



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:52 PM UTC

PDB ID : 1OVM / pdb\_00001ovm  
Title : Crystal structure of Indolepyruvate decarboxylase from *Enterobacter cloacae*  
Authors : Schutz, A.; Sandalova, T.; Ricagno, S.; Hubner, G.; Konig, S.; Schneider, G.  
Deposited on : 2003-03-27  
Resolution : 2.65 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

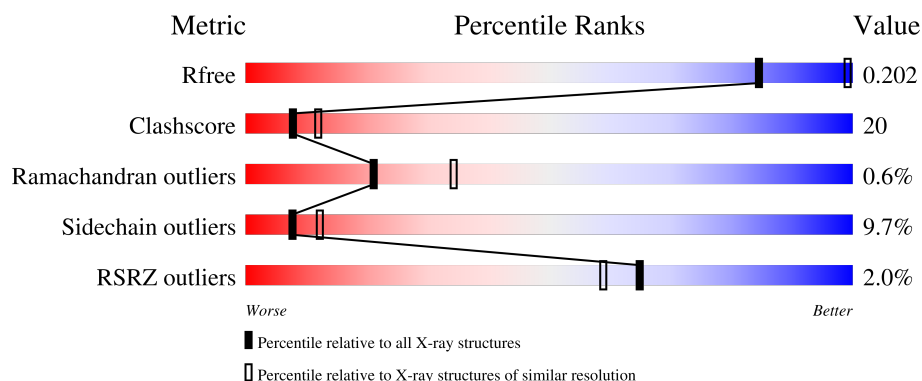
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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                      | 1110 (2.66-2.66)                                      |
| Clashscore            | 190562                      | 1141 (2.66-2.66)                                      |
| Ramachandran outliers | 187476                      | 1126 (2.66-2.66)                                      |
| Sidechain outliers    | 187428                      | 1126 (2.66-2.66)                                      |
| RSRZ outliers         | 180081                      | 1110 (2.66-2.66)                                      |

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     | 552    | <div> <div>2%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>6%</div> <div>.</div> </div> </div> |
| 1   | B     | 552    | <div> <div>2%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>6%</div> <div>.</div> </div> </div> |
| 1   | C     | 552    | <div> <div>3%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>6%</div> <div>.</div> </div> </div> |
| 1   | D     | 552    | <div> <div>%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>5%</div> <div>.</div> </div> </div>  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16859 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.

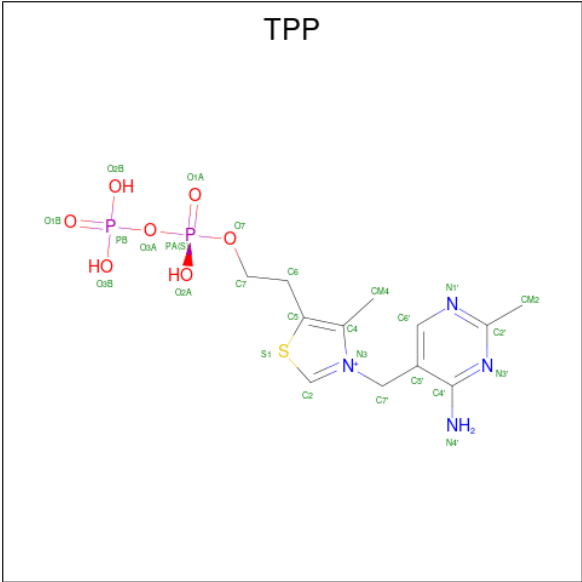
- Molecule 1 is a protein called Indole-3-pyruvate decarboxylase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 535      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4101  | 2596 | 718 | 764 | 23 |         |         |       |
| 1   | B     | 535      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4101  | 2596 | 718 | 764 | 23 |         |         |       |
| 1   | C     | 535      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4101  | 2596 | 718 | 764 | 23 |         |         |       |
| 1   | D     | 535      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4101  | 2596 | 718 | 764 | 23 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | P | S | 0       | 0       |
|     |       |          | 26    | 12 | 4 | 7 | 2 | 1 |         |         |
| 3   | B     | 1        | Total | C  | N | O | P | S | 0       | 0       |
|     |       |          | 26    | 12 | 4 | 7 | 2 | 1 |         |         |
| 3   | C     | 1        | Total | C  | N | O | P | S | 0       | 0       |
|     |       |          | 26    | 12 | 4 | 7 | 2 | 1 |         |         |
| 3   | D     | 1        | Total | C  | N | O | P | S | 0       | 0       |
|     |       |          | 26    | 12 | 4 | 7 | 2 | 1 |         |         |

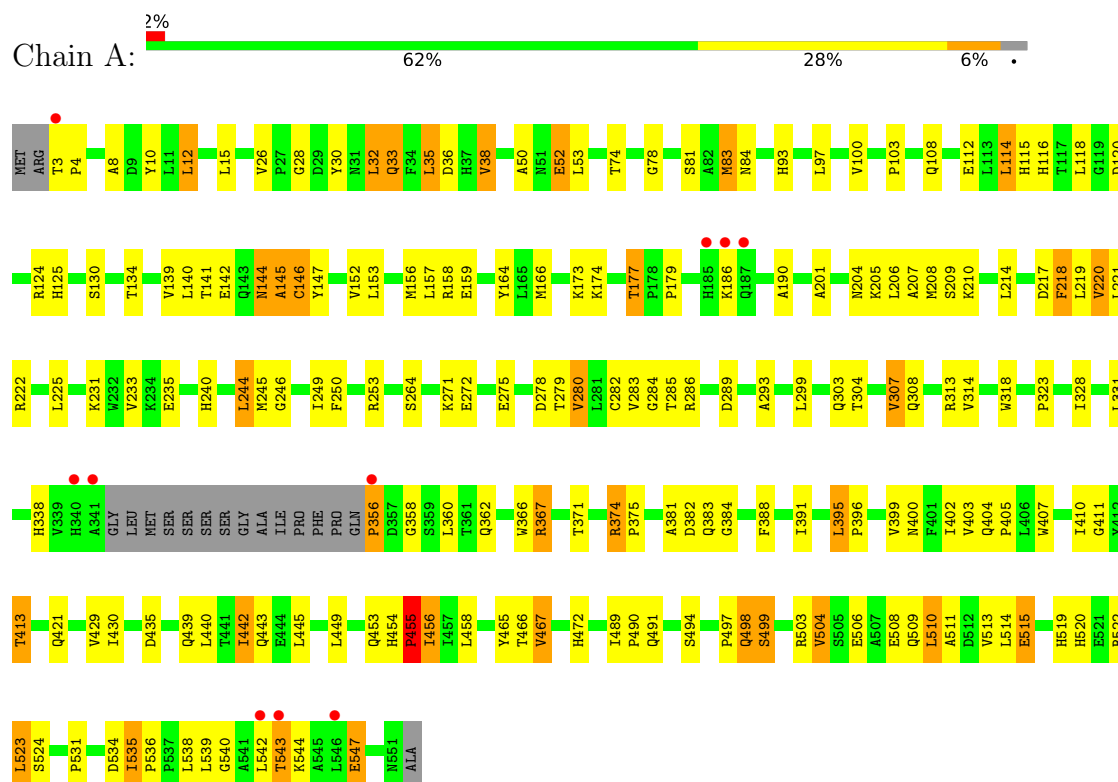
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 103      | Total | O   | 0       | 0       |
|     |       |          | 103   | 103 |         |         |
| 4   | B     | 96       | Total | O   | 0       | 0       |
|     |       |          | 96    | 96  |         |         |
| 4   | C     | 86       | Total | O   | 0       | 0       |
|     |       |          | 86    | 86  |         |         |
| 4   | D     | 62       | Total | O   | 0       | 0       |
|     |       |          | 62    | 62  |         |         |

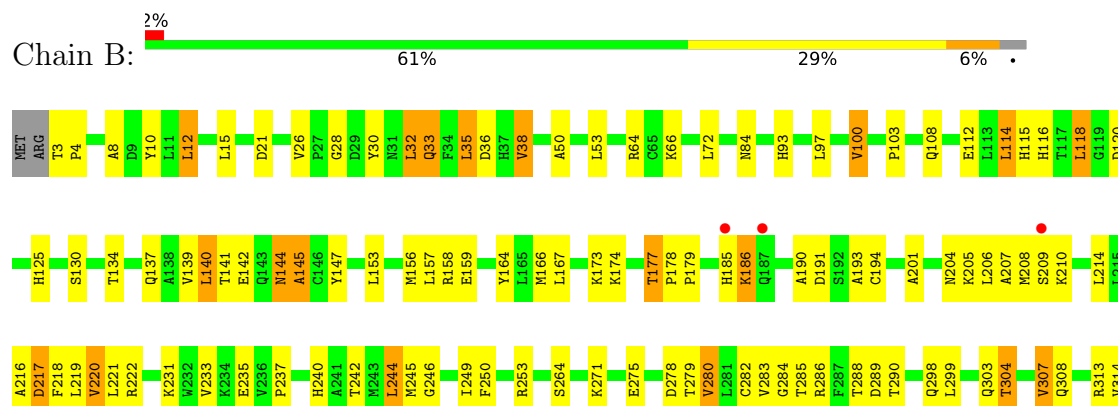
### 3 Residue-property plots

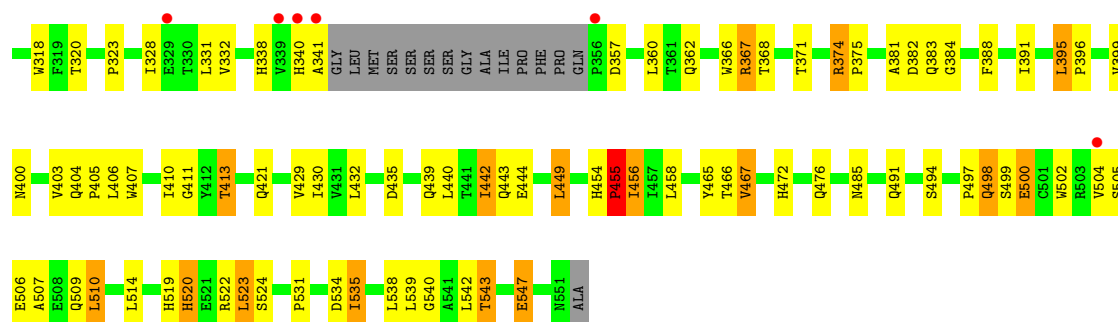
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Indole-3-pyruvate decarboxylase

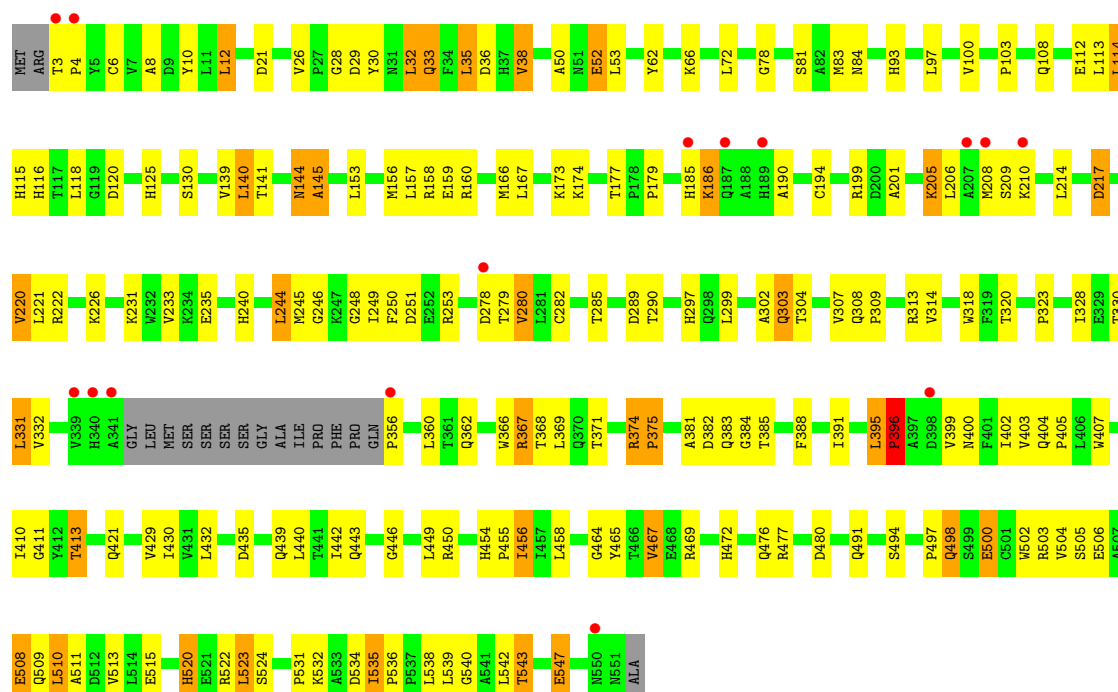


#### • Molecule 1: Indole-3-pyruvate decarboxylase

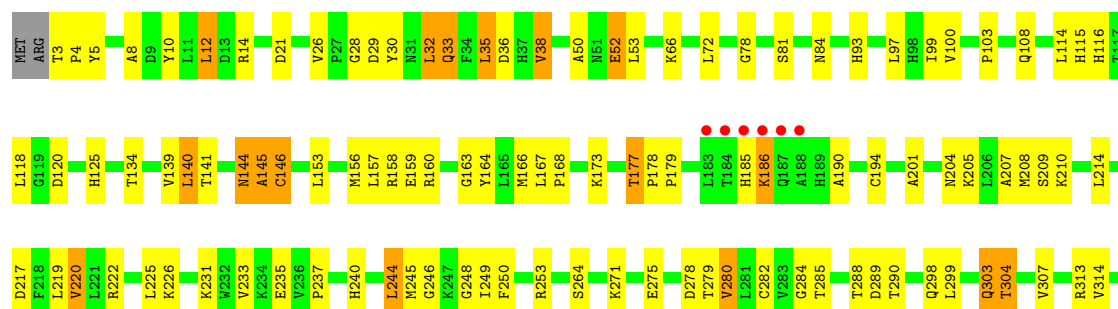


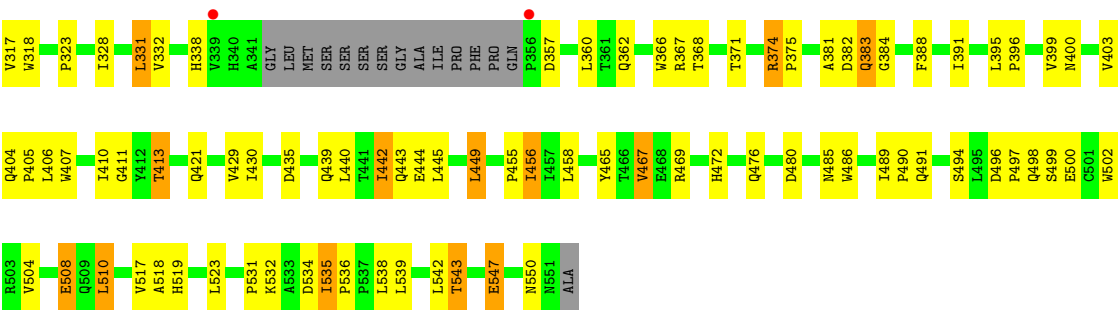


• Molecule 1: Indole-3-pyruvate decarboxylase



• Molecule 1: Indole-3-pyruvate decarboxylase





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 132.20Å 151.62Å 107.55Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.56 – 2.65<br>29.56 – 2.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (29.56-2.65)<br>99.9 (29.56-2.65)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.90 (at 2.64Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.205 , 0.236<br>0.208 , 0.202                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3198 reflections (5.05%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.237                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 44.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 16859                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 33.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: MG, TPP

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     | 0.52         | 0/4194         | 0.96        | 13/5711 (0.2%)  |
| 1   | B     | 0.49         | 1/4194 (0.0%)  | 0.97        | 12/5711 (0.2%)  |
| 1   | C     | 0.51         | 0/4194         | 0.98        | 14/5711 (0.2%)  |
| 1   | D     | 0.50         | 0/4194         | 0.97        | 15/5711 (0.3%)  |
| All | All   | 0.51         | 1/16776 (0.0%) | 0.97        | 54/22844 (0.2%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | B     | 454 | HIS  | C-N   | 5.15 | 1.40        | 1.33     |

