:ARG:HD3  | 2.02                     | 0.59              |
| 1:B:265:ILE:HD11 | 1:B:448:MET:CG   | 2.31                     | 0.59              |
| 1:B:321:ASN:HB3  | 1:B:324:HIS:HB2  | 1.84                     | 0.59              |
| 1:B:341:LEU:HD11 | 1:B:488:PHE:HA   | 1.84                     | 0.59              |
| 1:A:339:GLU:HG3  | 1:B:411:THR:HB   | 1.83                     | 0.59              |
| 1:C:270:VAL:O    | 1:C:391:ARG:HA   | 2.03                     | 0.59              |
| 1:A:267:ARG:NH1  | 1:B:407:SER:OG   | 2.36                     | 0.59              |
| 1:A:121:ARG:HG2  | 1:A:121:ARG:NH1  | 2.15                     | 0.59              |
| 1:A:483:ASN:ND2  | 1:B:478:SER:HB2  | 2.17                     | 0.59              |
| 1:A:253:PHE:C    | 1:A:253:PHE:CD2  | 2.81                     | 0.59              |
| 1:C:46:GLU:C     | 1:C:48:LYS:H     | 2.11                     | 0.59              |
| 1:C:199:ARG:HG2  | 1:C:199:ARG:NH1  | 2.18                     | 0.59              |
| 1:B:411:THR:H    | 1:B:416:ARG:HH22 | 1.49                     | 0.59              |
| 1:C:33:ILE:HG21  | 1:C:291:PHE:CE2  | 2.38                     | 0.59              |
| 1:A:321:ASN:HB3  | 1:A:324:HIS:HB2  | 1.83                     | 0.59              |
| 1:B:489:PHE:H    | 1:C:405:GLN:HE21 | 1.49                     | 0.59              |
| 1:C:61:LEU:HA    | 1:C:64:GLU:OE1   | 2.03                     | 0.58              |
| 1:C:382:ARG:HH11 | 1:C:382:ARG:HG2  | 1.68                     | 0.58              |
| 1:C:283:SER:O    | 1:C:286:ALA:HB3  | 2.04                     | 0.58              |
| 1:A:298:LEU:N    | 1:A:298:LEU:HD12 | 2.19                     | 0.58              |
| 1:C:438:SER:HB3  | 1:C:441:ARG:HG3  | 1.84                     | 0.58              |
| 1:A:408:ILE:HD11 | 1:C:339:GLU:C    | 2.29                     | 0.58              |
| 1:C:216:ARG:NH2  | 1:C:243:ARG:O    | 2.37                     | 0.58              |
| 1:A:150:ARG:O    | 1:A:154:LEU:HG   | 2.04                     | 0.58              |
| 1:B:317:ARG:O    | 1:B:320:GLU:HB2  | 2.04                     | 0.58              |
| 1:B:372:GLU:HA   | 1:B:372:GLU:OE1  | 2.04                     | 0.58              |
| 1:B:115:GLU:OE1  | 1:B:115:GLU:HA   | 2.04                     | 0.57              |
| 1:B:417:ASN:O    | 1:B:419:PRO:HD3  | 2.04                     | 0.57              |
| 1:A:267:ARG:HB2  | 1:A:393:GLY:HA3  | 1.86                     | 0.57              |
| 1:A:61:LEU:HA    | 1:A:64:GLU:OE1   | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:324:HIS:CD2  | 1:C:359:SER:H    | 2.22                     | 0.57              |
| 1:C:464:PHE:N    | 1:C:464:PHE:CD2  | 2.73                     | 0.57              |
| 1:A:46:GLU:O     | 1:A:48:LYS:HG2   | 2.05                     | 0.57              |
| 1:C:25:ILE:HG13  | 1:C:26:ARG:N     | 2.20                     | 0.57              |
| 1:C:197:ILE:HD12 | 1:C:248:PRO:HB3  | 1.86                     | 0.57              |
| 1:B:100:VAL:HG22 | 1:B:105:ARG:HD3  | 1.84                     | 0.57              |
| 1:B:355:ARG:HG2  | 1:B:489:PHE:HE2  | 1.68                     | 0.57              |
| 1:B:139:TRP:CZ2  | 1:B:277:PRO:HG3  | 2.40                     | 0.57              |
| 1:C:371:MET:O    | 1:C:371:MET:HG2  | 2.05                     | 0.57              |
| 1:B:411:THR:N    | 1:B:416:ARG:HH22 | 2.03                     | 0.56              |
| 1:A:100:VAL:O    | 1:A:101:ASP:C    | 2.48                     | 0.56              |
| 1:A:238:MET:O    | 1:A:242:VAL:HG23 | 2.06                     | 0.56              |
| 1:A:346:PHE:CE2  | 1:A:477:PRO:HB3  | 2.39                     | 0.56              |
| 1:A:390:THR:OG1  | 1:B:413:SER:HB2  | 2.05                     | 0.56              |
| 1:A:424:THR:O    | 1:A:427:ALA:HB3  | 2.05                     | 0.56              |
| 1:C:240:ASP:O    | 1:C:244:GLU:HG2  | 2.03                     | 0.56              |
| 1:A:71:PHE:CE1   | 1:A:117:ARG:HG2  | 2.40                     | 0.56              |
| 1:B:155:VAL:HG23 | 1:B:156:ARG:H    | 1.69                     | 0.56              |
| 1:B:448:MET:HB3  | 1:C:426:MET:HE1  | 1.86                     | 0.56              |
| 1:C:109:ILE:HD11 | 1:C:111:TYR:HB2  | 1.88                     | 0.56              |
| 1:B:366:ALA:HB3  | 1:B:369:GLU:HG3  | 1.87                     | 0.56              |
| 1:A:321:ASN:HD22 | 1:A:322:PRO:HD2  | 1.70                     | 0.56              |
| 1:B:321:ASN:OD1  | 1:B:324:HIS:ND1  | 2.37                     | 0.56              |
| 1:B:346:PHE:CE2  | 1:B:477:PRO:HB3  | 2.41                     | 0.56              |
| 1:C:21:ASN:CG    | 1:C:22:ALA:H     | 2.09                     | 0.56              |
| 1:C:190:VAL:HG13 | 1:C:256:LEU:HB3  | 1.88                     | 0.56              |
| 1:A:196:MET:CE   | 1:A:219:TYR:HB2  | 2.35                     | 0.56              |
| 1:A:339:GLU:OE1  | 1:A:340:ASP:N    | 2.35                     | 0.56              |
| 1:B:214:ARG:HG2  | 1:B:214:ARG:HH11 | 1.71                     | 0.56              |
| 1:C:475:ILE:O    | 1:C:477:PRO:HD3  | 2.05                     | 0.56              |
| 1:A:189:MET:CE   | 1:A:192:GLU:OE1  | 2.52                     | 0.56              |
| 1:C:231:GLN:HG3  | 1:C:395:ASN:CG   | 2.31                     | 0.56              |
| 1:A:31:LYS:HD3   | 1:A:292:GLU:OE2  | 2.05                     | 0.55              |
| 1:A:321:ASN:HD22 | 1:A:322:PRO:CD   | 2.20                     | 0.55              |
| 1:A:353:VAL:HG13 | 1:A:354:PRO:HD2  | 1.88                     | 0.55              |
| 1:A:370:ASN:HD22 | 1:A:372:GLU:HB3  | 1.70                     | 0.55              |
| 1:A:415:GLN:HE21 | 1:C:460:GLY:H    | 1.53                     | 0.55              |
| 1:A:417:ASN:HA   | 1:C:455:ASP:O    | 2.06                     | 0.55              |
| 1:A:230:PHE:HB3  | 1:A:235:GLN:HB3  | 1.88                     | 0.55              |
| 1:A:163:MET:HE3  | 1:A:261:ARG:CG   | 2.32                     | 0.55              |
| 1:B:21:ASN:HB3   | 1:B:24:GLU:CG    | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:39:PHE:CE2   | 1:B:67:VAL:HG21  | 2.42                     | 0.55              |
| 1:B:134:THR:CG2  | 1:B:177:GLY:H    | 2.19                     | 0.55              |
| 1:A:263:ALA:HA   | 1:A:266:LEU:O    | 2.06                     | 0.55              |
| 1:B:189:MET:HE2  | 1:B:189:MET:HA   | 1.87                     | 0.55              |
| 1:A:39:PHE:CZ    | 1:A:67:VAL:HG21  | 2.42                     | 0.55              |
| 1:B:454:GLU:H    | 1:B:454:GLU:CD   | 2.15                     | 0.55              |
| 1:C:369:GLU:HG3  | 1:C:370:ASN:H    | 1.72                     | 0.55              |
| 1:A:252:GLU:O    | 1:A:255:ASP:N    | 2.40                     | 0.55              |
| 1:B:465:GLU:HB2  | 1:B:468:ASP:HB2  | 1.88                     | 0.55              |
