



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:57 AM UTC

PDB ID : 3HKB / pdb\_00003hkb  
Title : Tubulin: RB3 Stathmin-like domain complex  
Authors : Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.  
Deposited on : 2009-05-23  
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

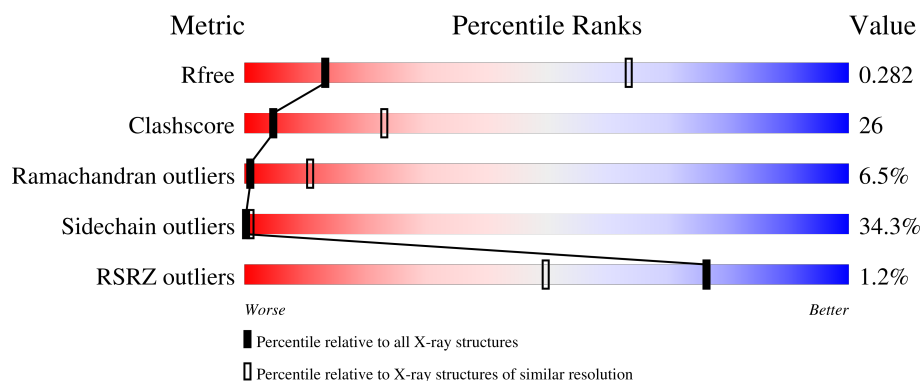
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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                      | 1062 (3.78-3.54)                                      |
| Clashscore            | 190562                      | 1009 (3.76-3.56)                                      |
| Ramachandran outliers | 187476                      | 1054 (3.78-3.54)                                      |
| Sidechain outliers    | 187428                      | 1052 (3.78-3.54)                                      |
| RSRZ outliers         | 180081                      | 1061 (3.78-3.54)                                      |

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     | 451    | <div> <div>44%</div> <div>35%</div> <div>14%</div> <div>• 5%</div> </div>               |
| 1   | C     | 451    | <div> <div>%</div> <div>47%</div> <div>34%</div> <div>12%</div> <div>• 5%</div> </div>  |
| 2   | B     | 445    | <div> <div>38%</div> <div>35%</div> <div>19%</div> <div>• 6%</div> </div>               |
| 2   | D     | 445    | <div> <div>3%</div> <div>38%</div> <div>38%</div> <div>18%</div> <div>• 6%</div> </div> |
| 3   | E     | 142    | <div> <div>%</div> <div>43%</div> <div>26%</div> <div>15%</div> <div>• 13%</div> </div> |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14125 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 Tubulin alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 427      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3307  | 2100 | 560 | 626 | 21 |         |         |       |
| 1   | C     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3296  | 2095 | 557 | 623 | 21 |         |         |       |

- Molecule 2 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 420      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3249  | 2044 | 548 | 633 | 24 |         |         |       |
| 2   | D     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3240  | 2038 | 546 | 632 | 24 |         |         |       |

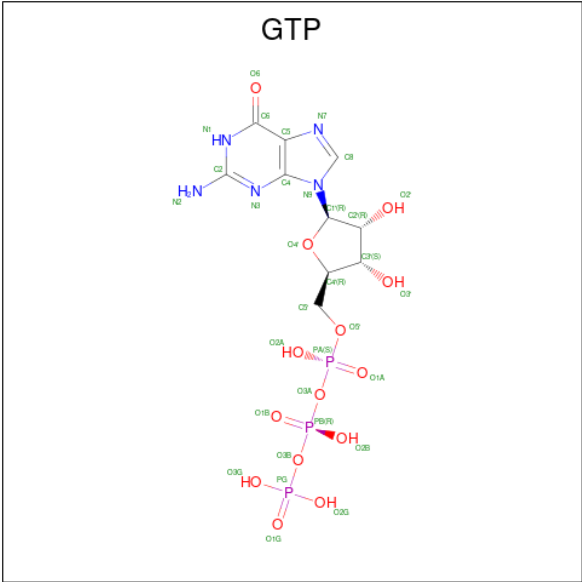
- Molecule 3 is a protein called Stathmin-4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | E     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 911   | 552 | 171 | 183 | 5 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 4       | ALA      | -      | expression tag | UNP P63043 |

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |         |
| 4   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |         |

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

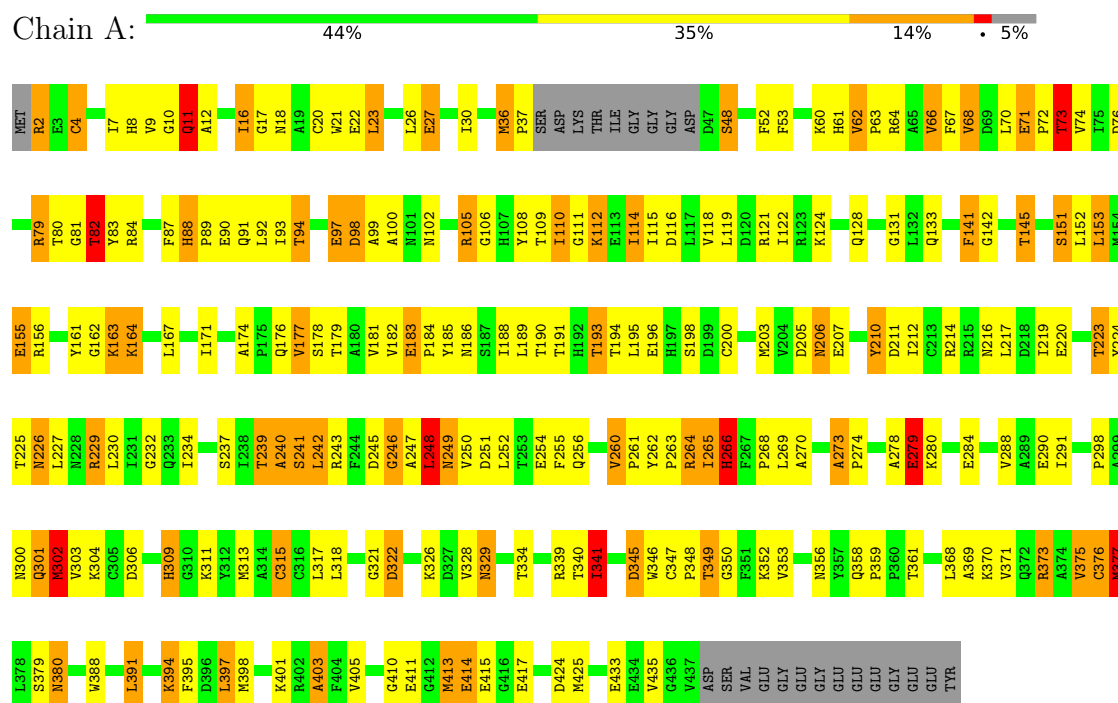
- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



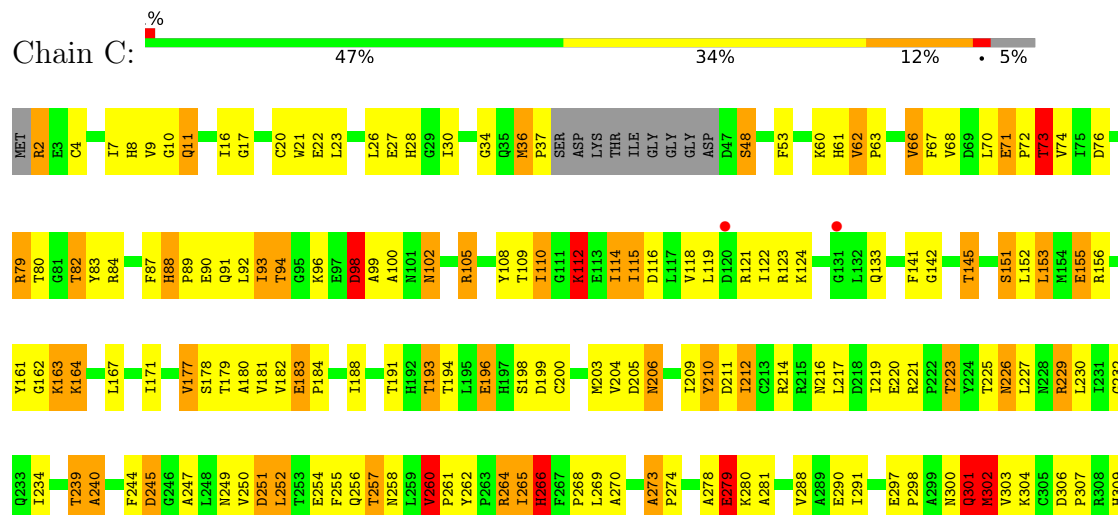
### 3 Residue-property plots

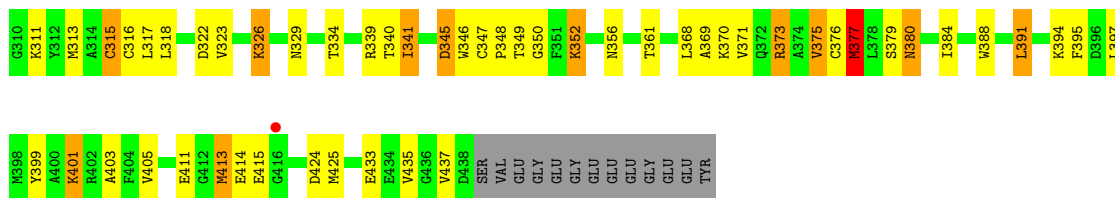
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Tubulin alpha chain



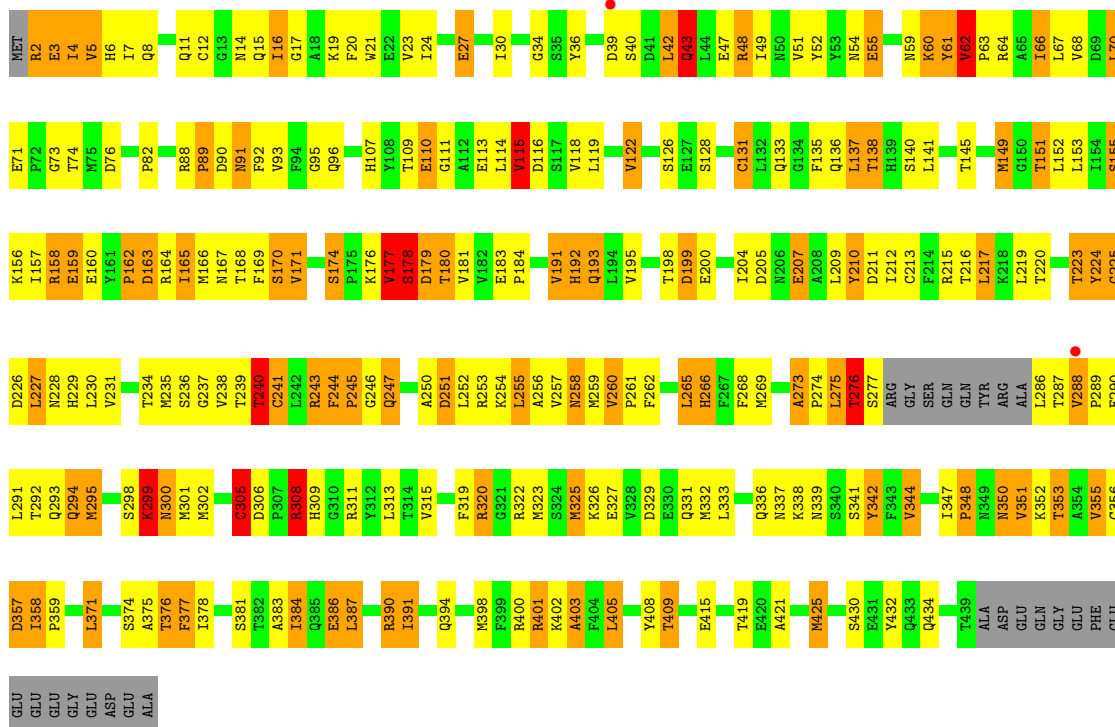
#### • Molecule 1: Tubulin alpha chain





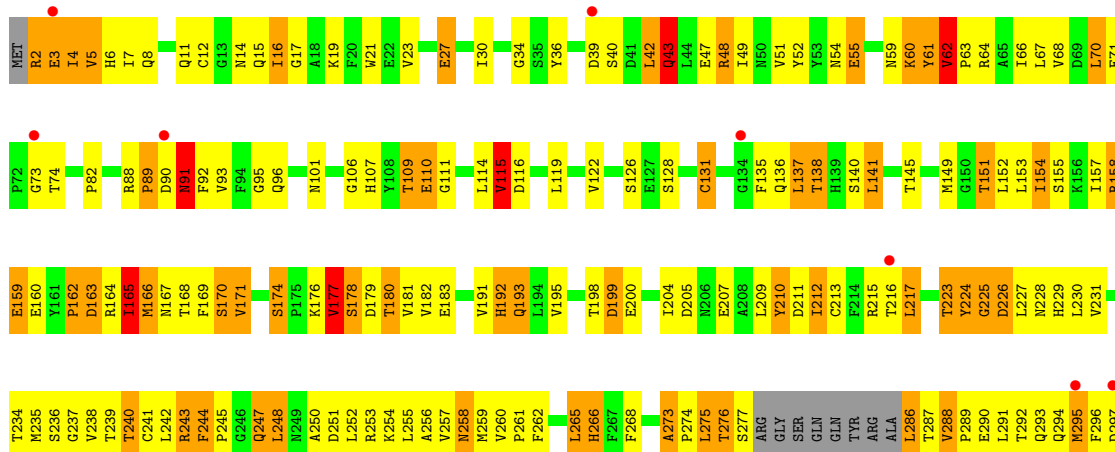
• Molecule 2: Tubulin beta chain

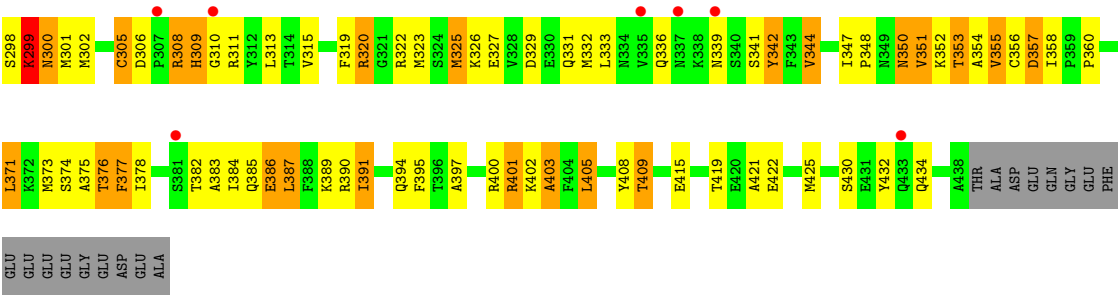
Chain B: 38% 35% 19% 6%



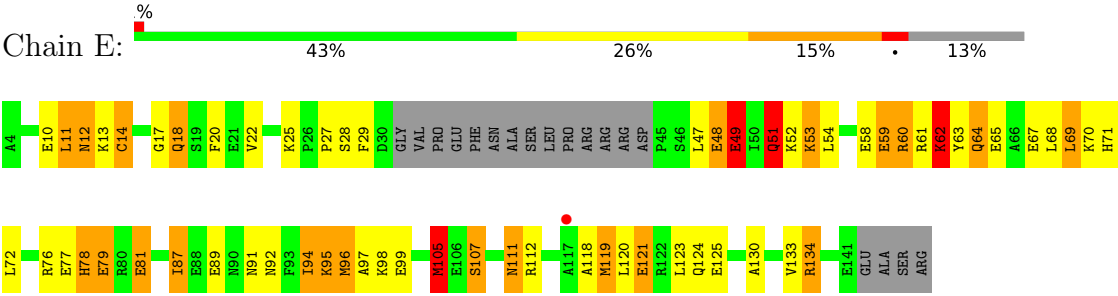
• Molecule 2: Tubulin beta chain

Chain D: 38% 38% 18% 6%





• Molecule 3: Stathmin-4





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 65                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 328.83Å 328.83Å 53.71Å<br>90.00° 90.00° 120.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.65<br>20.00 – 3.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.6 (20.00-3.65)<br>96.6 (20.00-3.65)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.06                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.27 (at 3.64Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.1.24                                               | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.254<br>0.246 , 0.282                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1812 reflections (4.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 150.2                                                       | Xtriage          |
| Anisotropy                                                              | 0.116                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 236.4                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | 0.035 for h,-h-k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 14125                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, GDP

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.85         | 2/3384 (0.1%)  | 1.13        | 7/4601 (0.2%)   |
| 1   | C     | 0.69         | 1/3373 (0.0%)  | 1.08        | 7/4588 (0.2%)   |
| 2   | B     | 0.73         | 3/3321 (0.1%)  | 1.10        | 9/4509 (0.2%)   |
| 2   | D     | 0.74         | 0/3312         | 1.09        | 8/4498 (0.2%)   |
| 3   | E     | 0.74         | 1/919 (0.1%)   | 1.19        | 6/1234 (0.5%)   |
| All | All   | 0.75         | 7/14309 (0.0%) | 1.11        | 37/19430 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 2   | B     | 0                   | 2                   |
| 2   | D     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 149 | MET  | SD-CE | -7.91 | 1.59        | 1.79     |
| 1   | A     | 302 | MET  | SD-CE | 7.87  | 1.99        | 1.79     |
| 1   | C     | 302 | MET  | SD-CE | 6.03  | 1.94        | 1.79     |
| 2   | B     | 425 | MET  | SD-CE | -5.78 | 1.65        | 1.79     |
| 1   | A     | 341 | ILE  | CA-CB | 5.43  | 1.61        | 1.54     |
| 2   | B     | 325 | MET  | SD-CE | 5.28  | 1.92        | 1.79     |
| 3   | E     | 105 | MET  | SD-CE | 5.22  | 1.92        | 1.79     |

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | E     | 51  | GLN  | N-CA-C  | -8.87 | 98.86       | 113.50   |
| 2   | B     | 199 | ASP  | N-CA-C  | -7.75 | 104.42      | 114.04   |
| 1   | A     | 16  | ILE  | N-CA-C  | -7.35 | 103.62      | 110.53   |
| 1   | A     | 102 | ASN  | N-CA-C  | 7.02  | 121.12      | 108.69   |
| 3   | E     | 69  | LEU  | N-CA-C  | -6.96 | 106.69      | 114.62   |
| 1   | A     | 93  | ILE  | N-CA-C  | 6.94  | 117.89      | 108.17   |
| 1   | C     | 102 | ASN  | N-CA-C  | 6.62  | 119.25      | 108.26   |
| 2   | B     | 260 | VAL  | N-CA-C  | 6.58  | 114.66      | 108.15   |
| 2   | D     | 199 | ASP  | N-CA-C  | -6.58 | 105.89      | 114.04   |
| 3   | E     | 52  | LYS  | N-CA-C  | -6.44 | 105.81      | 113.21   |
| 2   | B     | 308 | ARG  | N-CA-C  | -6.18 | 103.67      | 112.13   |
| 2   | B     | 338 | LYS  | N-CA-C  | -6.03 | 104.61      | 111.07   |
| 3   | E     | 78  | HIS  | N-CA-C  | -5.99 | 105.88      | 113.43   |
| 2   | B     | 337 | ASN  | N-CA-C  | -5.91 | 105.32      | 113.18   |
| 1   | C     | 339 | ARG  | N-CA-C  | 5.78  | 115.88      | 108.24   |
| 2   | D     | 166 | MET  | N-CA-C  | 5.73  | 117.75      | 108.41   |
| 1   | A     | 266 | HIS  | CB-CA-C | -5.69 | 98.11       | 109.99   |
| 2   | D     | 163 | ASP  | N-CA-C  | 5.68  | 122.89      | 110.80   |
| 2   | D     | 91  | ASN  | N-CA-C  | -5.66 | 105.12      | 113.61   |
| 1   | C     | 266 | HIS  | CB-CA-C | -5.63 | 98.22       | 109.99   |
| 2   | D     | 224 | TYR  | N-CA-C  | -5.53 | 106.38      | 113.01   |
| 3   | E     | 71  | HIS  | N-CA-C  | -5.52 | 105.76      | 112.88   |
| 2   | B     | 163 | ASP  | N-CA-C  | 5.51  | 122.53      | 110.80   |
| 1   | A     | 83  | TYR  | N-CA-C  | -5.46 | 105.21      | 113.51   |
| 3   | E     | 118 | ALA  | N-CA-C  | -5.43 | 106.82      | 113.50   |
| 1   | C     | 83  | TYR  | N-CA-C  | -5.42 | 105.27      | 113.51   |
| 2   | D     | 266 | HIS  | CA-C-N  | -5.25 | 114.99      | 123.23   |
| 2   | D     | 266 | HIS  | C-N-CA  | -5.25 | 114.99      | 123.23   |
| 2   | B     | 266 | HIS  | CA-C-N  | -5.18 | 115.09      | 123.23   |
| 2   | B     | 266 | HIS  | C-N-CA  | -5.18 | 115.09      | 123.23   |
| 1   | A     | 224 | TYR  | N-CA-C  | -5.16 | 105.34      | 111.69   |
| 1   | C     | 180 | ALA  | N-CA-C  | 5.16  | 118.62      | 109.96   |
| 1   | C     | 93  | ILE  | N-CA-C  | 5.12  | 115.96      | 108.53   |
| 1   | C     | 260 | VAL  | N-CA-C  | 5.12  | 113.57      | 107.73   |
| 2   | D     | 165 | ILE  | N-CA-C  | 5.12  | 116.56      | 109.45   |
| 2   | B     | 224 | TYR  | N-CA-C  | -5.09 | 106.90      | 113.01   |
| 1   | A     | 376 | CYS  | N-CA-C  | 5.07  | 121.14      | 114.75   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 266 | HIS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 162 | PRO  | Peptide |
| 2   | B     | 178 | SER  | Peptide |
| 1   | C     | 266 | HIS  | Peptide |
| 2   | D     | 162 | PRO  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3307  | 0        | 3182     | 168     | 0            |
| 1   | C     | 3296  | 0        | 3158     | 149     | 0            |
| 2   | B     | 3249  | 0        | 3069     | 192     | 0            |
| 2   | D     | 3240  | 0        | 3056     | 189     | 0            |
| 3   | E     | 911   | 0        | 792      | 44      | 0            |
| 4   | A     | 32    | 0        | 12       | 3       | 0            |
| 4   | C     | 32    | 0        | 12       | 2       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 28    | 0        | 12       | 1       | 0            |
| 6   | D     | 28    | 0        | 12       | 3       | 0            |
| All | All   | 14125 | 0        | 13305    | 701     | 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 26.