All (54) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 455 | PRO  | CA-N-CD    | -11.45 | 95.98       | 112.00   |
| 1   | C     | 303 | GLN  | OE1-CD-NE2 | -10.55 | 112.05      | 122.60   |
| 1   | A     | 303 | GLN  | OE1-CD-NE2 | -10.11 | 112.49      | 122.60   |
| 1   | D     | 303 | GLN  | OE1-CD-NE2 | -9.25  | 113.35      | 122.60   |
| 1   | D     | 383 | GLN  | OE1-CD-NE2 | -9.03  | 113.57      | 122.60   |
| 1   | B     | 455 | PRO  | CB-CA-C    | -8.08  | 100.39      | 110.98   |
| 1   | C     | 396 | PRO  | CA-N-CD    | -7.58  | 101.39      | 112.00   |
| 1   | B     | 395 | LEU  | N-CA-C     | 7.27   | 118.94      | 109.93   |
| 1   | C     | 395 | LEU  | CA-C-N     | 7.20   | 128.83      | 119.84   |
| 1   | C     | 395 | LEU  | C-N-CA     | 7.20   | 128.83      | 119.84   |
| 1   | D     | 404 | GLN  | CA-C-N     | 7.16   | 126.78      | 119.19   |
| 1   | D     | 404 | GLN  | C-N-CA     | 7.16   | 126.78      | 119.19   |
| 1   | A     | 303 | GLN  | CG-CD-NE2  | 7.12   | 127.08      | 116.40   |
| 1   | D     | 383 | GLN  | CG-CD-NE2  | 6.93   | 126.79      | 116.40   |
| 1   | B     | 404 | GLN  | CA-C-N     | 6.90   | 126.50      | 119.19   |
| 1   | B     | 404 | GLN  | C-N-CA     | 6.90   | 126.50      | 119.19   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 395 | LEU  | N-CA-C    | 6.88  | 118.45      | 109.93   |
| 1   | C     | 303 | GLN  | CG-CD-NE2 | 6.77  | 126.55      | 116.40   |
| 1   | C     | 413 | THR  | N-CA-C    | 6.73  | 118.62      | 111.28   |
| 1   | B     | 413 | THR  | N-CA-C    | 6.65  | 118.53      | 111.28   |
| 1   | D     | 395 | LEU  | CA-C-O    | 6.46  | 126.82      | 120.23   |
| 1   | A     | 455 | PRO  | CA-N-CD   | -6.45 | 102.97      | 112.00   |
| 1   | D     | 303 | GLN  | CG-CD-NE2 | 6.38  | 125.97      | 116.40   |
| 1   | B     | 499 | SER  | N-CA-C    | 6.17  | 118.15      | 108.96   |
| 1   | D     | 413 | THR  | N-CA-C    | 6.13  | 117.96      | 111.28   |
| 1   | A     | 413 | THR  | N-CA-C    | 6.04  | 117.87      | 111.28   |
| 1   | C     | 404 | GLN  | CA-C-N    | 6.00  | 125.56      | 119.19   |
| 1   | C     | 404 | GLN  | C-N-CA    | 6.00  | 125.56      | 119.19   |
| 1   | C     | 217 | ASP  | N-CA-C    | 5.82  | 115.97      | 108.34   |
| 1   | B     | 442 | ILE  | N-CA-C    | 5.72  | 117.14      | 110.62   |
| 1   | A     | 442 | ILE  | N-CA-C    | 5.69  | 117.11      | 110.62   |
| 1   | A     | 411 | GLY  | N-CA-C    | -5.61 | 107.30      | 114.37   |
| 1   | C     | 375 | PRO  | CB-CA-C   | 5.59  | 118.55      | 111.39   |
| 1   | B     | 455 | PRO  | N-CA-CB   | 5.56  | 108.50      | 103.33   |
| 1   | B     | 411 | GLY  | N-CA-C    | -5.41 | 107.47      | 113.79   |
| 1   | C     | 411 | GLY  | N-CA-C    | -5.40 | 107.57      | 114.37   |
| 1   | A     | 404 | GLN  | CA-C-N    | 5.36  | 124.87      | 119.19   |
| 1   | A     | 404 | GLN  | C-N-CA    | 5.36  | 124.87      | 119.19   |
| 1   | A     | 499 | SER  | N-CA-C    | 5.28  | 116.82      | 108.96   |
| 1   | D     | 146 | CYS  | N-CA-C    | 5.23  | 116.67      | 111.07   |
| 1   | A     | 445 | LEU  | N-CA-C    | -5.23 | 105.76      | 111.82   |
| 1   | B     | 304 | THR  | N-CA-C    | 5.22  | 117.79      | 109.81   |
| 1   | D     | 499 | SER  | N-CA-C    | 5.21  | 117.59      | 109.52   |
| 1   | C     | 402 | ILE  | N-CA-C    | 5.18  | 115.04      | 107.37   |
| 1   | D     | 442 | ILE  | N-CA-C    | 5.17  | 116.51      | 110.62   |
| 1   | C     | 464 | GLY  | N-CA-C    | 5.17  | 117.41      | 110.43   |
| 1   | D     | 486 | TRP  | N-CA-C    | 5.17  | 119.89      | 111.37   |
| 1   | D     | 317 | VAL  | N-CA-C    | 5.16  | 115.73      | 108.36   |
| 1   | A     | 146 | CYS  | N-CA-C    | 5.14  | 117.28      | 111.11   |
| 1   | A     | 402 | ILE  | N-CA-C    | 5.10  | 114.91      | 107.37   |
| 1   | C     | 251 | ASP  | CA-C-O    | -5.10 | 115.47      | 120.98   |
| 1   | B     | 217 | ASP  | N-CA-C    | 5.09  | 115.01      | 108.34   |
| 1   | D     | 304 | THR  | N-CA-C    | 5.04  | 117.81      | 109.85   |
| 1   | D     | 411 | GLY  | N-CA-C    | -5.03 | 108.03      | 114.37   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 4101  | 0        | 4037     | 162     | 0            |
| 1   | B     | 4101  | 0        | 4037     | 156     | 0            |
| 1   | C     | 4101  | 0        | 4037     | 182     | 0            |
| 1   | D     | 4101  | 0        | 4037     | 173     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 26    | 0        | 16       | 2       | 0            |
| 3   | B     | 26    | 0        | 16       | 1       | 0            |
| 3   | C     | 26    | 0        | 16       | 1       | 0            |
| 3   | D     | 26    | 0        | 16       | 1       | 0            |
| 4   | A     | 103   | 0        | 0        | 10      | 0            |
| 4   | B     | 96    | 0        | 0        | 7       | 0            |
| 4   | C     | 86    | 0        | 0        | 5       | 0            |
| 4   | D     | 62    | 0        | 0        | 8       | 0            |
| All | All   | 16859 | 0        | 16212    | 652     | 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 20.