| 1:C:353:VAL:HG22 | 1:C:354:PRO:CD   | 2.32                     | 0.55              |
| 1:A:311:GLN:HG3  | 1:A:313:TYR:CZ   | 2.42                     | 0.55              |
| 1:B:231:GLN:HE22 | 1:B:269:SER:HB3  | 1.70                     | 0.55              |
| 1:C:303:PRO:HG2  | 1:C:389:ARG:HH12 | 1.72                     | 0.55              |
| 1:A:243:ARG:O    | 1:A:243:ARG:HG2  | 2.06                     | 0.54              |
| 1:B:167:MET:HE1  | 1:B:187:GLY:HA3  | 1.89                     | 0.54              |
| 1:C:194:ILE:HD11 | 1:C:256:LEU:HB2  | 1.89                     | 0.54              |
| 1:A:97:TYR:CD1   | 1:A:97:TYR:N     | 2.74                     | 0.54              |
| 1:B:190:VAL:O    | 1:B:194:ILE:HD13 | 2.08                     | 0.54              |
| 1:C:43:MET:HE3   | 1:C:119:ILE:HG21 | 1.88                     | 0.54              |
| 1:C:198:LYS:HD3  | 1:C:201:ILE:CD1  | 2.37                     | 0.54              |
| 1:C:270:VAL:CG1  | 1:C:271:ALA:N    | 2.69                     | 0.54              |
| 1:B:56:LEU:HD11  | 1:B:315:LEU:HG   | 1.89                     | 0.54              |
| 1:A:162:ARG:HD3  | 1:B:402:SER:CB   | 2.38                     | 0.54              |
| 1:B:303:PRO:HG2  | 1:B:389:ARG:HH12 | 1.72                     | 0.54              |
| 1:B:339:GLU:OE2  | 1:C:416:ARG:NH1  | 2.40                     | 0.54              |
| 1:B:339:GLU:C    | 1:C:408:ILE:HD11 | 2.33                     | 0.54              |
| 1:B:416:ARG:HD2  | 1:B:418:LEU:CD2  | 2.38                     | 0.54              |
| 1:C:21:ASN:OD1   | 1:C:22:ALA:N     | 2.33                     | 0.54              |
| 1:C:107:GLU:O    | 1:C:109:ILE:N    | 2.41                     | 0.54              |
| 1:C:196:MET:O    | 1:C:197:ILE:C    | 2.50                     | 0.54              |
| 1:C:143:LEU:HA   | 1:C:332:ALA:CB   | 2.38                     | 0.54              |
| 1:C:38:ARG:HD2   | 1:C:123:ALA:O    | 2.08                     | 0.53              |
| 1:C:344:SER:O    | 1:C:347:ILE:HG22 | 2.08                     | 0.53              |
| 1:C:348:ARG:NH2  | 1:C:380:GLU:O    | 2.40                     | 0.53              |
| 1:C:58:GLN:HG3   | 1:C:315:LEU:HG   | 1.90                     | 0.53              |
| 1:C:321:ASN:HB3  | 1:C:324:HIS:CD2  | 2.42                     | 0.53              |
| 1:C:321:ASN:HB3  | 1:C:324:HIS:CG   | 2.43                     | 0.53              |
| 1:C:348:ARG:HA   | 1:C:383:SER:OG   | 2.07                     | 0.53              |
| 1:B:34:ASP:OD1   | 1:B:38:ARG:NH2   | 2.41                     | 0.53              |
| 1:A:167:MET:HG3  | 1:A:170:SER:HB3  | 1.91                     | 0.53              |
| 1:A:411:THR:O    | 1:C:389:ARG:HA   | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:420:PHE:HA   | 1:C:487:TYR:OH   | 2.09                     | 0.53              |
| 1:C:227:LYS:HB2  | 1:C:239:VAL:HG11 | 1.89                     | 0.53              |
| 1:C:252:GLU:H    | 1:C:252:GLU:CD   | 2.17                     | 0.53              |
| 1:A:460:GLY:H    | 1:B:415:GLN:NE2  | 2.07                     | 0.53              |
| 1:C:355:ARG:HB2  | 1:C:488:PHE:CE2  | 2.44                     | 0.53              |
| 1:B:197:ILE:HG23 | 1:B:248:PRO:HB2  | 1.91                     | 0.53              |
| 1:B:291:PHE:O    | 1:B:295:GLY:N    | 2.40                     | 0.53              |
| 1:C:121:ARG:HB3  | 1:C:126:GLY:HA2  | 1.91                     | 0.53              |
| 1:A:270:VAL:N    | 1:A:391:ARG:O    | 2.42                     | 0.53              |
| 1:C:33:ILE:HG23  | 1:C:281:TYR:CE2  | 2.43                     | 0.53              |
| 1:C:267:ARG:HG3  | 1:C:393:GLY:O    | 2.09                     | 0.53              |
| 1:B:355:ARG:HG2  | 1:B:489:PHE:CE2  | 2.43                     | 0.52              |
| 1:C:302:ASP:O    | 1:C:306:LEU:HD13 | 2.09                     | 0.52              |
| 1:A:189:MET:HE2  | 1:A:189:MET:HA   | 1.91                     | 0.52              |
| 1:A:232:THR:O    | 1:A:236:ARG:HG3  | 2.09                     | 0.52              |
| 1:A:339:GLU:OE1  | 1:B:416:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:134:THR:O    | 1:A:137:MET:HB3  | 2.10                     | 0.52              |
| 1:A:71:PHE:CD1   | 1:A:117:ARG:HG2  | 2.44                     | 0.52              |
| 1:A:100:VAL:HG12 | 1:A:101:ASP:N    | 2.22                     | 0.52              |
| 1:A:370:ASN:ND2  | 1:A:372:GLU:HB3  | 2.24                     | 0.52              |
| 1:C:174:ARG:HD3  | 1:C:175:ARG:H    | 1.75                     | 0.52              |
| 1:C:270:VAL:HG12 | 1:C:271:ALA:H    | 1.74                     | 0.52              |
| 1:A:106:ARG:NH2  | 1:A:371:MET:HE3  | 2.25                     | 0.52              |
| 1:B:265:ILE:HD11 | 1:B:448:MET:CB   | 2.39                     | 0.52              |
| 1:C:342:ARG:HB3  | 1:C:479:PHE:CD2  | 2.45                     | 0.52              |
| 1:A:69:SER:OG    | 1:A:92:THR:HG21  | 2.10                     | 0.52              |
| 1:C:247:ASN:O    | 1:C:248:PRO:C    | 2.53                     | 0.52              |
| 1:B:69:SER:OG    | 1:B:92:THR:CG2   | 2.58                     | 0.52              |
| 1:B:327:GLN:O    | 1:B:331:MET:HG3  | 2.09                     | 0.52              |
| 1:B:276:LEU:HD13 | 1:B:280:VAL:HG11 | 1.90                     | 0.52              |
| 1:B:385:TYR:HB3  | 1:B:463:VAL:HG12 | 1.92                     | 0.52              |
| 1:B:416:ARG:HD2  | 1:B:418:LEU:HD23 | 1.92                     | 0.52              |
| 1:A:39:PHE:CE2   | 1:A:67:VAL:HG21  | 2.45                     | 0.51              |
| 1:A:196:MET:HE1  | 1:A:219:TYR:CB   | 2.38                     | 0.51              |
| 1:A:342:ARG:HH22 | 1:B:417:ASN:ND2  | 2.08                     | 0.51              |
| 1:B:385:TYR:HB3  | 1:B:463:VAL:CG1  | 2.40                     | 0.51              |
| 1:C:261:ARG:O    | 1:C:264:LEU:HB2  | 2.10                     | 0.51              |
| 1:C:265:ILE:HD11 | 1:C:448:MET:CE   | 2.40                     | 0.51              |
| 1:A:111:TYR:CD2  | 1:A:116:ILE:HD11 | 2.45                     | 0.51              |
| 1:A:315:LEU:HB2  | 1:A:365:ILE:HD11 | 1.92                     | 0.51              |
| 1:A:343:VAL:HG13 | 1:A:344:SER:N    | 2.24                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:LEU:HD23  | 1:C:64:GLU:OE1   | 2.09                     | 0.51              |
| 1:A:35:GLY:HA3   | 1:A:124:ASN:OD1  | 2.11                     | 0.51              |
| 1:A:297:SER:C    | 1:A:298:LEU:HD12 | 2.35                     | 0.51              |
| 1:A:317:ARG:HB2  | 1:A:320:GLU:HG3  | 1.91                     | 0.51              |
| 1:B:155:VAL:CG2  | 1:B:156:ARG:N    | 2.71                     | 0.51              |
| 1:B:386:TRP:NE1  | 1:B:464:PHE:HB2  | 2.25                     | 0.51              |
| 1:B:406:ILE:O    | 1:B:420:PHE:HA   | 2.10                     | 0.51              |