All (701) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:180:THR:HA  | 1:C:352:LYS:NZ   | 1.68                     | 1.08              |
| 2:B:273:ALA:CB  | 2:B:274:PRO:HD3  | 1.84                     | 1.08              |
| 2:D:273:ALA:CB  | 2:D:274:PRO:HD3  | 1.84                     | 1.07              |
| 2:D:251:ASP:HB3 | 2:D:254:LYS:HB2  | 1.35                     | 1.04              |
| 1:A:273:ALA:CB  | 1:A:274:PRO:HD3  | 1.89                     | 1.03              |
| 2:B:140:SER:HA  | 2:B:171:VAL:HG23 | 1.42                     | 1.02              |
| 1:A:273:ALA:HB3 | 1:A:274:PRO:HD3  | 1.43                     | 1.01              |
| 2:B:273:ALA:HB1 | 2:B:274:PRO:HD3  | 1.43                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:273:ALA:HB1  | 2:D:274:PRO:HD3  | 1.39                     | 1.00              |
| 1:C:273:ALA:HB3  | 1:C:274:PRO:HD3  | 1.46                     | 0.98              |
| 1:A:206:ASN:HD21 | 4:A:600:GTP:HN22 | 1.11                     | 0.98              |
| 1:C:273:ALA:CB   | 1:C:274:PRO:HD3  | 1.93                     | 0.98              |
| 1:C:278:ALA:O    | 1:C:279:GLU:HB3  | 1.63                     | 0.97              |
| 2:D:244:PHE:HB3  | 2:D:245:PRO:HD3  | 1.46                     | 0.97              |
| 2:D:140:SER:HA   | 2:D:171:VAL:HG23 | 1.45                     | 0.96              |
| 1:A:79:ARG:HH22  | 1:A:94:THR:HG21  | 1.29                     | 0.96              |
| 1:A:278:ALA:O    | 1:A:279:GLU:HB3  | 1.64                     | 0.96              |
| 2:B:216:THR:HG21 | 2:B:299:LYS:HD3  | 1.47                     | 0.96              |
| 1:A:270:ALA:HB3  | 1:A:302:MET:HE2  | 1.48                     | 0.95              |
| 1:A:88:HIS:HB2   | 1:A:91:GLN:HE21  | 1.31                     | 0.94              |
| 2:D:54:ASN:HD22  | 2:D:64:ARG:HD3   | 1.33                     | 0.93              |
| 1:C:199:ASP:HB3  | 1:C:256:GLN:HE22 | 1.32                     | 0.93              |
| 1:A:133:GLN:HE21 | 1:A:252:LEU:HG   | 1.34                     | 0.92              |
| 2:B:158:ARG:O    | 2:B:159:GLU:HB2  | 1.69                     | 0.92              |
| 2:D:158:ARG:O    | 2:D:159:GLU:HB2  | 1.68                     | 0.91              |
| 1:C:88:HIS:HB2   | 1:C:91:GLN:HE21  | 1.35                     | 0.90              |
| 2:D:273:ALA:CB   | 2:D:274:PRO:CD   | 2.50                     | 0.90              |
| 1:A:322:ASP:O    | 1:A:373:ARG:NH1  | 2.04                     | 0.90              |
| 2:D:2:ARG:HD3    | 2:D:131:CYS:SG   | 2.13                     | 0.89              |
| 2:B:180:THR:HA   | 1:C:352:LYS:HZ2  | 1.38                     | 0.88              |
| 2:D:231:VAL:HG12 | 2:D:235:MET:HE2  | 1.53                     | 0.88              |
| 2:B:273:ALA:CB   | 2:B:274:PRO:CD   | 2.52                     | 0.87              |
| 2:B:2:ARG:HD3    | 2:B:131:CYS:SG   | 2.15                     | 0.87              |
| 1:C:270:ALA:HB3  | 1:C:302:MET:HE2  | 1.56                     | 0.86              |
| 3:E:11:LEU:O     | 3:E:12:ASN:HB3   | 1.76                     | 0.85              |
| 1:C:79:ARG:HH22  | 1:C:94:THR:HG21  | 1.40                     | 0.85              |
| 2:D:223:THR:HB   | 2:D:225:GLY:H    | 1.40                     | 0.85              |
| 1:A:229:ARG:HG2  | 1:A:229:ARG:HH11 | 1.41                     | 0.85              |
| 2:B:54:ASN:HD22  | 2:B:64:ARG:HD3   | 1.40                     | 0.84              |
| 2:D:251:ASP:CB   | 2:D:254:LYS:HB2  | 2.08                     | 0.83              |
| 1:A:273:ALA:HB3  | 1:A:274:PRO:CD   | 2.07                     | 0.83              |
| 2:D:11:GLN:HG3   | 2:D:74:THR:HG21  | 1.60                     | 0.83              |
| 2:B:180:THR:HA   | 1:C:352:LYS:HZ1  | 1.39                     | 0.82              |
| 3:E:96:MET:HE2   | 3:E:97:ALA:HB2   | 1.61                     | 0.82              |
| 1:C:322:ASP:O    | 1:C:373:ARG:NH1  | 2.12                     | 0.82              |
| 2:B:244:PHE:HB3  | 2:B:245:PRO:HD3  | 1.60                     | 0.81              |
| 1:A:347:CYS:O    | 3:E:27:PRO:HA    | 1.80                     | 0.81              |
| 1:C:206:ASN:HD21 | 4:C:600:GTP:HN22 | 1.27                     | 0.81              |
| 1:C:229:ARG:HG2  | 1:C:229:ARG:HH11 | 1.44                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:244:PHE:HB3  | 2:D:245:PRO:CD   | 2.10                     | 0.80              |
| 2:B:223:THR:HB   | 2:B:225:GLY:H    | 1.46                     | 0.80              |
| 1:A:27:GLU:OE2   | 1:A:243:ARG:NH2  | 2.15                     | 0.80              |
| 1:C:244:PHE:O    | 1:C:245:ASP:HB2  | 1.80                     | 0.80              |
| 1:A:79:ARG:NH2   | 1:A:94:THR:HG21  | 1.95                     | 0.79              |
| 1:C:346:TRP:HZ2  | 1:C:435:VAL:HG13 | 1.47                     | 0.79              |
| 1:A:273:ALA:CB   | 1:A:375:VAL:H    | 1.96                     | 0.79              |
| 1:A:273:ALA:CB   | 1:A:274:PRO:CD   | 2.58                     | 0.79              |
| 2:B:273:ALA:HB3  | 2:B:274:PRO:HD3  | 1.64                     | 0.79              |
| 2:B:138:THR:HG22 | 2:B:169:PHE:HB2  | 1.64                     | 0.79              |
| 1:A:315:CYS:SG   | 1:A:377:MET:HE1  | 2.23                     | 0.79              |
| 2:B:251:ASP:HB3  | 2:B:254:LYS:HB2  | 1.64                     | 0.79              |
| 2:D:138:THR:HG22 | 2:D:169:PHE:HB2  | 1.65                     | 0.78              |
| 1:A:8:HIS:CD2    | 1:A:17:GLY:HA3   | 2.18                     | 0.78              |
| 2:D:273:ALA:HB3  | 2:D:274:PRO:CD   | 2.13                     | 0.78              |
| 1:A:133:GLN:NE2  | 1:A:252:LEU:H    | 1.79                     | 0.78              |
| 2:B:11:GLN:HG3   | 2:B:74:THR:HG21  | 1.66                     | 0.78              |
| 2:D:216:THR:HG21 | 2:D:299:LYS:HD3  | 1.66                     | 0.78              |
| 2:D:311:ARG:HE   | 2:D:344:VAL:HG23 | 1.48                     | 0.78              |
| 1:C:100:ALA:HB1  | 2:D:253:ARG:HG2  | 1.66                     | 0.78              |
| 2:B:231:VAL:HG12 | 2:B:235:MET:HE2  | 1.65                     | 0.77              |
| 2:D:273:ALA:HB2  | 2:D:375:ALA:H    | 1.47                     | 0.77              |
| 1:A:278:ALA:HA   | 1:A:369:ALA:HB2  | 1.67                     | 0.77              |
| 1:C:191:THR:HG23 | 1:C:425:MET:HE3  | 1.67                     | 0.77              |
| 3:E:67:GLU:C     | 3:E:69:LEU:H     | 1.91                     | 0.77              |
| 1:C:273:ALA:HB3  | 1:C:274:PRO:CD   | 2.14                     | 0.77              |
| 2:D:238:VAL:HG13 | 2:D:378:ILE:HD11 | 1.66                     | 0.76              |
| 1:C:8:HIS:CD2    | 1:C:17:GLY:HA3   | 2.20                     | 0.76              |
| 2:D:229:HIS:CE1  | 2:D:277:SER:HB3  | 2.21                     | 0.76              |
| 1:C:315:CYS:SG   | 1:C:377:MET:HE1  | 2.25                     | 0.76              |
| 1:C:79:ARG:NH2   | 1:C:94:THR:HG21  | 2.01                     | 0.76              |
| 2:B:70:LEU:HA    | 2:B:95:GLY:HA3   | 1.67                     | 0.75              |
| 2:B:12:CYS:SG    | 2:B:171:VAL:HG21 | 2.25                     | 0.75              |
| 1:C:273:ALA:CB   | 1:C:274:PRO:CD   | 2.63                     | 0.75              |
| 1:C:273:ALA:CB   | 1:C:375:VAL:H    | 1.99                     | 0.75              |
| 2:D:332:MET:HG3  | 2:D:353:THR:HG21 | 1.69                     | 0.75              |
| 2:B:273:ALA:HB2  | 2:B:375:ALA:H    | 1.51                     | 0.75              |
| 2:B:180:THR:CA   | 1:C:352:LYS:HZ2  | 1.99                     | 0.74              |
| 2:B:273:ALA:HB3  | 2:B:274:PRO:CD   | 2.16                     | 0.74              |
| 1:C:142:GLY:HA3  | 1:C:183:GLU:HG3  | 1.70                     | 0.74              |
| 1:C:270:ALA:O    | 1:C:302:MET:HB2  | 1.88                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:165:ILE:HD11 | 2:D:252:LEU:HG   | 1.70                     | 0.73              |
| 1:A:142:GLY:HA3  | 1:A:183:GLU:HG3  | 1.69                     | 0.73              |
| 1:A:133:GLN:NE2  | 1:A:252:LEU:HG   | 2.02                     | 0.73              |
| 2:D:2:ARG:O      | 2:D:3:GLU:HB2    | 1.87                     | 0.73              |
| 2:D:260:VAL:HG11 | 2:D:266:HIS:HB3  | 1.69                     | 0.73              |
| 2:D:12:CYS:SG    | 2:D:171:VAL:HG21 | 2.30                     | 0.72              |
| 1:A:191:THR:HG23 | 1:A:425:MET:HE3  | 1.71                     | 0.72              |
| 1:A:273:ALA:HB1  | 1:A:274:PRO:HD3  | 1.71                     | 0.72              |
| 3:E:89:GLU:HA    | 3:E:92:ASN:HB2   | 1.70                     | 0.72              |
| 2:D:54:ASN:ND2   | 2:D:64:ARG:HD3   | 2.05                     | 0.72              |
| 2:B:220:THR:CG2  | 1:C:326:LYS:HG3  | 2.19                     | 0.72              |
| 2:B:291:LEU:HD21 | 2:B:375:ALA:HB2  | 1.72                     | 0.72              |
| 1:A:133:GLN:OE1  | 1:A:251:ASP:HB2  | 1.90                     | 0.71              |
| 1:A:206:ASN:HD21 | 4:A:600:GTP:N2   | 1.87                     | 0.71              |
| 2:B:165:ILE:HD11 | 2:B:252:LEU:HG   | 1.70                     | 0.71              |
| 2:D:70:LEU:HA    | 2:D:95:GLY:HA3   | 1.71                     | 0.71              |
| 1:A:346:TRP:HZ2  | 1:A:435:VAL:HG13 | 1.55                     | 0.71              |
| 1:C:266:HIS:O    | 1:C:268:PRO:HD3  | 1.90                     | 0.71              |
| 2:D:223:THR:HB   | 2:D:225:GLY:N    | 2.04                     | 0.71              |
| 2:B:114:LEU:O    | 2:B:116:ASP:N    | 2.24                     | 0.71              |
| 1:C:262:TYR:HB2  | 1:C:265:ILE:HD13 | 1.72                     | 0.71              |
| 1:A:273:ALA:HB2  | 1:A:375:VAL:H    | 1.56                     | 0.70              |
| 1:C:179:THR:HG22 | 2:D:248:LEU:HB2  | 1.73                     | 0.70              |
| 1:A:270:ALA:O    | 1:A:302:MET:HB2  | 1.91                     | 0.70              |
| 2:B:244:PHE:HB3  | 2:B:245:PRO:CD   | 2.21                     | 0.70              |
| 2:D:259:MET:HE2  | 2:D:378:ILE:HG22 | 1.72                     | 0.70              |
| 2:D:16:ILE:HG23  | 2:D:235:MET:HE1  | 1.74                     | 0.70              |
| 1:A:266:HIS:O    | 1:A:268:PRO:HD3  | 1.92                     | 0.70              |
| 2:D:114:LEU:O    | 2:D:116:ASP:N    | 2.25                     | 0.69              |
| 2:B:229:HIS:CE1  | 2:B:277:SER:HB3  | 2.27                     | 0.69              |
| 2:D:244:PHE:CB   | 2:D:245:PRO:CD   | 2.70                     | 0.69              |
| 2:D:319:PHE:HB2  | 2:D:355:VAL:HG12 | 1.74                     | 0.69              |
| 1:C:278:ALA:HA   | 1:C:369:ALA:HB2  | 1.75                     | 0.69              |
| 1:C:179:THR:O    | 2:D:352:LYS:HE2  | 1.92                     | 0.69              |
| 1:C:229:ARG:HH11 | 1:C:229:ARG:CG   | 2.04                     | 0.69              |
| 2:B:153:LEU:O    | 2:B:157:ILE:HG12 | 1.93                     | 0.69              |
| 2:D:5:VAL:HG22   | 2:D:135:PHE:CD2  | 2.27                     | 0.68              |
| 1:A:88:HIS:HB2   | 1:A:91:GLN:NE2   | 2.08                     | 0.68              |
| 2:D:158:ARG:O    | 2:D:159:GLU:CB   | 2.42                     | 0.68              |
| 2:B:2:ARG:O      | 2:B:3:GLU:HB2    | 1.91                     | 0.68              |
| 2:B:241:CYS:HB2  | 2:B:250:ALA:HB2  | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:167:LEU:HD13 | 1:C:252:LEU:HD11 | 1.74                     | 0.68              |
| 2:B:332:MET:HG3  | 2:B:353:THR:HG21 | 1.75                     | 0.68              |
| 1:C:264:ARG:NH2  | 1:C:424:ASP:OD1  | 2.28                     | 0.67              |
| 2:B:223:THR:HB   | 2:B:225:GLY:N    | 2.09                     | 0.67              |
| 1:C:70:LEU:HD13  | 1:C:145:THR:CB   | 2.25                     | 0.67              |
| 1:C:206:ASN:HD21 | 4:C:600:GTP:N2   | 1.93                     | 0.66              |
| 2:B:5:VAL:HG22   | 2:B:135:PHE:CD2  | 2.31                     | 0.66              |
| 2:B:301:MET:SD   | 2:B:377:PHE:HE2  | 2.18                     | 0.66              |
| 2:B:180:THR:CA   | 1:C:352:LYS:NZ   | 2.53                     | 0.66              |
| 2:B:260:VAL:HG11 | 2:B:266:HIS:HB3  | 1.78                     | 0.66              |
| 1:A:70:LEU:HD13  | 1:A:145:THR:HB   | 1.77                     | 0.65              |
| 1:C:88:HIS:HB2   | 1:C:91:GLN:NE2   | 2.11                     | 0.65              |
| 1:C:112:LYS:HE3  | 3:E:105:MET:HE3  | 1.78                     | 0.65              |
| 1:C:133:GLN:NE2  | 1:C:252:LEU:HB2  | 2.11                     | 0.65              |
| 1:C:249:ASN:HB3  | 1:C:255:PHE:CD2  | 2.32                     | 0.65              |
| 2:D:27:GLU:OE2   | 2:D:320:ARG:NH2  | 2.30                     | 0.65              |
| 2:B:237:GLY:HA3  | 2:B:376:THR:HG21 | 1.79                     | 0.65              |
| 1:C:70:LEU:HD13  | 1:C:145:THR:HB   | 1.79                     | 0.65              |
| 1:A:264:ARG:NH2  | 1:A:424:ASP:OD1  | 2.28                     | 0.65              |
| 2:B:158:ARG:O    | 2:B:159:GLU:CB   | 2.44                     | 0.65              |
| 1:A:66:VAL:HG11  | 1:A:122:ILE:HG12 | 1.79                     | 0.65              |
| 3:E:61:ARG:O     | 3:E:63:TYR:N     | 2.30                     | 0.64              |
| 2:B:54:ASN:ND2   | 2:B:64:ARG:HD3   | 2.12                     | 0.64              |
| 2:D:200:GLU:HB3  | 2:D:268:PHE:CE1  | 2.33                     | 0.64              |
| 3:E:61:ARG:C     | 3:E:63:TYR:H     | 2.04                     | 0.64              |
| 2:D:301:MET:SD   | 2:D:377:PHE:HE2  | 2.19                     | 0.64              |
| 1:A:229:ARG:HH11 | 1:A:229:ARG:CG   | 2.08                     | 0.64              |
| 2:D:325:MET:HE3  | 2:D:326:LYS:N    | 2.12                     | 0.64              |
| 1:A:71:GLU:HG3   | 1:A:73:THR:OG1   | 1.98                     | 0.64              |
| 1:C:167:LEU:HD13 | 1:C:252:LEU:CD1  | 2.27                     | 0.63              |
| 2:D:2:ARG:CD     | 2:D:131:CYS:SG   | 2.87                     | 0.63              |
| 1:A:99:ALA:CB    | 1:A:145:THR:HG22 | 2.29                     | 0.63              |
| 1:C:377:MET:O    | 1:C:377:MET:HG3  | 1.99                     | 0.63              |
| 1:C:249:ASN:HB3  | 1:C:255:PHE:HD2  | 1.63                     | 0.63              |
| 1:C:191:THR:HG23 | 1:C:425:MET:CE   | 2.28                     | 0.63              |
| 2:B:292:THR:HA   | 2:B:295:MET:HE3  | 1.80                     | 0.63              |
| 1:C:273:ALA:HB1  | 1:C:274:PRO:HD3  | 1.78                     | 0.62              |
| 2:D:244:PHE:CB   | 2:D:245:PRO:HD3  | 2.25                     | 0.62              |
| 1:C:121:ARG:HG3  | 1:C:121:ARG:HH11 | 1.64                     | 0.62              |
| 2:B:21:TRP:CZ3   | 2:B:63:PRO:HB3   | 2.34                     | 0.62              |
| 1:A:223:THR:O    | 1:A:227:LEU:HD13 | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:GLN:C    | 1:C:258:ASN:N    | 2.55                     | 0.62              |
| 3:E:51:GLN:C     | 3:E:53:LYS:H     | 2.07                     | 0.62              |
| 2:B:7:ILE:O      | 2:B:137:LEU:HA   | 2.00                     | 0.62              |
| 2:D:54:ASN:HD22  | 2:D:64:ARG:CD    | 2.08                     | 0.62              |
| 1:C:177:VAL:HG13 | 1:C:177:VAL:O    | 1.99                     | 0.62              |
| 1:A:241:SER:HB2  | 1:A:249:ASN:O    | 2.00                     | 0.62              |
| 2:B:6:HIS:CE1    | 2:B:8:GLN:HB2    | 2.35                     | 0.61              |
| 2:B:311:ARG:HE   | 2:B:344:VAL:HG23 | 1.65                     | 0.61              |
| 2:D:21:TRP:CZ3   | 2:D:63:PRO:HB3   | 2.35                     | 0.61              |
| 2:B:287:THR:HG22 | 2:B:290:GLU:HB2  | 1.82                     | 0.61              |
| 1:C:317:LEU:HD23 | 1:C:377:MET:HB2  | 1.81                     | 0.61              |
| 1:A:99:ALA:HB2   | 1:A:145:THR:HG22 | 1.82                     | 0.61              |
| 1:C:177:VAL:O    | 1:C:177:VAL:CG1  | 2.48                     | 0.61              |
| 2:D:151:THR:HB   | 2:D:193:GLN:HG2  | 1.82                     | 0.61              |
| 2:B:259:MET:HE2  | 2:B:378:ILE:HG22 | 1.82                     | 0.61              |
| 1:A:121:ARG:HG3  | 1:A:121:ARG:HH11 | 1.65                     | 0.61              |
| 1:A:246:GLY:HA2  | 3:E:14:CYS:SG    | 2.41                     | 0.61              |
| 1:C:435:VAL:HG12 | 1:C:435:VAL:O    | 2.00                     | 0.61              |
| 1:A:70:LEU:HD13  | 1:A:145:THR:CB   | 2.31                     | 0.61              |
| 1:C:273:ALA:HB2  | 1:C:375:VAL:H    | 1.66                     | 0.61              |
| 1:C:179:THR:HA   | 2:D:248:LEU:HD12 | 1.83                     | 0.61              |
| 2:B:174:SER:HB2  | 2:B:207:GLU:HB2  | 1.82                     | 0.61              |
| 1:C:70:LEU:N     | 1:C:70:LEU:HD12  | 2.16                     | 0.60              |
| 1:A:145:THR:HG23 | 4:A:600:GTP:O2B  | 2.00                     | 0.60              |
| 1:A:179:THR:O    | 2:B:352:LYS:HE2  | 2.02                     | 0.60              |
| 1:A:317:LEU:HD23 | 1:A:377:MET:HB2  | 1.84                     | 0.60              |
| 2:B:27:GLU:OE2   | 2:B:320:ARG:NH2  | 2.34                     | 0.60              |
| 2:D:153:LEU:O    | 2:D:157:ILE:HG12 | 2.01                     | 0.60              |
| 1:C:21:TRP:CZ3   | 1:C:63:PRO:HB3   | 2.36                     | 0.59              |
| 3:E:61:ARG:C     | 3:E:63:TYR:N     | 2.59                     | 0.59              |
| 2:B:145:THR:HG22 | 6:B:600:GDP:O3B  | 2.02                     | 0.59              |
| 2:D:169:PHE:CE2  | 2:D:235:MET:HG2  | 2.37                     | 0.59              |
| 2:D:287:THR:HG22 | 2:D:290:GLU:HB2  | 1.83                     | 0.59              |
| 2:B:224:TYR:O    | 2:B:228:ASN:ND2  | 2.35                     | 0.59              |
| 2:D:5:VAL:HG22   | 2:D:135:PHE:HD2  | 1.66                     | 0.59              |
| 2:D:383:ALA:O    | 2:D:386:GLU:HB2  | 2.02                     | 0.59              |
| 1:A:2:ARG:HA     | 1:A:2:ARG:NH1    | 2.16                     | 0.59              |
| 2:B:169:PHE:CE2  | 2:B:235:MET:HG2  | 2.38                     | 0.59              |
| 2:D:48:ARG:HH22  | 2:D:250:ALA:HB1  | 1.66                     | 0.59              |
| 2:D:223:THR:CB   | 2:D:225:GLY:H    | 2.13                     | 0.59              |
| 2:B:54:ASN:HD22  | 2:B:64:ARG:CD    | 2.13                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:114:ILE:O    | 1:C:118:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:79:ARG:HH22  | 1:A:94:THR:CG2   | 2.08                     | 0.59              |
| 2:B:291:LEU:HD21 | 2:B:375:ALA:CB   | 2.32                     | 0.59              |
| 2:B:59:ASN:O     | 2:B:60:LYS:O     | 2.21                     | 0.58              |
| 1:A:262:TYR:HB2  | 1:A:265:ILE:HD13 | 1.84                     | 0.58              |
| 2:B:14:ASN:HD22  | 2:B:67:LEU:HD23  | 1.68                     | 0.58              |
| 2:D:7:ILE:O      | 2:D:137:LEU:HA   | 2.04                     | 0.58              |
| 1:A:151:SER:OG   | 1:A:193:THR:HB   | 2.04                     | 0.58              |
| 2:B:210:TYR:HD1  | 2:B:210:TYR:C    | 2.12                     | 0.58              |
| 1:A:247:ALA:HB2  | 3:E:12:ASN:CG    | 2.28                     | 0.58              |
| 2:B:48:ARG:HH22  | 2:B:246:GLY:HA3  | 1.67                     | 0.58              |
| 1:C:79:ARG:HH22  | 1:C:94:THR:CG2   | 2.13                     | 0.58              |
| 2:D:70:LEU:HD11  | 2:D:149:MET:HE3  | 1.85                     | 0.58              |
| 2:B:229:HIS:HE1  | 2:B:276:THR:O    | 1.86                     | 0.57              |
| 2:D:114:LEU:HD23 | 2:D:149:MET:HE1  | 1.85                     | 0.57              |
| 1:A:21:TRP:CZ3   | 1:A:63:PRO:HB3   | 2.38                     | 0.57              |
| 2:B:274:PRO:C    | 2:B:275:LEU:HG   | 2.29                     | 0.57              |
| 1:C:99:ALA:HB2   | 1:C:145:THR:HG22 | 1.86                     | 0.57              |
| 2:D:237:GLY:HA3  | 2:D:376:THR:HG21 | 1.84                     | 0.57              |
| 2:D:4:ILE:HD11   | 2:D:52:TYR:CE2   | 2.39                     | 0.57              |
| 2:B:4:ILE:HD11   | 2:B:52:TYR:CE2   | 2.39                     | 0.57              |
| 1:C:100:ALA:CB   | 2:D:253:ARG:HG2  | 2.34                     | 0.57              |