All (652) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:97:LEU:HD13  | 1:D:156:MET:HE1  | 1.38                     | 1.02              |
| 1:D:141:THR:H    | 1:D:144:ASN:HD21 | 1.02                     | 0.99              |
| 1:A:141:THR:H    | 1:A:144:ASN:HD21 | 1.07                     | 0.98              |
| 1:D:282:CYS:HB3  | 1:D:285:THR:HG21 | 1.48                     | 0.96              |
| 1:C:141:THR:H    | 1:C:144:ASN:HD21 | 1.15                     | 0.94              |
| 1:B:282:CYS:HB3  | 1:B:285:THR:HG21 | 1.49                     | 0.93              |
| 1:C:205:LYS:HE2  | 1:C:279:THR:HG22 | 1.50                     | 0.93              |
| 1:A:535:ILE:HG13 | 1:A:539:LEU:HD23 | 1.52                     | 0.92              |
| 1:A:144:ASN:HD22 | 1:A:145:ALA:N    | 1.68                     | 0.92              |
| 1:C:210:LYS:HA   | 1:C:210:LYS:HE2  | 1.50                     | 0.90              |
| 1:C:282:CYS:HB3  | 1:C:285:THR:HG21 | 1.53                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:210:LYS:HE2  | 1:B:210:LYS:HA   | 1.53                     | 0.90              |
| 1:A:210:LYS:HE2  | 1:A:210:LYS:HA   | 1.53                     | 0.90              |
| 1:B:144:ASN:HD22 | 1:B:145:ALA:N    | 1.71                     | 0.89              |
| 1:B:535:ILE:HG13 | 1:B:539:LEU:HD23 | 1.51                     | 0.89              |
| 1:B:141:THR:H    | 1:B:144:ASN:HD21 | 1.20                     | 0.89              |
| 1:A:97:LEU:HD13  | 1:A:156:MET:HE1  | 1.53                     | 0.88              |
| 1:D:141:THR:H    | 1:D:144:ASN:ND2  | 1.71                     | 0.88              |
| 1:D:210:LYS:HE2  | 1:D:210:LYS:HA   | 1.54                     | 0.88              |
| 1:D:535:ILE:HG13 | 1:D:539:LEU:HD23 | 1.55                     | 0.88              |
| 1:A:282:CYS:HB3  | 1:A:285:THR:HG21 | 1.56                     | 0.88              |
| 1:C:535:ILE:HG13 | 1:C:539:LEU:HD23 | 1.55                     | 0.87              |
| 1:C:511:ALA:O    | 1:C:515:GLU:HG2  | 1.75                     | 0.87              |
| 1:C:504:VAL:HG13 | 1:C:509:GLN:HB2  | 1.54                     | 0.87              |
| 1:B:97:LEU:HD13  | 1:B:156:MET:HE1  | 1.55                     | 0.86              |
| 1:C:205:LYS:HE2  | 1:C:279:THR:CG2  | 2.05                     | 0.86              |
| 1:D:449:LEU:HD11 | 1:D:523:LEU:HD23 | 1.58                     | 0.85              |
| 1:C:97:LEU:HD13  | 1:C:156:MET:HE1  | 1.58                     | 0.84              |
| 1:A:141:THR:H    | 1:A:144:ASN:ND2  | 1.74                     | 0.84              |
| 1:D:201:ALA:HB1  | 1:D:314:VAL:HG21 | 1.58                     | 0.84              |
| 1:C:141:THR:H    | 1:C:144:ASN:ND2  | 1.76                     | 0.83              |
| 1:A:201:ALA:HB1  | 1:A:314:VAL:HG21 | 1.59                     | 0.82              |
| 1:C:201:ALA:HB1  | 1:C:314:VAL:HG21 | 1.61                     | 0.82              |
| 1:B:201:ALA:HB1  | 1:B:314:VAL:HG21 | 1.62                     | 0.82              |
| 1:C:144:ASN:HD22 | 1:C:145:ALA:N    | 1.79                     | 0.80              |
| 1:D:144:ASN:HD22 | 1:D:145:ALA:N    | 1.79                     | 0.79              |
| 1:B:141:THR:H    | 1:B:144:ASN:ND2  | 1.80                     | 0.78              |
| 1:D:384:GLY:HA2  | 1:D:467:VAL:HG11 | 1.64                     | 0.77              |
| 1:C:244:LEU:HD22 | 1:C:403:VAL:HG11 | 1.66                     | 0.76              |
| 1:A:511:ALA:O    | 1:A:515:GLU:HG2  | 1.85                     | 0.76              |
| 1:C:384:GLY:HA2  | 1:C:467:VAL:HG11 | 1.67                     | 0.76              |
| 1:B:253:ARG:HH21 | 1:B:396:PRO:HG3  | 1.51                     | 0.76              |
| 1:D:97:LEU:HD13  | 1:D:156:MET:CE   | 2.15                     | 0.76              |
| 1:C:36:ASP:OD2   | 1:D:472:HIS:HE1  | 1.69                     | 0.75              |
| 1:A:421:GLN:HE21 | 1:A:455:PRO:HD3  | 1.51                     | 0.75              |
| 1:B:244:LEU:HD22 | 1:B:403:VAL:HG11 | 1.68                     | 0.75              |
| 1:C:217:ASP:O    | 1:C:220:VAL:HG13 | 1.87                     | 0.74              |
| 1:D:449:LEU:CD1  | 1:D:523:LEU:HD23 | 2.17                     | 0.74              |
| 1:A:293:ALA:HA   | 1:A:542:LEU:HD23 | 1.67                     | 0.74              |
| 1:B:144:ASN:HD22 | 1:B:144:ASN:C    | 1.96                     | 0.74              |
| 1:A:205:LYS:HE3  | 1:A:279:THR:HG22 | 1.71                     | 0.73              |
| 1:D:467:VAL:HG12 | 1:D:539:LEU:HD21 | 1.68                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:491:GLN:HA   | 1:B:497:PRO:HG2  | 1.71                     | 0.73              |
| 1:A:491:GLN:HA   | 1:A:497:PRO:HG2  | 1.70                     | 0.72              |
| 1:A:36:ASP:OD2   | 1:B:472:HIS:HE1  | 1.71                     | 0.72              |
| 1:B:207:ALA:HA   | 1:B:338:HIS:CD2  | 2.25                     | 0.72              |
| 1:C:456:ILE:HD11 | 1:C:458:LEU:HD11 | 1.72                     | 0.72              |
| 1:C:362:GLN:NE2  | 1:C:366:TRP:HE1  | 1.88                     | 0.71              |
| 1:D:246:GLY:O    | 1:D:249:ILE:HG23 | 1.90                     | 0.71              |
| 1:D:205:LYS:HE3  | 1:D:279:THR:CG2  | 2.21                     | 0.71              |
| 1:D:449:LEU:CD1  | 1:D:523:LEU:CD2  | 2.69                     | 0.71              |
| 1:D:500:GLU:HB3  | 1:D:502:TRP:CH2  | 2.26                     | 0.70              |
| 1:B:205:LYS:HE3  | 1:B:279:THR:CG2  | 2.21                     | 0.70              |
| 1:A:384:GLY:HA2  | 1:A:467:VAL:HG11 | 1.72                     | 0.70              |
| 1:D:237:PRO:HA   | 4:D:609:HOH:O    | 1.91                     | 0.70              |
| 1:B:494:SER:HB3  | 1:B:497:PRO:HG3  | 1.74                     | 0.69              |
| 1:D:290:THR:HA   | 1:D:542:LEU:HD11 | 1.75                     | 0.69              |
| 1:C:491:GLN:HA   | 1:C:497:PRO:HG2  | 1.73                     | 0.69              |
| 1:A:205:LYS:HE3  | 1:A:279:THR:CG2  | 2.21                     | 0.69              |
| 1:B:467:VAL:HG12 | 1:B:539:LEU:HD21 | 1.74                     | 0.68              |
| 1:B:217:ASP:O    | 1:B:220:VAL:HG13 | 1.93                     | 0.68              |
| 1:C:356:PRO:HG3  | 1:C:367:ARG:NH1  | 2.09                     | 0.68              |
| 1:A:293:ALA:HA   | 1:A:542:LEU:CD2  | 2.24                     | 0.67              |
| 1:C:246:GLY:O    | 1:C:249:ILE:HG23 | 1.94                     | 0.67              |
| 1:D:531:PRO:HB2  | 1:D:534:ASP:HB2  | 1.76                     | 0.67              |
| 1:A:153:LEU:HD23 | 1:A:156:MET:HE3  | 1.77                     | 0.67              |
| 1:D:491:GLN:HA   | 1:D:497:PRO:HG2  | 1.77                     | 0.67              |
| 1:A:456:ILE:HD11 | 1:A:458:LEU:HD11 | 1.74                     | 0.67              |
| 1:C:455:PRO:HD2  | 1:C:523:LEU:HD22 | 1.75                     | 0.67              |
| 1:A:217:ASP:O    | 1:A:220:VAL:HG13 | 1.95                     | 0.67              |
| 1:B:246:GLY:O    | 1:B:249:ILE:HG23 | 1.94                     | 0.67              |
| 1:A:246:GLY:O    | 1:A:249:ILE:HG23 | 1.94                     | 0.67              |
| 1:A:494:SER:HB3  | 1:A:497:PRO:HG3  | 1.77                     | 0.67              |
| 1:B:290:THR:HA   | 1:B:542:LEU:HD11 | 1.77                     | 0.67              |
| 1:A:144:ASN:HD22 | 1:A:144:ASN:C    | 1.99                     | 0.67              |
| 1:A:253:ARG:HH21 | 1:A:396:PRO:HG3  | 1.60                     | 0.66              |
| 1:B:280:VAL:HG13 | 1:B:304:THR:HG22 | 1.77                     | 0.66              |
| 1:B:384:GLY:HA2  | 1:B:467:VAL:HG11 | 1.77                     | 0.66              |
| 1:A:531:PRO:HB2  | 1:A:534:ASP:HB2  | 1.78                     | 0.66              |
| 1:C:290:THR:HA   | 1:C:542:LEU:HD11 | 1.77                     | 0.66              |
| 1:C:467:VAL:HG12 | 1:C:539:LEU:HD21 | 1.77                     | 0.66              |
| 1:D:500:GLU:HB3  | 1:D:502:TRP:CZ3  | 2.31                     | 0.66              |
| 1:D:226:LYS:HE3  | 1:D:249:ILE:HA   | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:358:GLY:HA2  | 1:A:508:GLU:OE2  | 1.97                     | 0.65              |
| 1:D:205:LYS:HE3  | 1:D:279:THR:HG22 | 1.78                     | 0.65              |
| 1:D:455:PRO:HD2  | 1:D:523:LEU:HD13 | 1.77                     | 0.65              |
| 1:D:244:LEU:HD22 | 1:D:403:VAL:HG11 | 1.79                     | 0.65              |
| 1:D:449:LEU:HD13 | 1:D:523:LEU:HD22 | 1.78                     | 0.64              |
| 1:C:36:ASP:OD2   | 1:D:472:HIS:CE1  | 2.49                     | 0.64              |
| 1:D:455:PRO:HG2  | 1:D:523:LEU:CD1  | 2.26                     | 0.64              |
| 1:C:144:ASN:HD22 | 1:C:144:ASN:C    | 2.03                     | 0.64              |
| 1:D:449:LEU:HD13 | 1:D:523:LEU:CD2  | 2.27                     | 0.64              |
| 1:B:253:ARG:HD2  | 4:B:690:HOH:O    | 1.97                     | 0.64              |
| 1:C:469:ARG:NH2  | 1:C:480:ASP:OD1  | 2.31                     | 0.64              |
| 1:A:10:TYR:CE2   | 1:A:179:PRO:HG3  | 2.33                     | 0.64              |
| 1:D:467:VAL:CG1  | 1:D:539:LEU:HD21 | 2.27                     | 0.63              |
| 1:B:205:LYS:HE3  | 1:B:279:THR:HG22 | 1.81                     | 0.63              |
| 1:A:207:ALA:HA   | 1:A:338:HIS:CD2  | 2.33                     | 0.63              |
| 1:D:141:THR:N    | 1:D:144:ASN:HD21 | 1.84                     | 0.63              |
| 1:D:253:ARG:HH21 | 1:D:396:PRO:HG3  | 1.64                     | 0.63              |
| 1:A:28:GLY:O     | 1:A:32:LEU:HD13  | 1.98                     | 0.63              |
| 1:C:469:ARG:NH1  | 1:C:532:LYS:HG3  | 2.13                     | 0.63              |
| 1:B:467:VAL:CG1  | 1:B:539:LEU:HD21 | 2.29                     | 0.63              |
| 1:A:244:LEU:HD22 | 1:A:403:VAL:HG11 | 1.81                     | 0.62              |
| 1:A:141:THR:N    | 1:A:144:ASN:HD21 | 1.89                     | 0.62              |
| 1:A:472:HIS:HE1  | 1:B:36:ASP:OD2   | 1.82                     | 0.62              |
| 1:D:456:ILE:HD11 | 1:D:458:LEU:HD11 | 1.82                     | 0.62              |
| 1:A:421:GLN:NE2  | 1:A:455:PRO:HD3  | 2.15                     | 0.62              |
| 1:A:467:VAL:HG12 | 1:A:539:LEU:HD21 | 1.82                     | 0.62              |
| 1:C:446:GLY:HA3  | 4:D:604:HOH:O    | 2.00                     | 0.62              |
| 1:C:472:HIS:HE1  | 1:D:36:ASP:OD2   | 1.82                     | 0.61              |
| 1:D:217:ASP:O    | 1:D:220:VAL:HG13 | 1.99                     | 0.61              |
| 1:C:115:HIS:HD2  | 1:D:289:ASP:OD2  | 1.82                     | 0.61              |
| 1:D:382:ASP:CA   | 1:D:413:THR:HG21 | 2.30                     | 0.61              |
| 1:A:413:THR:HG22 | 4:A:628:HOH:O    | 1.99                     | 0.61              |
| 1:D:469:ARG:NH2  | 1:D:480:ASP:OD1  | 2.33                     | 0.61              |
| 1:B:531:PRO:HB2  | 1:B:534:ASP:HB2  | 1.83                     | 0.61              |
| 1:A:210:LYS:HE2  | 1:A:210:LYS:CA   | 2.30                     | 0.60              |
| 1:D:280:VAL:HG13 | 1:D:304:THR:HG22 | 1.81                     | 0.60              |
| 1:B:539:LEU:O    | 1:B:543:THR:HB   | 2.01                     | 0.60              |
| 1:D:494:SER:HB3  | 1:D:497:PRO:HG3  | 1.82                     | 0.60              |
| 1:A:108:GLN:HE22 | 1:A:166:MET:HE3  | 1.66                     | 0.60              |
| 1:D:10:TYR:CE2   | 1:D:179:PRO:HG3  | 2.37                     | 0.60              |
| 1:C:382:ASP:CA   | 1:C:413:THR:HG21 | 2.32                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:368:THR:HG21 | 1:D:510:LEU:HD13 | 1.83                     | 0.60              |
| 1:C:28:GLY:O     | 1:C:32:LEU:HD13  | 2.02                     | 0.60              |
| 1:A:97:LEU:HD13  | 1:A:156:MET:CE   | 2.27                     | 0.60              |
| 1:A:52:GLU:HG2   | 1:A:81:SER:HB2   | 1.83                     | 0.59              |
| 1:D:28:GLY:O     | 1:D:32:LEU:HD13  | 2.02                     | 0.59              |
| 1:A:35:LEU:O     | 1:A:38:VAL:HG13  | 2.03                     | 0.59              |
| 1:A:36:ASP:OD2   | 1:B:472:HIS:CE1  | 2.55                     | 0.59              |
| 1:B:320:THR:OG1  | 1:D:146:CYS:SG   | 2.61                     | 0.59              |
| 1:A:3:THR:N      | 1:A:4:PRO:HD3    | 2.18                     | 0.59              |
| 1:A:233:VAL:HG21 | 1:A:240:HIS:CE1  | 2.37                     | 0.59              |
| 1:C:52:GLU:HG2   | 1:C:81:SER:HB2   | 1.84                     | 0.59              |
| 1:C:190:ALA:HB2  | 1:C:323:PRO:HD2  | 1.85                     | 0.59              |
| 1:B:500:GLU:HB3  | 1:B:502:TRP:CZ3  | 2.38                     | 0.59              |
| 1:B:8:ALA:O      | 1:B:12:LEU:HD22  | 2.02                     | 0.59              |
| 1:D:3:THR:N      | 1:D:4:PRO:HD3    | 2.18                     | 0.59              |
| 1:D:360:LEU:HD11 | 1:D:504:VAL:HG12 | 1.84                     | 0.59              |
| 1:B:3:THR:N      | 1:B:4:PRO:HD3    | 2.18                     | 0.58              |
| 1:D:190:ALA:HB2  | 1:D:323:PRO:HD2  | 1.83                     | 0.58              |
| 1:D:282:CYS:HB3  | 1:D:285:THR:CG2  | 2.29                     | 0.58              |
| 1:B:190:ALA:HB2  | 1:B:323:PRO:HD2  | 1.85                     | 0.58              |
| 1:D:233:VAL:HG21 | 1:D:240:HIS:CE1  | 2.37                     | 0.58              |
| 1:D:8:ALA:O      | 1:D:12:LEU:HD22  | 2.03                     | 0.58              |
| 1:A:356:PRO:HB3  | 4:A:655:HOH:O    | 2.03                     | 0.58              |
| 1:D:469:ARG:NH1  | 4:D:602:HOH:O    | 2.36                     | 0.58              |
| 1:A:120:ASP:OD2  | 1:A:125:HIS:HE1  | 1.86                     | 0.58              |
| 1:D:382:ASP:N    | 1:D:413:THR:HG21 | 2.19                     | 0.58              |
| 1:A:124:ARG:NH2  | 4:A:693:HOH:O    | 2.36                     | 0.58              |
| 1:C:382:ASP:N    | 1:C:413:THR:HG21 | 2.19                     | 0.58              |
| 1:B:314:VAL:O    | 1:B:314:VAL:HG23 | 2.04                     | 0.58              |
| 1:C:244:LEU:HD13 | 1:C:405:PRO:HG3  | 1.86                     | 0.58              |
| 1:C:313:ARG:HD3  | 1:C:318:TRP:CE2  | 2.38                     | 0.58              |
| 1:D:93:HIS:O     | 1:D:222:ARG:HD2  | 2.03                     | 0.58              |
| 1:D:144:ASN:HD22 | 1:D:144:ASN:C    | 2.08                     | 0.58              |
| 1:B:28:GLY:O     | 1:B:32:LEU:HD13  | 2.03                     | 0.58              |
| 1:A:362:GLN:NE2  | 1:A:366:TRP:HE1  | 2.03                     | 0.57              |
| 1:C:226:LYS:HE3  | 1:C:249:ILE:HA   | 1.85                     | 0.57              |
| 1:C:531:PRO:HB2  | 1:C:534:ASP:HB2  | 1.86                     | 0.57              |
| 1:D:209:SER:HB2  | 1:D:279:THR:HG21 | 1.85                     | 0.57              |
| 1:D:413:THR:HG22 | 4:D:618:HOH:O    | 2.03                     | 0.57              |
| 1:A:225:LEU:HD13 | 1:A:328:ILE:HD12 | 1.86                     | 0.57              |
| 1:A:253:ARG:HG2  | 1:A:253:ARG:HH11 | 1.68                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:456:ILE:O    | 1:B:456:ILE:HG13 | 2.03                     | 0.57              |
| 1:C:233:VAL:HG21 | 1:C:240:HIS:CE1  | 2.40                     | 0.57              |
| 1:A:367:ARG:NH1  | 4:A:630:HOH:O    | 2.37                     | 0.57              |
| 1:B:253:ARG:NH2  | 1:B:396:PRO:HG3  | 2.17                     | 0.57              |
| 1:C:500:GLU:HG3  | 1:C:522:ARG:NH1  | 2.19                     | 0.57              |
| 1:A:190:ALA:HB2  | 1:A:323:PRO:HD2  | 1.87                     | 0.57              |
| 1:A:467:VAL:CG1  | 1:A:539:LEU:HD21 | 2.35                     | 0.57              |
| 1:A:84:ASN:ND2   | 1:A:407:TRP:HE1  | 2.02                     | 0.57              |
| 1:D:30:TYR:CZ    | 1:D:103:PRO:HG3  | 2.40                     | 0.57              |
| 1:B:118:LEU:HB2  | 4:B:617:HOH:O    | 2.03                     | 0.57              |
| 1:B:207:ALA:HA   | 1:B:338:HIS:NE2  | 2.19                     | 0.57              |
| 1:C:539:LEU:O    | 1:C:543:THR:HB   | 2.04                     | 0.56              |
| 1:C:368:THR:HG21 | 1:C:510:LEU:CD1  | 2.35                     | 0.56              |
| 1:A:144:ASN:ND2  | 1:A:144:ASN:C    | 2.60                     | 0.56              |
| 1:B:523:LEU:HD13 | 1:B:524:SER:N    | 2.20                     | 0.56              |
| 1:C:97:LEU:HD13  | 1:C:156:MET:CE   | 2.34                     | 0.56              |
| 1:C:467:VAL:CG1  | 1:C:539:LEU:HD21 | 2.35                     | 0.56              |
| 1:C:494:SER:HB3  | 1:C:497:PRO:HG3  | 1.86                     | 0.56              |
| 1:D:362:GLN:NE2  | 1:D:366:TRP:HE1  | 2.02                     | 0.56              |
| 1:D:469:ARG:NH1  | 1:D:532:LYS:HG3  | 2.21                     | 0.56              |
| 1:A:201:ALA:CB   | 1:A:314:VAL:HG21 | 2.32                     | 0.56              |
| 1:C:141:THR:N    | 1:C:144:ASN:HD21 | 1.94                     | 0.56              |
| 1:B:190:ALA:HB2  | 1:B:323:PRO:CD   | 2.36                     | 0.56              |
| 1:B:194:CYS:HA   | 1:D:177:THR:HG21 | 1.88                     | 0.56              |
| 1:D:108:GLN:HE22 | 1:D:166:MET:HE3  | 1.71                     | 0.56              |
| 1:B:368:THR:HG21 | 1:B:510:LEU:HD13 | 1.88                     | 0.55              |
| 1:C:153:LEU:HD23 | 1:C:156:MET:HE3  | 1.87                     | 0.55              |
| 1:B:201:ALA:CB   | 1:B:314:VAL:HG21 | 2.36                     | 0.55              |
| 1:A:539:LEU:O    | 1:A:543:THR:HB   | 2.06                     | 0.55              |
| 1:B:144:ASN:ND2  | 1:B:144:ASN:C    | 2.61                     | 0.55              |
| 1:C:120:ASP:OD2  | 1:C:125:HIS:HE1  | 1.90                     | 0.55              |
| 1:D:539:LEU:O    | 1:D:543:THR:HB   | 2.06                     | 0.55              |
| 1:A:209:SER:HB2  | 1:A:279:THR:HG21 | 1.87                     | 0.55              |
| 1:C:112:GLU:HB2  | 1:C:114:LEU:HD13 | 1.88                     | 0.55              |
| 1:C:210:LYS:HE2  | 1:C:210:LYS:CA   | 2.31                     | 0.55              |
| 1:B:357:ASP:HA   | 1:B:507:ALA:HB3  | 1.88                     | 0.55              |
| 1:C:454:HIS:ND1  | 1:C:522:ARG:HA   | 2.20                     | 0.55              |
| 1:D:190:ALA:HB2  | 1:D:323:PRO:CD   | 2.37                     | 0.55              |
| 1:A:314:VAL:HG23 | 1:A:314:VAL:O    | 2.07                     | 0.54              |
| 1:B:371:THR:O    | 1:B:374:ARG:NH2  | 2.41                     | 0.54              |
| 1:D:280:VAL:HG11 | 1:D:299:LEU:HD22 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:35:LEU:O     | 1:B:38:VAL:HG13  | 2.07                     | 0.54              |
| 1:B:466:THR:HG22 | 4:B:603:HOH:O    | 2.05                     | 0.54              |
| 1:C:253:ARG:NH2  | 1:C:396:PRO:HD3  | 2.22                     | 0.54              |
| 1:C:440:LEU:HG   | 1:D:50:ALA:O     | 2.08                     | 0.54              |
| 1:B:210:LYS:HE2  | 1:B:210:LYS:CA   | 2.31                     | 0.54              |
| 1:C:84:ASN:ND2   | 1:C:407:TRP:HE1  | 2.06                     | 0.54              |
| 1:C:93:HIS:O     | 1:C:222:ARG:HD2  | 2.07                     | 0.54              |
| 1:B:421:GLN:HE21 | 1:B:455:PRO:HD3  | 1.72                     | 0.54              |
| 1:C:52:GLU:CD    | 1:C:52:GLU:H     | 2.13                     | 0.54              |
| 1:B:280:VAL:HG11 | 1:B:299:LEU:HD22 | 1.88                     | 0.54              |
| 1:C:158:ARG:HD2  | 1:C:159:GLU:OE2  | 2.07                     | 0.54              |
| 1:D:517:VAL:O    | 1:D:519:HIS:N    | 2.41                     | 0.54              |
| 1:B:139:VAL:HG13 | 1:B:166:MET:HE2  | 1.89                     | 0.54              |
| 1:B:388:PHE:CD2  | 1:B:539:LEU:HD13 | 2.42                     | 0.54              |
| 1:C:21:ASP:OD2   | 1:C:66:LYS:NZ    | 2.39                     | 0.54              |
| 1:C:30:TYR:CZ    | 1:C:103:PRO:HG3  | 2.42                     | 0.54              |
| 1:D:245:MET:HG2  | 1:D:405:PRO:HD2  | 1.89                     | 0.54              |
| 1:A:139:VAL:HG13 | 1:A:166:MET:HE2  | 1.89                     | 0.54              |
| 1:A:289:ASP:OD2  | 1:B:115:HIS:HD2  | 1.89                     | 0.54              |
| 1:C:10:TYR:CE2   | 1:C:179:PRO:HG3  | 2.43                     | 0.54              |
| 1:D:210:LYS:HE2  | 1:D:210:LYS:CA   | 2.32                     | 0.54              |
| 1:A:158:ARG:HD2  | 1:A:159:GLU:OE2  | 2.08                     | 0.54              |
| 1:A:456:ILE:HD11 | 1:A:458:LEU:CD1  | 2.37                     | 0.54              |
| 1:A:190:ALA:HB2  | 1:A:323:PRO:CD   | 2.39                     | 0.53              |
| 1:A:245:MET:HG2  | 1:A:405:PRO:HD2  | 1.91                     | 0.53              |
| 1:C:108:GLN:HE22 | 1:C:166:MET:HE3  | 1.72                     | 0.53              |
| 1:C:371:THR:O    | 1:C:374:ARG:NH2  | 2.41                     | 0.53              |
| 1:D:35:LEU:O     | 1:D:38:VAL:HG13  | 2.07                     | 0.53              |
| 1:C:289:ASP:OD2  | 1:D:115:HIS:HD2  | 1.90                     | 0.53              |
| 1:B:158:ARG:HD2  | 1:B:159:GLU:OE2  | 2.09                     | 0.53              |
| 1:C:362:GLN:HE21 | 1:C:366:TRP:HE1  | 1.54                     | 0.53              |
| 1:A:465:TYR:HB3  | 3:A:600:TPP:H62  | 1.90                     | 0.53              |
| 1:B:153:LEU:HD23 | 1:B:156:MET:HE3  | 1.91                     | 0.53              |
| 1:C:50:ALA:O     | 1:D:440:LEU:HG   | 2.09                     | 0.53              |
| 1:C:356:PRO:HG3  | 1:C:367:ARG:HH12 | 1.73                     | 0.53              |
| 1:C:456:ILE:O    | 1:C:456:ILE:HG13 | 2.07                     | 0.53              |
| 1:B:282:CYS:HB3  | 1:B:285:THR:CG2  | 2.30                     | 0.53              |
| 1:B:382:ASP:CA   | 1:B:413:THR:HG21 | 2.39                     | 0.53              |
| 1:C:205:LYS:NZ   | 1:C:302:ALA:O    | 2.40                     | 0.53              |
| 1:A:367:ARG:HG2  | 1:A:367:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:97:LEU:HD13  | 1:B:156:MET:CE   | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:440:LEU:HG   | 1:B:50:ALA:O     | 2.09                     | 0.52              |
| 1:B:233:VAL:HG21 | 1:B:240:HIS:CE1  | 2.44                     | 0.52              |
| 1:B:382:ASP:CG   | 1:B:413:THR:HG23 | 2.35                     | 0.52              |
| 1:C:3:THR:N      | 1:C:4:PRO:HD3    | 2.23                     | 0.52              |
| 1:C:314:VAL:HG23 | 1:C:314:VAL:O    | 2.07                     | 0.52              |
| 1:A:50:ALA:O     | 1:B:440:LEU:HG   | 2.10                     | 0.52              |
| 1:C:465:TYR:HB3  | 3:C:600:TPP:H62  | 1.90                     | 0.52              |
| 1:D:120:ASP:OD2  | 1:D:125:HIS:HE1  | 1.92                     | 0.52              |
| 1:D:357:ASP:HB2  | 1:D:508:GLU:HG3  | 1.91                     | 0.52              |
| 1:A:371:THR:O    | 1:A:374:ARG:NH2  | 2.42                     | 0.52              |
| 1:B:153:LEU:HA   | 1:B:156:MET:HE3  | 1.90                     | 0.52              |
| 1:B:362:GLN:NE2  | 1:B:366:TRP:HE1  | 2.06                     | 0.52              |
| 1:C:280:VAL:HG13 | 1:C:304:THR:HG22 | 1.92                     | 0.52              |
| 1:C:201:ALA:CB   | 1:C:314:VAL:HG21 | 2.37                     | 0.52              |
| 1:A:472:HIS:CE1  | 1:B:36:ASP:OD2   | 2.63                     | 0.52              |
| 1:C:209:SER:HB2  | 1:C:279:THR:HG21 | 1.90                     | 0.52              |
| 1:D:201:ALA:CB   | 1:D:314:VAL:HG21 | 2.33                     | 0.52              |
| 1:A:221:LEU:HD21 | 1:A:249:ILE:HG22 | 1.92                     | 0.52              |
| 1:B:465:TYR:HB3  | 3:B:600:TPP:H62  | 1.91                     | 0.52              |
| 1:C:144:ASN:ND2  | 1:C:144:ASN:C    | 2.68                     | 0.52              |
| 1:D:421:GLN:HG2  | 1:D:429:VAL:HG21 | 1.91                     | 0.52              |
| 1:D:449:LEU:CD1  | 1:D:523:LEU:HD22 | 2.38                     | 0.52              |
| 1:C:384:GLY:HA2  | 1:C:467:VAL:CG1  | 2.40                     | 0.51              |
| 1:C:455:PRO:HD2  | 1:C:523:LEU:CD2  | 2.38                     | 0.51              |
| 1:C:456:ILE:HD11 | 1:C:458:LEU:CD1  | 2.40                     | 0.51              |
| 1:C:506:GLU:HB2  | 1:C:509:GLN:HG3  | 1.93                     | 0.51              |
| 1:D:217:ASP:OD2  | 1:D:245:MET:HB2  | 2.09                     | 0.51              |
| 1:D:368:THR:HG21 | 1:D:510:LEU:CD1  | 2.38                     | 0.51              |
| 1:C:280:VAL:HG11 | 1:C:299:LEU:HD22 | 1.91                     | 0.51              |
| 1:D:84:ASN:ND2   | 1:D:407:TRP:HE1  | 2.08                     | 0.51              |
| 1:A:374:ARG:HG3  | 1:A:375:PRO:HD2  | 1.92                     | 0.51              |
| 1:B:141:THR:N    | 1:B:144:ASN:HD21 | 2.00                     | 0.51              |
| 1:C:115:HIS:O    | 1:C:116:HIS:HB2  | 2.09                     | 0.51              |
| 1:D:21:ASP:OD2   | 1:D:66:LYS:NZ    | 2.38                     | 0.51              |
| 1:D:445:LEU:HD11 | 1:D:523:LEU:HD21 | 1.91                     | 0.51              |
| 1:D:465:TYR:HB3  | 3:D:600:TPP:H62  | 1.92                     | 0.51              |
| 1:C:504:VAL:HG13 | 1:C:509:GLN:CB   | 2.34                     | 0.51              |
| 1:A:280:VAL:HG11 | 1:A:299:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:382:ASP:CG   | 1:A:413:THR:HG23 | 2.36                     | 0.51              |
| 1:A:388:PHE:CD2  | 1:A:539:LEU:HD13 | 2.46                     | 0.51              |
| 1:B:177:THR:HG21 | 1:D:194:CYS:HA   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:244:LEU:HD13 | 1:D:405:PRO:HG3  | 1.91                     | 0.51              |
| 1:D:374:ARG:HG3  | 1:D:375:PRO:HD2  | 1.92                     | 0.51              |
| 1:B:374:ARG:HG3  | 1:B:375:PRO:HD2  | 1.93                     | 0.51              |
| 1:C:368:THR:HG21 | 1:C:510:LEU:HD12 | 1.93                     | 0.51              |
| 1:D:153:LEU:HD23 | 1:D:156:MET:HE3  | 1.92                     | 0.51              |
| 1:C:190:ALA:HB2  | 1:C:323:PRO:CD   | 2.40                     | 0.51              |
| 1:C:421:GLN:HG2  | 1:C:429:VAL:HG21 | 1.92                     | 0.51              |
| 1:C:504:VAL:HG12 | 1:C:505:SER:N    | 2.25                     | 0.51              |
| 1:D:382:ASP:HA   | 1:D:413:THR:HG21 | 1.92                     | 0.51              |
| 1:D:391:ILE:HG21 | 1:D:538:LEU:HD22 | 1.93                     | 0.51              |
| 1:C:8:ALA:O      | 1:C:12:LEU:HD22  | 2.11                     | 0.51              |
| 1:B:506:GLU:HG2  | 1:B:509:GLN:OE1  | 2.10                     | 0.51              |
| 1:A:115:HIS:HD2  | 1:B:289:ASP:OD2  | 1.94                     | 0.50              |
| 1:D:374:ARG:HG3  | 1:D:375:PRO:CD   | 2.41                     | 0.50              |
| 1:B:209:SER:HB2  | 1:B:279:THR:HG21 | 1.93                     | 0.50              |
| 1:B:367:ARG:HG2  | 1:B:367:ARG:HH11 | 1.76                     | 0.50              |
| 1:D:371:THR:O    | 1:D:374:ARG:NH2  | 2.44                     | 0.50              |
| 1:A:382:ASP:CA   | 1:A:413:THR:HG21 | 2.41                     | 0.50              |
| 1:A:456:ILE:HD12 | 1:A:456:ILE:C    | 2.36                     | 0.50              |
| 1:A:456:ILE:O    | 1:A:456:ILE:HG13 | 2.12                     | 0.50              |
| 1:C:245:MET:HG2  | 1:C:405:PRO:HD2  | 1.92                     | 0.50              |
| 1:A:97:LEU:HD22  | 1:A:153:LEU:HD21 | 1.94                     | 0.50              |
| 1:B:21:ASP:OD2   | 1:B:66:LYS:NZ    | 2.40                     | 0.50              |
| 1:D:264:SER:HA   | 1:D:271:LYS:HE2  | 1.94                     | 0.50              |
| 1:B:10:TYR:CE2   | 1:B:179:PRO:HG3  | 2.47                     | 0.50              |
| 1:B:30:TYR:CZ    | 1:B:103:PRO:HG3  | 2.47                     | 0.50              |
| 1:B:253:ARG:HH11 | 1:B:253:ARG:HG2  | 1.76                     | 0.50              |
| 1:B:400:ASN:C    | 1:B:400:ASN:HD22 | 2.20                     | 0.50              |
| 1:C:500:GLU:HB3  | 1:C:502:TRP:CH2  | 2.47                     | 0.50              |
| 1:D:388:PHE:CD2  | 1:D:539:LEU:HD13 | 2.46                     | 0.50              |
| 1:A:253:ARG:NH2  | 1:A:396:PRO:HG3  | 2.26                     | 0.50              |