| 1:C:341:LEU:CB   | 1:C:486:SER:HA   | 2.32                     | 0.51              |
| 1:A:296:TYR:CE1  | 1:A:302:ASP:HB3  | 2.46                     | 0.51              |
| 1:A:171:THR:O    | 1:A:173:PRO:HD3  | 2.11                     | 0.51              |
| 1:B:343:VAL:HG23 | 1:B:344:SER:N    | 2.26                     | 0.51              |
| 1:B:461:ARG:HD2  | 1:B:461:ARG:N    | 2.26                     | 0.51              |
| 1:C:319:ASN:N    | 1:C:319:ASN:HD22 | 2.08                     | 0.51              |
| 1:A:458:PHE:HB2  | 1:B:414:VAL:O    | 2.11                     | 0.51              |
| 1:C:331:MET:HE1  | 1:C:488:PHE:CD1  | 2.46                     | 0.51              |
| 1:A:53:GLU:OE2   | 1:A:99:ARG:N     | 2.41                     | 0.51              |
| 1:A:291:PHE:O    | 1:A:295:GLY:N    | 2.42                     | 0.51              |
| 1:B:321:ASN:HD22 | 1:B:322:PRO:N    | 2.09                     | 0.51              |
| 1:C:24:GLU:O     | 1:C:25:ILE:C     | 2.54                     | 0.51              |
| 1:C:422:ARG:HG2  | 1:C:422:ARG:NH1  | 2.26                     | 0.51              |
| 1:A:238:MET:HE2  | 1:A:259:LEU:HD13 | 1.92                     | 0.51              |
| 1:B:408:ILE:O    | 1:B:408:ILE:HG22 | 2.09                     | 0.51              |
| 1:C:57:ILE:HG22  | 1:C:58:GLN:N     | 2.26                     | 0.51              |
| 1:A:38:ARG:NH1   | 1:A:123:ALA:O    | 2.44                     | 0.50              |
| 1:A:253:PHE:O    | 1:A:257:ILE:HG13 | 2.11                     | 0.50              |
| 1:C:421:ASP:OD1  | 1:C:424:THR:HG23 | 2.10                     | 0.50              |
| 1:A:56:LEU:O     | 1:A:57:ILE:C     | 2.54                     | 0.50              |
| 1:B:423:PRO:O    | 1:B:425:ILE:N    | 2.44                     | 0.50              |
| 1:C:345:SER:CB   | 1:C:352:VAL:H    | 2.24                     | 0.50              |
| 1:A:106:ARG:NH1  | 1:A:367:SER:HA   | 2.26                     | 0.50              |
| 1:A:137:MET:CE   | 1:A:175:ARG:HE   | 2.25                     | 0.50              |
| 1:A:168:GLN:O    | 1:A:184:LYS:HA   | 2.11                     | 0.50              |
| 1:C:291:PHE:HE2  | 1:C:306:LEU:HD21 | 1.75                     | 0.50              |
| 1:A:223:CYS:O    | 1:A:226:LEU:HB3  | 2.11                     | 0.50              |
| 1:A:29:VAL:O     | 1:A:32:MET:HG3   | 2.10                     | 0.50              |
| 1:A:406:ILE:O    | 1:A:406:ILE:HG22 | 2.10                     | 0.50              |
| 1:B:303:PRO:CG   | 1:B:389:ARG:HH12 | 2.24                     | 0.50              |
| 1:B:324:HIS:HD2  | 1:B:358:LEU:HA   | 1.75                     | 0.50              |
| 1:A:311:GLN:HG3  | 1:A:313:TYR:OH   | 2.12                     | 0.50              |
| 1:C:250:ASN:HA   | 1:C:253:PHE:HB3  | 1.93                     | 0.50              |
| 1:A:146:ALA:HB2  | 1:A:337:ALA:HB2  | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:ASP:HB2  | 1:A:303:PRO:HD3  | 1.93                     | 0.50              |
| 1:C:100:VAL:HG23 | 1:C:100:VAL:O    | 2.11                     | 0.50              |
| 1:A:321:ASN:HD22 | 1:A:322:PRO:N    | 2.09                     | 0.50              |
| 1:B:457:SER:O    | 1:C:415:GLN:HA   | 2.12                     | 0.50              |
| 1:C:321:ASN:HD22 | 1:C:322:PRO:HD2  | 1.76                     | 0.50              |
| 1:B:60:SER:OG    | 1:B:278:ALA:HB3  | 2.11                     | 0.50              |
| 1:B:134:THR:HG23 | 1:B:177:GLY:H    | 1.76                     | 0.50              |
| 1:A:308:GLN:HE22 | 1:A:383:SER:N    | 2.01                     | 0.49              |
| 1:A:402:SER:HB3  | 1:C:162:ARG:NE   | 2.27                     | 0.49              |
| 1:C:164:CYS:C    | 1:C:166:LEU:N    | 2.68                     | 0.49              |
| 1:C:37:GLY:O     | 1:C:41:ILE:HG13  | 2.12                     | 0.49              |
| 1:C:38:ARG:CD    | 1:C:123:ALA:O    | 2.60                     | 0.49              |
| 1:C:394:GLY:O    | 1:C:395:ASN:O    | 2.30                     | 0.49              |
| 1:A:483:ASN:ND2  | 1:B:476:VAL:O    | 2.46                     | 0.49              |
| 1:C:100:VAL:O    | 1:C:103:LYS:O    | 2.30                     | 0.49              |
| 1:A:118:ARG:HH21 | 1:A:122:GLN:HG3  | 1.77                     | 0.49              |
| 1:B:316:ILE:CG1  | 1:B:320:GLU:HB3  | 2.42                     | 0.49              |
| 1:B:452:ARG:NH1  | 1:C:449:GLU:OE2  | 2.42                     | 0.49              |
| 1:C:300:GLY:O    | 1:C:303:PRO:HD2  | 2.12                     | 0.49              |
| 1:C:410:PRO:HA   | 1:C:416:ARG:HH21 | 1.77                     | 0.49              |
| 1:A:58:GLN:HE21  | 1:A:58:GLN:HA    | 1.77                     | 0.49              |
| 1:B:30:GLY:O     | 1:B:34:ASP:HB2   | 2.12                     | 0.49              |
| 1:C:243:ARG:O    | 1:C:243:ARG:HG3  | 2.11                     | 0.49              |
| 1:A:483:ASN:HD21 | 1:B:478:SER:HB2  | 1.77                     | 0.49              |
| 1:B:488:PHE:H    | 1:C:405:GLN:NE2  | 2.11                     | 0.49              |
| 1:C:104:TRP:CZ2  | 1:C:376:SER:CB   | 2.96                     | 0.49              |
| 1:A:162:ARG:HG2  | 1:B:404:GLY:O    | 2.13                     | 0.49              |
| 1:C:33:ILE:HD12  | 1:C:281:TYR:CE2  | 2.40                     | 0.49              |
| 1:C:143:LEU:HA   | 1:C:332:ALA:HB1  | 1.95                     | 0.49              |
| 1:C:195:ARG:CG   | 1:C:196:MET:N    | 2.76                     | 0.49              |
| 1:C:289:TYR:CZ   | 1:C:294:GLU:HG2  | 2.48                     | 0.49              |
| 1:C:291:PHE:CE2  | 1:C:306:LEU:HD21 | 2.48                     | 0.49              |
| 1:A:406:ILE:HG23 | 1:A:421:ASP:HB3  | 1.94                     | 0.49              |
| 1:C:52:TYR:HE2   | 1:C:104:TRP:HH2  | 1.59                     | 0.49              |
| 1:C:247:ASN:C    | 1:C:247:ASN:HD22 | 2.20                     | 0.49              |
| 1:A:26:ARG:NH1   | 1:A:295:GLY:C    | 2.71                     | 0.48              |
| 1:B:92:THR:CG2   | 1:B:93:GLY:N     | 2.74                     | 0.48              |
| 1:B:234:ALA:HB1  | 1:B:444:ILE:CG1  | 2.41                     | 0.48              |
| 1:C:22:ALA:O     | 1:C:25:ILE:HG12  | 2.13                     | 0.48              |
| 1:B:37:GLY:O     | 1:B:41:ILE:HG13  | 2.13                     | 0.48              |
| 1:A:166:LEU:HD21 | 1:A:264:LEU:HD23 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:267:ARG:HH21 | 1:B:418:LEU:HB2  | 1.77                     | 0.48              |
| 1:B:190:VAL:HG13 | 1:B:256:LEU:HB3  | 1.94                     | 0.48              |
| 1:B:326:SER:HA   | 1:B:379:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:43:MET:CE    | 1:C:119:ILE:HG21 | 2.44                     | 0.48              |
| 1:C:171:THR:O    | 1:C:171:THR:CG2  | 2.60                     | 0.48              |