| 2:D:48:ARG:NH2   | 2:D:250:ALA:HB1  | 2.20                     | 0.57              |
| 2:D:198:THR:OG1  | 2:D:266:HIS:CE1  | 2.58                     | 0.57              |
| 2:D:224:TYR:O    | 2:D:228:ASN:ND2  | 2.38                     | 0.57              |
| 1:A:177:VAL:O    | 1:A:177:VAL:HG13 | 2.04                     | 0.57              |
| 2:B:319:PHE:HB2  | 2:B:355:VAL:HG12 | 1.85                     | 0.57              |
| 2:B:210:TYR:C    | 2:B:210:TYR:CD1  | 2.83                     | 0.56              |
| 2:D:273:ALA:HB3  | 2:D:274:PRO:HD3  | 1.67                     | 0.56              |
| 3:E:17:GLY:O     | 3:E:18:GLN:HB2   | 2.03                     | 0.56              |
| 3:E:67:GLU:C     | 3:E:69:LEU:N     | 2.61                     | 0.56              |
| 2:B:70:LEU:HD11  | 2:B:149:MET:HE3  | 1.85                     | 0.56              |
| 2:B:200:GLU:OE2  | 2:B:255:LEU:HD12 | 2.05                     | 0.56              |
| 2:B:2:ARG:CD     | 2:B:131:CYS:SG   | 2.92                     | 0.56              |
| 2:B:5:VAL:HG22   | 2:B:135:PHE:HD2  | 1.70                     | 0.56              |
| 2:B:200:GLU:HB3  | 2:B:268:PHE:CE1  | 2.40                     | 0.56              |
| 2:D:141:LEU:HD13 | 2:D:170:SER:HB3  | 1.86                     | 0.56              |
| 2:B:229:HIS:CE1  | 2:B:276:THR:O    | 2.58                     | 0.56              |
| 2:B:357:ASP:OD2  | 2:B:357:ASP:N    | 2.38                     | 0.56              |
| 2:D:180:THR:HG22 | 2:D:182:VAL:HG22 | 1.86                     | 0.56              |
| 3:E:11:LEU:O     | 3:E:12:ASN:CB    | 2.52                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:210:TYR:HD1  | 2:D:210:TYR:C    | 2.13                     | 0.56              |
| 3:E:12:ASN:OD1   | 3:E:12:ASN:C     | 2.49                     | 0.56              |
| 1:A:191:THR:HG23 | 1:A:425:MET:CE   | 2.35                     | 0.56              |
| 1:C:256:GLN:C    | 1:C:258:ASN:H    | 2.11                     | 0.56              |
| 2:B:174:SER:O    | 2:B:178:SER:HB3  | 2.06                     | 0.56              |
| 1:C:99:ALA:CB    | 1:C:145:THR:HG22 | 2.36                     | 0.56              |
| 3:E:76:ARG:C     | 3:E:78:HIS:H     | 2.14                     | 0.56              |
| 1:A:205:ASP:HB2  | 1:A:303:VAL:HA   | 1.88                     | 0.56              |
| 1:C:273:ALA:HB3  | 1:C:375:VAL:H    | 1.71                     | 0.56              |
| 2:D:88:ARG:O     | 2:D:91:ASN:HB2   | 2.05                     | 0.56              |
| 2:D:210:TYR:C    | 2:D:210:TYR:CD1  | 2.84                     | 0.55              |
| 2:D:274:PRO:C    | 2:D:275:LEU:HG   | 2.31                     | 0.55              |
| 2:D:291:LEU:HD21 | 2:D:375:ALA:HB2  | 1.88                     | 0.55              |
| 2:D:336:GLN:OE1  | 2:D:351:VAL:HG11 | 2.05                     | 0.55              |
| 2:B:287:THR:HG23 | 2:B:289:PRO:HD2  | 1.88                     | 0.55              |
| 2:D:295:MET:O    | 2:D:295:MET:HG2  | 2.06                     | 0.55              |
| 2:B:88:ARG:O     | 2:B:91:ASN:HB2   | 2.07                     | 0.55              |
| 2:D:89:PRO:O     | 2:D:92:PHE:HD1   | 1.89                     | 0.55              |
| 2:B:205:ASP:OD1  | 2:B:207:GLU:HB3  | 2.07                     | 0.55              |
| 2:D:224:TYR:OH   | 6:D:600:GDP:H2'  | 2.07                     | 0.55              |
| 2:D:261:PRO:HB2  | 2:D:262:PHE:CD1  | 2.41                     | 0.55              |
| 2:B:401:ARG:NH1  | 2:B:401:ARG:HG3  | 2.22                     | 0.54              |
| 1:C:96:LYS:HD3   | 2:D:131:CYS:HB2  | 1.89                     | 0.54              |
| 1:A:36:MET:O     | 1:A:36:MET:HG3   | 2.06                     | 0.54              |
| 2:B:250:ALA:O    | 2:B:251:ASP:HB2  | 2.08                     | 0.54              |
| 1:A:250:VAL:O    | 1:A:250:VAL:HG22 | 2.08                     | 0.54              |
| 1:C:53:PHE:HD2   | 1:C:61:HIS:O     | 1.90                     | 0.54              |
| 2:D:213:CYS:HA   | 2:D:217:LEU:HB2  | 1.89                     | 0.54              |
| 1:A:114:ILE:O    | 1:A:118:VAL:HG23 | 2.07                     | 0.54              |
| 1:C:264:ARG:O    | 1:C:265:ILE:C    | 2.51                     | 0.54              |
| 2:B:383:ALA:O    | 2:B:386:GLU:HB2  | 2.08                     | 0.53              |
| 1:C:66:VAL:HG11  | 1:C:122:ILE:HG12 | 1.89                     | 0.53              |
| 1:A:410:GLY:HA2  | 3:E:64:GLN:HE22  | 1.73                     | 0.53              |
| 1:C:229:ARG:HG2  | 1:C:229:ARG:NH1  | 2.20                     | 0.53              |
| 2:D:136:GLN:HB3  | 2:D:167:ASN:HB3  | 1.90                     | 0.53              |
| 2:B:336:GLN:OE1  | 2:B:351:VAL:HG11 | 2.09                     | 0.53              |
| 2:D:174:SER:HB2  | 2:D:207:GLU:HB2  | 1.90                     | 0.53              |
| 2:D:114:LEU:HB3  | 2:D:149:MET:CE   | 2.38                     | 0.53              |
| 2:D:192:HIS:CD2  | 2:D:421:ALA:HA   | 2.44                     | 0.53              |
| 2:B:347:ILE:HG22 | 2:B:350:ASN:HB3  | 1.91                     | 0.53              |
| 2:B:401:ARG:HG3  | 2:B:401:ARG:HH11 | 1.73                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:205:ASP:OD1  | 2:D:207:GLU:HB3  | 2.09                     | 0.53              |
| 1:A:398:MET:HG3  | 2:B:348:PRO:HD3  | 1.90                     | 0.53              |
| 2:D:200:GLU:HA   | 2:D:266:HIS:HB2  | 1.90                     | 0.53              |
| 1:A:100:ALA:HB1  | 2:B:253:ARG:HG2  | 1.90                     | 0.53              |
| 1:C:88:HIS:O     | 1:C:91:GLN:HG2   | 2.09                     | 0.53              |
| 2:D:305:CYS:HB3  | 2:D:386:GLU:HB3  | 1.90                     | 0.53              |
| 2:B:20:PHE:O     | 2:B:24:ILE:HG23  | 2.09                     | 0.53              |
| 1:A:249:ASN:N    | 1:A:254:GLU:OE1  | 2.42                     | 0.53              |
| 1:A:398:MET:HG3  | 2:B:348:PRO:CD   | 2.39                     | 0.52              |
| 2:B:89:PRO:O     | 2:B:92:PHE:HD1   | 1.91                     | 0.52              |
| 2:B:261:PRO:HB2  | 2:B:262:PHE:CD1  | 2.44                     | 0.52              |
| 2:D:6:HIS:CE1    | 2:D:8:GLN:HB2    | 2.45                     | 0.52              |
| 2:D:51:VAL:HG12  | 2:D:52:TYR:CD1   | 2.45                     | 0.52              |
| 2:D:234:THR:O    | 2:D:238:VAL:HG23 | 2.10                     | 0.52              |
| 2:B:342:TYR:N    | 2:B:342:TYR:HD2  | 2.07                     | 0.52              |
| 2:D:126:SER:C    | 2:D:128:SER:H    | 2.16                     | 0.52              |
| 2:D:292:THR:HA   | 2:D:295:MET:HE3  | 1.90                     | 0.52              |
| 1:A:211:ASP:OD1  | 1:A:304:LYS:HE3  | 2.08                     | 0.52              |
| 2:B:14:ASN:ND2   | 2:B:67:LEU:HD23  | 2.24                     | 0.52              |
| 2:D:217:LEU:HD21 | 2:D:276:THR:HB   | 1.92                     | 0.52              |
| 2:D:342:TYR:HD2  | 2:D:342:TYR:N    | 2.07                     | 0.52              |
| 2:B:8:GLN:OE1    | 2:B:67:LEU:HD23  | 2.10                     | 0.52              |
| 1:A:229:ARG:HG2  | 1:A:229:ARG:NH1  | 2.19                     | 0.52              |
| 2:B:16:ILE:HG23  | 2:B:235:MET:HE1  | 1.91                     | 0.52              |
| 2:B:151:THR:HB   | 2:B:193:GLN:HG2  | 1.92                     | 0.52              |
| 1:A:8:HIS:CD2    | 1:A:17:GLY:CA    | 2.92                     | 0.52              |
| 1:A:87:PHE:N     | 1:A:87:PHE:CD2   | 2.77                     | 0.52              |
| 1:A:88:HIS:O     | 1:A:91:GLN:HG2   | 2.10                     | 0.52              |
| 1:A:188:ILE:HD12 | 1:A:425:MET:HG3  | 1.91                     | 0.52              |
| 1:A:210:TYR:CE1  | 1:A:214:ARG:HD3  | 2.45                     | 0.52              |
| 2:B:391:ILE:HG13 | 2:B:425:MET:HE1  | 1.91                     | 0.52              |
| 2:D:336:GLN:OE1  | 2:D:351:VAL:CG1  | 2.58                     | 0.52              |
| 1:A:105:ARG:HD2  | 1:A:411:GLU:OE1  | 2.10                     | 0.52              |
| 1:A:377:MET:O    | 1:A:377:MET:HG3  | 2.08                     | 0.52              |
| 2:B:234:THR:O    | 2:B:238:VAL:HG23 | 2.10                     | 0.51              |
| 1:C:102:ASN:OD1  | 1:C:105:ARG:HB2  | 2.11                     | 0.51              |
| 2:B:166:MET:HB2  | 2:B:199:ASP:OD1  | 2.10                     | 0.51              |
| 2:D:8:GLN:OE1    | 2:D:67:LEU:HD23  | 2.10                     | 0.51              |
| 1:C:395:PHE:C    | 1:C:395:PHE:CD2  | 2.87                     | 0.51              |
| 2:D:166:MET:HB2  | 2:D:199:ASP:OD1  | 2.09                     | 0.51              |
| 2:D:342:TYR:N    | 2:D:342:TYR:CD2  | 2.79                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:64:ARG:HG3   | 1:A:64:ARG:HH11  | 1.75                     | 0.51              |
| 2:B:401:ARG:HH11 | 2:B:401:ARG:CG   | 2.23                     | 0.51              |
| 1:C:346:TRP:HZ2  | 1:C:435:VAL:CG1  | 2.22                     | 0.51              |
| 2:D:229:HIS:HE1  | 2:D:276:THR:O    | 1.93                     | 0.51              |
| 2:B:213:CYS:HA   | 2:B:217:LEU:HB2  | 1.92                     | 0.51              |
| 3:E:60:ARG:HG3   | 3:E:60:ARG:HH11  | 1.76                     | 0.51              |
| 2:B:198:THR:OG1  | 2:B:266:HIS:CE1  | 2.64                     | 0.51              |
| 1:C:183:GLU:HB3  | 1:C:184:PRO:HD3  | 1.91                     | 0.51              |
| 1:C:376:CYS:O    | 1:C:377:MET:C    | 2.54                     | 0.51              |
| 1:A:291:ILE:HD12 | 1:A:375:VAL:CG2  | 2.41                     | 0.50              |
| 2:B:88:ARG:NH1   | 2:B:91:ASN:OD1   | 2.45                     | 0.50              |
| 1:C:121:ARG:HG3  | 1:C:121:ARG:NH1  | 2.26                     | 0.50              |
| 1:A:186:ASN:O    | 1:A:190:THR:HG22 | 2.11                     | 0.50              |
| 2:B:223:THR:CB   | 2:B:225:GLY:H    | 2.20                     | 0.50              |
| 2:B:342:TYR:N    | 2:B:342:TYR:CD2  | 2.79                     | 0.50              |
| 1:C:221:ARG:CB   | 2:D:325:MET:HE1  | 2.42                     | 0.50              |
| 2:D:114:LEU:HB3  | 2:D:149:MET:HE1  | 1.94                     | 0.50              |
| 2:D:256:ALA:O    | 2:D:260:VAL:HG22 | 2.10                     | 0.50              |
| 2:D:292:THR:HA   | 2:D:295:MET:CE   | 2.41                     | 0.50              |
| 3:E:60:ARG:HG3   | 3:E:60:ARG:NH1   | 2.26                     | 0.50              |
| 2:D:391:ILE:HG13 | 2:D:425:MET:HE1  | 1.92                     | 0.50              |
| 1:A:239:THR:O    | 1:A:242:LEU:N    | 2.38                     | 0.50              |
| 2:B:36:TYR:OH    | 2:B:40:SER:O     | 2.25                     | 0.50              |
| 2:B:70:LEU:C     | 2:B:95:GLY:HA3   | 2.37                     | 0.50              |
| 2:B:70:LEU:CA    | 2:B:95:GLY:HA3   | 2.38                     | 0.50              |
| 2:B:238:VAL:HG13 | 2:B:378:ILE:HD11 | 1.92                     | 0.50              |
| 1:C:205:ASP:HB2  | 1:C:303:VAL:HA   | 1.94                     | 0.50              |
| 2:D:265:LEU:HB3  | 2:D:432:TYR:CE2  | 2.45                     | 0.50              |
| 2:B:251:ASP:O    | 2:B:253:ARG:N    | 2.42                     | 0.50              |
| 2:B:295:MET:O    | 2:B:295:MET:HG2  | 2.10                     | 0.50              |
| 1:A:306:ASP:O    | 1:A:309:HIS:HB3  | 2.12                     | 0.50              |
| 2:B:192:HIS:CD2  | 2:B:421:ALA:HA   | 2.47                     | 0.50              |
| 1:C:260:VAL:O    | 1:C:260:VAL:CG2  | 2.60                     | 0.50              |
| 2:D:298:SER:C    | 2:D:300:ASN:H    | 2.19                     | 0.50              |
| 2:B:141:LEU:HD13 | 2:B:170:SER:HB3  | 1.92                     | 0.50              |
| 2:B:336:GLN:OE1  | 2:B:351:VAL:CG1  | 2.59                     | 0.50              |
| 1:C:115:ILE:HG13 | 1:C:152:LEU:HD23 | 1.94                     | 0.50              |
| 1:A:298:PRO:HA   | 1:A:301:GLN:NE2  | 2.26                     | 0.49              |
| 2:B:387:LEU:O    | 2:B:390:ARG:HG3  | 2.12                     | 0.49              |
| 2:D:174:SER:O    | 2:D:178:SER:HB3  | 2.12                     | 0.49              |
| 3:E:130:ALA:HB1  | 3:E:134:ARG:HH12 | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:PHE:HD2   | 1:A:61:HIS:O     | 1.95                     | 0.49              |
| 2:B:204:ILE:HD13 | 2:B:231:VAL:HG13 | 1.94                     | 0.49              |
| 2:D:4:ILE:O      | 2:D:4:ILE:HG12   | 2.12                     | 0.49              |
| 2:D:16:ILE:HG12  | 2:D:231:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:239:THR:O    | 1:A:240:ALA:C    | 2.54                     | 0.49              |
| 1:A:435:VAL:HG12 | 1:A:435:VAL:O    | 2.12                     | 0.49              |
| 2:B:114:LEU:HD23 | 2:B:149:MET:HE1  | 1.94                     | 0.49              |
| 2:B:256:ALA:O    | 2:B:260:VAL:HG22 | 2.13                     | 0.49              |
| 1:A:376:CYS:O    | 1:A:377:MET:C    | 2.55                     | 0.49              |
| 2:D:14:ASN:HD22  | 2:D:67:LEU:HD23  | 1.77                     | 0.49              |
| 2:D:225:GLY:C    | 2:D:227:LEU:H    | 2.21                     | 0.49              |
| 1:A:329:ASN:ND2  | 3:E:20:PHE:CE1   | 2.80                     | 0.49              |
| 2:B:156:LYS:HE3  | 3:E:76:ARG:NE    | 2.28                     | 0.49              |
| 1:A:273:ALA:HB3  | 1:A:375:VAL:H    | 1.77                     | 0.49              |
| 2:B:4:ILE:HD11   | 2:B:52:TYR:CZ    | 2.48                     | 0.49              |
| 2:B:200:GLU:HA   | 2:B:266:HIS:HB2  | 1.95                     | 0.49              |
| 2:D:311:ARG:NE   | 2:D:344:VAL:HG23 | 2.23                     | 0.49              |
| 1:A:167:LEU:HD22 | 1:A:252:LEU:HD22 | 1.94                     | 0.48              |
| 1:A:181:VAL:H    | 2:B:258:ASN:HD21 | 1.59                     | 0.48              |
| 1:A:397:LEU:CD2  | 2:B:348:PRO:HG3  | 2.43                     | 0.48              |
| 2:D:52:TYR:CE1   | 2:D:243:ARG:HD3  | 2.48                     | 0.48              |
| 1:A:177:VAL:O    | 1:A:177:VAL:CG1  | 2.62                     | 0.48              |
| 1:C:36:MET:O     | 1:C:36:MET:HG3   | 2.14                     | 0.48              |
| 2:D:200:GLU:HG2  | 2:D:268:PHE:HE1  | 1.78                     | 0.48              |
| 2:D:36:TYR:OH    | 2:D:40:SER:O     | 2.28                     | 0.48              |
| 1:A:2:ARG:HB2    | 1:A:131:GLY:O    | 2.13                     | 0.48              |
| 1:C:265:ILE:HG22 | 1:C:265:ILE:O    | 2.13                     | 0.48              |
| 2:D:107:HIS:O    | 2:D:152:LEU:HD22 | 2.13                     | 0.48              |
| 3:E:94:ILE:O     | 3:E:98:LYS:N     | 2.45                     | 0.48              |
| 1:A:163:LYS:O    | 1:A:164:LYS:C    | 2.57                     | 0.48              |
| 2:B:211:ASP:O    | 2:B:215:ARG:N    | 2.36                     | 0.48              |
| 2:B:403:ALA:C    | 2:B:405:LEU:H    | 2.22                     | 0.48              |
| 1:C:211:ASP:OD1  | 1:C:304:LYS:HE3  | 2.13                     | 0.48              |
| 1:C:260:VAL:O    | 1:C:260:VAL:HG23 | 2.12                     | 0.48              |
| 1:A:183:GLU:HB3  | 1:A:184:PRO:HD3  | 1.94                     | 0.48              |
| 1:A:313:MET:HE3  | 1:A:380:ASN:ND2  | 2.28                     | 0.48              |
| 1:A:70:LEU:N     | 1:A:70:LEU:HD12  | 2.29                     | 0.48              |
| 1:A:223:THR:HB   | 1:A:226:ASN:H    | 1.78                     | 0.48              |
| 2:B:179:ASP:C    | 1:C:352:LYS:HE3  | 2.39                     | 0.48              |
| 1:C:212:ILE:O    | 1:C:216:ASN:HB2  | 2.14                     | 0.48              |
| 2:D:4:ILE:HD11   | 2:D:52:TYR:CZ    | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:TRP:HE3  | 1:A:346:TRP:O    | 1.96                     | 0.48              |
| 2:D:5:VAL:CG2    | 2:D:135:PHE:HD2  | 2.27                     | 0.48              |
| 2:D:247:GLN:CD   | 2:D:354:ALA:HB1  | 2.38                     | 0.48              |
| 1:A:121:ARG:HG3  | 1:A:121:ARG:NH1  | 2.28                     | 0.48              |
| 2:B:244:PHE:CB   | 2:B:245:PRO:CD   | 2.89                     | 0.48              |
| 2:D:296:PHE:HE1  | 2:D:332:MET:HE1  | 1.79                     | 0.48              |
| 2:B:225:GLY:C    | 2:B:227:LEU:H    | 2.22                     | 0.47              |
| 2:B:325:MET:HE3  | 2:B:326:LYS:N    | 2.29                     | 0.47              |
| 2:D:395:PHE:CE2  | 2:D:422:GLU:HB2  | 2.49                     | 0.47              |
| 1:A:388:TRP:CE3  | 1:A:388:TRP:HA   | 2.49                     | 0.47              |
| 1:A:62:VAL:HA    | 1:A:63:PRO:HD3   | 1.82                     | 0.47              |
| 1:A:189:LEU:HD21 | 1:A:413:MET:HE1  | 1.96                     | 0.47              |
| 2:D:59:ASN:O     | 2:D:60:LYS:O     | 2.31                     | 0.47              |
| 1:C:88:HIS:H     | 1:C:91:GLN:NE2   | 2.12                     | 0.47              |
| 1:C:223:THR:O    | 1:C:227:LEU:HD13 | 2.13                     | 0.47              |
| 2:D:320:ARG:HA   | 2:D:356:CYS:O    | 2.14                     | 0.47              |
| 2:B:298:SER:C    | 2:B:300:ASN:H    | 2.22                     | 0.47              |
| 1:A:30:ILE:HA    | 1:A:36:MET:HB3   | 1.95                     | 0.47              |
| 2:B:114:LEU:HB3  | 2:B:149:MET:CE   | 2.44                     | 0.47              |
| 2:B:292:THR:HA   | 2:B:295:MET:CE   | 2.43                     | 0.47              |
| 1:C:313:MET:HG2  | 1:C:380:ASN:O    | 2.15                     | 0.47              |
| 2:D:27:GLU:CD    | 2:D:320:ARG:HH22 | 2.23                     | 0.47              |
| 2:D:88:ARG:NH1   | 2:D:91:ASN:OD1   | 2.48                     | 0.47              |
| 2:D:204:ILE:HD13 | 2:D:231:VAL:HG13 | 1.95                     | 0.47              |
| 2:D:239:THR:O    | 2:D:242:LEU:N    | 2.45                     | 0.47              |
| 2:D:296:PHE:CE1  | 2:D:332:MET:HE1  | 2.49                     | 0.47              |
| 2:B:315:VAL:HG13 | 2:B:377:PHE:HD1  | 1.79                     | 0.47              |
| 2:B:4:ILE:O      | 2:B:4:ILE:HG12   | 2.15                     | 0.47              |
| 2:B:42:LEU:O     | 2:B:43:GLN:C     | 2.57                     | 0.47              |
| 2:B:107:HIS:O    | 2:B:152:LEU:HD22 | 2.15                     | 0.47              |
| 2:D:347:ILE:HG22 | 2:D:350:ASN:HB3  | 1.97                     | 0.47              |
| 1:A:317:LEU:CD2  | 1:A:377:MET:HB2  | 2.45                     | 0.46              |
| 1:C:264:ARG:O    | 1:C:266:HIS:N    | 2.48                     | 0.46              |
| 2:D:169:PHE:CD2  | 2:D:235:MET:HG2  | 2.50                     | 0.46              |
| 1:A:298:PRO:O    | 1:A:301:GLN:HB2  | 2.15                     | 0.46              |
| 2:D:42:LEU:O     | 2:D:43:GLN:C     | 2.58                     | 0.46              |
| 1:C:28:HIS:CE1   | 1:C:244:PHE:CZ   | 3.04                     | 0.46              |
| 1:C:317:LEU:CD2  | 1:C:377:MET:HB2  | 2.45                     | 0.46              |
| 1:C:244:PHE:O    | 1:C:245:ASP:CB   | 2.57                     | 0.46              |
| 1:A:264:ARG:O    | 1:A:265:ILE:C    | 2.57                     | 0.46              |
| 2:B:408:TYR:O    | 2:B:409:THR:C    | 2.59                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:14:ASN:ND2   | 2:D:67:LEU:HD23  | 2.30                     | 0.46              |
| 2:D:259:MET:HB3  | 2:D:268:PHE:CZ   | 2.51                     | 0.46              |
| 2:D:401:ARG:HG3  | 2:D:401:ARG:NH1  | 2.29                     | 0.46              |
| 2:D:239:THR:O    | 2:D:240:THR:C    | 2.58                     | 0.46              |
| 1:A:97:GLU:HG3   | 1:A:98:ASP:N     | 2.31                     | 0.46              |
| 2:B:126:SER:C    | 2:B:128:SER:H    | 2.23                     | 0.46              |
| 1:C:71:GLU:HG3   | 1:C:73:THR:OG1   | 2.15                     | 0.46              |
| 2:D:11:GLN:HG3   | 2:D:74:THR:CG2   | 2.41                     | 0.46              |
| 2:D:138:THR:CG2  | 2:D:169:PHE:HB2  | 2.43                     | 0.46              |
| 2:D:145:THR:HG22 | 6:D:600:GDP:O3B  | 2.16                     | 0.46              |
| 2:D:177:VAL:O    | 2:D:177:VAL:CG1  | 2.64                     | 0.46              |
| 2:D:178:SER:HB2  | 2:D:183:GLU:OE1  | 2.15                     | 0.46              |