| 1:B:504:VAL:HG13 | 1:B:509:GLN:HB2  | 1.94                     | 0.50              |
| 1:C:375:PRO:HG3  | 1:C:396:PRO:HB3  | 1.94                     | 0.50              |
| 1:D:456:ILE:O    | 1:D:456:ILE:HG13 | 2.12                     | 0.50              |
| 1:A:400:ASN:HD22 | 1:A:400:ASN:C    | 2.19                     | 0.49              |
| 1:B:245:MET:HG2  | 1:B:405:PRO:HD2  | 1.93                     | 0.49              |
| 1:C:498:GLN:O    | 1:C:522:ARG:HB2  | 2.12                     | 0.49              |
| 1:B:120:ASP:OD2  | 1:B:125:HIS:HE1  | 1.95                     | 0.49              |
| 1:B:430:ILE:N    | 1:B:430:ILE:HD12 | 2.28                     | 0.49              |
| 1:C:253:ARG:HG2  | 1:C:253:ARG:HH11 | 1.77                     | 0.49              |
| 1:C:253:ARG:HH21 | 1:C:396:PRO:HG3  | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:144:ASN:ND2  | 1:D:144:ASN:C    | 2.71                     | 0.49              |
| 1:D:253:ARG:HG2  | 1:D:253:ARG:HH11 | 1.78                     | 0.49              |
| 1:A:286:ARG:NH1  | 1:A:308:GLN:OE1  | 2.45                     | 0.49              |
| 1:B:523:LEU:CD1  | 1:B:523:LEU:C    | 2.85                     | 0.49              |
| 1:A:8:ALA:O      | 1:A:12:LEU:HD22  | 2.13                     | 0.49              |
| 1:C:314:VAL:O    | 1:C:314:VAL:CG2  | 2.61                     | 0.49              |
| 1:C:367:ARG:HG2  | 1:C:367:ARG:HH11 | 1.78                     | 0.49              |
| 1:A:523:LEU:HD13 | 1:A:524:SER:N    | 2.28                     | 0.49              |
| 1:B:93:HIS:O     | 1:B:222:ARG:HD2  | 2.13                     | 0.48              |
| 1:C:52:GLU:CG    | 1:C:81:SER:HB2   | 2.43                     | 0.48              |
| 1:C:217:ASP:OD2  | 1:C:245:MET:HB2  | 2.13                     | 0.48              |
| 1:C:360:LEU:HD12 | 1:C:505:SER:HA   | 1.95                     | 0.48              |
| 1:C:391:ILE:HD13 | 1:C:538:LEU:HD22 | 1.95                     | 0.48              |
| 1:C:523:LEU:HD13 | 1:C:524:SER:N    | 2.28                     | 0.48              |
| 1:A:244:LEU:HD13 | 1:A:405:PRO:HG3  | 1.95                     | 0.48              |
| 1:A:382:ASP:N    | 1:A:413:THR:HG21 | 2.28                     | 0.48              |
| 1:B:142:GLU:OE2  | 1:B:174:LYS:HE2  | 2.12                     | 0.48              |
| 1:B:410:ILE:HG13 | 1:B:440:LEU:HD22 | 1.95                     | 0.48              |
| 1:B:522:ARG:HD3  | 4:B:686:HOH:O    | 2.12                     | 0.48              |
| 1:D:382:ASP:CG   | 1:D:413:THR:HG23 | 2.38                     | 0.48              |
| 1:A:33:GLN:NE2   | 1:A:173:LYS:HE2  | 2.28                     | 0.48              |
| 1:A:467:VAL:HG22 | 3:A:600:TPP:O2B  | 2.12                     | 0.48              |
| 1:B:15:LEU:HD11  | 1:B:97:LEU:HD23  | 1.95                     | 0.48              |
| 1:B:204:ASN:O    | 1:B:208:MET:HG3  | 2.14                     | 0.48              |
| 1:B:382:ASP:HA   | 1:B:413:THR:HG21 | 1.96                     | 0.48              |
| 1:C:282:CYS:HB3  | 1:C:285:THR:CG2  | 2.35                     | 0.48              |
| 1:B:314:VAL:O    | 1:B:314:VAL:CG2  | 2.62                     | 0.48              |
| 1:C:382:ASP:HA   | 1:C:413:THR:HG21 | 1.94                     | 0.48              |
| 1:D:489:ILE:HB   | 1:D:490:PRO:HD3  | 1.96                     | 0.48              |
| 1:A:52:GLU:HG2   | 1:A:81:SER:CB    | 2.44                     | 0.48              |
| 1:D:314:VAL:O    | 1:D:314:VAL:HG23 | 2.12                     | 0.48              |
| 1:D:328:ILE:O    | 1:D:332:VAL:HG23 | 2.14                     | 0.48              |
| 1:B:382:ASP:N    | 1:B:413:THR:HG21 | 2.29                     | 0.48              |
| 1:C:440:LEU:HD12 | 1:C:440:LEU:H    | 1.79                     | 0.48              |
| 1:C:455:PRO:CD   | 1:C:523:LEU:HD22 | 2.42                     | 0.48              |
| 1:D:139:VAL:HG13 | 1:D:166:MET:HE2  | 1.94                     | 0.48              |
| 1:A:93:HIS:O     | 1:A:222:ARG:HD2  | 2.13                     | 0.48              |
| 1:A:217:ASP:OD2  | 1:A:245:MET:HB2  | 2.13                     | 0.48              |
| 1:B:115:HIS:O    | 1:B:116:HIS:HB2  | 2.14                     | 0.48              |
| 1:B:271:LYS:O    | 1:B:275:GLU:HB2  | 2.14                     | 0.48              |
| 1:C:139:VAL:HG13 | 1:C:166:MET:HE2  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:472:HIS:CE1  | 1:D:36:ASP:OD2   | 2.66                     | 0.48              |
| 1:A:153:LEU:HD23 | 1:A:156:MET:CE   | 2.44                     | 0.48              |
| 1:A:374:ARG:HG3  | 1:A:375:PRO:CD   | 2.43                     | 0.48              |
| 1:B:108:GLN:HE22 | 1:B:166:MET:HE3  | 1.78                     | 0.48              |
| 1:C:231:LYS:HE2  | 1:C:235:GLU:OE2  | 2.14                     | 0.48              |
| 1:D:225:LEU:HD13 | 1:D:328:ILE:HD12 | 1.95                     | 0.48              |
| 1:D:504:VAL:HG11 | 1:D:510:LEU:HB2  | 1.96                     | 0.48              |
| 1:C:33:GLN:NE2   | 1:C:173:LYS:HE2  | 2.28                     | 0.47              |
| 1:C:509:GLN:O    | 1:C:513:VAL:HG23 | 2.14                     | 0.47              |
| 1:C:35:LEU:O     | 1:C:38:VAL:HG13  | 2.15                     | 0.47              |
| 1:C:221:LEU:HD21 | 1:C:249:ILE:HG22 | 1.96                     | 0.47              |
| 1:C:400:ASN:C    | 1:C:400:ASN:HD22 | 2.19                     | 0.47              |
| 1:A:153:LEU:HA   | 1:A:156:MET:HE3  | 1.96                     | 0.47              |
| 1:A:83:MET:HE3   | 4:A:652:HOH:O    | 2.15                     | 0.47              |
| 1:C:477:ARG:NH2  | 4:D:613:HOH:O    | 2.47                     | 0.47              |
| 1:D:178:PRO:HA   | 1:D:179:PRO:HD3  | 1.85                     | 0.47              |
| 1:D:430:ILE:HD12 | 1:D:430:ILE:N    | 2.29                     | 0.47              |
| 1:C:328:ILE:O    | 1:C:332:VAL:HG23 | 2.15                     | 0.47              |
| 1:C:435:ASP:O    | 1:C:439:GLN:HG3  | 2.15                     | 0.47              |
| 1:D:381:ALA:C    | 1:D:413:THR:HG21 | 2.39                     | 0.47              |
| 1:A:271:LYS:O    | 1:A:275:GLU:HB2  | 2.14                     | 0.47              |
| 1:A:283:VAL:HG13 | 1:A:307:VAL:CG2  | 2.45                     | 0.47              |
| 1:B:84:ASN:ND2   | 1:B:407:TRP:HE1  | 2.12                     | 0.47              |
| 1:B:275:GLU:OE1  | 1:B:298:GLN:HB2  | 2.14                     | 0.47              |
| 1:B:519:HIS:O    | 1:B:520:HIS:C    | 2.57                     | 0.47              |
| 1:D:29:ASP:C     | 1:D:29:ASP:OD1   | 2.56                     | 0.47              |
| 1:D:244:LEU:HG   | 1:D:391:ILE:HD12 | 1.97                     | 0.47              |
| 1:A:83:MET:HG2   | 4:A:704:HOH:O    | 2.14                     | 0.47              |
| 1:A:144:ASN:ND2  | 1:A:145:ALA:N    | 2.50                     | 0.47              |
| 1:B:456:ILE:HD11 | 1:B:458:LEU:HD11 | 1.95                     | 0.47              |
| 1:C:534:ASP:O    | 1:C:535:ILE:HD12 | 2.14                     | 0.47              |
| 1:D:391:ILE:HG21 | 1:D:538:LEU:CD2  | 2.45                     | 0.47              |
| 1:C:508:GLU:CD   | 1:C:508:GLU:H    | 2.22                     | 0.47              |
| 1:B:178:PRO:HA   | 1:B:179:PRO:HD3  | 1.85                     | 0.47              |
| 1:C:153:LEU:HA   | 1:C:156:MET:HE3  | 1.95                     | 0.47              |
| 1:B:435:ASP:O    | 1:B:439:GLN:HG3  | 2.15                     | 0.47              |
| 1:C:253:ARG:HE   | 1:C:396:PRO:HG3  | 1.80                     | 0.47              |
| 1:D:360:LEU:CD1  | 1:D:504:VAL:HG12 | 2.45                     | 0.47              |
| 1:B:547:GLU:O    | 1:B:547:GLU:HG3  | 2.14                     | 0.46              |
| 1:D:400:ASN:C    | 1:D:400:ASN:HD22 | 2.21                     | 0.46              |
| 1:C:52:GLU:HG2   | 1:C:81:SER:CB    | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:369:LEU:HD21 | 1:C:432:LEU:HD21 | 1.96                     | 0.46              |
| 1:A:410:ILE:HG13 | 1:A:440:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:391:ILE:HG21 | 1:B:538:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:442:ILE:HG23 | 1:B:443:GLN:N    | 2.31                     | 0.46              |
| 1:C:382:ASP:CG   | 1:C:413:THR:HG23 | 2.40                     | 0.46              |
| 1:A:499:SER:HB3  | 1:A:523:LEU:HB3  | 1.96                     | 0.46              |
| 1:C:375:PRO:HD3  | 1:C:396:PRO:CB   | 2.46                     | 0.46              |
| 1:C:381:ALA:C    | 1:C:413:THR:HG21 | 2.40                     | 0.46              |
| 1:C:382:ASP:OD1  | 1:C:410:ILE:HA   | 2.16                     | 0.46              |
| 1:D:35:LEU:HA    | 1:D:38:VAL:CG1   | 2.45                     | 0.46              |
| 1:B:217:ASP:OD2  | 1:B:245:MET:HB2  | 2.15                     | 0.46              |
| 1:C:504:VAL:HG11 | 1:C:510:LEU:N    | 2.30                     | 0.46              |
| 1:C:6:CYS:HB2    | 1:C:174:LYS:O    | 2.16                     | 0.46              |
| 1:D:226:LYS:HE3  | 1:D:248:GLY:O    | 2.16                     | 0.46              |
| 1:D:279:THR:HA   | 1:D:303:GLN:O    | 2.16                     | 0.46              |
| 1:D:442:ILE:HG23 | 1:D:443:GLN:N    | 2.29                     | 0.46              |
| 1:A:280:VAL:HG13 | 1:A:304:THR:HG22 | 1.97                     | 0.46              |
| 1:D:52:GLU:CD    | 1:D:52:GLU:H     | 2.23                     | 0.46              |
| 1:D:219:LEU:HB2  | 1:D:284:GLY:CA   | 2.46                     | 0.46              |
| 1:A:146:CYS:HB2  | 1:C:320:THR:OG1  | 2.16                     | 0.46              |
| 1:B:142:GLU:CD   | 1:B:174:LYS:HE2  | 2.41                     | 0.46              |
| 1:B:340:HIS:O    | 1:B:341:ALA:C    | 2.58                     | 0.46              |
| 1:D:231:LYS:HE2  | 1:D:235:GLU:OE2  | 2.16                     | 0.46              |
| 1:D:237:PRO:HD2  | 4:D:652:HOH:O    | 2.16                     | 0.46              |
| 1:A:204:ASN:O    | 1:A:208:MET:HG3  | 2.16                     | 0.46              |
| 1:C:395:LEU:HA   | 1:C:396:PRO:HD2  | 1.88                     | 0.46              |
| 1:A:382:ASP:HA   | 1:A:413:THR:HG21 | 1.97                     | 0.45              |
| 1:C:374:ARG:HG3  | 1:C:375:PRO:HD2  | 1.98                     | 0.45              |
| 1:C:476:GLN:HA   | 1:C:476:GLN:OE1  | 2.17                     | 0.45              |
| 1:A:362:GLN:NE2  | 1:A:536:PRO:HG3  | 2.32                     | 0.45              |
| 1:D:476:GLN:OE1  | 1:D:476:GLN:HA   | 2.15                     | 0.45              |
| 1:A:391:ILE:HD13 | 1:A:538:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:454:HIS:N    | 1:A:455:PRO:CD   | 2.80                     | 0.45              |
| 1:A:519:HIS:O    | 1:A:520:HIS:C    | 2.60                     | 0.45              |
| 1:C:303:GLN:O    | 1:C:303:GLN:HG2  | 2.17                     | 0.45              |
| 1:D:185:HIS:O    | 1:D:186:LYS:C    | 2.59                     | 0.45              |
| 1:D:288:THR:HG21 | 1:D:406:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:314:VAL:O    | 1:A:314:VAL:CG2  | 2.64                     | 0.45              |
| 1:A:453:GLN:C    | 1:A:455:PRO:HD2  | 2.40                     | 0.45              |
| 1:D:382:ASP:OD1  | 1:D:410:ILE:HA   | 2.17                     | 0.45              |
| 1:A:264:SER:HA   | 1:A:271:LYS:HE2  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:52:GLU:CG    | 1:A:81:SER:HB2   | 2.46                     | 0.45              |
| 1:C:498:GLN:OE1  | 1:C:498:GLN:HA   | 2.15                     | 0.45              |
| 1:D:367:ARG:HH11 | 1:D:367:ARG:HG2  | 1.81                     | 0.45              |
| 1:A:15:LEU:HD11  | 1:A:97:LEU:HD23  | 1.99                     | 0.45              |
| 1:C:249:ILE:HD11 | 1:C:250:PHE:CE2  | 2.52                     | 0.45              |
| 1:D:313:ARG:HD3  | 1:D:318:TRP:CE2  | 2.52                     | 0.45              |
| 1:C:244:LEU:HD13 | 1:C:405:PRO:CG   | 2.46                     | 0.45              |
| 1:C:410:ILE:HG13 | 1:C:440:LEU:HD22 | 1.99                     | 0.45              |
| 1:D:547:GLU:O    | 1:D:547:GLU:HG3  | 2.16                     | 0.45              |
| 1:C:540:GLY:O    | 1:C:543:THR:HG22 | 2.17                     | 0.45              |
| 1:D:207:ALA:HA   | 1:D:338:HIS:CD2  | 2.52                     | 0.45              |
| 1:A:35:LEU:HA    | 1:A:38:VAL:CG1   | 2.46                     | 0.45              |
| 1:A:421:GLN:HG2  | 1:A:429:VAL:HG21 | 1.99                     | 0.45              |
| 1:B:421:GLN:HG2  | 1:B:429:VAL:HG21 | 1.99                     | 0.45              |
| 1:C:440:LEU:HD12 | 1:C:440:LEU:N    | 2.31                     | 0.44              |
| 1:D:440:LEU:N    | 1:D:440:LEU:HD12 | 2.32                     | 0.44              |
| 1:A:112:GLU:HB2  | 1:A:114:LEU:HD13 | 1.99                     | 0.44              |
| 1:B:279:THR:HA   | 1:B:303:GLN:O    | 2.18                     | 0.44              |
| 1:B:381:ALA:C    | 1:B:413:THR:HG21 | 2.43                     | 0.44              |
| 1:C:388:PHE:CD2  | 1:C:539:LEU:HD13 | 2.52                     | 0.44              |
| 1:A:84:ASN:HD21  | 1:A:407:TRP:HE1  | 1.65                     | 0.44              |
| 1:A:435:ASP:O    | 1:A:439:GLN:HG3  | 2.17                     | 0.44              |
| 1:B:360:LEU:HD11 | 1:B:504:VAL:HG12 | 1.99                     | 0.44              |
| 1:C:84:ASN:HD21  | 1:C:407:TRP:HE1  | 1.65                     | 0.44              |
| 1:A:52:GLU:HG3   | 1:A:78:GLY:O     | 2.16                     | 0.44              |
| 1:A:381:ALA:C    | 1:A:413:THR:HG21 | 2.43                     | 0.44              |
| 1:D:253:ARG:NH2  | 1:D:396:PRO:HG3  | 2.29                     | 0.44              |
| 1:C:313:ARG:HB2  | 1:C:318:TRP:CD2  | 2.53                     | 0.44              |
| 1:D:496:ASP:OD1  | 1:D:498:GLN:NE2  | 2.50                     | 0.44              |
| 1:A:523:LEU:CD1  | 1:A:523:LEU:C    | 2.91                     | 0.44              |
| 1:D:204:ASN:O    | 1:D:208:MET:HG3  | 2.17                     | 0.44              |
| 1:D:158:ARG:HD2  | 1:D:159:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:313:ARG:HB2  | 1:A:318:TRP:CD2  | 2.53                     | 0.44              |
| 1:C:523:LEU:CD1  | 1:C:523:LEU:C    | 2.91                     | 0.44              |
| 1:A:177:THR:HG21 | 1:C:194:CYS:HA   | 2.00                     | 0.44              |
| 1:B:35:LEU:HA    | 1:B:38:VAL:HG13  | 2.00                     | 0.44              |
| 1:A:430:ILE:HD12 | 1:A:430:ILE:N    | 2.33                     | 0.43              |
| 1:D:249:ILE:HD11 | 1:D:250:PHE:CE2  | 2.52                     | 0.43              |
| 1:B:244:LEU:HG   | 1:B:391:ILE:HD12 | 2.00                     | 0.43              |
| 1:D:5:TYR:CE1    | 1:D:178:PRO:HG3  | 2.52                     | 0.43              |
| 1:D:382:ASP:HA   | 1:D:413:THR:CG2  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:33:GLN:NE2   | 1:B:173:LYS:HE2  | 2.33                     | 0.43              |
| 1:B:381:ALA:HA   | 1:B:432:LEU:O    | 2.18                     | 0.43              |
| 1:C:29:ASP:HB2   | 4:C:681:HOH:O    | 2.18                     | 0.43              |
| 1:D:35:LEU:HA    | 1:D:38:VAL:HG13  | 2.00                     | 0.43              |
| 1:D:314:VAL:O    | 1:D:314:VAL:CG2  | 2.66                     | 0.43              |
| 1:D:362:GLN:NE2  | 1:D:536:PRO:HG3  | 2.33                     | 0.43              |
| 1:D:435:ASP:O    | 1:D:439:GLN:HG3  | 2.18                     | 0.43              |
| 1:B:249:ILE:HD11 | 1:B:250:PHE:CE2  | 2.53                     | 0.43              |
| 1:B:283:VAL:HG13 | 1:B:307:VAL:CG2  | 2.48                     | 0.43              |
| 1:D:455:PRO:CD   | 1:D:523:LEU:HD13 | 2.46                     | 0.43              |
| 1:D:485:ASN:ND2  | 4:D:629:HOH:O    | 2.46                     | 0.43              |
| 1:A:547:GLU:O    | 1:A:547:GLU:HG3  | 2.18                     | 0.43              |
| 1:D:156:MET:HE2  | 1:D:163:GLY:HA3  | 2.00                     | 0.43              |
| 1:B:374:ARG:HG3  | 1:B:375:PRO:CD   | 2.48                     | 0.43              |
| 1:B:395:LEU:HA   | 1:B:396:PRO:HD3  | 1.76                     | 0.43              |
| 1:A:225:LEU:HD13 | 1:A:328:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:506:GLU:HB2  | 1:A:509:GLN:HG3  | 2.01                     | 0.43              |
| 1:A:540:GLY:O    | 1:A:543:THR:HG22 | 2.19                     | 0.43              |
| 1:B:112:GLU:HB2  | 1:B:114:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:35:LEU:HA    | 1:C:38:VAL:HG13  | 2.01                     | 0.43              |
| 1:C:308:GLN:HB3  | 1:C:309:PRO:CD   | 2.48                     | 0.43              |
| 1:C:442:ILE:HG23 | 1:C:443:GLN:N    | 2.33                     | 0.43              |
| 1:D:33:GLN:NE2   | 1:D:173:LYS:HE2  | 2.33                     | 0.43              |
| 1:B:177:THR:HA   | 1:B:178:PRO:HD3  | 1.91                     | 0.43              |
| 1:B:510:LEU:HD22 | 1:B:514:LEU:HG   | 2.00                     | 0.43              |
| 1:B:313:ARG:HD3  | 1:B:318:TRP:CE2  | 2.53                     | 0.43              |
| 1:B:360:LEU:HD12 | 1:B:505:SER:HA   | 2.01                     | 0.43              |
| 1:C:160:ARG:HD2  | 1:C:222:ARG:O    | 2.18                     | 0.43              |
| 1:C:500:GLU:HB3  | 1:C:502:TRP:CZ3  | 2.54                     | 0.43              |
| 1:D:72:LEU:HD12  | 1:D:99:ILE:O     | 2.19                     | 0.43              |
| 1:D:115:HIS:O    | 1:D:116:HIS:HB2  | 2.19                     | 0.43              |
| 1:A:115:HIS:O    | 1:A:116:HIS:HB2  | 2.18                     | 0.42              |
| 1:A:403:VAL:HG13 | 1:A:405:PRO:HD3  | 1.99                     | 0.42              |
| 1:A:522:ARG:HD3  | 4:A:677:HOH:O    | 2.18                     | 0.42              |
| 1:B:137:GLN:HA   | 1:B:164:TYR:O    | 2.18                     | 0.42              |
| 1:C:308:GLN:HB3  | 1:C:309:PRO:HD2  | 2.01                     | 0.42              |
| 1:D:28:GLY:O     | 1:D:29:ASP:C     | 2.61                     | 0.42              |
| 1:D:134:THR:HG21 | 1:D:164:TYR:HB2  | 2.00                     | 0.42              |
| 1:B:449:LEU:HD12 | 1:B:449:LEU:HA   | 1.92                     | 0.42              |
| 1:B:476:GLN:OE1  | 1:B:476:GLN:HA   | 2.18                     | 0.42              |
| 1:A:382:ASP:OD1  | 1:A:410:ILE:HA   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:489:ILE:HB   | 1:A:490:PRO:HD3  | 2.00                     | 0.42              |
| 1:B:219:LEU:HB2  | 1:B:284:GLY:CA   | 2.49                     | 0.42              |
| 1:B:523:LEU:HD13 | 1:B:523:LEU:C    | 2.43                     | 0.42              |
| 1:C:504:VAL:CG1  | 1:C:505:SER:N    | 2.82                     | 0.42              |
| 1:D:52:GLU:CG    | 1:D:81:SER:HB2   | 2.49                     | 0.42              |
| 1:A:510:LEU:HD22 | 1:A:514:LEU:HG   | 2.00                     | 0.42              |
| 1:C:52:GLU:CD    | 1:C:52:GLU:N     | 2.77                     | 0.42              |
| 1:B:100:VAL:HG11 | 1:B:164:TYR:CZ   | 2.54                     | 0.42              |
| 1:B:144:ASN:HA   | 1:B:147:TYR:CE2  | 2.55                     | 0.42              |
| 1:C:303:GLN:O    | 1:C:303:GLN:CG   | 2.67                     | 0.42              |
| 1:D:384:GLY:HA2  | 1:D:467:VAL:CG1  | 2.42                     | 0.42              |
| 1:D:391:ILE:HD13 | 1:D:538:LEU:HD22 | 2.02                     | 0.42              |
| 1:A:125:HIS:HB2  | 4:A:637:HOH:O    | 2.19                     | 0.42              |
| 1:B:35:LEU:HA    | 1:B:38:VAL:CG1   | 2.50                     | 0.42              |
| 1:A:231:LYS:HE2  | 1:A:235:GLU:OE2  | 2.18                     | 0.42              |
| 1:B:153:LEU:HD23 | 1:B:156:MET:CE   | 2.49                     | 0.42              |
| 1:B:288:THR:HG21 | 1:B:406:LEU:HD13 | 2.01                     | 0.42              |
| 1:C:403:VAL:HG13 | 1:C:405:PRO:HD3  | 2.01                     | 0.42              |
| 1:C:226:LYS:HE3  | 1:C:248:GLY:O    | 2.20                     | 0.42              |
| 1:C:331:LEU:HD12 | 1:C:331:LEU:HA   | 1.85                     | 0.42              |
| 1:D:455:PRO:CG   | 1:D:523:LEU:CD1  | 2.97                     | 0.42              |
| 1:A:134:THR:HG21 | 1:A:164:TYR:HB2  | 2.02                     | 0.42              |
| 1:A:283:VAL:HA   | 1:A:307:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:440:LEU:N    | 1:A:440:LEU:HD12 | 2.35                     | 0.42              |
| 1:B:264:SER:HA   | 1:B:271:LYS:HE2  | 2.02                     | 0.42              |
| 1:B:286:ARG:NH1  | 1:B:308:GLN:OE1  | 2.53                     | 0.42              |
| 1:C:93:HIS:HD2   | 4:C:680:HOH:O    | 2.02                     | 0.42              |
| 1:D:52:GLU:HG2   | 1:D:81:SER:HB2   | 2.02                     | 0.42              |
| 1:A:108:GLN:HE22 | 1:A:166:MET:CE   | 2.33                     | 0.42              |
| 1:A:282:CYS:HB3  | 1:A:285:THR:CG2  | 2.38                     | 0.42              |
| 1:A:384:GLY:HA2  | 1:A:467:VAL:CG1  | 2.44                     | 0.42              |
| 1:B:191:ASP:OD2  | 1:B:193:ALA:HB3  | 2.20                     | 0.42              |
| 1:D:153:LEU:HA   | 1:D:156:MET:HE3  | 2.02                     | 0.42              |
| 1:A:142:GLU:OE2  | 1:A:174:LYS:HE2  | 2.19                     | 0.41              |
| 1:A:144:ASN:HA   | 1:A:147:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:360:LEU:HD11 | 1:A:504:VAL:CG1  | 2.50                     | 0.41              |
| 1:B:235:GLU:O    | 1:B:237:PRO:HD3  | 2.20                     | 0.41              |
| 1:B:384:GLY:HA2  | 1:B:467:VAL:CG1  | 2.48                     | 0.41              |
| 1:C:469:ARG:HH11 | 1:C:532:LYS:HG3  | 1.83                     | 0.41              |
| 1:D:33:GLN:HE21  | 1:D:33:GLN:HB3   | 1.51                     | 0.41              |
| 1:A:244:LEU:HG   | 1:A:391:ILE:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:216:ALA:O    | 1:B:242:THR:HA   | 2.19                     | 0.41              |
| 1:C:253:ARG:CZ   | 1:C:396:PRO:HD3  | 2.50                     | 0.41              |
| 1:A:218:PHE:HB3  | 1:A:245:MET:HB3  | 2.02                     | 0.41              |
| 1:C:455:PRO:HG2  | 1:C:523:LEU:HD22 | 2.02                     | 0.41              |
| 1:C:504:VAL:HG11 | 1:C:510:LEU:HB2  | 2.01                     | 0.41              |
| 1:D:517:VAL:C    | 1:D:519:HIS:H    | 2.28                     | 0.41              |
| 1:A:442:ILE:HG23 | 1:A:443:GLN:N    | 2.34                     | 0.41              |
| 1:A:466:THR:HG22 | 4:A:603:HOH:O    | 2.21                     | 0.41              |
| 1:A:498:GLN:OE1  | 1:A:498:GLN:HA   | 2.19                     | 0.41              |
| 1:D:3:THR:N      | 4:D:657:HOH:O    | 2.53                     | 0.41              |
| 1:A:52:GLU:CD    | 1:A:52:GLU:H     | 2.26                     | 0.41              |
| 1:C:385:THR:HG22 | 1:C:536:PRO:HD3  | 2.02                     | 0.41              |
| 1:D:331:LEU:HD12 | 1:D:331:LEU:HA   | 1.84                     | 0.41              |
| 1:B:231:LYS:HE2  | 1:B:235:GLU:OE2  | 2.20                     | 0.41              |
| 1:D:140:LEU:HD23 | 1:D:167:LEU:HD13 | 2.01                     | 0.41              |
| 1:D:275:GLU:OE1  | 1:D:298:GLN:HB2  | 2.21                     | 0.41              |
| 1:A:144:ASN:O    | 1:A:145:ALA:C    | 2.63                     | 0.41              |
| 1:B:221:LEU:HD21 | 1:B:249:ILE:HG22 | 2.02                     | 0.41              |
| 1:C:52:GLU:HG3   | 1:C:78:GLY:O     | 2.21                     | 0.41              |
| 1:C:93:HIS:CD2   | 4:C:680:HOH:O    | 2.73                     | 0.41              |
| 1:D:35:LEU:HA    | 1:D:35:LEU:HD12  | 1.89                     | 0.41              |
| 1:D:547:GLU:HA   | 1:D:550:ASN:HD22 | 1.85                     | 0.41              |
| 1:A:74:THR:HG22  | 4:A:607:HOH:O    | 2.19                     | 0.41              |
| 1:A:395:LEU:HA   | 1:A:396:PRO:HD3  | 1.75                     | 0.41              |
| 1:B:64:ARG:HD3   | 4:B:681:HOH:O    | 2.20                     | 0.41              |
| 1:B:185:HIS:O    | 1:B:186:LYS:C    | 2.63                     | 0.41              |
| 1:C:410:ILE:HG13 | 1:C:410:ILE:O    | 2.19                     | 0.41              |
| 1:D:14:ARG:HB3   | 1:D:153:LEU:CD1  | 2.51                     | 0.41              |
| 1:D:455:PRO:O    | 1:D:523:LEU:HD12 | 2.21                     | 0.41              |
| 1:A:543:THR:CG2  | 1:A:544:LYS:N    | 2.84                     | 0.41              |
| 1:B:134:THR:HG21 | 1:B:164:TYR:HB2  | 2.02                     | 0.41              |
| 1:C:199:ARG:HG3  | 1:C:330:THR:HG23 | 2.03                     | 0.41              |
| 1:C:455:PRO:CG   | 1:C:523:LEU:HD22 | 2.51                     | 0.41              |
| 1:D:219:LEU:HB2  | 1:D:284:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:249:ILE:HD11 | 1:A:250:PHE:CE2  | 2.56                     | 0.40              |
| 1:B:140:LEU:HD23 | 1:B:167:LEU:HD13 | 2.03                     | 0.40              |
| 1:B:498:GLN:HA   | 1:B:498:GLN:OE1  | 2.20                     | 0.40              |
| 1:C:28:GLY:O     | 1:C:29:ASP:C     | 2.64                     | 0.40              |
| 1:C:159:GLU:O    | 1:C:160:ARG:HB2  | 2.21                     | 0.40              |
| 1:D:159:GLU:O    | 1:D:160:ARG:HB2  | 2.20                     | 0.40              |
| 1:D:166:MET:O    | 1:D:168:PRO:HD3  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:360:LEU:CD1  | 1:A:504:VAL:HG12 | 2.52                     | 0.40              |
| 1:C:520:HIS:O    | 1:C:520:HIS:CD2  | 2.74                     | 0.40              |
| 1:C:547:GLU:O    | 1:C:547:GLU:HG3  | 2.19                     | 0.40              |
| 1:D:403:VAL:C    | 1:D:405:PRO:HD3  | 2.45                     | 0.40              |
| 1:B:218:PHE:HB3  | 1:B:245:MET:HB3  | 2.04                     | 0.40              |
| 1:B:485:ASN:ND2  | 4:B:606:HOH:O    | 2.53                     | 0.40              |
| 1:B:540:GLY:O    | 1:B:543:THR:HG22 | 2.22                     | 0.40              |
| 1:C:35:LEU:HA    | 1:C:38:VAL:CG1   | 2.52                     | 0.40              |
| 1:C:62:TYR:CZ    | 1:C:66:LYS:HD3   | 2.56                     | 0.40              |
| 1:C:403:VAL:C    | 1:C:405:PRO:HD3  | 2.47                     | 0.40              |
| 1:D:209:SER:HB2  | 1:D:279:THR:CG2  | 2.51                     | 0.40              |
| 1:D:440:LEU:HD12 | 1:D:440:LEU:H    | 1.87                     | 0.40              |
| 1:C:140:LEU:HD23 | 1:C:167:LEU:HD13 | 2.04                     | 0.40              |
| 1:C:297:HIS:H    | 1:C:297:HIS:HD1  | 1.69                     | 0.40              |
| 1:D:282:CYS:CB   | 1:D:285:THR:HG21 | 2.35                     | 0.40              |
| 1:A:30:TYR:CZ    | 1:A:103:PRO:HG3  | 2.57                     | 0.40              |
| 1:A:219:LEU:HB2  | 1:A:284:GLY:CA   | 2.52                     | 0.40              |
| 1:A:233:VAL:HG21 | 1:A:240:HIS:ND1  | 2.36                     | 0.40              |
| 1:B:328:ILE:O    | 1:B:332:VAL:HG23 | 2.22                     | 0.40              |
| 1:B:382:ASP:HB3  | 4:B:616:HOH:O    | 2.22                     | 0.40              |
| 1:B:391:ILE:HG21 | 1:B:538:LEU:CD2  | 2.51                     | 0.40              |
| 1:C:113:LEU:HA   | 4:C:650:HOH:O    | 2.20                     | 0.40              |
| 1:C:185:HIS:O    | 1:C:186:LYS:C    | 2.65                     | 0.40              |
| 1:C:430:ILE:N    | 1:C:430:ILE:HD12 | 2.35                     | 0.40              |
| 1:C:450:ARG:NH1  | 4:C:616:HOH:O    | 2.52                     | 0.40              |
| 1:D:52:GLU:HG3   | 1:D:78:GLY:O     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | A     | 531/552 (96%)   | 511 (96%)  | 17 (3%) | 3 (1%)   | 21          | 34 |
| 1   | B     | 531/552 (96%)   | 507 (96%)  | 21 (4%) | 3 (1%)   | 21          | 34 |
| 1   | C     | 531/552 (96%)   | 506 (95%)  | 22 (4%) | 3 (1%)   | 21          | 34 |
| 1   | D     | 531/552 (96%)   | 505 (95%)  | 23 (4%) | 3 (1%)   | 21          | 34 |
| All | All   | 2124/2208 (96%) | 2029 (96%) | 83 (4%) | 12 (1%)  | 21          | 34 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | ALA  |
| 1   | B     | 145 | ALA  |
| 1   | C     | 145 | ALA  |
| 1   | D     | 145 | ALA  |
| 1   | D     | 518 | ALA  |
| 1   | A     | 218 | PHE  |
| 1   | D     | 186 | LYS  |
| 1   | B     | 186 | LYS  |
| 1   | C     | 186 | LYS  |
| 1   | A     | 186 | LYS  |
| 1   | B     | 520 | HIS  |
| 1   | C     | 520 | HIS  |