| 1:C:370:ASN:OD1  | 1:C:373:THR:HG23 | 2.12                     | 0.48              |
| 1:A:63:ILE:O     | 1:A:67:VAL:HG23  | 2.12                     | 0.48              |
| 1:A:298:LEU:N    | 1:A:298:LEU:CD1  | 2.76                     | 0.48              |
| 1:A:345:SER:HA   | 1:A:352:VAL:HG23 | 1.96                     | 0.48              |
| 1:A:56:LEU:HG    | 1:A:58:GLN:HG2   | 1.95                     | 0.48              |
| 1:B:97:TYR:CD1   | 1:B:97:TYR:N     | 2.81                     | 0.48              |
| 1:B:168:GLN:O    | 1:B:184:LYS:HA   | 2.13                     | 0.48              |
| 1:B:301:ILE:O    | 1:B:302:ASP:C    | 2.54                     | 0.48              |
| 1:B:321:ASN:ND2  | 1:B:322:PRO:HD2  | 2.27                     | 0.48              |
| 1:B:453:PRO:O    | 1:C:417:ASN:HB2  | 2.12                     | 0.48              |
| 1:C:98:ARG:NE    | 1:C:107:GLU:OE2  | 2.44                     | 0.48              |
| 1:C:113:LYS:H    | 1:C:113:LYS:CD   | 2.22                     | 0.48              |
| 1:C:265:ILE:HG13 | 1:C:266:LEU:N    | 2.27                     | 0.48              |
| 1:A:189:MET:HB2  | 1:A:226:LEU:HD23 | 1.95                     | 0.48              |
| 1:B:68:LEU:C     | 1:B:175:ARG:HH22 | 2.22                     | 0.48              |
| 1:B:157:THR:HG22 | 1:B:194:ILE:HG21 | 1.96                     | 0.48              |
| 1:C:321:ASN:HD22 | 1:C:322:PRO:CD   | 2.26                     | 0.48              |
| 1:A:365:ILE:HG12 | 1:A:374:MET:HE3  | 1.96                     | 0.48              |
| 1:B:156:ARG:NH1  | 1:B:195:ARG:NH1  | 2.61                     | 0.48              |
| 1:B:258:PHE:O    | 1:B:261:ARG:HB3  | 2.14                     | 0.48              |
| 1:C:174:ARG:HD3  | 1:C:175:ARG:N    | 2.28                     | 0.48              |
| 1:C:164:CYS:C    | 1:C:166:LEU:H    | 2.21                     | 0.48              |
| 1:C:340:ASP:HA   | 1:C:486:SER:HB2  | 1.96                     | 0.48              |
| 1:C:477:PRO:HB2  | 1:C:479:PHE:CE1  | 2.49                     | 0.48              |
| 1:B:214:ARG:HG2  | 1:B:214:ARG:NH1  | 2.27                     | 0.47              |
| 1:B:455:ASP:O    | 1:C:417:ASN:HA   | 2.13                     | 0.47              |
| 1:C:121:ARG:O    | 1:C:126:GLY:N    | 2.37                     | 0.47              |
| 1:C:341:LEU:HD12 | 1:C:485:GLY:O    | 2.14                     | 0.47              |
| 1:A:477:PRO:HG3  | 1:B:414:VAL:HG11 | 1.96                     | 0.47              |
| 1:B:37:GLY:HA2   | 1:B:282:GLY:N    | 2.29                     | 0.47              |
| 1:B:386:TRP:HB3  | 1:B:466:LEU:CD2  | 2.43                     | 0.47              |
| 1:C:297:SER:O    | 1:C:303:PRO:HG3  | 2.14                     | 0.47              |
| 1:B:143:LEU:HD11 | 1:B:363:VAL:HG21 | 1.97                     | 0.47              |
| 1:C:22:ALA:O     | 1:C:25:ILE:CG1   | 2.62                     | 0.47              |
| 1:C:230:PHE:CD1  | 1:C:235:GLN:HB3  | 2.49                     | 0.47              |
| 1:A:226:LEU:HD12 | 1:A:239:VAL:HG13 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:PRO:HD3  | 1:A:373:THR:O    | 2.14                     | 0.47              |
| 1:B:293:ARG:HG3  | 1:B:293:ARG:HH11 | 1.80                     | 0.47              |
| 1:B:124:ASN:O    | 1:B:127:ASP:OD2  | 2.32                     | 0.47              |
| 1:B:395:ASN:HD22 | 1:B:395:ASN:C    | 2.22                     | 0.47              |
| 1:C:406:ILE:HG13 | 1:C:421:ASP:HB3  | 1.95                     | 0.47              |
| 1:B:62:THR:HG23  | 1:B:94:GLY:HA3   | 1.97                     | 0.47              |
| 1:B:92:THR:OG1   | 1:B:113:LYS:HG2  | 2.15                     | 0.47              |
| 1:B:348:ARG:HG2  | 1:B:348:ARG:NH1  | 2.29                     | 0.47              |
| 1:C:331:MET:HE1  | 1:C:488:PHE:CE1  | 2.50                     | 0.47              |
| 1:A:40:TYR:CE2   | 1:A:279:CYS:HA   | 2.50                     | 0.47              |
| 1:A:316:ILE:HG22 | 1:A:376:SER:HA   | 1.95                     | 0.47              |
| 1:A:443:GLU:O    | 1:A:447:LEU:HG   | 2.15                     | 0.47              |
| 1:B:155:VAL:CG2  | 1:B:156:ARG:H    | 2.27                     | 0.47              |
| 1:B:166:LEU:HB3  | 1:B:187:GLY:H    | 1.78                     | 0.47              |
| 1:B:449:GLU:OE2  | 1:C:446:ARG:NH1  | 2.40                     | 0.47              |
| 1:C:49:LEU:HD22  | 1:C:53:GLU:HB3   | 1.97                     | 0.47              |
| 1:C:115:GLU:OE2  | 1:C:118:ARG:NH2  | 2.48                     | 0.47              |
| 1:C:141:SER:OG   | 1:C:169:GLY:HA2  | 2.14                     | 0.47              |
| 1:C:143:LEU:HD12 | 1:C:143:LEU:O    | 2.13                     | 0.47              |
| 1:C:208:ARG:HG2  | 1:C:208:ARG:HH11 | 1.80                     | 0.47              |
| 1:A:174:ARG:HD3  | 1:A:175:ARG:H    | 1.80                     | 0.47              |
| 1:A:417:ASN:C    | 1:A:417:ASN:OD1  | 2.58                     | 0.47              |
| 1:B:100:VAL:O    | 1:B:101:ASP:C    | 2.56                     | 0.47              |
| 1:C:258:PHE:HE2  | 1:C:444:ILE:HD12 | 1.80                     | 0.47              |
| 1:A:106:ARG:HH12 | 1:A:367:SER:HA   | 1.79                     | 0.47              |
| 1:A:368:ASN:N    | 1:A:368:ASN:HD22 | 2.13                     | 0.47              |
| 1:B:190:VAL:HG12 | 1:B:194:ILE:HD13 | 1.97                     | 0.47              |
| 1:C:92:THR:HG21  | 1:C:116:ILE:HD12 | 1.96                     | 0.47              |
| 1:C:106:ARG:NH1  | 1:C:367:SER:HA   | 2.22                     | 0.47              |
| 1:C:135:HIS:HE1  | 1:C:298:LEU:CD2  | 2.27                     | 0.47              |
| 1:A:112:ASP:O    | 1:A:113:LYS:C    | 2.56                     | 0.47              |
| 1:B:343:VAL:HG11 | 1:C:416:ARG:HH11 | 1.80                     | 0.47              |
| 1:C:345:SER:HB3  | 1:C:352:VAL:H    | 1.79                     | 0.47              |
| 1:A:267:ARG:HH21 | 1:B:418:LEU:CB   | 2.27                     | 0.46              |
| 1:C:385:TYR:HB3  | 1:C:463:VAL:CG1  | 2.45                     | 0.46              |
| 1:A:143:LEU:HA   | 1:A:332:ALA:HB2  | 1.96                     | 0.46              |
| 1:A:297:SER:O    | 1:A:303:PRO:HG3  | 2.16                     | 0.46              |
| 1:A:386:TRP:NE1  | 1:A:464:PHE:HB2  | 2.30                     | 0.46              |
| 1:B:96:ILE:HG13  | 1:B:109:ILE:CD1  | 2.40                     | 0.46              |
| 1:C:438:SER:HB3  | 1:C:441:ARG:CG   | 2.44                     | 0.46              |
| 1:A:170:SER:HA   | 1:A:188:THR:HG23 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:304:PHE:CE2  | 1:A:386:TRP:HA   | 2.50                     | 0.46              |
| 1:B:93:GLY:HA2   | 1:B:109:ILE:O    | 2.15                     | 0.46              |
| 1:C:265:ILE:CG1  | 1:C:266:LEU:H    | 2.29                     | 0.46              |