| 2:B:115:VAL:HG12 | 2:B:116:ASP:N    | 2.30                     | 0.46              |
| 2:D:225:GLY:O    | 2:D:227:LEU:N    | 2.41                     | 0.46              |
| 1:A:190:THR:O    | 1:A:193:THR:N    | 2.49                     | 0.45              |
| 1:A:212:ILE:O    | 1:A:216:ASN:HB2  | 2.16                     | 0.45              |
| 2:B:259:MET:HB3  | 2:B:268:PHE:CZ   | 2.51                     | 0.45              |
| 1:C:210:TYR:CE1  | 1:C:214:ARG:HD3  | 2.51                     | 0.45              |
| 1:A:7:ILE:HG21   | 1:A:153:LEU:HD11 | 1.98                     | 0.45              |
| 2:D:54:ASN:ND2   | 2:D:64:ARG:HH11  | 2.14                     | 0.45              |
| 2:D:229:HIS:CE1  | 2:D:276:THR:O    | 2.69                     | 0.45              |
| 2:D:291:LEU:HD21 | 2:D:375:ALA:CB   | 2.46                     | 0.45              |
| 2:D:401:ARG:CG   | 2:D:401:ARG:HH11 | 2.29                     | 0.45              |
| 1:A:397:LEU:HD23 | 2:B:348:PRO:HG3  | 1.97                     | 0.45              |
| 2:B:5:VAL:CG2    | 2:B:135:PHE:HD2  | 2.29                     | 0.45              |
| 2:B:48:ARG:NH2   | 2:B:246:GLY:HA3  | 2.30                     | 0.45              |
| 2:B:308:ARG:HH11 | 2:B:308:ARG:CG   | 2.29                     | 0.45              |
| 3:E:94:ILE:HG22  | 3:E:95:LYS:H     | 1.81                     | 0.45              |
| 2:B:239:THR:O    | 2:B:240:THR:C    | 2.59                     | 0.45              |
| 1:A:105:ARG:HG2  | 1:A:110:ILE:HG22 | 1.99                     | 0.45              |
| 1:A:302:MET:HE3  | 1:A:302:MET:HB3  | 1.69                     | 0.45              |
| 1:C:152:LEU:HA   | 1:C:155:GLU:HG3  | 1.98                     | 0.45              |
| 3:E:67:GLU:O     | 3:E:69:LEU:N     | 2.45                     | 0.45              |
| 3:E:119:MET:O    | 3:E:119:MET:HG3  | 2.12                     | 0.45              |
| 1:A:247:ALA:HB2  | 3:E:12:ASN:OD1   | 2.16                     | 0.45              |
| 1:C:251:ASP:OD1  | 1:C:252:LEU:N    | 2.49                     | 0.45              |
| 1:C:298:PRO:C    | 1:C:300:ASN:H    | 2.25                     | 0.45              |
| 1:A:99:ALA:HB3   | 1:A:145:THR:HG22 | 1.99                     | 0.45              |
| 2:B:62:VAL:O     | 2:B:62:VAL:CG2   | 2.64                     | 0.45              |
| 2:B:177:VAL:O    | 2:B:177:VAL:CG1  | 2.65                     | 0.45              |
| 2:D:16:ILE:HG22  | 2:D:17:GLY:N     | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:308:ARG:HH11 | 2:D:308:ARG:CG   | 2.29                     | 0.45              |
| 2:B:110:GLU:H    | 2:B:110:GLU:HG2  | 1.64                     | 0.45              |
| 2:D:54:ASN:CG    | 2:D:64:ARG:HH11  | 2.25                     | 0.45              |
| 2:D:126:SER:C    | 2:D:128:SER:N    | 2.75                     | 0.45              |
| 2:D:265:LEU:HB3  | 2:D:432:TYR:CZ   | 2.52                     | 0.45              |
| 2:D:297:ASP:HB3  | 2:D:300:ASN:HB2  | 1.99                     | 0.45              |
| 1:A:242:LEU:HD21 | 1:A:255:PHE:HE2  | 1.82                     | 0.45              |
| 1:C:67:PHE:HB2   | 1:C:92:LEU:HD22  | 1.99                     | 0.45              |
| 1:C:223:THR:HB   | 1:C:226:ASN:H    | 1.80                     | 0.45              |
| 2:D:177:VAL:O    | 2:D:177:VAL:HG12 | 2.16                     | 0.45              |
| 1:A:161:TYR:HB3  | 1:A:164:LYS:HG3  | 1.99                     | 0.44              |
| 2:D:212:ILE:CD1  | 2:D:215:ARG:HH22 | 2.31                     | 0.44              |
| 2:D:274:PRO:HG2  | 2:D:286:LEU:HD13 | 1.99                     | 0.44              |
| 1:C:2:ARG:HA     | 1:C:2:ARG:NH1    | 2.32                     | 0.44              |
| 1:C:388:TRP:HA   | 1:C:388:TRP:CE3  | 2.52                     | 0.44              |
| 2:D:287:THR:HG23 | 2:D:289:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:88:HIS:H     | 1:A:91:GLN:NE2   | 2.15                     | 0.44              |
| 1:A:189:LEU:CD2  | 1:A:413:MET:HE1  | 2.46                     | 0.44              |
| 1:C:87:PHE:N     | 1:C:87:PHE:CD2   | 2.85                     | 0.44              |
| 2:D:385:GLN:HE21 | 2:D:389:LYS:HE3  | 1.81                     | 0.44              |
| 3:E:107:SER:O    | 3:E:111:ASN:HB2  | 2.17                     | 0.44              |
| 1:A:273:ALA:HB2  | 1:A:375:VAL:N    | 2.27                     | 0.44              |
| 2:B:398:MET:HE2  | 1:C:348:PRO:HD3  | 2.00                     | 0.44              |
| 1:C:34:GLY:O     | 1:C:61:HIS:HB2   | 2.18                     | 0.44              |
| 2:D:12:CYS:SG    | 6:D:600:GDP:C4   | 3.11                     | 0.44              |
| 2:D:315:VAL:HG13 | 2:D:377:PHE:HD1  | 1.82                     | 0.44              |
| 1:A:375:VAL:HG12 | 1:A:376:CYS:H    | 1.83                     | 0.44              |
| 2:D:211:ASP:O    | 2:D:215:ARG:N    | 2.36                     | 0.44              |
| 3:E:94:ILE:CG2   | 3:E:95:LYS:N     | 2.80                     | 0.44              |
| 2:B:178:SER:HB2  | 2:B:183:GLU:OE1  | 2.17                     | 0.44              |
| 2:D:55:GLU:HB3   | 2:D:61:TYR:CD2   | 2.53                     | 0.44              |
| 2:B:52:TYR:CE1   | 2:B:243:ARG:HD3  | 2.53                     | 0.44              |
| 1:C:163:LYS:O    | 1:C:164:LYS:C    | 2.60                     | 0.44              |
| 1:C:209:ILE:HD11 | 1:C:302:MET:SD   | 2.57                     | 0.44              |
| 2:D:351:VAL:HG22 | 2:D:351:VAL:O    | 2.17                     | 0.44              |
| 2:B:156:LYS:HE3  | 3:E:76:ARG:HE    | 1.82                     | 0.44              |
| 2:D:357:ASP:OD2  | 2:D:357:ASP:N    | 2.48                     | 0.44              |
| 1:A:8:HIS:HE1    | 1:A:21:TRP:HE1   | 1.66                     | 0.43              |
| 1:A:229:ARG:CG   | 1:A:229:ARG:NH1  | 2.78                     | 0.43              |
| 1:A:298:PRO:C    | 1:A:300:ASN:H    | 2.26                     | 0.43              |
| 1:A:306:ASP:O    | 1:A:309:HIS:CB   | 2.66                     | 0.43              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:414:GLU:N    | 3:E:60:ARG:HH21 | 2.16                     | 0.43              |
| 1:C:281:ALA:HB2  | 1:C:369:ALA:HB1 | 1.99                     | 0.43              |
| 1:A:264:ARG:O    | 1:A:266:HIS:CD2 | 2.70                     | 0.43              |
| 1:A:313:MET:HG2  | 1:A:380:ASN:O   | 2.17                     | 0.43              |
| 2:D:306:ASP:C    | 2:D:308:ARG:H   | 2.26                     | 0.43              |
| 1:A:321:GLY:HA2  | 1:A:359:PRO:HA  | 2.00                     | 0.43              |
| 2:D:115:VAL:HG12 | 2:D:116:ASP:N   | 2.33                     | 0.43              |
| 2:D:403:ALA:C    | 2:D:405:LEU:H   | 2.26                     | 0.43              |
| 2:D:408:TYR:O    | 2:D:409:THR:C   | 2.61                     | 0.43              |
| 3:E:48:GLU:O     | 3:E:49:GLU:C    | 2.61                     | 0.43              |
| 1:A:87:PHE:HD2   | 1:A:87:PHE:H    | 1.66                     | 0.43              |
| 2:B:288:VAL:HB   | 2:B:289:PRO:HD3 | 2.00                     | 0.43              |
| 1:A:11:GLN:CG    | 1:A:12:ALA:N    | 2.80                     | 0.43              |
| 2:B:155:SER:O    | 3:E:76:ARG:NH2  | 2.52                     | 0.43              |
| 2:B:306:ASP:C    | 2:B:308:ARG:H   | 2.26                     | 0.43              |
| 3:E:51:GLN:C     | 3:E:53:LYS:N    | 2.76                     | 0.43              |
| 1:A:141:PHE:HD2  | 1:A:141:PHE:HA  | 1.69                     | 0.43              |
| 2:B:171:VAL:HA   | 2:B:204:ILE:O   | 2.18                     | 0.43              |
| 1:C:36:MET:HG2   | 1:C:61:HIS:CD2  | 2.54                     | 0.43              |
| 2:B:66:ILE:HD11  | 2:B:122:VAL:HA  | 1.99                     | 0.43              |
| 1:C:108:TYR:CE1  | 1:C:413:MET:HG3 | 2.54                     | 0.43              |
| 1:C:298:PRO:O    | 1:C:301:GLN:HB2 | 2.18                     | 0.43              |
| 2:D:308:ARG:O    | 2:D:310:GLY:N   | 2.52                     | 0.43              |
| 2:B:191:VAL:CG1  | 2:B:425:MET:HG3 | 2.47                     | 0.43              |
| 1:C:70:LEU:N     | 1:C:70:LEU:CD1  | 2.81                     | 0.43              |
| 1:C:133:GLN:HE21 | 1:C:252:LEU:HG  | 1.84                     | 0.43              |
| 2:D:320:ARG:NH1  | 2:D:360:PRO:HG3 | 2.33                     | 0.43              |
| 2:D:387:LEU:O    | 2:D:390:ARG:HG3 | 2.19                     | 0.43              |
| 1:A:68:VAL:HG11  | 1:A:118:VAL:CG2 | 2.49                     | 0.43              |
| 1:C:151:SER:OG   | 1:C:193:THR:HB  | 2.19                     | 0.43              |
| 1:A:394:LYS:HG3  | 2:B:348:PRO:HG2 | 2.01                     | 0.43              |
| 2:B:240:THR:HG21 | 2:B:320:ARG:CZ  | 2.49                     | 0.43              |
| 1:C:161:TYR:HB3  | 1:C:164:LYS:HG3 | 2.01                     | 0.43              |
| 1:C:239:THR:O    | 1:C:240:ALA:C   | 2.61                     | 0.43              |
| 1:A:248:LEU:HD23 | 1:A:248:LEU:HA  | 1.92                     | 0.42              |
| 1:C:164:LYS:H    | 1:C:164:LYS:HG2 | 1.70                     | 0.42              |
| 1:C:347:CYS:HB3  | 1:C:348:PRO:HD2 | 2.00                     | 0.42              |
| 1:A:88:HIS:CD2   | 1:A:89:PRO:HD2  | 2.55                     | 0.42              |
| 1:A:349:THR:OG1  | 3:E:25:LYS:N    | 2.51                     | 0.42              |
| 1:C:260:VAL:HA   | 1:C:261:PRO:HD3 | 1.93                     | 0.42              |
| 1:C:297:GLU:HA   | 1:C:298:PRO:HD2 | 1.92                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:391:LEU:HD12 | 1:C:391:LEU:HA   | 1.83                     | 0.42              |
| 1:A:264:ARG:O    | 1:A:266:HIS:N    | 2.52                     | 0.42              |
| 2:B:136:GLN:HB3  | 2:B:167:ASN:HB3  | 2.01                     | 0.42              |
| 1:C:30:ILE:HA    | 1:C:36:MET:HB3   | 2.00                     | 0.42              |
| 2:D:3:GLU:CG     | 2:D:64:ARG:NH2   | 2.82                     | 0.42              |
| 2:D:3:GLU:HG3    | 2:D:64:ARG:NH2   | 2.35                     | 0.42              |
| 2:D:110:GLU:H    | 2:D:110:GLU:HG2  | 1.65                     | 0.42              |
| 2:D:288:VAL:HB   | 2:D:289:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:152:LEU:HD11 | 3:E:54:LEU:HD22  | 2.01                     | 0.42              |
| 1:A:262:TYR:O    | 1:A:263:PRO:C    | 2.62                     | 0.42              |
| 2:B:305:CYS:HB3  | 2:B:386:GLU:HB3  | 2.01                     | 0.42              |
| 1:C:249:ASN:HA   | 1:C:255:PHE:HA   | 2.00                     | 0.42              |
| 1:C:346:TRP:HE3  | 1:C:346:TRP:O    | 2.01                     | 0.42              |
| 2:D:401:ARG:HG3  | 2:D:401:ARG:HH11 | 1.85                     | 0.42              |
| 3:E:76:ARG:HD3   | 3:E:79:GLU:OE1   | 2.19                     | 0.42              |
| 1:A:36:MET:HA    | 1:A:37:PRO:HD3   | 1.88                     | 0.42              |
| 1:A:81:GLY:O     | 1:A:82:THR:C     | 2.63                     | 0.42              |
| 1:A:108:TYR:CE1  | 1:A:413:MET:HG3  | 2.53                     | 0.42              |
| 2:B:183:GLU:N    | 2:B:184:PRO:HD2  | 2.34                     | 0.42              |
| 1:A:185:TYR:OH   | 1:A:403:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:391:LEU:HD12 | 1:A:391:LEU:HA   | 1.73                     | 0.42              |
| 2:B:114:LEU:HB3  | 2:B:149:MET:HE1  | 2.02                     | 0.42              |
| 2:B:247:GLN:H    | 2:B:247:GLN:HE21 | 1.66                     | 0.42              |
| 2:B:403:ALA:O    | 2:B:405:LEU:N    | 2.53                     | 0.42              |
| 1:C:105:ARG:HD2  | 1:C:411:GLU:OE1  | 2.19                     | 0.42              |
| 2:D:141:LEU:HA   | 2:D:141:LEU:HD12 | 1.79                     | 0.42              |
| 2:D:192:HIS:HD2  | 2:D:421:ALA:HA   | 1.83                     | 0.42              |
| 2:B:16:ILE:HG22  | 2:B:17:GLY:N     | 2.34                     | 0.42              |
| 2:B:320:ARG:HA   | 2:B:356:CYS:O    | 2.20                     | 0.42              |
| 3:E:121:GLU:O    | 3:E:121:GLU:HG3  | 2.17                     | 0.42              |
| 1:A:265:ILE:O    | 1:A:265:ILE:HG22 | 2.20                     | 0.42              |
| 2:B:179:ASP:O    | 1:C:352:LYS:HE3  | 2.20                     | 0.42              |
| 1:C:181:VAL:H    | 2:D:258:ASN:HD21 | 1.67                     | 0.42              |
| 1:C:346:TRP:CZ2  | 1:C:435:VAL:HG13 | 2.39                     | 0.42              |
| 2:D:226:ASP:OD1  | 2:D:226:ASP:N    | 2.53                     | 0.42              |
| 2:D:382:THR:HG22 | 2:D:432:TYR:HD2  | 1.84                     | 0.42              |
| 2:D:394:GLN:O    | 2:D:397:ALA:HB3  | 2.19                     | 0.42              |
| 2:B:7:ILE:HG22   | 2:B:137:LEU:HD13 | 2.02                     | 0.42              |
| 1:C:7:ILE:HG21   | 1:C:153:LEU:HD11 | 2.01                     | 0.42              |
| 1:C:8:HIS:HE1    | 1:C:21:TRP:HE1   | 1.68                     | 0.42              |
| 1:C:291:ILE:HD12 | 1:C:375:VAL:CG2  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:LEU:HA   | 1:A:155:GLU:HG3  | 2.02                     | 0.42              |
| 1:A:174:ALA:CB   | 1:A:207:GLU:HB2  | 2.49                     | 0.42              |
| 1:A:358:GLN:HA   | 1:A:359:PRO:HD3  | 1.84                     | 0.42              |
| 2:B:294:GLN:HG3  | 2:B:300:ASN:ND2  | 2.35                     | 0.42              |
| 2:B:66:ILE:HD13  | 2:B:122:VAL:HG12 | 2.03                     | 0.41              |
| 2:B:381:SER:O    | 2:B:384:ILE:HB   | 2.20                     | 0.41              |
| 1:C:105:ARG:HG2  | 1:C:110:ILE:HG22 | 2.02                     | 0.41              |
| 2:B:4:ILE:HG22   | 2:B:133:GLN:CB   | 2.50                     | 0.41              |
| 2:B:265:LEU:HB3  | 2:B:432:TYR:CE2  | 2.54                     | 0.41              |
| 3:E:58:GLU:O     | 3:E:62:LYS:HB2   | 2.20                     | 0.41              |
| 1:A:23:LEU:HD23  | 1:A:27:GLU:OE1   | 2.20                     | 0.41              |
| 1:A:64:ARG:HG3   | 1:A:64:ARG:NH1   | 2.34                     | 0.41              |
| 1:A:79:ARG:HH12  | 1:A:94:THR:HG22  | 1.85                     | 0.41              |
| 1:A:181:VAL:HG23 | 2:B:258:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:346:TRP:HZ2  | 1:A:435:VAL:CG1  | 2.31                     | 0.41              |
| 2:D:151:THR:O    | 2:D:154:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:67:PHE:HB2   | 1:A:92:LEU:HD22  | 2.03                     | 0.41              |
| 2:B:27:GLU:CD    | 2:B:320:ARG:HH22 | 2.27                     | 0.41              |
| 2:B:169:PHE:CD2  | 2:B:235:MET:HG2  | 2.54                     | 0.41              |
| 2:D:12:CYS:HB3   | 2:D:140:SER:HB3  | 2.03                     | 0.41              |
| 1:A:79:ARG:HH12  | 1:A:94:THR:CG2   | 2.33                     | 0.41              |
| 1:A:210:TYR:HE1  | 1:A:214:ARG:HH11 | 1.68                     | 0.41              |
| 1:A:260:VAL:HA   | 1:A:261:PRO:HD3  | 1.91                     | 0.41              |
| 1:A:328:VAL:HG11 | 1:A:353:VAL:HG11 | 2.02                     | 0.41              |
| 2:B:51:VAL:HG12  | 2:B:52:TYR:CD1   | 2.56                     | 0.41              |
| 1:C:188:ILE:HD12 | 1:C:425:MET:HG3  | 2.01                     | 0.41              |
| 1:C:204:VAL:HG22 | 1:C:302:MET:HE1  | 2.03                     | 0.41              |
| 2:B:111:GLY:C    | 2:B:113:GLU:N    | 2.78                     | 0.41              |
| 2:B:401:ARG:NH1  | 2:B:401:ARG:CG   | 2.83                     | 0.41              |
| 1:C:123:ARG:HD2  | 1:C:161:TYR:OH   | 2.20                     | 0.41              |
| 2:D:106:GLY:O    | 2:D:111:GLY:HA3  | 2.21                     | 0.41              |
| 1:A:174:ALA:HB1  | 1:A:207:GLU:HB2  | 2.03                     | 0.41              |
| 2:B:62:VAL:HA    | 2:B:63:PRO:HD2   | 1.80                     | 0.41              |
| 2:B:217:LEU:C    | 2:B:219:LEU:H    | 2.29                     | 0.41              |
| 1:C:98:ASP:OD2   | 2:D:251:ASP:OD1  | 2.39                     | 0.41              |
| 1:C:322:ASP:O    | 1:C:323:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:395:PHE:CD2  | 1:A:395:PHE:C    | 2.99                     | 0.41              |
| 2:B:55:GLU:HB3   | 2:B:61:TYR:CD2   | 2.56                     | 0.41              |
| 2:B:211:ASP:HB3  | 2:B:215:ARG:NH1  | 2.35                     | 0.41              |
| 2:B:358:ILE:HA   | 2:B:359:PRO:HD3  | 1.87                     | 0.41              |
| 1:C:196:GLU:H    | 1:C:196:GLU:HG3  | 1.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:306:ASP:O    | 1:C:309:HIS:HB3  | 2.20                     | 0.41              |
| 2:D:62:VAL:O     | 2:D:62:VAL:CG2   | 2.68                     | 0.41              |
| 1:A:8:HIS:CE1    | 1:A:21:TRP:HE1   | 2.39                     | 0.41              |
| 1:A:106:GLY:O    | 1:A:111:GLY:HA3  | 2.21                     | 0.41              |
| 1:A:413:MET:HE3  | 1:A:417:GLU:CD   | 2.46                     | 0.41              |
| 2:B:12:CYS:HB3   | 2:B:140:SER:HB3  | 2.02                     | 0.41              |
| 2:B:177:VAL:O    | 2:B:177:VAL:HG12 | 2.21                     | 0.41              |
| 1:C:8:HIS:CD2    | 1:C:17:GLY:CA    | 2.98                     | 0.41              |
| 1:C:302:MET:HB3  | 1:C:302:MET:HE3  | 1.58                     | 0.41              |
| 2:D:5:VAL:CG2    | 2:D:135:PHE:CD2  | 3.02                     | 0.41              |
| 2:D:308:ARG:NH1  | 2:D:308:ARG:HG3  | 2.35                     | 0.41              |
| 1:A:142:GLY:CA   | 1:A:183:GLU:HG3  | 2.45                     | 0.41              |
| 1:A:205:ASP:CB   | 1:A:303:VAL:HA   | 2.50                     | 0.41              |
| 2:B:225:GLY:O    | 2:B:227:LEU:N    | 2.45                     | 0.41              |
| 2:B:239:THR:O    | 2:B:241:CYS:N    | 2.53                     | 0.41              |
| 1:C:88:HIS:CD2   | 1:C:89:PRO:HD2   | 2.57                     | 0.41              |
| 3:E:87:ILE:O     | 3:E:91:ASN:HB2   | 2.21                     | 0.41              |
| 1:A:251:ASP:O    | 1:A:252:LEU:C    | 2.65                     | 0.40              |
| 2:B:20:PHE:HD2   | 2:B:235:MET:HB3  | 1.85                     | 0.40              |
| 1:C:306:ASP:HA   | 1:C:307:PRO:HD3  | 1.75                     | 0.40              |
| 3:E:111:ASN:HD22 | 3:E:111:ASN:HA   | 1.62                     | 0.40              |
| 1:A:52:PHE:HE1   | 1:A:242:LEU:HD12 | 1.86                     | 0.40              |
| 1:C:273:ALA:HB2  | 1:C:375:VAL:N    | 2.35                     | 0.40              |
| 1:A:394:LYS:HG3  | 2:B:348:PRO:CG   | 2.51                     | 0.40              |
| 2:B:2:ARG:NH1    | 2:B:133:GLN:HA   | 2.37                     | 0.40              |
| 2:B:76:ASP:OD1   | 2:B:76:ASP:N     | 2.55                     | 0.40              |
| 1:C:20:CYS:HB3   | 1:C:232:GLY:HA2  | 2.04                     | 0.40              |
| 1:C:167:LEU:CD1  | 1:C:252:LEU:CD1  | 2.98                     | 0.40              |
| 1:A:380:ASN:HD22 | 1:A:380:ASN:C    | 2.28                     | 0.40              |
| 2:D:223:THR:HB   | 2:D:225:GLY:CA   | 2.51                     | 0.40              |
| 3:E:78:HIS:HA    | 3:E:81:GLU:HB2   | 2.03                     | 0.40              |
| 1:A:20:CYS:HB3   | 1:A:232:GLY:HA2  | 2.02                     | 0.40              |
| 2:B:287:THR:O    | 2:B:288:VAL:HB   | 2.22                     | 0.40              |
| 1:C:36:MET:HA    | 1:C:37:PRO:HD3   | 1.93                     | 0.40              |
| 1:C:399:TYR:C    | 1:C:401:LYS:H    | 2.30                     | 0.40              |
| 2:D:240:THR:HG21 | 2:D:320:ARG:CZ   | 2.52                     | 0.40              |
| 3:E:59:GLU:OE1   | 3:E:59:GLU:HA    | 2.12                     | 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     | 423/451 (94%)   | 357 (84%)  | 41 (10%)  | 25 (6%)  | 1           | 12 |
| 1   | C     | 424/451 (94%)   | 356 (84%)  | 42 (10%)  | 26 (6%)  | 1           | 11 |
| 2   | B     | 416/445 (94%)   | 326 (78%)  | 60 (14%)  | 30 (7%)  | 1           | 9  |
| 2   | D     | 415/445 (93%)   | 325 (78%)  | 62 (15%)  | 28 (7%)  | 1           | 10 |
| 3   | E     | 120/142 (84%)   | 91 (76%)   | 21 (18%)  | 8 (7%)   | 1           | 10 |
| All | All   | 1798/1934 (93%) | 1455 (81%) | 226 (13%) | 117 (6%) | 1           | 11 |