### 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     | 426/439 (97%)   | 380 (89%)  | 46 (11%)  | 6           | 9  |
| 1   | B     | 426/439 (97%)   | 386 (91%)  | 40 (9%)   | 8           | 13 |
| 1   | C     | 426/439 (97%)   | 381 (89%)  | 45 (11%)  | 6           | 10 |
| 1   | D     | 426/439 (97%)   | 392 (92%)  | 34 (8%)   | 11          | 19 |
| All | All   | 1704/1756 (97%) | 1539 (90%) | 165 (10%) | 8           | 12 |

All (165) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | LEU  |
| 1   | A     | 26  | VAL  |
| 1   | A     | 32  | LEU  |
| 1   | A     | 33  | GLN  |
| 1   | A     | 35  | LEU  |
| 1   | A     | 38  | VAL  |
| 1   | A     | 52  | GLU  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 83  | MET  |
| 1   | A     | 100 | VAL  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 118 | LEU  |
| 1   | A     | 130 | SER  |
| 1   | A     | 140 | LEU  |
| 1   | A     | 144 | ASN  |
| 1   | A     | 152 | VAL  |
| 1   | A     | 157 | LEU  |
| 1   | A     | 177 | THR  |
| 1   | A     | 206 | LEU  |
| 1   | A     | 214 | LEU  |
| 1   | A     | 220 | VAL  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 272 | GLU  |
| 1   | A     | 278 | ASP  |
| 1   | A     | 280 | VAL  |
| 1   | A     | 307 | VAL  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 356 | PRO  |
| 1   | A     | 367 | ARG  |
| 1   | A     | 374 | ARG  |
| 1   | A     | 383 | GLN  |
| 1   | A     | 399 | VAL  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 455 | PRO  |
| 1   | A     | 456 | ILE  |
| 1   | A     | 467 | VAL  |
| 1   | A     | 498 | GLN  |
| 1   | A     | 503 | ARG  |
| 1   | A     | 504 | VAL  |
| 1   | A     | 510 | LEU  |
| 1   | A     | 513 | VAL  |
| 1   | A     | 515 | GLU  |
| 1   | A     | 523 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 535 | ILE  |
| 1   | A     | 543 | THR  |
| 1   | A     | 547 | GLU  |
| 1   | B     | 12  | LEU  |
| 1   | B     | 26  | VAL  |
| 1   | B     | 32  | LEU  |
| 1   | B     | 33  | GLN  |
| 1   | B     | 35  | LEU  |
| 1   | B     | 38  | VAL  |
| 1   | B     | 53  | LEU  |
| 1   | B     | 72  | LEU  |
| 1   | B     | 100 | VAL  |
| 1   | B     | 114 | LEU  |
| 1   | B     | 118 | LEU  |
| 1   | B     | 130 | SER  |
| 1   | B     | 140 | LEU  |
| 1   | B     | 144 | ASN  |
| 1   | B     | 157 | LEU  |
| 1   | B     | 177 | THR  |
| 1   | B     | 206 | LEU  |
| 1   | B     | 214 | LEU  |
| 1   | B     | 220 | VAL  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 278 | ASP  |
| 1   | B     | 280 | VAL  |
| 1   | B     | 307 | VAL  |
| 1   | B     | 331 | LEU  |
| 1   | B     | 367 | ARG  |
| 1   | B     | 374 | ARG  |
| 1   | B     | 383 | GLN  |
| 1   | B     | 399 | VAL  |
| 1   | B     | 444 | GLU  |
| 1   | B     | 449 | LEU  |
| 1   | B     | 455 | PRO  |
| 1   | B     | 456 | ILE  |
| 1   | B     | 467 | VAL  |
| 1   | B     | 498 | GLN  |
| 1   | B     | 500 | GLU  |
| 1   | B     | 510 | LEU  |
| 1   | B     | 523 | LEU  |
| 1   | B     | 535 | ILE  |
| 1   | B     | 543 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 547 | GLU  |
| 1   | C     | 12  | LEU  |
| 1   | C     | 26  | VAL  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 33  | GLN  |
| 1   | C     | 35  | LEU  |
| 1   | C     | 38  | VAL  |
| 1   | C     | 52  | GLU  |
| 1   | C     | 53  | LEU  |
| 1   | C     | 72  | LEU  |
| 1   | C     | 83  | MET  |
| 1   | C     | 100 | VAL  |
| 1   | C     | 114 | LEU  |
| 1   | C     | 118 | LEU  |
| 1   | C     | 130 | SER  |
| 1   | C     | 140 | LEU  |
| 1   | C     | 144 | ASN  |
| 1   | C     | 157 | LEU  |
| 1   | C     | 177 | THR  |
| 1   | C     | 205 | LYS  |
| 1   | C     | 206 | LEU  |
| 1   | C     | 208 | MET  |
| 1   | C     | 214 | LEU  |
| 1   | C     | 220 | VAL  |
| 1   | C     | 244 | LEU  |
| 1   | C     | 278 | ASP  |
| 1   | C     | 280 | VAL  |
| 1   | C     | 307 | VAL  |
| 1   | C     | 331 | LEU  |
| 1   | C     | 367 | ARG  |
| 1   | C     | 374 | ARG  |
| 1   | C     | 383 | GLN  |
| 1   | C     | 396 | PRO  |
| 1   | C     | 399 | VAL  |
| 1   | C     | 449 | LEU  |
| 1   | C     | 456 | ILE  |
| 1   | C     | 467 | VAL  |
| 1   | C     | 498 | GLN  |
| 1   | C     | 500 | GLU  |
| 1   | C     | 503 | ARG  |
| 1   | C     | 508 | GLU  |
| 1   | C     | 510 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 523 | LEU  |
| 1   | C     | 535 | ILE  |
| 1   | C     | 543 | THR  |
| 1   | C     | 547 | GLU  |
| 1   | D     | 12  | LEU  |
| 1   | D     | 26  | VAL  |
| 1   | D     | 32  | LEU  |
| 1   | D     | 33  | GLN  |
| 1   | D     | 35  | LEU  |
| 1   | D     | 38  | VAL  |
| 1   | D     | 52  | GLU  |
| 1   | D     | 53  | LEU  |
| 1   | D     | 100 | VAL  |
| 1   | D     | 114 | LEU  |
| 1   | D     | 118 | LEU  |
| 1   | D     | 140 | LEU  |
| 1   | D     | 144 | ASN  |
| 1   | D     | 157 | LEU  |
| 1   | D     | 177 | THR  |
| 1   | D     | 214 | LEU  |
| 1   | D     | 220 | VAL  |
| 1   | D     | 244 | LEU  |
| 1   | D     | 278 | ASP  |
| 1   | D     | 280 | VAL  |
| 1   | D     | 307 | VAL  |
| 1   | D     | 331 | LEU  |
| 1   | D     | 374 | ARG  |
| 1   | D     | 383 | GLN  |
| 1   | D     | 399 | VAL  |
| 1   | D     | 444 | GLU  |
| 1   | D     | 449 | LEU  |
| 1   | D     | 456 | ILE  |
| 1   | D     | 467 | VAL  |
| 1   | D     | 508 | GLU  |
| 1   | D     | 510 | LEU  |
| 1   | D     | 535 | ILE  |
| 1   | D     | 543 | THR  |
| 1   | D     | 547 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | GLN  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 84  | ASN  |
| 1   | A     | 115 | HIS  |
| 1   | A     | 125 | HIS  |
| 1   | A     | 137 | GLN  |
| 1   | A     | 144 | ASN  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 223 | HIS  |
| 1   | A     | 310 | HIS  |
| 1   | A     | 325 | ASN  |
| 1   | A     | 362 | GLN  |
| 1   | A     | 383 | GLN  |
| 1   | A     | 400 | ASN  |
| 1   | A     | 472 | HIS  |
| 1   | A     | 485 | ASN  |
| 1   | A     | 520 | HIS  |
| 1   | A     | 550 | ASN  |
| 1   | B     | 33  | GLN  |
| 1   | B     | 54  | ASN  |
| 1   | B     | 84  | ASN  |
| 1   | B     | 108 | GLN  |
| 1   | B     | 115 | HIS  |
| 1   | B     | 125 | HIS  |
| 1   | B     | 137 | GLN  |
| 1   | B     | 144 | ASN  |
| 1   | B     | 181 | ASN  |
| 1   | B     | 223 | HIS  |
| 1   | B     | 362 | GLN  |
| 1   | B     | 383 | GLN  |
| 1   | B     | 400 | ASN  |
| 1   | B     | 472 | HIS  |
| 1   | B     | 485 | ASN  |
| 1   | C     | 33  | GLN  |
| 1   | C     | 54  | ASN  |
| 1   | C     | 84  | ASN  |
| 1   | C     | 93  | HIS  |
| 1   | C     | 109 | GLN  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 125 | HIS  |
| 1   | C     | 137 | GLN  |
| 1   | C     | 144 | ASN  |
| 1   | C     | 181 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 223 | HIS  |
| 1   | C     | 310 | HIS  |
| 1   | C     | 340 | HIS  |
| 1   | C     | 362 | GLN  |
| 1   | C     | 400 | ASN  |
| 1   | C     | 472 | HIS  |
| 1   | C     | 485 | ASN  |
| 1   | C     | 488 | HIS  |
| 1   | C     | 520 | HIS  |
| 1   | C     | 550 | ASN  |
| 1   | D     | 33  | GLN  |
| 1   | D     | 54  | ASN  |
| 1   | D     | 84  | ASN  |
| 1   | D     | 115 | HIS  |
| 1   | D     | 125 | HIS  |
| 1   | D     | 137 | GLN  |
| 1   | D     | 144 | ASN  |
| 1   | D     | 181 | ASN  |
| 1   | D     | 223 | HIS  |
| 1   | D     | 325 | ASN  |
| 1   | D     | 337 | GLN  |
| 1   | D     | 338 | HIS  |
| 1   | D     | 340 | HIS  |
| 1   | D     | 362 | GLN  |
| 1   | D     | 400 | ASN  |
| 1   | D     | 472 | HIS  |
| 1   | D     | 485 | ASN  |
| 1   | D     | 498 | GLN  |
| 1   | D     | 550 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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 |
| 3   | TPP  | A     | 600 | 2    | 26,27,27     | 3.04 | 8 (30%)  | 38,40,40    | 1.84 | 11 (28%) |
| 3   | TPP  | B     | 600 | 2    | 26,27,27     | 2.97 | 8 (30%)  | 38,40,40    | 1.79 | 10 (26%) |
| 3   | TPP  | C     | 600 | 2    | 26,27,27     | 2.97 | 7 (26%)  | 38,40,40    | 1.80 | 9 (23%)  |
| 3   | TPP  | D     | 600 | 2    | 26,27,27     | 2.89 | 6 (23%)  | 38,40,40    | 1.75 | 9 (23%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | TPP  | A     | 600 | 2    | -       | 7/17/17/17 | 0/2/2/2 |
| 3   | TPP  | B     | 600 | 2    | -       | 7/17/17/17 | 0/2/2/2 |
| 3   | TPP  | C     | 600 | 2    | -       | 4/17/17/17 | 0/2/2/2 |
| 3   | TPP  | D     | 600 | 2    | -       | 4/17/17/17 | 0/2/2/2 |