| 1:A:342:ARG:HB3  | 1:A:479:PHE:HE2  | 1.73                     | 0.46              |
| 1:B:302:ASP:N    | 1:B:303:PRO:HD2  | 2.31                     | 0.46              |
| 1:C:204:ARG:O    | 1:C:205:ASN:HB2  | 2.15                     | 0.46              |
| 1:A:39:PHE:CZ    | 1:A:67:VAL:CG2   | 2.99                     | 0.46              |
| 1:A:487:TYR:HB3  | 1:B:405:GLN:HB2  | 1.96                     | 0.46              |
| 1:C:129:ALA:O    | 1:C:133:LEU:HG   | 2.16                     | 0.46              |
| 1:B:296:TYR:CE1  | 1:B:302:ASP:HB3  | 2.51                     | 0.46              |
| 1:B:300:GLY:O    | 1:B:303:PRO:HD2  | 2.16                     | 0.46              |
| 1:B:393:GLY:HA2  | 1:C:410:PRO:HG3  | 1.97                     | 0.46              |
| 1:C:111:TYR:HB3  | 1:C:116:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:58:GLN:HG3   | 1:B:315:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:423:PRO:O    | 1:B:424:THR:C    | 2.57                     | 0.46              |
| 1:A:232:THR:OG1  | 1:A:235:GLN:CG   | 2.61                     | 0.46              |
| 1:A:253:PHE:C    | 1:A:253:PHE:HD2  | 2.21                     | 0.46              |
| 1:A:324:HIS:HD2  | 1:A:358:LEU:HA   | 1.81                     | 0.46              |
| 1:B:234:ALA:HB1  | 1:B:444:ILE:HG12 | 1.97                     | 0.46              |
| 1:C:342:ARG:C    | 1:C:344:SER:N    | 2.73                     | 0.46              |
| 1:C:56:LEU:HD22  | 1:C:104:TRP:CZ3  | 2.50                     | 0.46              |
| 1:A:53:GLU:OE2   | 1:A:98:ARG:HA    | 2.15                     | 0.45              |
| 1:C:34:ASP:OD2   | 1:C:291:PHE:HB2  | 2.16                     | 0.45              |
| 1:C:95:PRO:HB2   | 1:C:97:TYR:HE2   | 1.81                     | 0.45              |
| 1:A:402:SER:HB3  | 1:C:162:ARG:CZ   | 2.47                     | 0.45              |
| 1:C:164:CYS:O    | 1:C:166:LEU:N    | 2.49                     | 0.45              |
| 1:C:457:SER:O    | 1:C:458:PHE:HB2  | 2.16                     | 0.45              |
| 1:A:143:LEU:HA   | 1:A:332:ALA:CB   | 2.47                     | 0.45              |
| 1:A:426:MET:HE2  | 1:A:426:MET:CA   | 2.44                     | 0.45              |
| 1:C:342:ARG:C    | 1:C:344:SER:H    | 2.23                     | 0.45              |
| 1:C:406:ILE:HD11 | 1:C:425:ILE:HG13 | 1.99                     | 0.45              |
| 1:B:232:THR:OG1  | 1:B:235:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:276:LEU:HD22 | 1:B:307:LEU:HD21 | 1.99                     | 0.45              |
| 1:C:247:ASN:N    | 1:C:248:PRO:HD3  | 2.31                     | 0.45              |
| 1:C:270:VAL:CG1  | 1:C:271:ALA:H    | 2.29                     | 0.45              |
| 1:B:170:SER:HA   | 1:B:188:THR:HG23 | 1.99                     | 0.45              |
| 1:A:39:PHE:CE1   | 1:A:43:MET:HE2   | 2.51                     | 0.45              |
| 1:A:121:ARG:O    | 1:A:122:GLN:C    | 2.60                     | 0.45              |
| 1:A:321:ASN:HD22 | 1:A:321:ASN:C    | 2.24                     | 0.45              |
| 1:C:33:ILE:HG23  | 1:C:281:TYR:HD2  | 1.79                     | 0.45              |
| 1:A:269:SER:HA   | 1:A:391:ARG:O    | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:160:ASP:C    | 1:B:162:ARG:H    | 2.24                     | 0.45              |
| 1:C:215:THR:O    | 1:C:218:ALA:N    | 2.50                     | 0.45              |
| 1:B:193:LEU:O    | 1:B:197:ILE:HG12 | 2.16                     | 0.45              |
| 1:B:255:ASP:O    | 1:B:258:PHE:HB3  | 2.17                     | 0.45              |
| 1:A:56:LEU:O     | 1:A:58:GLN:N     | 2.49                     | 0.45              |
| 1:A:232:THR:HG1  | 1:A:235:GLN:HG3  | 1.80                     | 0.45              |
| 1:A:407:SER:HG   | 1:C:267:ARG:NH1  | 2.12                     | 0.45              |
| 1:B:141:SER:HB2  | 1:B:172:LEU:HD12 | 1.98                     | 0.45              |
| 1:C:230:PHE:CE1  | 1:C:259:LEU:HD12 | 2.52                     | 0.45              |
| 1:C:356:GLY:O    | 1:C:357:LYS:HG3  | 2.17                     | 0.45              |
| 1:A:92:THR:CA    | 1:A:113:LYS:HZ3  | 2.30                     | 0.45              |
| 1:A:174:ARG:CD   | 1:A:175:ARG:H    | 2.30                     | 0.45              |
| 1:A:184:LYS:HD3  | 1:A:189:MET:HE3  | 1.98                     | 0.45              |
| 1:B:232:THR:CG2  | 1:B:235:GLN:HE21 | 2.30                     | 0.45              |
| 1:B:440:MET:HE2  | 1:B:440:MET:HA   | 1.99                     | 0.45              |
| 1:B:451:ALA:O    | 1:B:452:ARG:HD3  | 2.17                     | 0.45              |
| 1:C:25:ILE:O     | 1:C:29:VAL:HG23  | 2.17                     | 0.45              |
| 1:C:58:GLN:HA    | 1:C:58:GLN:HE21  | 1.82                     | 0.44              |
| 1:C:456:VAL:O    | 1:C:456:VAL:HG13 | 2.17                     | 0.44              |
| 1:A:111:TYR:HD2  | 1:A:116:ILE:HD11 | 1.81                     | 0.44              |
| 1:C:116:ILE:O    | 1:C:119:ILE:HG22 | 2.16                     | 0.44              |
| 1:C:193:LEU:HD21 | 1:C:222:MET:HB2  | 1.98                     | 0.44              |
| 1:A:68:LEU:HD21  | 1:A:133:LEU:O    | 2.17                     | 0.44              |
| 1:A:487:TYR:N    | 1:A:487:TYR:CD2  | 2.84                     | 0.44              |
| 1:C:30:GLY:HA2   | 1:C:291:PHE:HB3  | 1.98                     | 0.44              |
| 1:C:44:CYS:SG    | 1:C:49:LEU:HD12  | 2.58                     | 0.44              |
| 1:C:58:GLN:HE21  | 1:C:58:GLN:CA    | 2.29                     | 0.44              |
| 1:C:135:HIS:CE1  | 1:C:298:LEU:HD21 | 2.53                     | 0.44              |
| 1:B:37:GLY:CA    | 1:B:282:GLY:HA2  | 2.47                     | 0.44              |
| 1:B:408:ILE:HD12 | 1:B:419:PRO:HB2  | 1.98                     | 0.44              |
| 1:A:34:ASP:OD2   | 1:A:291:PHE:HB2  | 2.17                     | 0.44              |
| 1:C:58:GLN:HE22  | 1:C:363:VAL:HG13 | 1.81                     | 0.44              |
| 1:C:154:LEU:CD2  | 1:C:167:MET:HE3  | 2.34                     | 0.44              |
| 1:C:301:ILE:HG12 | 1:C:305:ARG:HG3  | 1.99                     | 0.44              |
| 1:A:386:TRP:CE2  | 1:A:464:PHE:HB2  | 2.53                     | 0.44              |
| 1:B:41:ILE:HD11  | 1:B:286:ALA:N    | 2.32                     | 0.44              |
| 1:C:160:ASP:O    | 1:C:163:MET:HG3  | 2.18                     | 0.44              |
| 1:A:47:LEU:HD11  | 1:A:109:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:342:ARG:HH22 | 1:B:417:ASN:HD21 | 1.65                     | 0.44              |
| 1:C:46:GLU:C     | 1:C:48:LYS:N     | 2.72                     | 0.44              |
| 1:C:406:ILE:O    | 1:C:406:ILE:HG12 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:422:ARG:HB3  | 1:C:423:PRO:CD   | 2.45                     | 0.44              |