All (117) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | GLN  |
| 1   | A     | 48  | SER  |
| 1   | A     | 72  | PRO  |
| 1   | A     | 73  | THR  |
| 1   | A     | 82  | THR  |
| 1   | A     | 264 | ARG  |
| 1   | A     | 265 | ILE  |
| 1   | A     | 273 | ALA  |
| 1   | A     | 345 | ASP  |
| 1   | A     | 403 | ALA  |
| 2   | B     | 3   | GLU  |
| 2   | B     | 43  | GLN  |
| 2   | B     | 60  | LYS  |
| 2   | B     | 62  | VAL  |
| 2   | B     | 82  | PRO  |
| 2   | B     | 115 | VAL  |
| 2   | B     | 163 | ASP  |
| 2   | B     | 244 | PHE  |
| 2   | B     | 251 | ASP  |
| 2   | B     | 273 | ALA  |
| 2   | B     | 276 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 288 | VAL  |
| 2   | B     | 348 | PRO  |
| 2   | B     | 371 | LEU  |
| 1   | C     | 11  | GLN  |
| 1   | C     | 48  | SER  |
| 1   | C     | 72  | PRO  |
| 1   | C     | 73  | THR  |
| 1   | C     | 82  | THR  |
| 1   | C     | 245 | ASP  |
| 1   | C     | 264 | ARG  |
| 1   | C     | 265 | ILE  |
| 1   | C     | 273 | ALA  |
| 1   | C     | 345 | ASP  |
| 1   | C     | 403 | ALA  |
| 1   | C     | 437 | VAL  |
| 2   | D     | 3   | GLU  |
| 2   | D     | 43  | GLN  |
| 2   | D     | 60  | LYS  |
| 2   | D     | 62  | VAL  |
| 2   | D     | 82  | PRO  |
| 2   | D     | 115 | VAL  |
| 2   | D     | 163 | ASP  |
| 2   | D     | 244 | PHE  |
| 2   | D     | 273 | ALA  |
| 2   | D     | 276 | THR  |
| 2   | D     | 288 | VAL  |
| 2   | D     | 348 | PRO  |
| 2   | D     | 371 | LEU  |
| 3   | E     | 18  | GLN  |
| 3   | E     | 29  | PHE  |
| 3   | E     | 49  | GLU  |
| 1   | A     | 18  | ASN  |
| 1   | A     | 162 | GLY  |
| 1   | A     | 240 | ALA  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 350 | GLY  |
| 1   | A     | 377 | MET  |
| 2   | B     | 34  | GLY  |
| 2   | B     | 73  | GLY  |
| 2   | B     | 159 | GLU  |
| 2   | B     | 299 | LYS  |
| 2   | B     | 403 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 98  | ASP  |
| 1   | C     | 162 | GLY  |
| 1   | C     | 279 | GLU  |
| 1   | C     | 350 | GLY  |
| 1   | C     | 377 | MET  |
| 2   | D     | 73  | GLY  |
| 2   | D     | 159 | GLU  |
| 2   | D     | 299 | LYS  |
| 2   | D     | 309 | HIS  |
| 2   | D     | 403 | ALA  |
| 3   | E     | 12  | ASN  |
| 3   | E     | 62  | LYS  |
| 3   | E     | 68  | LEU  |
| 1   | A     | 248 | LEU  |
| 2   | B     | 217 | LEU  |
| 2   | B     | 226 | ASP  |
| 2   | B     | 245 | PRO  |
| 2   | B     | 322 | ARG  |
| 1   | C     | 164 | LYS  |
| 2   | D     | 34  | GLY  |
| 2   | D     | 89  | PRO  |
| 2   | D     | 217 | LEU  |
| 2   | D     | 226 | ASP  |
| 2   | D     | 402 | LYS  |
| 3   | E     | 47  | LEU  |
| 2   | B     | 89  | PRO  |
| 2   | B     | 162 | PRO  |
| 2   | B     | 240 | THR  |
| 2   | B     | 402 | LYS  |
| 1   | C     | 10  | GLY  |
| 1   | C     | 112 | LYS  |
| 1   | C     | 240 | ALA  |
| 1   | C     | 247 | ALA  |
| 1   | C     | 257 | THR  |
| 1   | C     | 341 | ILE  |
| 2   | D     | 109 | THR  |
| 2   | D     | 162 | PRO  |
| 2   | D     | 322 | ARG  |
| 1   | A     | 10  | GLY  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 164 | LYS  |
| 1   | A     | 309 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 341 | ILE  |
| 2   | B     | 305 | CYS  |
| 2   | D     | 225 | GLY  |
| 1   | A     | 4   | CYS  |
| 2   | B     | 225 | GLY  |
| 1   | C     | 301 | GLN  |
| 3   | E     | 95  | LYS  |
| 2   | B     | 177 | VAL  |
| 2   | D     | 177 | VAL  |
| 1   | A     | 348 | PRO  |
| 1   | A     | 246 | GLY  |
| 1   | C     | 62  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric | Outliers  | Percentiles |   |
|-----|-------|-----------------|-----------|-----------|-------------|---|
| 1   | A     | 349/378 (92%)   | 231 (66%) | 118 (34%) | 0           | 1 |
| 1   | C     | 345/378 (91%)   | 232 (67%) | 113 (33%) | 0           | 1 |
| 2   | B     | 349/383 (91%)   | 230 (66%) | 119 (34%) | 0           | 1 |
| 2   | D     | 348/383 (91%)   | 230 (66%) | 118 (34%) | 0           | 1 |
| 3   | E     | 79/126 (63%)    | 43 (54%)  | 36 (46%)  | 0           | 0 |
| All | All   | 1470/1648 (89%) | 966 (66%) | 504 (34%) | 0           | 1 |