All (29) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | A     | 600 | TPP  | C5'-C4' | 9.85 | 1.59        | 1.42     |
| 3   | C     | 600 | TPP  | C5'-C4' | 9.79 | 1.59        | 1.42     |
| 3   | B     | 600 | TPP  | C5'-C4' | 9.28 | 1.58        | 1.42     |
| 3   | D     | 600 | TPP  | C5'-C4' | 9.10 | 1.57        | 1.42     |
| 3   | B     | 600 | TPP  | C6'-C5' | 8.44 | 1.54        | 1.37     |
| 3   | D     | 600 | TPP  | C6'-C5' | 8.33 | 1.54        | 1.37     |
| 3   | C     | 600 | TPP  | C6'-C5' | 8.28 | 1.54        | 1.37     |
| 3   | A     | 600 | TPP  | C6'-C5' | 8.06 | 1.53        | 1.37     |
| 3   | A     | 600 | TPP  | C4'-N3' | 4.87 | 1.41        | 1.35     |
| 3   | B     | 600 | TPP  | C4'-N3' | 4.51 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | D     | 600 | TPP  | C4'-N3' | 4.24  | 1.40        | 1.35     |
| 3   | C     | 600 | TPP  | C4'-N3' | 4.04  | 1.40        | 1.35     |
| 3   | C     | 600 | TPP  | C7'-N3  | 3.49  | 1.56        | 1.48     |
| 3   | B     | 600 | TPP  | C7'-N3  | 3.24  | 1.55        | 1.48     |
| 3   | A     | 600 | TPP  | C7'-N3  | 3.04  | 1.55        | 1.48     |
| 3   | D     | 600 | TPP  | C7'-N3  | 2.90  | 1.54        | 1.48     |
| 3   | A     | 600 | TPP  | C4-N3   | -2.57 | 1.34        | 1.39     |
| 3   | D     | 600 | TPP  | C4-N3   | -2.53 | 1.34        | 1.39     |
| 3   | A     | 600 | TPP  | C6'-N1' | 2.50  | 1.39        | 1.34     |
| 3   | B     | 600 | TPP  | PB-O2B  | -2.48 | 1.45        | 1.54     |
| 3   | C     | 600 | TPP  | C6'-N1' | 2.47  | 1.39        | 1.34     |
| 3   | B     | 600 | TPP  | C6'-N1' | 2.42  | 1.39        | 1.34     |
| 3   | A     | 600 | TPP  | PA-O2A  | -2.34 | 1.44        | 1.55     |
| 3   | C     | 600 | TPP  | C4-N3   | -2.32 | 1.35        | 1.39     |
| 3   | C     | 600 | TPP  | PA-O2A  | -2.28 | 1.44        | 1.55     |
| 3   | B     | 600 | TPP  | PA-O2A  | -2.26 | 1.44        | 1.55     |
| 3   | D     | 600 | TPP  | C6'-N1' | 2.25  | 1.39        | 1.34     |
| 3   | A     | 600 | TPP  | PB-O2B  | -2.10 | 1.47        | 1.54     |
| 3   | B     | 600 | TPP  | C2'-N1' | 2.09  | 1.37        | 1.34     |