| 1:C:438:SER:HB3  | 1:C:441:ARG:CD   | 2.47                     | 0.44              |
| 1:A:50:SER:OG    | 1:A:53:GLU:HG3   | 2.18                     | 0.44              |
| 1:A:197:ILE:HG23 | 1:A:201:ILE:CG1  | 2.45                     | 0.44              |
| 1:B:269:SER:HB2  | 1:B:391:ARG:O    | 2.17                     | 0.44              |
| 1:C:293:ARG:HG2  | 1:C:293:ARG:HH11 | 1.83                     | 0.44              |
| 1:C:485:GLY:O    | 1:C:487:TYR:N    | 2.51                     | 0.44              |
| 1:A:172:LEU:HD12 | 1:A:173:PRO:HD2  | 2.00                     | 0.44              |
| 1:A:416:ARG:HG2  | 1:C:343:VAL:HG11 | 1.99                     | 0.44              |
| 1:B:118:ARG:HD2  | 1:B:119:ILE:N    | 2.33                     | 0.44              |
| 1:A:114:GLU:HA   | 1:A:117:ARG:NE   | 2.24                     | 0.43              |
| 1:A:185:GLY:HA2  | 1:A:270:VAL:HG21 | 2.00                     | 0.43              |
| 1:B:459:GLN:H    | 1:B:459:GLN:NE2  | 2.14                     | 0.43              |
| 1:C:204:ARG:O    | 1:C:205:ASN:CB   | 2.66                     | 0.43              |
| 1:B:63:ILE:O     | 1:B:67:VAL:HG23  | 2.18                     | 0.43              |
| 1:B:343:VAL:HG11 | 1:C:416:ARG:CD   | 2.47                     | 0.43              |
| 1:C:98:ARG:HB2   | 1:C:105:ARG:HB2  | 1.99                     | 0.43              |
| 1:A:145:ASP:OD2  | 1:A:169:GLY:N    | 2.48                     | 0.43              |
| 1:B:312:VAL:O    | 1:B:379:LEU:HB2  | 2.18                     | 0.43              |
| 1:C:58:GLN:CA    | 1:C:58:GLN:NE2   | 2.81                     | 0.43              |
| 1:C:61:LEU:HD12  | 1:C:364:GLN:HG2  | 2.00                     | 0.43              |
| 1:C:293:ARG:C    | 1:C:295:GLY:N    | 2.77                     | 0.43              |
| 1:C:470:LYS:O    | 1:C:471:ALA:C    | 2.61                     | 0.43              |
| 1:A:159:MET:HE3  | 1:A:190:VAL:HG12 | 1.99                     | 0.43              |
| 1:B:384:ARG:HG2  | 1:B:384:ARG:HH11 | 1.84                     | 0.43              |
| 1:C:61:LEU:O     | 1:C:65:ARG:HG3   | 2.18                     | 0.43              |
| 1:C:195:ARG:HG2  | 1:C:196:MET:N    | 2.33                     | 0.43              |
| 1:C:240:ASP:HA   | 1:C:243:ARG:HH12 | 1.80                     | 0.43              |
| 1:B:235:GLN:O    | 1:B:239:VAL:HG23 | 2.18                     | 0.43              |
| 1:C:46:GLU:O     | 1:C:48:LYS:N     | 2.51                     | 0.43              |
| 1:A:51:ASP:O     | 1:A:55:ARG:HG3   | 2.19                     | 0.43              |
| 1:A:420:PHE:CD1  | 1:C:265:ILE:HG22 | 2.53                     | 0.43              |
| 1:B:115:GLU:OE1  | 1:B:115:GLU:CA   | 2.66                     | 0.43              |
| 1:C:320:GLU:OE1  | 1:C:325:LYS:NZ   | 2.51                     | 0.43              |
| 1:C:446:ARG:O    | 1:C:449:GLU:HB3  | 2.19                     | 0.43              |
| 1:B:37:GLY:HA2   | 1:B:282:GLY:CA   | 2.49                     | 0.43              |
| 1:C:205:ASN:N    | 1:C:205:ASN:ND2  | 2.64                     | 0.43              |
| 1:B:39:PHE:CZ    | 1:B:67:VAL:CG2   | 3.01                     | 0.43              |
| 1:B:103:LYS:HD3  | 1:B:372:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:321:ASN:HD22 | 1:B:321:ASN:C    | 2.27                     | 0.43              |
| 1:C:32:MET:O     | 1:C:36:ILE:HG13  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:216:ARG:NH1  | 1:C:245:SER:O    | 2.49                     | 0.43              |
| 1:C:462:GLY:O    | 1:C:464:PHE:CE2  | 2.71                     | 0.43              |
| 1:B:327:GLN:NE2  | 1:B:353:VAL:O    | 2.49                     | 0.43              |
| 1:C:52:TYR:HE2   | 1:C:104:TRP:CH2  | 2.36                     | 0.43              |
| 1:C:194:ILE:HD12 | 1:C:253:PHE:CD1  | 2.49                     | 0.43              |
| 1:C:338:PHE:CD1  | 1:C:338:PHE:N    | 2.87                     | 0.43              |
| 1:C:382:ARG:HG2  | 1:C:382:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:33:ILE:HG22  | 1:A:34:ASP:N     | 2.34                     | 0.42              |
| 1:A:235:GLN:HE21 | 1:A:266:LEU:HB2  | 1.83                     | 0.42              |
| 1:A:223:CYS:O    | 1:A:227:LYS:N    | 2.45                     | 0.42              |
| 1:B:242:VAL:O    | 1:B:242:VAL:HG12 | 2.20                     | 0.42              |
| 1:B:365:ILE:HG21 | 1:B:371:MET:HE1  | 2.01                     | 0.42              |
| 1:C:21:ASN:CG    | 1:C:22:ALA:N     | 2.77                     | 0.42              |
| 1:C:97:TYR:HA    | 1:C:105:ARG:O    | 2.19                     | 0.42              |
| 1:A:37:GLY:HA3   | 1:A:285:VAL:CG2  | 2.46                     | 0.42              |
| 1:A:40:TYR:CE1   | 1:A:63:ILE:HD12  | 2.54                     | 0.42              |
| 1:A:303:PRO:HD2  | 1:A:389:ARG:HH22 | 1.84                     | 0.42              |
| 1:A:451:ALA:C    | 1:A:452:ARG:HD3  | 2.44                     | 0.42              |
| 1:A:453:PRO:HG3  | 1:B:420:PHE:CD1  | 2.53                     | 0.42              |
| 1:C:438:SER:HB3  | 1:C:441:ARG:HD2  | 2.01                     | 0.42              |
| 1:A:58:GLN:HE21  | 1:A:58:GLN:CA    | 2.31                     | 0.42              |
| 1:C:120:TRP:CZ2  | 1:C:129:ALA:HB3  | 2.55                     | 0.42              |
| 1:C:139:TRP:CZ2  | 1:C:143:LEU:HD22 | 2.54                     | 0.42              |
| 1:A:33:ILE:HG21  | 1:A:291:PHE:CG   | 2.54                     | 0.42              |
| 1:B:262:SER:C    | 1:B:264:LEU:H    | 2.27                     | 0.42              |
| 1:B:343:VAL:HG11 | 1:C:416:ARG:HD3  | 2.01                     | 0.42              |
| 1:C:317:ARG:HB2  | 1:C:318:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:58:GLN:HA    | 1:A:58:GLN:NE2   | 2.34                     | 0.42              |
| 1:C:213:ARG:O    | 1:C:217:ILE:HG13 | 2.19                     | 0.42              |
| 1:C:237:THR:O    | 1:C:241:GLN:HG3  | 2.19                     | 0.42              |
| 1:C:316:ILE:HG13 | 1:C:320:GLU:OE1  | 2.19                     | 0.42              |
| 1:A:159:MET:SD   | 1:A:191:MET:HG3  | 2.60                     | 0.42              |
| 1:A:452:ARG:HA   | 1:A:453:PRO:HD3  | 1.95                     | 0.42              |
| 1:C:265:ILE:CG1  | 1:C:266:LEU:N    | 2.83                     | 0.42              |
| 1:A:124:ASN:O    | 1:A:127:ASP:HB2  | 2.20                     | 0.42              |
| 1:A:221:ARG:O    | 1:A:224:ASN:N    | 2.53                     | 0.42              |
| 1:A:317:ARG:HB2  | 1:A:320:GLU:CG   | 2.49                     | 0.42              |
| 1:A:331:MET:HE1  | 1:A:488:PHE:CD1  | 2.55                     | 0.42              |
| 1:A:388:ILE:O    | 1:A:389:ARG:C    | 2.60                     | 0.42              |
| 1:A:487:TYR:O    | 1:A:488:PHE:C    | 2.61                     | 0.42              |