All (504) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | ARG  |
| 1   | A     | 4   | CYS  |
| 1   | A     | 9   | VAL  |
| 1   | A     | 11  | GLN  |
| 1   | A     | 16  | ILE  |
| 1   | A     | 22  | GLU  |
| 1   | A     | 23  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | LEU  |
| 1   | A     | 27  | GLU  |
| 1   | A     | 36  | MET  |
| 1   | A     | 48  | SER  |
| 1   | A     | 60  | LYS  |
| 1   | A     | 62  | VAL  |
| 1   | A     | 66  | VAL  |
| 1   | A     | 68  | VAL  |
| 1   | A     | 71  | GLU  |
| 1   | A     | 73  | THR  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 76  | ASP  |
| 1   | A     | 79  | ARG  |
| 1   | A     | 80  | THR  |
| 1   | A     | 82  | THR  |
| 1   | A     | 84  | ARG  |
| 1   | A     | 88  | HIS  |
| 1   | A     | 90  | GLU  |
| 1   | A     | 94  | THR  |
| 1   | A     | 97  | GLU  |
| 1   | A     | 98  | ASP  |
| 1   | A     | 105 | ARG  |
| 1   | A     | 109 | THR  |
| 1   | A     | 110 | ILE  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 114 | ILE  |
| 1   | A     | 115 | ILE  |
| 1   | A     | 116 | ASP  |
| 1   | A     | 119 | LEU  |
| 1   | A     | 124 | LYS  |
| 1   | A     | 128 | GLN  |
| 1   | A     | 141 | PHE  |
| 1   | A     | 145 | THR  |
| 1   | A     | 151 | SER  |
| 1   | A     | 153 | LEU  |
| 1   | A     | 155 | GLU  |
| 1   | A     | 156 | ARG  |
| 1   | A     | 163 | LYS  |
| 1   | A     | 171 | ILE  |
| 1   | A     | 176 | GLN  |
| 1   | A     | 177 | VAL  |
| 1   | A     | 178 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 182 | VAL  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 193 | THR  |
| 1   | A     | 194 | THR  |
| 1   | A     | 195 | LEU  |
| 1   | A     | 196 | GLU  |
| 1   | A     | 198 | SER  |
| 1   | A     | 200 | CYS  |
| 1   | A     | 203 | MET  |
| 1   | A     | 206 | ASN  |
| 1   | A     | 210 | TYR  |
| 1   | A     | 217 | LEU  |
| 1   | A     | 219 | ILE  |
| 1   | A     | 220 | GLU  |
| 1   | A     | 223 | THR  |
| 1   | A     | 225 | THR  |
| 1   | A     | 226 | ASN  |
| 1   | A     | 229 | ARG  |
| 1   | A     | 230 | LEU  |
| 1   | A     | 234 | ILE  |
| 1   | A     | 237 | SER  |
| 1   | A     | 239 | THR  |
| 1   | A     | 241 | SER  |
| 1   | A     | 242 | LEU  |
| 1   | A     | 245 | ASP  |
| 1   | A     | 248 | LEU  |
| 1   | A     | 249 | ASN  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 260 | VAL  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 280 | LYS  |
| 1   | A     | 284 | GLU  |
| 1   | A     | 288 | VAL  |
| 1   | A     | 290 | GLU  |
| 1   | A     | 301 | GLN  |
| 1   | A     | 302 | MET  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 315 | CYS  |
| 1   | A     | 318 | LEU  |
| 1   | A     | 322 | ASP  |
| 1   | A     | 326 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 329 | ASN  |
| 1   | A     | 334 | THR  |
| 1   | A     | 339 | ARG  |
| 1   | A     | 340 | THR  |
| 1   | A     | 341 | ILE  |
| 1   | A     | 345 | ASP  |
| 1   | A     | 349 | THR  |
| 1   | A     | 352 | LYS  |
| 1   | A     | 356 | ASN  |
| 1   | A     | 361 | THR  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 370 | LYS  |
| 1   | A     | 371 | VAL  |
| 1   | A     | 373 | ARG  |
| 1   | A     | 375 | VAL  |
| 1   | A     | 377 | MET  |
| 1   | A     | 379 | SER  |
| 1   | A     | 380 | ASN  |
| 1   | A     | 391 | LEU  |
| 1   | A     | 394 | LYS  |
| 1   | A     | 397 | LEU  |
| 1   | A     | 401 | LYS  |
| 1   | A     | 405 | VAL  |
| 1   | A     | 413 | MET  |
| 1   | A     | 414 | GLU  |
| 1   | A     | 415 | GLU  |
| 1   | A     | 433 | GLU  |
| 2   | B     | 2   | ARG  |
| 2   | B     | 4   | ILE  |
| 2   | B     | 5   | VAL  |
| 2   | B     | 15  | GLN  |
| 2   | B     | 16  | ILE  |
| 2   | B     | 19  | LYS  |
| 2   | B     | 23  | VAL  |
| 2   | B     | 27  | GLU  |
| 2   | B     | 30  | ILE  |
| 2   | B     | 39  | ASP  |
| 2   | B     | 42  | LEU  |
| 2   | B     | 43  | GLN  |
| 2   | B     | 47  | GLU  |
| 2   | B     | 48  | ARG  |
| 2   | B     | 49  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 55  | GLU  |
| 2   | B     | 61  | TYR  |
| 2   | B     | 62  | VAL  |
| 2   | B     | 66  | ILE  |
| 2   | B     | 68  | VAL  |
| 2   | B     | 70  | LEU  |
| 2   | B     | 71  | GLU  |
| 2   | B     | 90  | ASP  |
| 2   | B     | 91  | ASN  |
| 2   | B     | 93  | VAL  |
| 2   | B     | 96  | GLN  |
| 2   | B     | 109 | THR  |
| 2   | B     | 110 | GLU  |
| 2   | B     | 115 | VAL  |
| 2   | B     | 118 | VAL  |
| 2   | B     | 119 | LEU  |
| 2   | B     | 122 | VAL  |
| 2   | B     | 131 | CYS  |
| 2   | B     | 137 | LEU  |
| 2   | B     | 138 | THR  |
| 2   | B     | 151 | THR  |
| 2   | B     | 155 | SER  |
| 2   | B     | 158 | ARG  |
| 2   | B     | 160 | GLU  |
| 2   | B     | 164 | ARG  |
| 2   | B     | 165 | ILE  |
| 2   | B     | 168 | THR  |
| 2   | B     | 170 | SER  |
| 2   | B     | 171 | VAL  |
| 2   | B     | 174 | SER  |
| 2   | B     | 176 | LYS  |
| 2   | B     | 177 | VAL  |
| 2   | B     | 178 | SER  |
| 2   | B     | 179 | ASP  |
| 2   | B     | 180 | THR  |
| 2   | B     | 181 | VAL  |
| 2   | B     | 191 | VAL  |
| 2   | B     | 192 | HIS  |
| 2   | B     | 193 | GLN  |
| 2   | B     | 195 | VAL  |
| 2   | B     | 207 | GLU  |
| 2   | B     | 209 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 210 | TYR  |
| 2   | B     | 212 | ILE  |
| 2   | B     | 223 | THR  |
| 2   | B     | 227 | LEU  |
| 2   | B     | 230 | LEU  |
| 2   | B     | 236 | SER  |
| 2   | B     | 240 | THR  |
| 2   | B     | 241 | CYS  |
| 2   | B     | 243 | ARG  |
| 2   | B     | 247 | GLN  |
| 2   | B     | 255 | LEU  |
| 2   | B     | 257 | VAL  |
| 2   | B     | 258 | ASN  |
| 2   | B     | 265 | LEU  |
| 2   | B     | 269 | MET  |
| 2   | B     | 275 | LEU  |
| 2   | B     | 276 | THR  |
| 2   | B     | 286 | LEU  |
| 2   | B     | 293 | GLN  |
| 2   | B     | 294 | GLN  |
| 2   | B     | 295 | MET  |
| 2   | B     | 299 | LYS  |
| 2   | B     | 300 | ASN  |
| 2   | B     | 302 | MET  |
| 2   | B     | 305 | CYS  |
| 2   | B     | 308 | ARG  |
| 2   | B     | 309 | HIS  |
| 2   | B     | 313 | LEU  |
| 2   | B     | 320 | ARG  |
| 2   | B     | 323 | MET  |
| 2   | B     | 327 | GLU  |
| 2   | B     | 329 | ASP  |
| 2   | B     | 331 | GLN  |
| 2   | B     | 333 | LEU  |
| 2   | B     | 339 | ASN  |
| 2   | B     | 341 | SER  |
| 2   | B     | 342 | TYR  |
| 2   | B     | 344 | VAL  |
| 2   | B     | 350 | ASN  |
| 2   | B     | 351 | VAL  |
| 2   | B     | 353 | THR  |
| 2   | B     | 355 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 357 | ASP  |
| 2   | B     | 358 | ILE  |
| 2   | B     | 371 | LEU  |
| 2   | B     | 374 | SER  |
| 2   | B     | 376 | THR  |
| 2   | B     | 377 | PHE  |
| 2   | B     | 384 | ILE  |
| 2   | B     | 386 | GLU  |
| 2   | B     | 387 | LEU  |
| 2   | B     | 390 | ARG  |
| 2   | B     | 391 | ILE  |
| 2   | B     | 394 | GLN  |
| 2   | B     | 400 | ARG  |
| 2   | B     | 401 | ARG  |
| 2   | B     | 405 | LEU  |
| 2   | B     | 409 | THR  |
| 2   | B     | 415 | GLU  |
| 2   | B     | 419 | THR  |
| 2   | B     | 430 | SER  |
| 2   | B     | 434 | GLN  |
| 1   | C     | 2   | ARG  |
| 1   | C     | 4   | CYS  |
| 1   | C     | 9   | VAL  |
| 1   | C     | 11  | GLN  |
| 1   | C     | 16  | ILE  |
| 1   | C     | 22  | GLU  |
| 1   | C     | 23  | LEU  |
| 1   | C     | 26  | LEU  |
| 1   | C     | 27  | GLU  |
| 1   | C     | 36  | MET  |
| 1   | C     | 48  | SER  |
| 1   | C     | 60  | LYS  |
| 1   | C     | 62  | VAL  |
| 1   | C     | 66  | VAL  |
| 1   | C     | 68  | VAL  |
| 1   | C     | 71  | GLU  |
| 1   | C     | 73  | THR  |
| 1   | C     | 74  | VAL  |
| 1   | C     | 76  | ASP  |
| 1   | C     | 79  | ARG  |
| 1   | C     | 80  | THR  |
| 1   | C     | 82  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 84  | ARG  |
| 1   | C     | 88  | HIS  |
| 1   | C     | 90  | GLU  |
| 1   | C     | 93  | ILE  |
| 1   | C     | 94  | THR  |
| 1   | C     | 98  | ASP  |
| 1   | C     | 105 | ARG  |
| 1   | C     | 109 | THR  |
| 1   | C     | 110 | ILE  |
| 1   | C     | 112 | LYS  |
| 1   | C     | 114 | ILE  |
| 1   | C     | 115 | ILE  |
| 1   | C     | 116 | ASP  |
| 1   | C     | 119 | LEU  |
| 1   | C     | 124 | LYS  |
| 1   | C     | 141 | PHE  |
| 1   | C     | 145 | THR  |
| 1   | C     | 151 | SER  |
| 1   | C     | 153 | LEU  |
| 1   | C     | 155 | GLU  |
| 1   | C     | 156 | ARG  |
| 1   | C     | 163 | LYS  |
| 1   | C     | 171 | ILE  |
| 1   | C     | 177 | VAL  |
| 1   | C     | 178 | SER  |
| 1   | C     | 182 | VAL  |
| 1   | C     | 183 | GLU  |
| 1   | C     | 193 | THR  |
| 1   | C     | 194 | THR  |
| 1   | C     | 196 | GLU  |
| 1   | C     | 198 | SER  |
| 1   | C     | 200 | CYS  |
| 1   | C     | 203 | MET  |
| 1   | C     | 206 | ASN  |
| 1   | C     | 210 | TYR  |
| 1   | C     | 212 | ILE  |
| 1   | C     | 217 | LEU  |
| 1   | C     | 219 | ILE  |
| 1   | C     | 220 | GLU  |
| 1   | C     | 223 | THR  |
| 1   | C     | 225 | THR  |
| 1   | C     | 226 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 229 | ARG  |
| 1   | C     | 230 | LEU  |
| 1   | C     | 234 | ILE  |
| 1   | C     | 239 | THR  |
| 1   | C     | 250 | VAL  |
| 1   | C     | 251 | ASP  |
| 1   | C     | 252 | LEU  |
| 1   | C     | 254 | GLU  |
| 1   | C     | 257 | THR  |
| 1   | C     | 260 | VAL  |
| 1   | C     | 269 | LEU  |
| 1   | C     | 279 | GLU  |
| 1   | C     | 280 | LYS  |
| 1   | C     | 288 | VAL  |
| 1   | C     | 290 | GLU  |
| 1   | C     | 301 | GLN  |
| 1   | C     | 302 | MET  |
| 1   | C     | 311 | LYS  |
| 1   | C     | 315 | CYS  |
| 1   | C     | 316 | CYS  |
| 1   | C     | 318 | LEU  |
| 1   | C     | 326 | LYS  |
| 1   | C     | 329 | ASN  |
| 1   | C     | 334 | THR  |
| 1   | C     | 340 | THR  |
| 1   | C     | 341 | ILE  |
| 1   | C     | 345 | ASP  |
| 1   | C     | 349 | THR  |
| 1   | C     | 352 | LYS  |
| 1   | C     | 356 | ASN  |
| 1   | C     | 361 | THR  |
| 1   | C     | 368 | LEU  |
| 1   | C     | 370 | LYS  |
| 1   | C     | 371 | VAL  |
| 1   | C     | 373 | ARG  |
| 1   | C     | 375 | VAL  |
| 1   | C     | 377 | MET  |
| 1   | C     | 379 | SER  |
| 1   | C     | 380 | ASN  |
| 1   | C     | 384 | ILE  |
| 1   | C     | 391 | LEU  |
| 1   | C     | 394 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 397 | LEU  |
| 1   | C     | 401 | LYS  |
| 1   | C     | 405 | VAL  |
| 1   | C     | 413 | MET  |
| 1   | C     | 414 | GLU  |
| 1   | C     | 415 | GLU  |
| 1   | C     | 433 | GLU  |
| 2   | D     | 2   | ARG  |
| 2   | D     | 4   | ILE  |
| 2   | D     | 5   | VAL  |
| 2   | D     | 15  | GLN  |
| 2   | D     | 16  | ILE  |
| 2   | D     | 19  | LYS  |
| 2   | D     | 23  | VAL  |
| 2   | D     | 27  | GLU  |
| 2   | D     | 30  | ILE  |
| 2   | D     | 39  | ASP  |
| 2   | D     | 42  | LEU  |
| 2   | D     | 43  | GLN  |
| 2   | D     | 47  | GLU  |
| 2   | D     | 48  | ARG  |
| 2   | D     | 49  | ILE  |
| 2   | D     | 55  | GLU  |
| 2   | D     | 61  | TYR  |
| 2   | D     | 62  | VAL  |
| 2   | D     | 66  | ILE  |
| 2   | D     | 68  | VAL  |
| 2   | D     | 70  | LEU  |
| 2   | D     | 71  | GLU  |
| 2   | D     | 90  | ASP  |
| 2   | D     | 91  | ASN  |
| 2   | D     | 93  | VAL  |
| 2   | D     | 96  | GLN  |
| 2   | D     | 101 | ASN  |
| 2   | D     | 109 | THR  |
| 2   | D     | 110 | GLU  |
| 2   | D     | 115 | VAL  |
| 2   | D     | 119 | LEU  |
| 2   | D     | 122 | VAL  |
| 2   | D     | 131 | CYS  |
| 2   | D     | 137 | LEU  |
| 2   | D     | 138 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 141 | LEU  |
| 2   | D     | 151 | THR  |
| 2   | D     | 154 | ILE  |
| 2   | D     | 155 | SER  |
| 2   | D     | 158 | ARG  |
| 2   | D     | 160 | GLU  |
| 2   | D     | 164 | ARG  |
| 2   | D     | 165 | ILE  |
| 2   | D     | 168 | THR  |
| 2   | D     | 170 | SER  |
| 2   | D     | 171 | VAL  |
| 2   | D     | 174 | SER  |
| 2   | D     | 176 | LYS  |
| 2   | D     | 177 | VAL  |
| 2   | D     | 178 | SER  |
| 2   | D     | 179 | ASP  |
| 2   | D     | 180 | THR  |
| 2   | D     | 181 | VAL  |
| 2   | D     | 191 | VAL  |
| 2   | D     | 192 | HIS  |
| 2   | D     | 193 | GLN  |
| 2   | D     | 195 | VAL  |
| 2   | D     | 209 | LEU  |
| 2   | D     | 210 | TYR  |
| 2   | D     | 212 | ILE  |
| 2   | D     | 223 | THR  |
| 2   | D     | 230 | LEU  |
| 2   | D     | 236 | SER  |
| 2   | D     | 240 | THR  |
| 2   | D     | 241 | CYS  |
| 2   | D     | 243 | ARG  |
| 2   | D     | 247 | GLN  |
| 2   | D     | 248 | LEU  |
| 2   | D     | 255 | LEU  |
| 2   | D     | 257 | VAL  |
| 2   | D     | 258 | ASN  |
| 2   | D     | 265 | LEU  |
| 2   | D     | 275 | LEU  |
| 2   | D     | 286 | LEU  |
| 2   | D     | 293 | GLN  |
| 2   | D     | 294 | GLN  |
| 2   | D     | 295 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 299 | LYS  |
| 2   | D     | 300 | ASN  |
| 2   | D     | 302 | MET  |
| 2   | D     | 305 | CYS  |
| 2   | D     | 308 | ARG  |
| 2   | D     | 309 | HIS  |
| 2   | D     | 313 | LEU  |
| 2   | D     | 320 | ARG  |
| 2   | D     | 323 | MET  |
| 2   | D     | 325 | MET  |
| 2   | D     | 327 | GLU  |
| 2   | D     | 329 | ASP  |
| 2   | D     | 331 | GLN  |
| 2   | D     | 333 | LEU  |
| 2   | D     | 339 | ASN  |
| 2   | D     | 341 | SER  |
| 2   | D     | 342 | TYR  |
| 2   | D     | 344 | VAL  |
| 2   | D     | 350 | ASN  |
| 2   | D     | 351 | VAL  |
| 2   | D     | 353 | THR  |
| 2   | D     | 355 | VAL  |
| 2   | D     | 357 | ASP  |
| 2   | D     | 358 | ILE  |
| 2   | D     | 371 | LEU  |
| 2   | D     | 373 | MET  |
| 2   | D     | 374 | SER  |
| 2   | D     | 376 | THR  |
| 2   | D     | 377 | PHE  |
| 2   | D     | 384 | ILE  |
| 2   | D     | 386 | GLU  |
| 2   | D     | 387 | LEU  |
| 2   | D     | 391 | ILE  |
| 2   | D     | 400 | ARG  |
| 2   | D     | 401 | ARG  |
| 2   | D     | 405 | LEU  |
| 2   | D     | 409 | THR  |
| 2   | D     | 415 | GLU  |
| 2   | D     | 419 | THR  |
| 2   | D     | 430 | SER  |
| 2   | D     | 434 | GLN  |
| 3   | E     | 10  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E     | 11  | LEU  |
| 3   | E     | 13  | LYS  |
| 3   | E     | 14  | CYS  |
| 3   | E     | 22  | VAL  |
| 3   | E     | 28  | SER  |
| 3   | E     | 48  | GLU  |
| 3   | E     | 49  | GLU  |
| 3   | E     | 51  | GLN  |
| 3   | E     | 53  | LYS  |
| 3   | E     | 59  | GLU  |
| 3   | E     | 60  | ARG  |
| 3   | E     | 62  | LYS  |
| 3   | E     | 64  | GLN  |
| 3   | E     | 65  | GLU  |
| 3   | E     | 70  | LYS  |
| 3   | E     | 72  | LEU  |
| 3   | E     | 77  | GLU  |
| 3   | E     | 79  | GLU  |
| 3   | E     | 81  | GLU  |
| 3   | E     | 87  | ILE  |
| 3   | E     | 94  | ILE  |
| 3   | E     | 96  | MET  |
| 3   | E     | 99  | GLU  |
| 3   | E     | 105 | MET  |
| 3   | E     | 107 | SER  |
| 3   | E     | 111 | ASN  |
| 3   | E     | 112 | ARG  |
| 3   | E     | 119 | MET  |
| 3   | E     | 120 | LEU  |
| 3   | E     | 121 | GLU  |
| 3   | E     | 123 | LEU  |
| 3   | E     | 124 | GLN  |
| 3   | E     | 125 | GLU  |
| 3   | E     | 133 | VAL  |
| 3   | E     | 134 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | HIS  |
| 1   | A     | 50  | ASN  |
| 1   | A     | 61  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 88  | HIS  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 139 | HIS  |
| 1   | A     | 206 | ASN  |
| 1   | A     | 216 | ASN  |
| 1   | A     | 258 | ASN  |
| 1   | A     | 266 | HIS  |
| 1   | A     | 283 | HIS  |
| 1   | A     | 372 | GLN  |
| 1   | A     | 380 | ASN  |
| 2   | B     | 6   | HIS  |
| 2   | B     | 14  | ASN  |
| 2   | B     | 15  | GLN  |
| 2   | B     | 54  | ASN  |
| 2   | B     | 139 | HIS  |
| 2   | B     | 197 | ASN  |
| 2   | B     | 229 | HIS  |
| 2   | B     | 247 | GLN  |
| 2   | B     | 258 | ASN  |
| 2   | B     | 266 | HIS  |
| 2   | B     | 294 | GLN  |
| 2   | B     | 349 | ASN  |
| 2   | B     | 350 | ASN  |
| 2   | B     | 380 | ASN  |
| 2   | B     | 424 | ASN  |
| 2   | B     | 433 | GLN  |
| 2   | B     | 436 | GLN  |
| 1   | C     | 8   | HIS  |
| 1   | C     | 50  | ASN  |
| 1   | C     | 61  | HIS  |
| 1   | C     | 88  | HIS  |
| 1   | C     | 91  | GLN  |
| 1   | C     | 133 | GLN  |
| 1   | C     | 139 | HIS  |
| 1   | C     | 206 | ASN  |
| 1   | C     | 216 | ASN  |
| 1   | C     | 256 | GLN  |
| 1   | C     | 258 | ASN  |
| 1   | C     | 266 | HIS  |
| 1   | C     | 283 | HIS  |
| 1   | C     | 380 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 6   | HIS  |
| 2   | D     | 14  | ASN  |
| 2   | D     | 15  | GLN  |
| 2   | D     | 54  | ASN  |
| 2   | D     | 229 | HIS  |
| 2   | D     | 258 | ASN  |
| 2   | D     | 266 | HIS  |
| 2   | D     | 294 | GLN  |
| 2   | D     | 339 | ASN  |
| 2   | D     | 350 | ASN  |
| 2   | D     | 380 | ASN  |
| 2   | D     | 424 | ASN  |
| 2   | D     | 433 | GLN  |
| 2   | D     | 436 | GLN  |
| 3   | E     | 64  | GLN  |
| 3   | E     | 108 | ASN  |
| 3   | E     | 111 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | GDP  | D     | 600 | -    | 29,30,30     | 1.01 | 2 (6%)   | 45,47,47    | 1.80 | 12 (26%) |
| 6   | GDP  | B     | 600 | -    | 29,30,30     | 0.84 | 1 (3%)   | 45,47,47    | 1.85 | 10 (22%) |
| 4   | GTP  | C     | 600 | -    | 33,34,34     | 1.05 | 3 (9%)   | 50,54,54    | 1.64 | 9 (18%)  |
| 4   | GTP  | A     | 600 | -    | 33,34,34     | 1.20 | 5 (15%)  | 50,54,54    | 1.55 | 10 (20%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | GDP  | D     | 600 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 6   | GDP  | B     | 600 | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 4   | GTP  | C     | 600 | -    | -       | 7/22/38/38 | 0/3/3/3 |
| 4   | GTP  | A     | 600 | -    | -       | 5/22/38/38 | 0/3/3/3 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | A     | 600 | GTP  | PB-O3B  | 3.54  | 1.63        | 1.59     |
| 6   | D     | 600 | GDP  | PA-O3A  | 3.04  | 1.62        | 1.59     |
| 4   | C     | 600 | GTP  | PB-O3B  | 2.89  | 1.62        | 1.59     |
| 4   | A     | 600 | GTP  | PB-O3A  | 2.59  | 1.62        | 1.59     |
| 4   | C     | 600 | GTP  | PB-O3A  | 2.30  | 1.62        | 1.59     |
| 4   | A     | 600 | GTP  | O4'-C4' | -2.20 | 1.40        | 1.45     |
| 4   | A     | 600 | GTP  | PA-O3A  | 2.18  | 1.61        | 1.59     |
| 6   | B     | 600 | GDP  | C2-N3   | 2.18  | 1.38        | 1.33     |
| 6   | D     | 600 | GDP  | C5-N7   | -2.17 | 1.34        | 1.39     |
| 4   | C     | 600 | GTP  | C2-N3   | 2.07  | 1.38        | 1.33     |
| 4   | A     | 600 | GTP  | C2-N3   | 2.02  | 1.38        | 1.33     |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | B     | 600 | GDP  | C5-C4-N3 | -5.51 | 119.63      | 128.39   |
| 4   | C     | 600 | GTP  | C5-C4-N3 | -5.05 | 120.35      | 128.39   |
| 6   | B     | 600 | GDP  | C2-N3-C4 | 4.88  | 120.71      | 112.30   |
| 4   | C     | 600 | GTP  | C2-N3-C4 | 4.87  | 120.69      | 112.30   |
| 6   | D     | 600 | GDP  | C2-N3-C4 | 4.80  | 120.56      | 112.30   |
| 6   | D     | 600 | GDP  | C5-C4-N3 | -4.73 | 120.86      | 128.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | A     | 600 | GTP  | C5-C4-N3    | -4.53 | 121.17      | 128.39   |
| 4   | A     | 600 | GTP  | C2-N3-C4    | 4.00  | 119.19      | 112.30   |
| 6   | B     | 600 | GDP  | N9-C4-N3    | 3.51  | 132.97      | 125.95   |
| 4   | C     | 600 | GTP  | N9-C4-N3    | 3.28  | 132.51      | 125.95   |
| 6   | D     | 600 | GDP  | N9-C8-N7    | -3.25 | 107.37      | 113.40   |
| 6   | D     | 600 | GDP  | N9-C4-N3    | 3.09  | 132.13      | 125.95   |
| 6   | B     | 600 | GDP  | C2-N1-C6    | -3.06 | 119.56      | 125.11   |
| 6   | D     | 600 | GDP  | C8-N7-C5    | 3.01  | 109.62      | 104.26   |
| 4   | C     | 600 | GTP  | C2-N1-C6    | -2.95 | 119.76      | 125.11   |
| 6   | B     | 600 | GDP  | O6-C6-C5    | -2.93 | 118.80      | 126.53   |
| 6   | D     | 600 | GDP  | C2'-C3'-C4' | 2.73  | 107.88      | 102.61   |
| 6   | B     | 600 | GDP  | O3B-PB-O3A  | 2.73  | 113.78      | 104.64   |
| 4   | C     | 600 | GTP  | N9-C8-N7    | -2.72 | 108.35      | 113.40   |
| 4   | C     | 600 | GTP  | O6-C6-C5    | -2.72 | 119.36      | 126.53   |
| 6   | B     | 600 | GDP  | C8-N7-C5    | 2.70  | 109.07      | 104.26   |
| 6   | B     | 600 | GDP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 4   | C     | 600 | GTP  | C5-C6-N1    | 2.63  | 119.96      | 113.25   |
| 4   | A     | 600 | GTP  | C2'-C1'-N9  | 2.63  | 120.58      | 113.25   |
| 6   | B     | 600 | GDP  | C5-C6-N1    | 2.63  | 119.95      | 113.25   |
| 4   | C     | 600 | GTP  | C8-N7-C5    | 2.55  | 108.81      | 104.26   |
| 6   | D     | 600 | GDP  | C2-N1-C6    | -2.50 | 120.57      | 125.11   |
| 4   | A     | 600 | GTP  | C2-N1-C6    | -2.48 | 120.61      | 125.11   |
| 6   | D     | 600 | GDP  | O6-C6-C5    | -2.44 | 120.08      | 126.53   |
| 4   | A     | 600 | GTP  | N2-C2-N1    | 2.35  | 121.71      | 116.76   |
| 6   | D     | 600 | GDP  | C5-C6-N1    | 2.29  | 119.09      | 113.25   |
| 4   | A     | 600 | GTP  | N9-C4-N3    | 2.24  | 130.42      | 125.95   |
| 6   | D     | 600 | GDP  | N1-C2-N3    | -2.21 | 119.28      | 123.32   |
| 4   | A     | 600 | GTP  | O5'-C5'-C4' | -2.19 | 101.53      | 108.99   |
| 4   | C     | 600 | GTP  | O3G-PG-O3B  | 2.15  | 111.85      | 104.64   |
| 4   | A     | 600 | GTP  | O6-C6-C5    | -2.14 | 120.88      | 126.53   |
| 4   | A     | 600 | GTP  | C5-C6-N1    | 2.06  | 118.50      | 113.25   |
| 6   | D     | 600 | GDP  | N2-C2-N1    | 2.05  | 121.09      | 116.76   |
| 6   | B     | 600 | GDP  | O2B-PB-O3A  | 2.04  | 111.46      | 104.64   |
| 6   | D     | 600 | GDP  | C4-C5-N7    | -2.02 | 107.47      | 110.67   |
| 4   | A     | 600 | GTP  | C8-N7-C5    | 2.00  | 107.83      | 104.26   |