All (39) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 600 | TPP  | C6'-N1'-C2' | 4.06  | 122.74      | 116.07   |
| 3   | C     | 600 | TPP  | O2A-PA-O3A  | -3.81 | 96.97       | 107.27   |
| 3   | C     | 600 | TPP  | C6'-N1'-C2' | 3.70  | 122.15      | 116.07   |
| 3   | B     | 600 | TPP  | C6'-N1'-C2' | 3.65  | 122.06      | 116.07   |
| 3   | B     | 600 | TPP  | O2A-PA-O3A  | -3.64 | 97.44       | 107.27   |
| 3   | D     | 600 | TPP  | C6'-N1'-C2' | 3.61  | 122.00      | 116.07   |
| 3   | A     | 600 | TPP  | O2A-PA-O3A  | -3.58 | 97.61       | 107.27   |
| 3   | B     | 600 | TPP  | O3A-PB-O1B  | -3.40 | 93.14       | 111.04   |
| 3   | A     | 600 | TPP  | C6'-C5'-C4' | -3.40 | 111.37      | 115.55   |
| 3   | D     | 600 | TPP  | C6'-C5'-C4' | -3.40 | 111.37      | 115.55   |
| 3   | A     | 600 | TPP  | O3A-PB-O1B  | -3.35 | 93.39       | 111.04   |
| 3   | B     | 600 | TPP  | C6'-C5'-C4' | -3.33 | 111.46      | 115.55   |
| 3   | D     | 600 | TPP  | O3A-PB-O1B  | -3.29 | 93.71       | 111.04   |
| 3   | D     | 600 | TPP  | O2A-PA-O3A  | -3.23 | 98.53       | 107.27   |
| 3   | C     | 600 | TPP  | C6'-C5'-C4' | -3.19 | 111.62      | 115.55   |
| 3   | C     | 600 | TPP  | O3A-PB-O1B  | -3.17 | 94.35       | 111.04   |
| 3   | C     | 600 | TPP  | C2'-N3'-C4' | 3.01  | 122.73      | 118.10   |
| 3   | D     | 600 | TPP  | C2'-N3'-C4' | 2.98  | 122.68      | 118.10   |
| 3   | A     | 600 | TPP  | C2-S1-C5    | -2.96 | 89.26       | 91.22    |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 600 | TPP  | C2'-N3'-C4' | 2.91  | 122.57      | 118.10   |
| 3   | B     | 600 | TPP  | C2'-N3'-C4' | 2.90  | 122.55      | 118.10   |
| 3   | D     | 600 | TPP  | C2-S1-C5    | -2.82 | 89.35       | 91.22    |
| 3   | C     | 600 | TPP  | O2A-PA-O7   | -2.68 | 95.43       | 107.57   |
| 3   | B     | 600 | TPP  | C2-S1-C5    | -2.65 | 89.46       | 91.22    |
| 3   | C     | 600 | TPP  | O3B-PB-O1B  | 2.63  | 121.07      | 110.83   |
| 3   | B     | 600 | TPP  | O3B-PB-O1B  | 2.58  | 120.88      | 110.83   |
| 3   | C     | 600 | TPP  | C2-S1-C5    | -2.54 | 89.53       | 91.22    |
| 3   | B     | 600 | TPP  | O2A-PA-O7   | -2.52 | 96.12       | 107.57   |
| 3   | D     | 600 | TPP  | O3B-PB-O1B  | 2.51  | 120.60      | 110.83   |
| 3   | A     | 600 | TPP  | O3B-PB-O1B  | 2.39  | 120.17      | 110.83   |
| 3   | D     | 600 | TPP  | O2A-PA-O7   | -2.37 | 96.81       | 107.57   |
| 3   | A     | 600 | TPP  | O2A-PA-O7   | -2.35 | 96.93       | 107.57   |
| 3   | D     | 600 | TPP  | O7-PA-O1A   | 2.24  | 117.80      | 108.94   |
| 3   | A     | 600 | TPP  | O7-PA-O1A   | 2.23  | 117.75      | 108.94   |
| 3   | C     | 600 | TPP  | O7-PA-O1A   | 2.16  | 117.51      | 108.94   |
| 3   | B     | 600 | TPP  | O7-PA-O1A   | 2.16  | 117.49      | 108.94   |
| 3   | A     | 600 | TPP  | C2-N3-C4    | -2.05 | 111.29      | 114.06   |
| 3   | A     | 600 | TPP  | C7'-C5'-C4' | 2.05  | 126.10      | 122.36   |
| 3   | B     | 600 | TPP  | C2-N3-C4    | -2.00 | 111.35      | 114.06   |

There are no chirality outliers.

All (22) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | A     | 600 | TPP  | PA-O3A-PB-O2B |
| 3   | A     | 600 | TPP  | PA-O3A-PB-O3B |
| 3   | B     | 600 | TPP  | C7-O7-PA-O1A  |
| 3   | B     | 600 | TPP  | PA-O3A-PB-O3B |
| 3   | C     | 600 | TPP  | C7-O7-PA-O1A  |
| 3   | D     | 600 | TPP  | C7-O7-PA-O1A  |
| 3   | A     | 600 | TPP  | PB-O3A-PA-O1A |
| 3   | B     | 600 | TPP  | PB-O3A-PA-O1A |
| 3   | B     | 600 | TPP  | PA-O3A-PB-O2B |
| 3   | B     | 600 | TPP  | C5-C6-C7-O7   |
| 3   | C     | 600 | TPP  | C5-C6-C7-O7   |
| 3   | D     | 600 | TPP  | C5-C6-C7-O7   |
| 3   | D     | 600 | TPP  | PB-O3A-PA-O2A |
| 3   | A     | 600 | TPP  | C7-O7-PA-O1A  |
| 3   | B     | 600 | TPP  | PB-O3A-PA-O2A |
| 3   | C     | 600 | TPP  | PB-O3A-PA-O2A |
| 3   | A     | 600 | TPP  | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | A     | 600 | TPP  | PA-O3A-PB-O1B |
| 3   | A     | 600 | TPP  | C5-C6-C7-O7   |
| 3   | D     | 600 | TPP  | PB-O3A-PA-O1A |
| 3   | B     | 600 | TPP  | PA-O3A-PB-O1B |
| 3   | C     | 600 | TPP  | PB-O3A-PA-O1A |

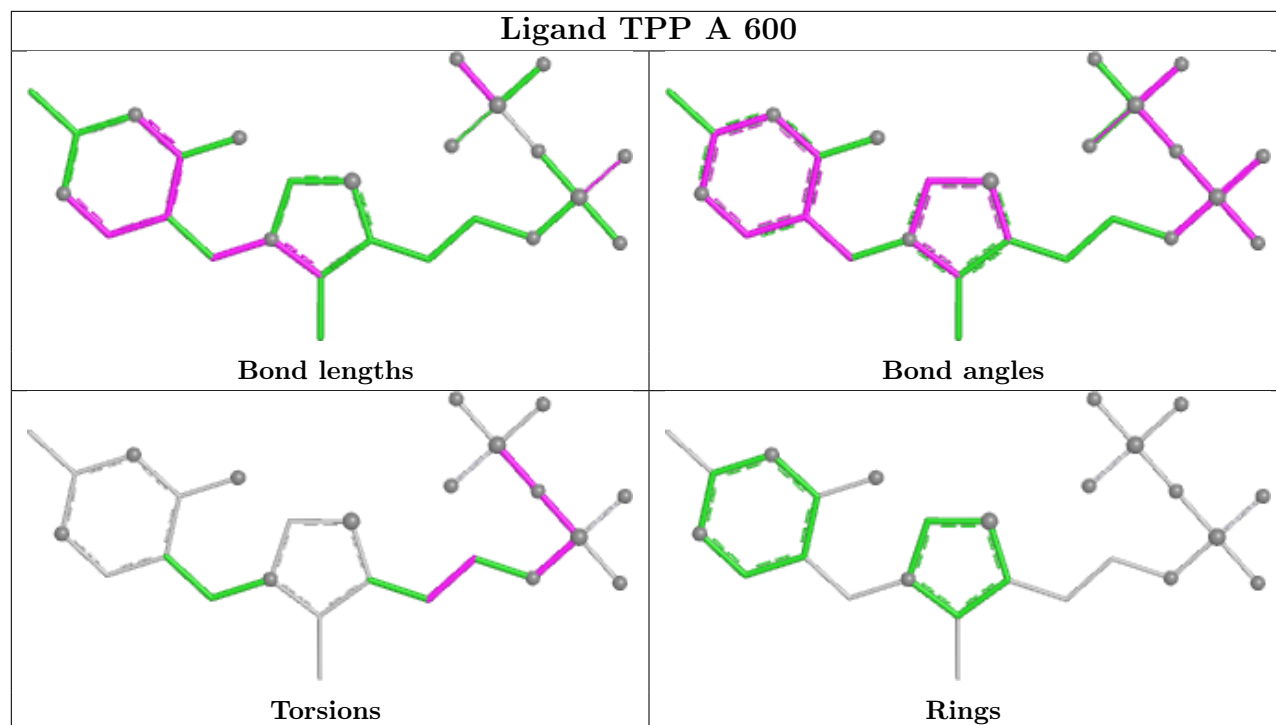
There are no ring outliers.