| 1:B:92:THR:HG22  | 1:B:93:GLY:H     | 1.80                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:114:GLU:HA   | 1:B:117:ARG:NE   | 2.34                     | 0.42              |
| 1:B:238:MET:SD   | 1:B:259:LEU:CD1  | 3.08                     | 0.42              |
| 1:C:172:LEU:HD12 | 1:C:172:LEU:HA   | 1.88                     | 0.42              |
| 1:C:361:ARG:HA   | 1:C:361:ARG:HD3  | 1.80                     | 0.42              |
| 1:A:174:ARG:HD3  | 1:A:174:ARG:H    | 1.82                     | 0.42              |
| 1:A:230:PHE:CE2  | 1:A:259:LEU:HG   | 2.55                     | 0.42              |
| 1:A:317:ARG:HB3  | 1:A:318:PRO:HD2  | 2.01                     | 0.42              |
| 1:B:317:ARG:O    | 1:B:318:PRO:C    | 2.62                     | 0.42              |
| 1:B:320:GLU:OE1  | 1:B:360:THR:HG23 | 2.19                     | 0.42              |
| 1:C:60:SER:HB3   | 1:C:279:CYS:HB3  | 2.02                     | 0.42              |
| 1:C:370:ASN:ND2  | 1:C:372:GLU:H    | 2.18                     | 0.42              |
| 1:A:60:SER:O     | 1:A:64:GLU:HG3   | 2.20                     | 0.42              |
| 1:A:114:GLU:HB3  | 1:A:117:ARG:NH2  | 2.26                     | 0.42              |
| 1:A:122:GLN:OE1  | 1:A:122:GLN:HA   | 2.20                     | 0.42              |
| 1:A:424:THR:O    | 1:A:427:ALA:CB   | 2.68                     | 0.42              |
| 1:B:68:LEU:HB3   | 1:B:175:ARG:NH2  | 2.34                     | 0.42              |
| 1:B:149:GLN:HG2  | 1:B:151:THR:HG23 | 2.02                     | 0.42              |
| 1:B:343:VAL:HG21 | 1:C:416:ARG:NH1  | 2.34                     | 0.42              |
| 1:B:395:ASN:C    | 1:B:395:ASN:ND2  | 2.75                     | 0.42              |
| 1:C:192:GLU:HA   | 1:C:195:ARG:HD3  | 2.00                     | 0.42              |
| 1:C:265:ILE:HD11 | 1:C:448:MET:CG   | 2.50                     | 0.42              |
| 1:A:230:PHE:CZ   | 1:A:259:LEU:HG   | 2.55                     | 0.41              |
| 1:A:324:HIS:CD2  | 1:A:358:LEU:HA   | 2.55                     | 0.41              |
| 1:A:346:PHE:HE2  | 1:A:463:VAL:HG21 | 1.85                     | 0.41              |
| 1:A:449:GLU:C    | 1:A:451:ALA:H    | 2.28                     | 0.41              |
| 1:B:234:ALA:CB   | 1:B:444:ILE:HG12 | 2.50                     | 0.41              |
| 1:B:317:ARG:HG2  | 1:B:317:ARG:H    | 1.62                     | 0.41              |
| 1:C:150:ARG:HA   | 1:C:150:ARG:HD3  | 1.81                     | 0.41              |
| 1:B:64:GLU:O     | 1:B:68:LEU:HG    | 2.20                     | 0.41              |
| 1:B:217:ILE:CG1  | 1:B:218:ALA:H    | 2.28                     | 0.41              |
| 1:B:273:LYS:HB3  | 1:B:298:LEU:HD23 | 2.01                     | 0.41              |
| 1:B:303:PRO:HG2  | 1:B:389:ARG:NH1  | 2.35                     | 0.41              |
| 1:C:341:LEU:HD23 | 1:C:341:LEU:HA   | 1.91                     | 0.41              |
| 1:C:464:PHE:CE1  | 1:C:471:ALA:HB1  | 2.55                     | 0.41              |
| 1:A:317:ARG:HD3  | 1:A:369:GLU:CD   | 2.45                     | 0.41              |
| 1:A:425:ILE:C    | 1:A:427:ALA:H    | 2.29                     | 0.41              |
| 1:C:56:LEU:HG    | 1:C:58:GLN:HG2   | 2.02                     | 0.41              |
| 1:C:159:MET:HE1  | 1:C:187:GLY:O    | 2.21                     | 0.41              |
| 1:C:265:ILE:HD11 | 1:C:448:MET:HG2  | 2.03                     | 0.41              |
| 1:C:381:LEU:C    | 1:C:382:ARG:HD2  | 2.46                     | 0.41              |
| 1:C:385:TYR:HB3  | 1:C:463:VAL:HG12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:386:TRP:HB3  | 1:B:466:LEU:HD21 | 2.02                     | 0.41              |
| 1:C:166:LEU:HB3  | 1:C:187:GLY:H    | 1.86                     | 0.41              |
| 1:A:114:GLU:O    | 1:A:115:GLU:C    | 2.64                     | 0.41              |
| 1:A:151:THR:O    | 1:A:155:VAL:HG22 | 2.20                     | 0.41              |
| 1:A:264:LEU:O    | 1:A:267:ARG:NH1  | 2.54                     | 0.41              |
| 1:A:473:SER:HA   | 1:A:474:PRO:HD3  | 1.63                     | 0.41              |
| 1:B:281:TYR:O    | 1:B:282:GLY:C    | 2.61                     | 0.41              |
| 1:C:113:LYS:HD2  | 1:C:113:LYS:N    | 2.30                     | 0.41              |
| 1:C:121:ARG:HG3  | 1:C:121:ARG:NH1  | 2.36                     | 0.41              |
| 1:C:138:ILE:O    | 1:C:139:TRP:C    | 2.64                     | 0.41              |
| 1:C:174:ARG:HD3  | 1:C:174:ARG:N    | 2.36                     | 0.41              |
| 1:C:265:ILE:HD11 | 1:C:448:MET:HB3  | 2.03                     | 0.41              |
| 1:C:324:HIS:HD2  | 1:C:359:SER:H    | 1.67                     | 0.41              |
| 1:C:340:ASP:CG   | 1:C:486:SER:HB3  | 2.46                     | 0.41              |
| 1:A:272:HIS:NE2  | 1:B:410:PRO:O    | 2.51                     | 0.41              |
| 1:B:41:ILE:CD1   | 1:B:286:ALA:HB2  | 2.51                     | 0.41              |
| 1:B:62:THR:O     | 1:B:66:MET:HG3   | 2.21                     | 0.41              |
| 1:B:217:ILE:CG1  | 1:B:218:ALA:N    | 2.79                     | 0.41              |
| 1:C:109:ILE:C    | 1:C:109:ILE:HD13 | 2.46                     | 0.41              |
| 1:C:255:ASP:O    | 1:C:258:PHE:HB3  | 2.21                     | 0.41              |
| 1:A:155:VAL:HG12 | 1:A:161:PRO:HD3  | 2.03                     | 0.40              |
| 1:A:257:ILE:O    | 1:A:260:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:315:LEU:HD12 | 1:A:365:ILE:CD1  | 2.50                     | 0.40              |
| 1:B:66:MET:HA    | 1:B:92:THR:HG21  | 2.02                     | 0.40              |
| 1:B:234:ALA:O    | 1:B:235:GLN:C    | 2.64                     | 0.40              |
| 1:C:215:THR:O    | 1:C:216:ARG:C    | 2.63                     | 0.40              |
| 1:C:258:PHE:C    | 1:C:260:ALA:N    | 2.79                     | 0.40              |
| 1:A:157:THR:HB   | 1:A:159:MET:HG3  | 2.04                     | 0.40              |
| 1:A:406:ILE:HG23 | 1:A:421:ASP:CB   | 2.51                     | 0.40              |
| 1:A:407:SER:OG   | 1:A:408:ILE:N    | 2.54                     | 0.40              |
| 1:B:238:MET:SD   | 1:B:259:LEU:HD11 | 2.62                     | 0.40              |
| 1:C:34:ASP:O     | 1:C:38:ARG:HG3   | 2.22                     | 0.40              |
| 1:C:44:CYS:C     | 1:C:46:GLU:N     | 2.78                     | 0.40              |
| 1:C:97:TYR:N     | 1:C:97:TYR:CD2   | 2.88                     | 0.40              |
| 1:C:104:TRP:HZ2  | 1:C:376:SER:CB   | 2.35                     | 0.40              |
| 1:C:485:GLY:C    | 1:C:487:TYR:H    | 2.29                     | 0.40              |
| 1:A:239:VAL:HG22 | 1:A:259:LEU:HD21 | 2.04                     | 0.40              |
| 1:A:302:ASP:N    | 1:A:303:PRO:CD   | 2.84                     | 0.40              |