There are no chirality outliers.

All (19) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 4   | A     | 600 | GTP  | C5'-O5'-PA-O3A |
| 4   | A     | 600 | GTP  | C5'-O5'-PA-O1A |

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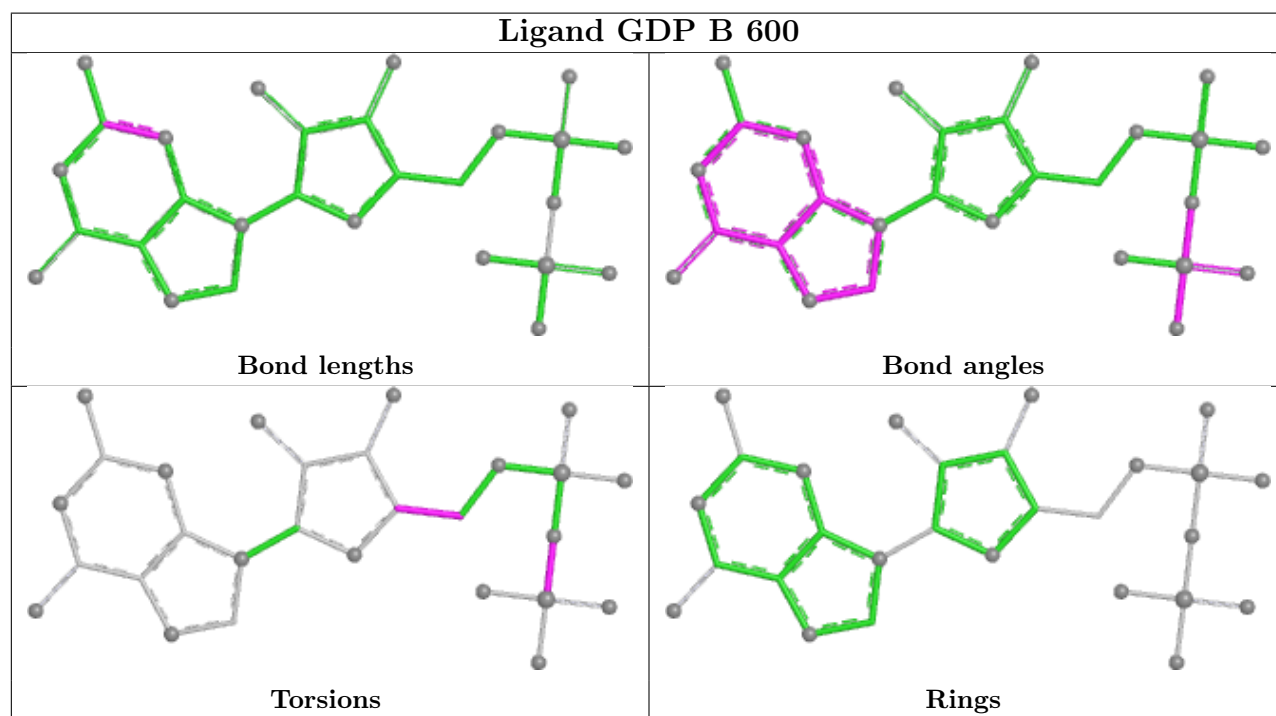
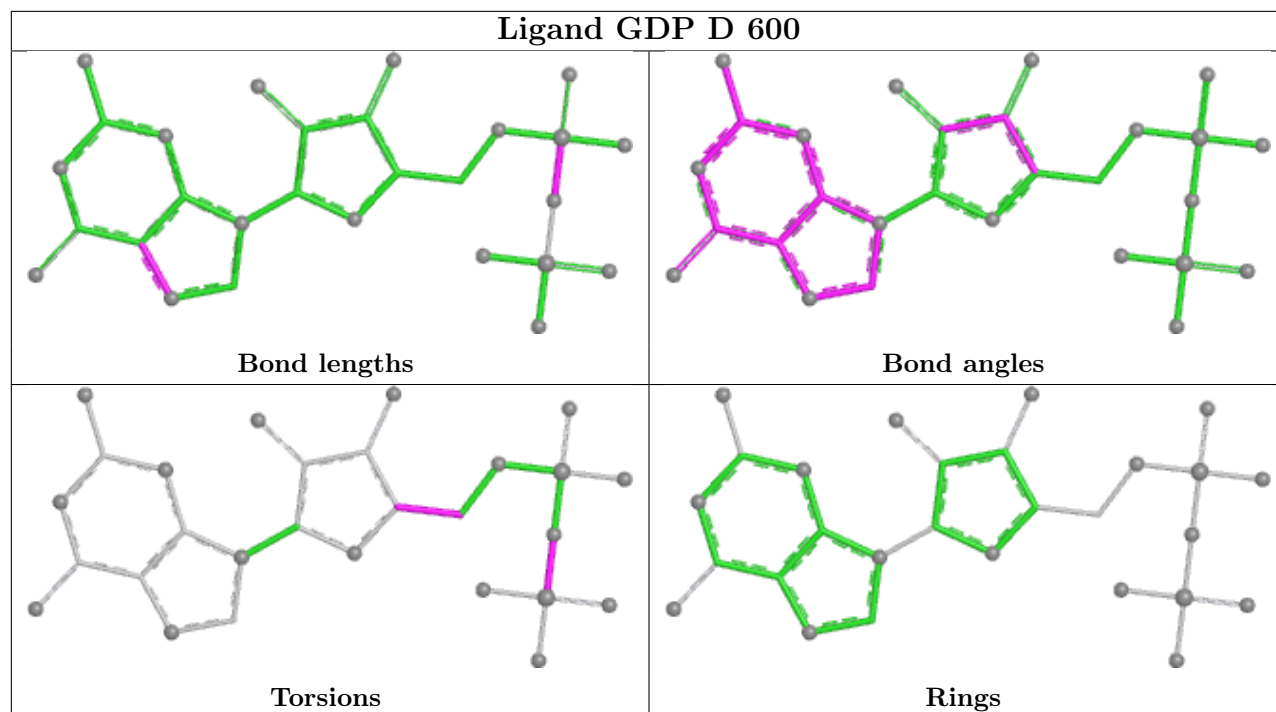
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | C     | 600 | GTP  | PB-O3B-PG-O3G   |
| 4   | C     | 600 | GTP  | C5'-O5'-PA-O3A  |
| 4   | C     | 600 | GTP  | C5'-O5'-PA-O1A  |
| 6   | B     | 600 | GDP  | O4'-C4'-C5'-O5' |
| 6   | D     | 600 | GDP  | PA-O3A-PB-O2B   |
| 6   | D     | 600 | GDP  | O4'-C4'-C5'-O5' |
| 6   | B     | 600 | GDP  | C3'-C4'-C5'-O5' |
| 6   | D     | 600 | GDP  | C3'-C4'-C5'-O5' |
| 6   | B     | 600 | GDP  | PA-O3A-PB-O1B   |
| 4   | A     | 600 | GTP  | C5'-O5'-PA-O2A  |
| 4   | C     | 600 | GTP  | C5'-O5'-PA-O2A  |
| 4   | A     | 600 | GTP  | PG-O3B-PB-O2B   |
| 4   | C     | 600 | GTP  | PB-O3A-PA-O2A   |
| 4   | A     | 600 | GTP  | PG-O3B-PB-O1B   |
| 4   | C     | 600 | GTP  | PB-O3B-PG-O1G   |
| 6   | D     | 600 | GDP  | PA-O3A-PB-O1B   |
| 4   | C     | 600 | GTP  | PB-O3A-PA-O1A   |

There are no ring outliers.