4 monomers are involved in 5 short contacts:

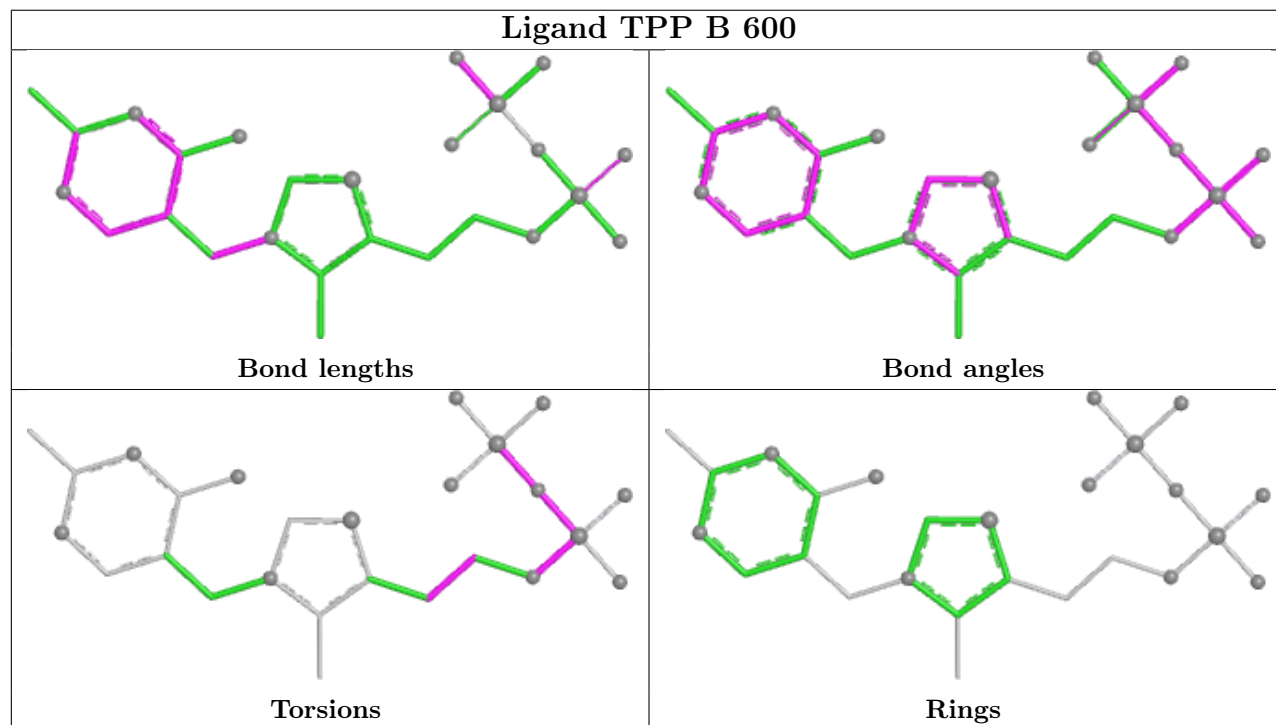
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 600 | TPP  | 2       | 0            |
| 3   | B     | 600 | TPP  | 1       | 0            |
| 3   | C     | 600 | TPP  | 1       | 0            |
| 3   | D     | 600 | TPP  | 1       | 0            |

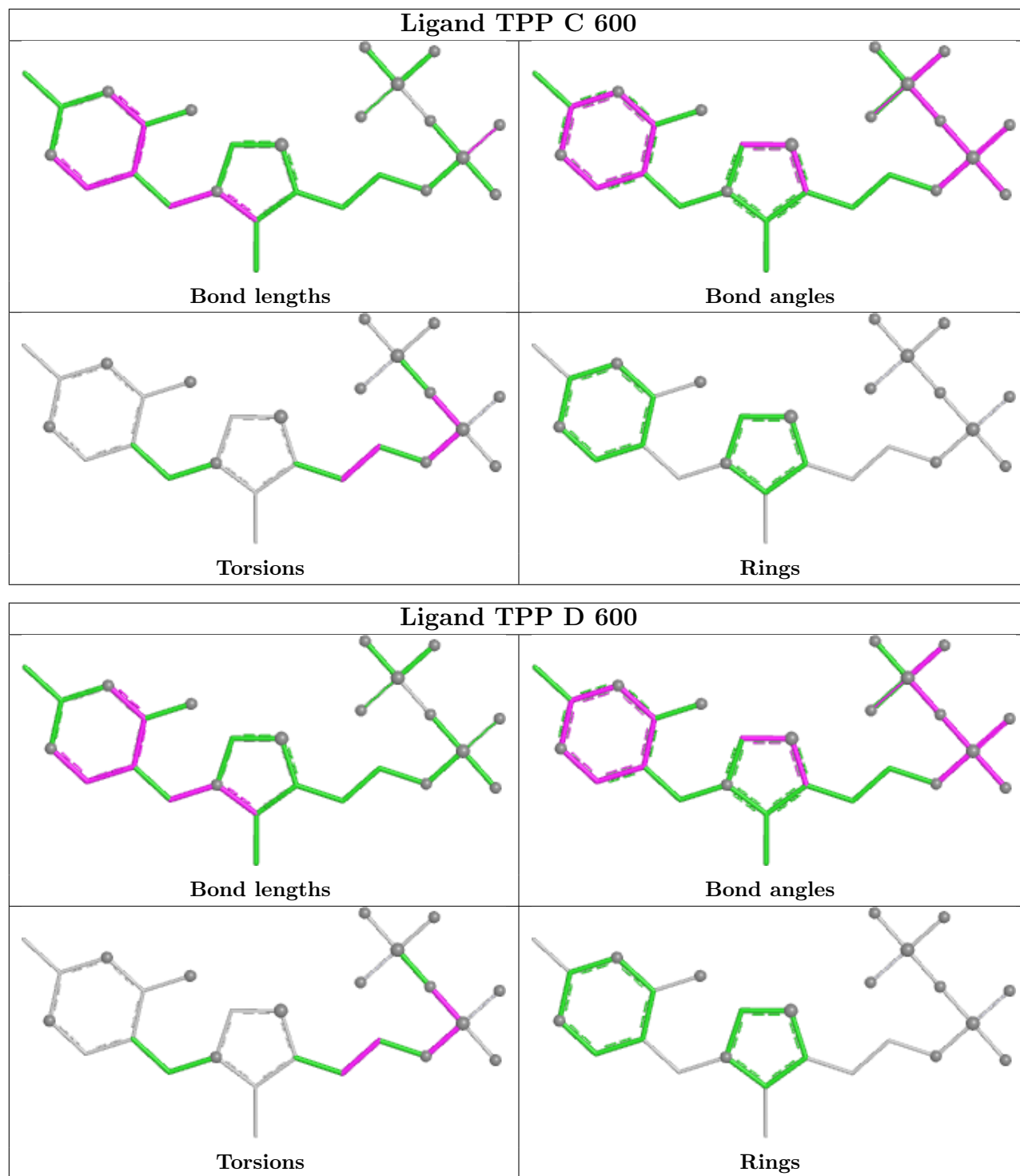
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 TPP A 600



## Ligand TPP B 600





## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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     | 535/552 (96%)   | -0.06  | 10 (1%) 66 61 | 14, 30, 54, 82        | 0     |
| 1   | B     | 535/552 (96%)   | -0.02  | 9 (1%) 69 64  | 16, 30, 54, 87        | 0     |
| 1   | C     | 535/552 (96%)   | 0.08   | 15 (2%) 55 48 | 16, 31, 55, 84        | 0     |
| 1   | D     | 535/552 (96%)   | 0.11   | 8 (1%) 72 67  | 17, 33, 58, 84        | 0     |
| All | All   | 2140/2208 (96%) | 0.03   | 42 (1%) 65 59 | 14, 31, 57, 87        | 0     |

All (42) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 341 | ALA  | 5.5  |
| 1   | C     | 208 | MET  | 5.0  |
| 1   | D     | 356 | PRO  | 4.2  |
| 1   | C     | 207 | ALA  | 4.2  |
| 1   | B     | 356 | PRO  | 4.1  |
| 1   | C     | 341 | ALA  | 3.8  |
| 1   | A     | 356 | PRO  | 3.6  |
| 1   | D     | 185 | HIS  | 3.4  |
| 1   | A     | 340 | HIS  | 3.4  |
| 1   | C     | 356 | PRO  | 3.4  |
| 1   | C     | 339 | VAL  | 3.3  |
| 1   | C     | 3   | THR  | 3.3  |
| 1   | A     | 341 | ALA  | 3.2  |
| 1   | B     | 209 | SER  | 3.0  |
| 1   | B     | 340 | HIS  | 3.0  |
| 1   | B     | 187 | GLN  | 3.0  |
| 1   | B     | 339 | VAL  | 3.0  |
| 1   | C     | 187 | GLN  | 2.9  |
| 1   | D     | 184 | THR  | 2.9  |
| 1   | D     | 183 | LEU  | 2.9  |
| 1   | C     | 185 | HIS  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 4   | PRO  | 2.8  |
| 1   | C     | 340 | HIS  | 2.8  |
| 1   | D     | 187 | GLN  | 2.7  |
| 1   | A     | 185 | HIS  | 2.7  |
| 1   | A     | 187 | GLN  | 2.7  |
| 1   | B     | 185 | HIS  | 2.6  |
| 1   | D     | 186 | LYS  | 2.6  |
| 1   | A     | 542 | LEU  | 2.6  |
| 1   | A     | 186 | LYS  | 2.6  |
| 1   | A     | 546 | LEU  | 2.4  |
| 1   | C     | 398 | ASP  | 2.4  |
| 1   | D     | 339 | VAL  | 2.4  |
| 1   | C     | 550 | ASN  | 2.3  |
| 1   | A     | 3   | THR  | 2.2  |
| 1   | C     | 210 | LYS  | 2.2  |
| 1   | D     | 188 | ALA  | 2.2  |
| 1   | A     | 543 | THR  | 2.2  |
| 1   | C     | 278 | ASP  | 2.2  |
| 1   | B     | 329 | GLU  | 2.0  |
| 1   | C     | 189 | HIS  | 2.0  |
| 1   | B     | 504 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MG   | C     | 601 | 1/1   | 0.82 | 0.11 | 29,29,29,29                 | 0     |
| 2   | MG   | A     | 601 | 1/1   | 0.93 | 0.10 | 23,23,23,23                 | 0     |

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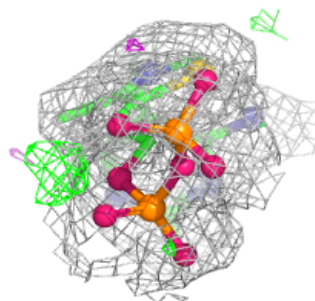
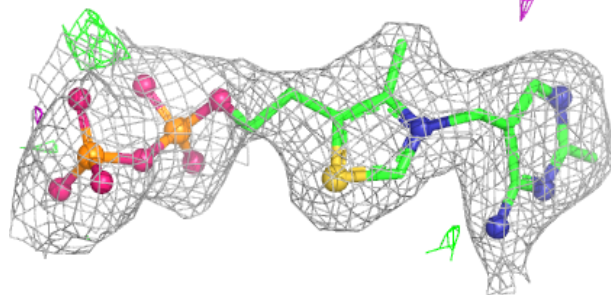
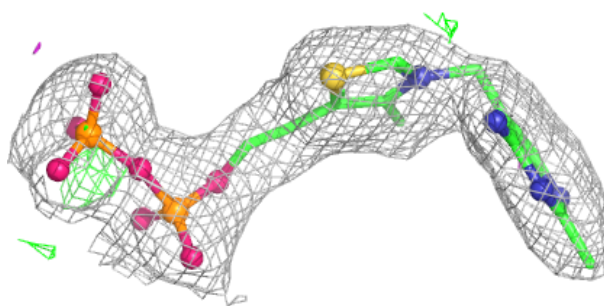
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MG   | D     | 601 | 1/1   | 0.95 | 0.12 | 27,27,27,27                 | 0     |
| 3   | TPP  | C     | 600 | 26/26 | 0.96 | 0.08 | 21,28,31,33                 | 0     |
| 3   | TPP  | D     | 600 | 26/26 | 0.96 | 0.07 | 22,28,31,32                 | 0     |
| 3   | TPP  | B     | 600 | 26/26 | 0.97 | 0.07 | 18,23,27,30                 | 0     |
| 3   | TPP  | A     | 600 | 26/26 | 0.98 | 0.06 | 19,24,26,28                 | 0     |
| 2   | MG   | B     | 601 | 1/1   | 0.98 | 0.10 | 19,19,19,19                 | 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.

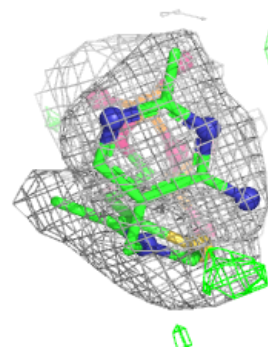
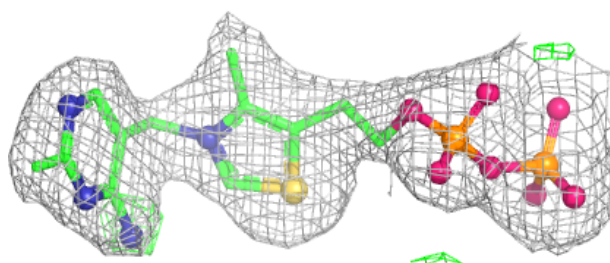
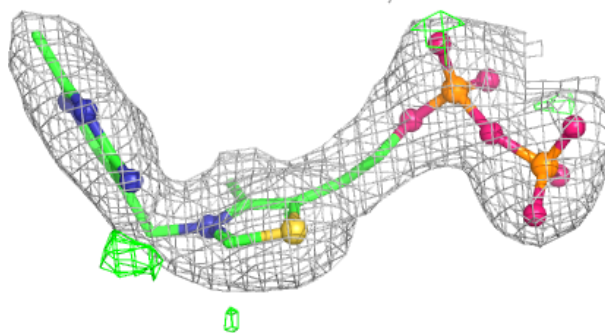
**Electron density around TPP C 600:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

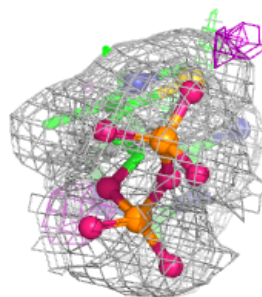
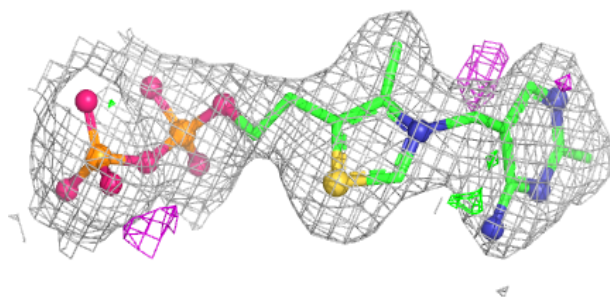
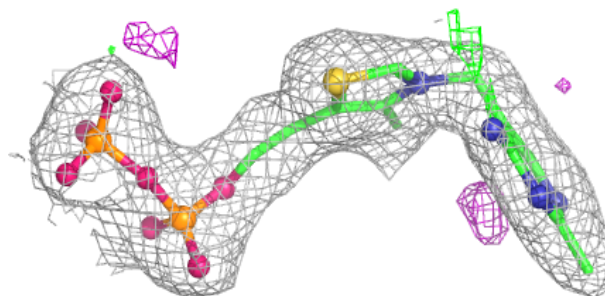


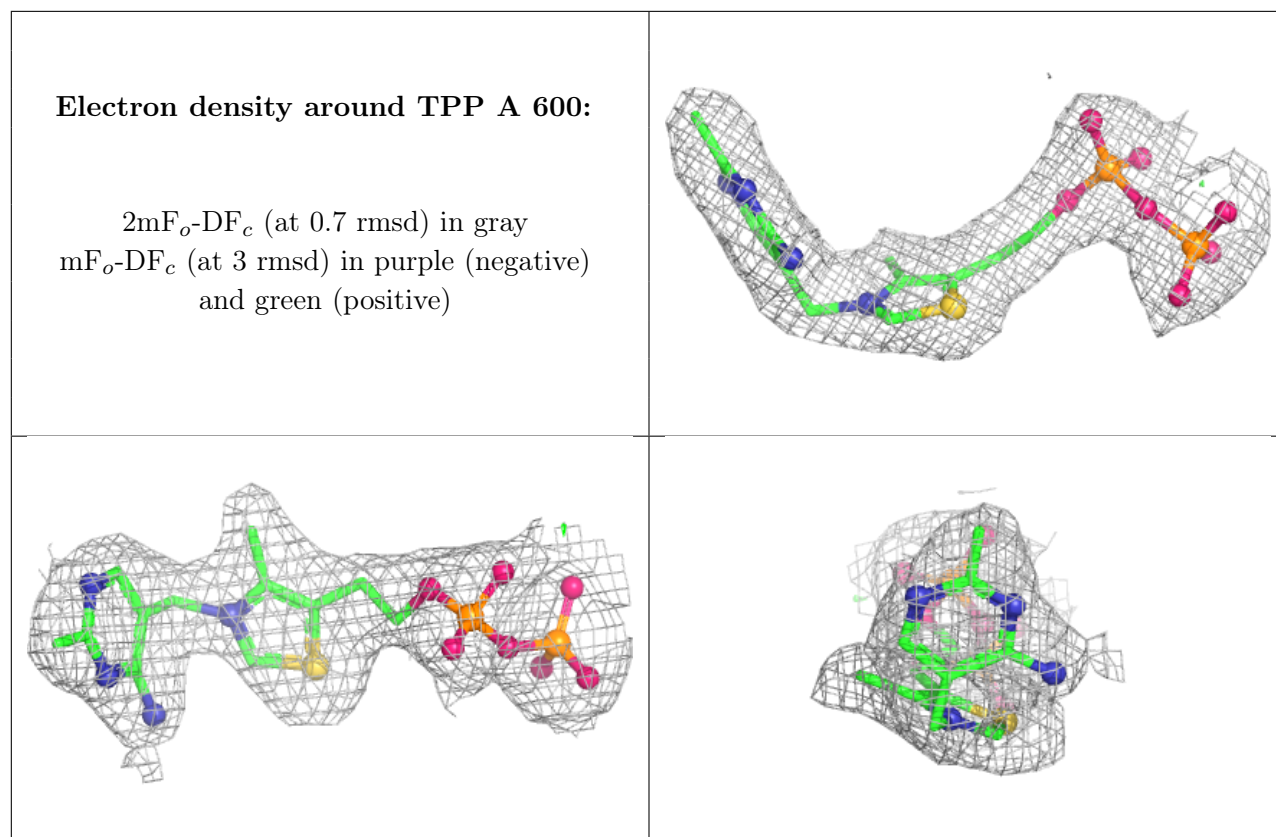
**Electron density around TPP D 600:**

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

**Electron density around TPP 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.