| 1:A:408:ILE:HD11 | 1:C:340:ASP:N    | 2.36                     | 0.40              |
| 1:B:231:GLN:NE2  | 1:B:269:SER:CB   | 2.78                     | 0.40              |
| 1:B:339:GLU:OE2  | 1:B:343:VAL:HG21 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:358:LEU:HD12 | 1:B:358:LEU:HA   | 1.97                     | 0.40              |
| 1:C:100:VAL:O    | 1:C:101:ASP:C    | 2.65                     | 0.40              |
| 1:C:121:ARG:HG3  | 1:C:121:ARG:HH11 | 1.86                     | 0.40              |
| 1:C:205:ASN:N    | 1:C:205:ASN:HD22 | 2.17                     | 0.40              |
| 1:C:235:GLN:O    | 1:C:239:VAL:HG23 | 2.20                     | 0.40              |
| 1:C:331:MET:SD   | 1:C:488:PHE:CE1  | 3.15                     | 0.40              |
| 1:A:168:GLN:NE2  | 1:A:183:VAL:HG22 | 2.36                     | 0.40              |
| 1:A:415:GLN:CD   | 1:C:459:GLN:HA   | 2.46                     | 0.40              |
| 1:C:195:ARG:HG2  | 1:C:196:MET:H    | 1.87                     | 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     | 416/499 (83%)   | 361 (87%)  | 50 (12%)  | 5 (1%)   | 10          | 42 |
| 1   | B     | 416/499 (83%)   | 360 (86%)  | 43 (10%)  | 13 (3%)  | 3           | 22 |
| 1   | C     | 428/499 (86%)   | 349 (82%)  | 68 (16%)  | 11 (3%)  | 4           | 26 |
| All | All   | 1260/1497 (84%) | 1070 (85%) | 161 (13%) | 29 (2%)  | 5           | 29 |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 423 | PRO  |
| 1   | C     | 203 | ASP  |
| 1   | C     | 395 | ASN  |
| 1   | C     | 486 | SER  |
| 1   | A     | 233 | ALA  |
| 1   | A     | 472 | THR  |
| 1   | B     | 150 | ARG  |
| 1   | B     | 177 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 424 | THR  |
| 1   | C     | 25  | ILE  |
| 1   | A     | 101 | ASP  |
| 1   | A     | 250 | ASN  |
| 1   | B     | 101 | ASP  |
| 1   | B     | 341 | LEU  |
| 1   | C     | 108 | LEU  |
| 1   | C     | 421 | ASP  |
| 1   | C     | 480 | ASP  |
| 1   | B     | 340 | ASP  |
| 1   | B     | 469 | GLU  |
| 1   | A     | 448 | MET  |
| 1   | B     | 318 | PRO  |
| 1   | C     | 47  | LEU  |
| 1   | C     | 266 | LEU  |
| 1   | B     | 427 | ALA  |
| 1   | C     | 406 | ILE  |
| 1   | C     | 423 | PRO  |
| 1   | B     | 248 | PRO  |
| 1   | B     | 425 | ILE  |
| 1   | B     | 356 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 362/425 (85%)   | 343 (95%)  | 19 (5%)  | 21          | 54 |
| 1   | B     | 362/425 (85%)   | 344 (95%)  | 18 (5%)  | 22          | 55 |
| 1   | C     | 370/425 (87%)   | 341 (92%)  | 29 (8%)  | 11          | 41 |
| All | All   | 1094/1275 (86%) | 1028 (94%) | 66 (6%)  | 17          | 50 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | LYS  |
| 1   | A     | 108 | LEU  |
| 1   | A     | 111 | TYR  |
| 1   | A     | 112 | ASP  |
| 1   | A     | 118 | ARG  |
| 1   | A     | 139 | TRP  |
| 1   | A     | 174 | ARG  |
| 1   | A     | 244 | GLU  |
| 1   | A     | 246 | ARG  |
| 1   | A     | 253 | PHE  |
| 1   | A     | 267 | ARG  |
| 1   | A     | 339 | GLU  |
| 1   | A     | 390 | THR  |
| 1   | A     | 416 | ARG  |
| 1   | A     | 454 | GLU  |
| 1   | A     | 456 | VAL  |
| 1   | A     | 483 | ASN  |
| 1   | A     | 484 | GLU  |
| 1   | B     | 58  | GLN  |
| 1   | B     | 107 | GLU  |
| 1   | B     | 114 | GLU  |
| 1   | B     | 115 | GLU  |
| 1   | B     | 139 | TRP  |
| 1   | B     | 220 | GLU  |
| 1   | B     | 259 | LEU  |
| 1   | B     | 308 | GLN  |
| 1   | B     | 312 | VAL  |
| 1   | B     | 363 | VAL  |
| 1   | B     | 368 | ASN  |
| 1   | B     | 389 | ARG  |
| 1   | B     | 390 | THR  |
| 1   | B     | 408 | ILE  |
| 1   | B     | 438 | SER  |
| 1   | B     | 459 | GLN  |
| 1   | B     | 479 | PHE  |
| 1   | B     | 483 | ASN  |
| 1   | C     | 46  | GLU  |
| 1   | C     | 57  | ILE  |
| 1   | C     | 58  | GLN  |
| 1   | C     | 59  | ASN  |
| 1   | C     | 60  | SER  |
| 1   | C     | 96  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 99  | ARG  |
| 1   | C     | 105 | ARG  |
| 1   | C     | 109 | ILE  |
| 1   | C     | 113 | LYS  |
| 1   | C     | 199 | ARG  |
| 1   | C     | 226 | LEU  |
| 1   | C     | 243 | ARG  |
| 1   | C     | 247 | ASN  |
| 1   | C     | 259 | LEU  |
| 1   | C     | 265 | ILE  |
| 1   | C     | 309 | ASN  |
| 1   | C     | 314 | SER  |
| 1   | C     | 316 | ILE  |
| 1   | C     | 371 | MET  |
| 1   | C     | 372 | GLU  |
| 1   | C     | 375 | GLU  |
| 1   | C     | 389 | ARG  |
| 1   | C     | 390 | THR  |
| 1   | C     | 406 | ILE  |
| 1   | C     | 446 | ARG  |
| 1   | C     | 469 | GLU  |
| 1   | C     | 481 | MET  |
| 1   | C     | 483 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | ASN  |
| 1   | A     | 168 | GLN  |
| 1   | A     | 224 | ASN  |
| 1   | A     | 272 | HIS  |
| 1   | A     | 308 | GLN  |
| 1   | A     | 319 | ASN  |
| 1   | A     | 321 | ASN  |
| 1   | A     | 324 | HIS  |
| 1   | A     | 368 | ASN  |
| 1   | A     | 370 | ASN  |
| 1   | A     | 415 | GLN  |
| 1   | A     | 459 | GLN  |
| 1   | A     | 483 | ASN  |
| 1   | B     | 21  | ASN  |
| 1   | B     | 122 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 142 | ASN  |
| 1   | B     | 235 | GLN  |
| 1   | B     | 241 | GLN  |
| 1   | B     | 308 | GLN  |
| 1   | B     | 309 | ASN  |
| 1   | B     | 311 | GLN  |
| 1   | B     | 321 | ASN  |
| 1   | B     | 395 | ASN  |
| 1   | B     | 415 | GLN  |
| 1   | B     | 459 | GLN  |
| 1   | B     | 483 | ASN  |
| 1   | C     | 125 | ASN  |
| 1   | C     | 140 | HIS  |
| 1   | C     | 142 | ASN  |
| 1   | C     | 205 | ASN  |
| 1   | C     | 247 | ASN  |
| 1   | C     | 308 | GLN  |
| 1   | C     | 309 | ASN  |
| 1   | C     | 319 | ASN  |
| 1   | C     | 321 | ASN  |
| 1   | C     | 324 | HIS  |
| 1   | C     | 364 | GLN  |
| 1   | C     | 370 | ASN  |
| 1   | C     | 405 | GLN  |
| 1   | C     | 409 | GLN  |
| 1   | C     | 459 | 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | C     | 2                |
| 1   | B     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 201:ILE   | C      | 202:ASN   | N      | 1.15         |
| 1     | C     | 202:ASN   | C      | 203:ASP   | N      | 1.15         |
| 1     | B     | 201:ILE   | C      | 202:ASN   | N      | 1.03         |

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 425/499 (85%)   | -0.08  | 3 (0%) 84 69 | 31, 69, 113, 124      | 0       |
| 1   | B     | 425/499 (85%)   | -0.13  | 4 (0%) 81 64 | 35, 68, 104, 126      | 0       |
| 1   | C     | 435/499 (87%)   | -0.05  | 1 (0%) 91 85 | 39, 82, 118, 132      | 0       |
| All | All   | 1285/1497 (85%) | -0.09  | 8 (0%) 85 73 | 31, 73, 111, 132      | 0       |

All (8) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 460 | GLY  | 2.8  |
| 1   | B     | 185 | GLY  | 2.7  |
| 1   | A     | 256 | LEU  | 2.7  |
| 1   | B     | 186 | VAL  | 2.6  |
| 1   | C     | 57  | ILE  | 2.5  |
| 1   | A     | 192 | GLU  | 2.4  |
| 1   | A     | 254 | GLU  | 2.2  |
| 1   | B     | 485 | 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.