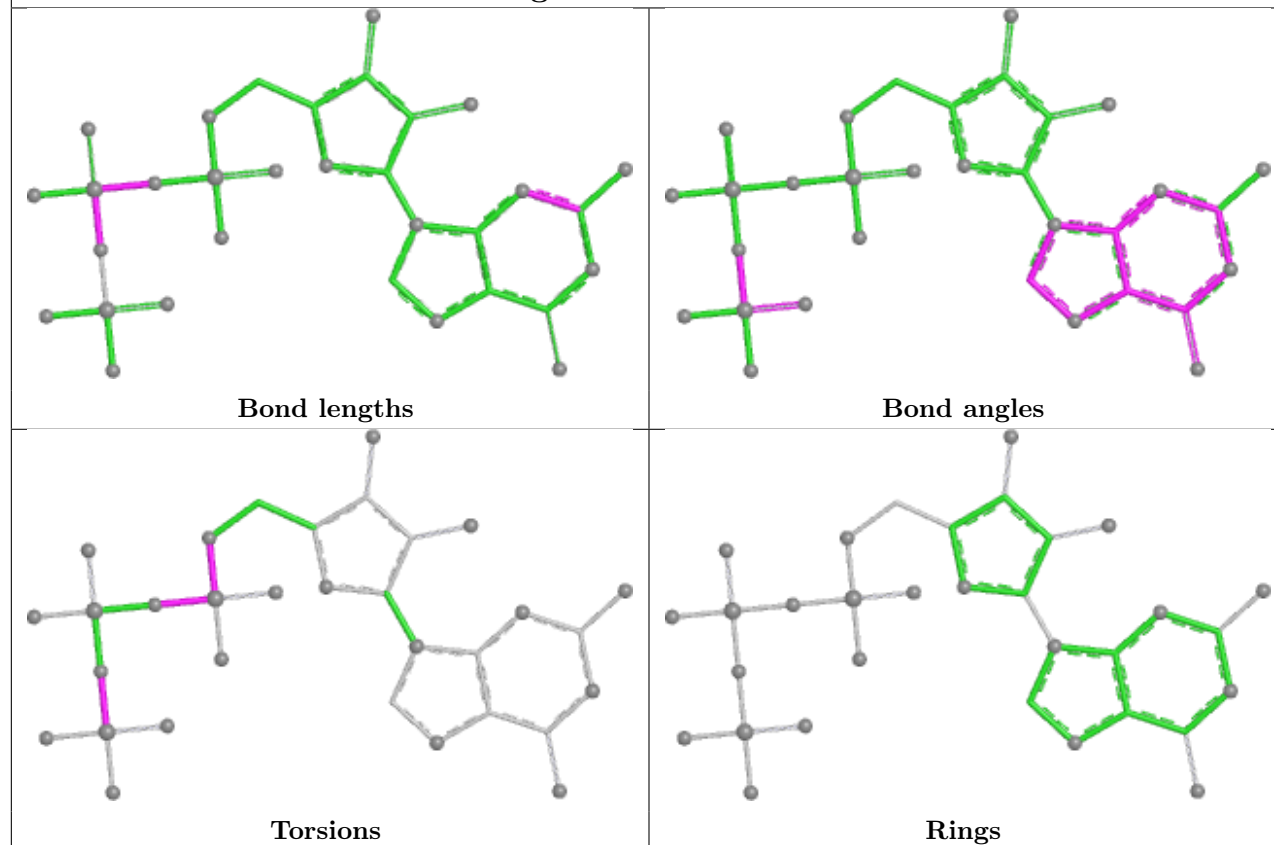
4 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | D     | 600 | GDP  | 3       | 0            |
| 6   | B     | 600 | GDP  | 1       | 0            |
| 4   | C     | 600 | GTP  | 2       | 0            |
| 4   | A     | 600 | GTP  | 3       | 0            |

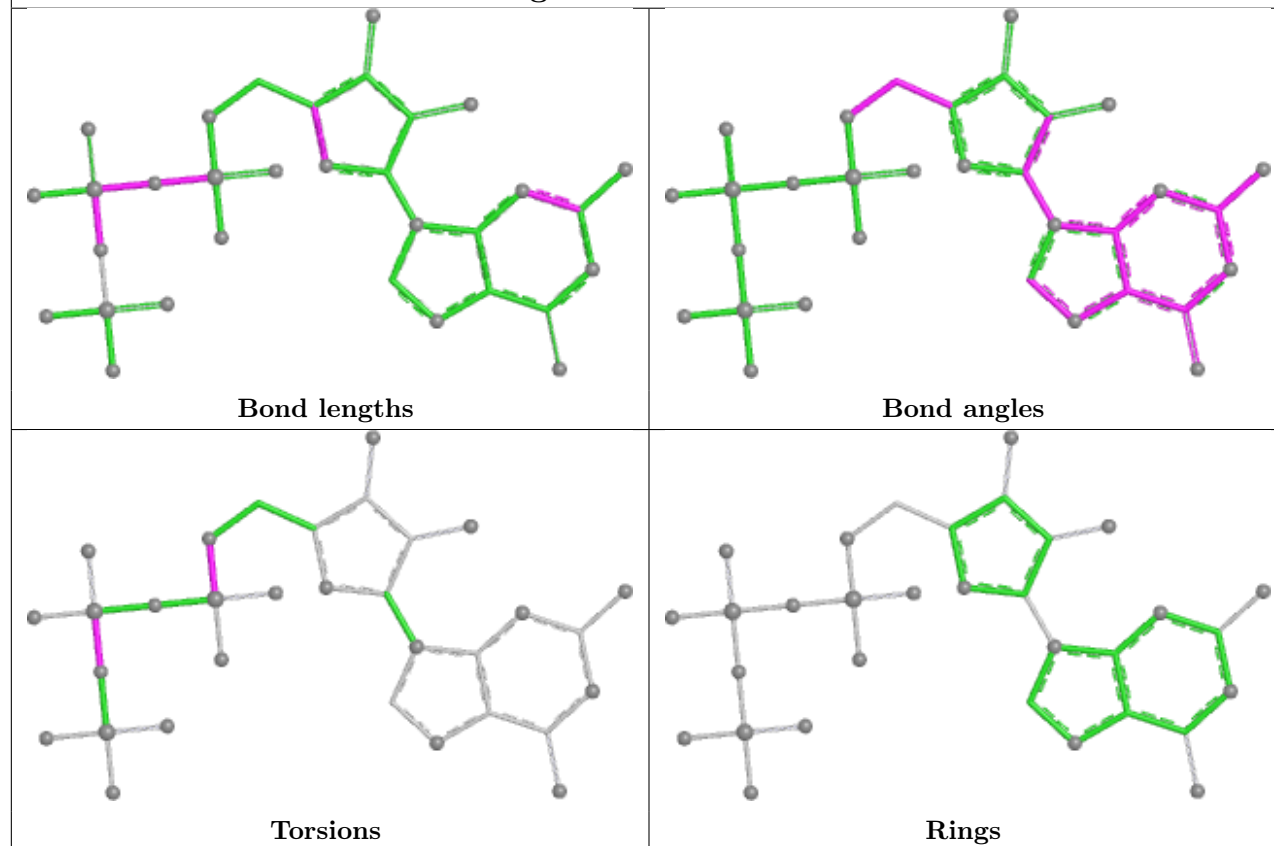
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand GTP C 600



## Ligand GTP A 600



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                                 | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------------------|-----------------------|-------|
| 1   | A     | 427/451 (94%)   | -0.95  | 0 <span>100</span> <span>100</span>     | 57, 61, 64, 70        | 0     |
| 1   | C     | 428/451 (94%)   | -0.31  | 3 (0%) <span>84</span> <span>61</span>  | 57, 61, 65, 76        | 0     |
| 2   | B     | 420/445 (94%)   | -0.71  | 2 (0%) <span>87</span> <span>67</span>  | 59, 62, 71, 87        | 0     |
| 2   | D     | 419/445 (94%)   | -0.01  | 15 (3%) <span>46</span> <span>27</span> | 59, 62, 72, 87        | 0     |
| 3   | E     | 124/142 (87%)   | -0.60  | 1 (0%) <span>82</span> <span>59</span>  | 47, 62, 73, 80        | 0     |
| All | All   | 1818/1934 (94%) | -0.50  | 21 (1%) <span>76</span> <span>50</span> | 47, 61, 68, 87        | 0     |

All (21) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 381 | SER  | 3.2  |
| 2   | D     | 307 | PRO  | 2.7  |
| 2   | D     | 73  | GLY  | 2.7  |
| 2   | D     | 134 | GLY  | 2.7  |
| 2   | D     | 3   | GLU  | 2.7  |
| 2   | D     | 297 | ASP  | 2.7  |
| 1   | C     | 131 | GLY  | 2.7  |
| 2   | B     | 39  | ASP  | 2.7  |
| 2   | D     | 339 | ASN  | 2.6  |
| 2   | D     | 310 | GLY  | 2.6  |
| 2   | B     | 288 | VAL  | 2.5  |
| 1   | C     | 120 | ASP  | 2.4  |
| 2   | D     | 90  | ASP  | 2.4  |
| 2   | D     | 216 | THR  | 2.3  |
| 2   | D     | 39  | ASP  | 2.2  |
| 2   | D     | 337 | ASN  | 2.2  |
| 2   | D     | 295 | MET  | 2.2  |
| 2   | D     | 335 | VAL  | 2.2  |
| 1   | C     | 416 | GLY  | 2.1  |
| 2   | D     | 433 | GLN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | E     | 117 | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

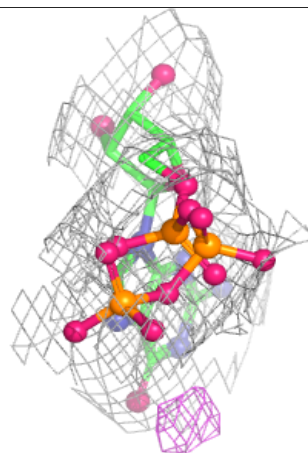
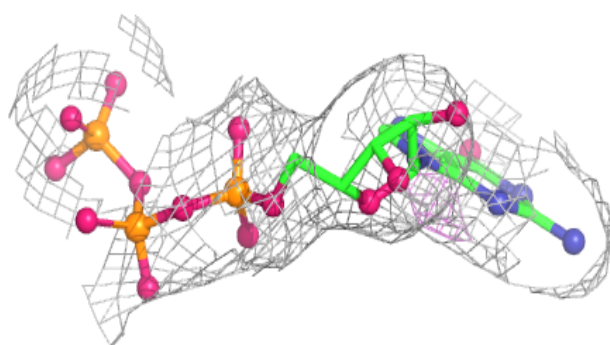
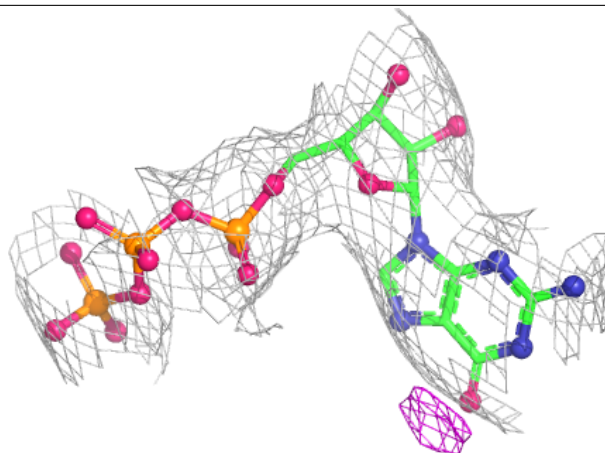
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | GTP  | A     | 600 | 32/32 | 0.99 | 0.04 | 53,59,62,63                | 0     |
| 4   | GTP  | C     | 600 | 32/32 | 0.99 | 0.04 | 53,56,57,57                | 0     |
| 5   | MG   | A     | 601 | 1/1   | 0.99 | 0.03 | 40,40,40,40                | 0     |
| 6   | GDP  | B     | 600 | 28/28 | 0.99 | 0.04 | 48,51,59,60                | 0     |
| 6   | GDP  | D     | 600 | 28/28 | 0.99 | 0.04 | 55,58,63,63                | 0     |
| 5   | MG   | C     | 601 | 1/1   | 1.00 | 0.04 | 40,40,40,40                | 0     |

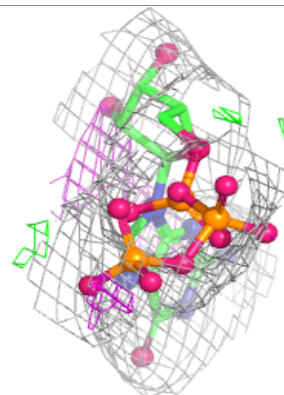
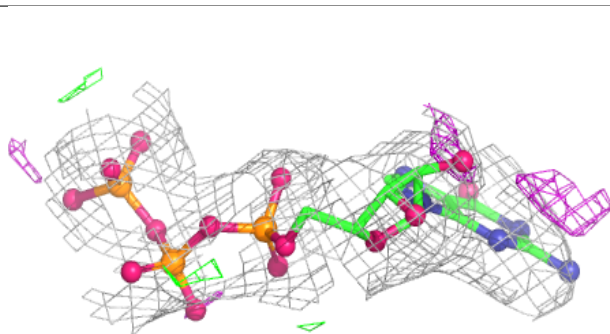
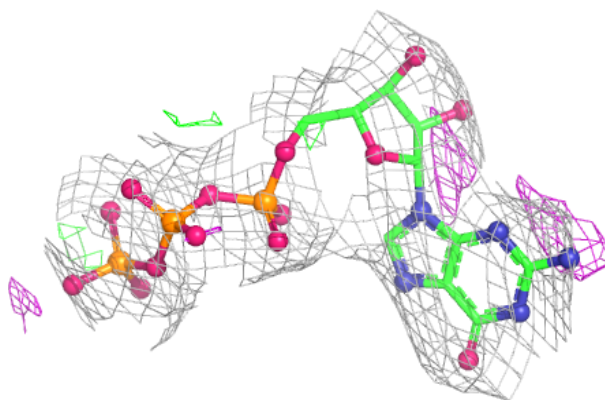
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GTP A 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GTP C 600:**

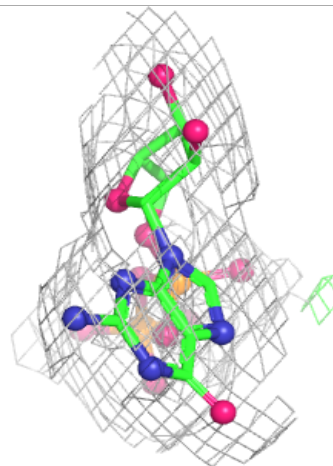
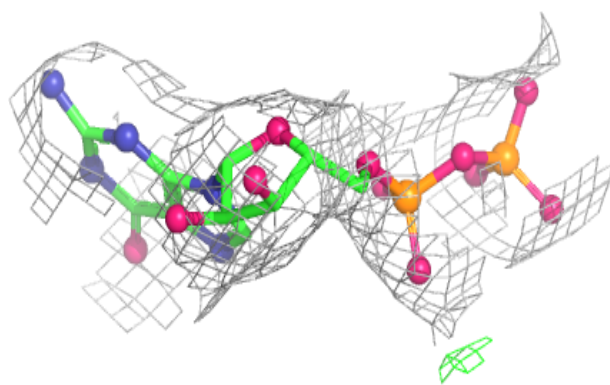
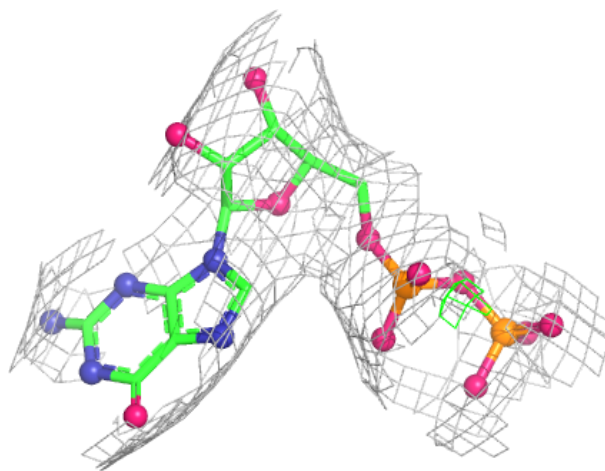
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





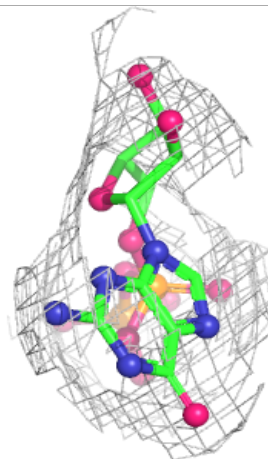
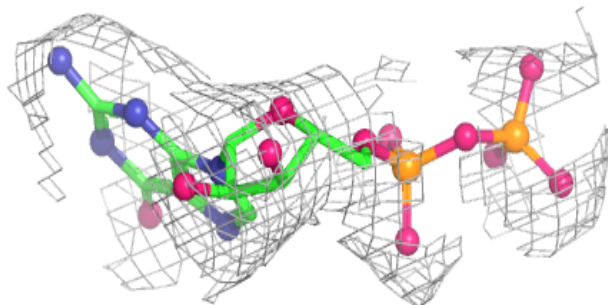
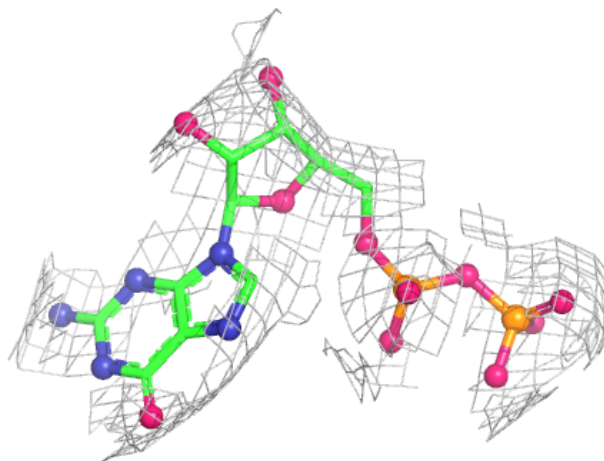
**Electron density around GDP B 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GDP D 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.