



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:01 AM UTC

PDB ID : 5EOM / pdb\_00005eom  
Title : Structure of full-length human MAB21L1 with bound CTP  
Authors : de Oliveira Mann, C.C.; Witte, G.; Hopfner, K.-P.  
Deposited on : 2015-11-10  
Resolution : 2.55 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:

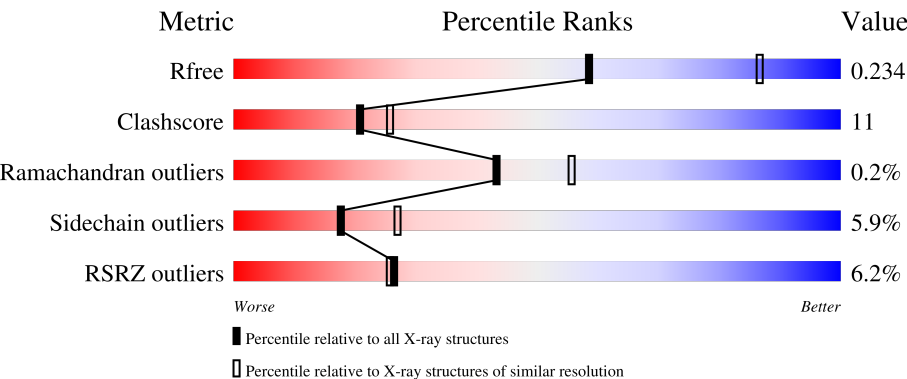
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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 <sub>free</sub>     | 180053                      | 1091 (2.54-2.54)                                      |
| Clashscore            | 190562                      | 1120 (2.54-2.54)                                      |
| Ramachandran outliers | 187476                      | 1106 (2.54-2.54)                                      |
| Sidechain outliers    | 187428                      | 1106 (2.54-2.54)                                      |
| RSRZ outliers         | 180081                      | 1091 (2.54-2.54)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 1   | A     | 362    | <div><div>4%</div><div><div></div><div>80%</div><div>14%</div><div>• •</div></div></div>   |
| 1   | B     | 362    | <div><div>5%</div><div><div></div><div>72%</div><div>22%</div><div>• •</div></div></div>   |
| 1   | C     | 362    | <div><div>2%</div><div><div></div><div>79%</div><div>17%</div><div>• •</div></div></div>   |
| 1   | D     | 362    | <div><div>7%</div><div><div></div><div>71%</div><div>22%</div><div>• 6%</div></div></div>  |
| 1   | E     | 362    | <div><div>4%</div><div><div></div><div>73%</div><div>19%</div><div>• • •</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 362    |                  |
| 1   | G     | 362    |                  |
| 1   | H     | 362    |                  |
| 1   | I     | 362    |                  |
| 1   | J     | 362    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CIT  | C     | 401 | -         | -        | X       | -                |
| 2   | CIT  | F     | 401 | -         | X        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28115 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 Protein mab-21-like 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 349      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2821  | 1790 | 506 | 505 | 20 |         |         |       |
| 1   | B     | 349      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2792  | 1771 | 494 | 507 | 20 |         |         |       |
| 1   | D     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2749  | 1748 | 492 | 490 | 19 |         |         |       |
| 1   | E     | 348      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2806  | 1779 | 503 | 507 | 17 |         |         |       |
| 1   | F     | 339      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2721  | 1732 | 482 | 490 | 17 |         |         |       |
| 1   | G     | 352      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2824  | 1790 | 506 | 508 | 20 |         |         |       |
| 1   | H     | 345      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2767  | 1759 | 491 | 497 | 20 |         |         |       |
| 1   | I     | 346      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2783  | 1767 | 499 | 499 | 18 |         |         |       |
| 1   | J     | 286      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2304  | 1467 | 415 | 407 | 15 |         |         |       |
| 1   | C     | 353      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2846  | 1804 | 510 | 511 | 21 |         |         |       |

There are 40 discrepancies between the modelled and reference sequences:

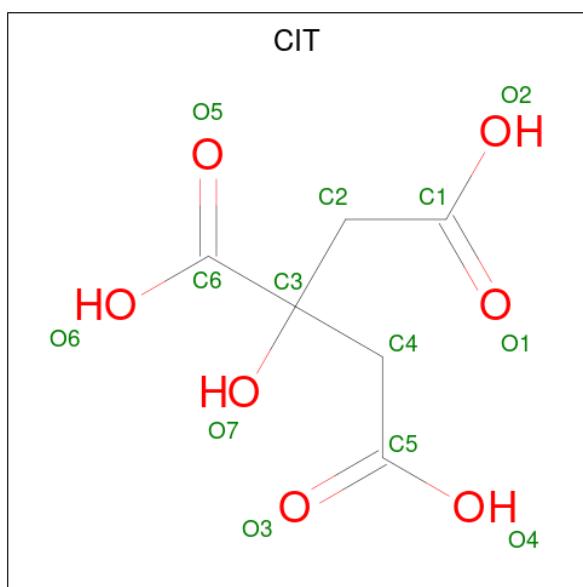
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| A     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| A     | 0       | MET      | -      | expression tag | UNP Q13394 |
| A     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| B     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| B     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| B     | 0       | MET      | -      | expression tag | UNP Q13394 |
| B     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| D     | -2      | GLY      | -      | expression tag | UNP Q13394 |

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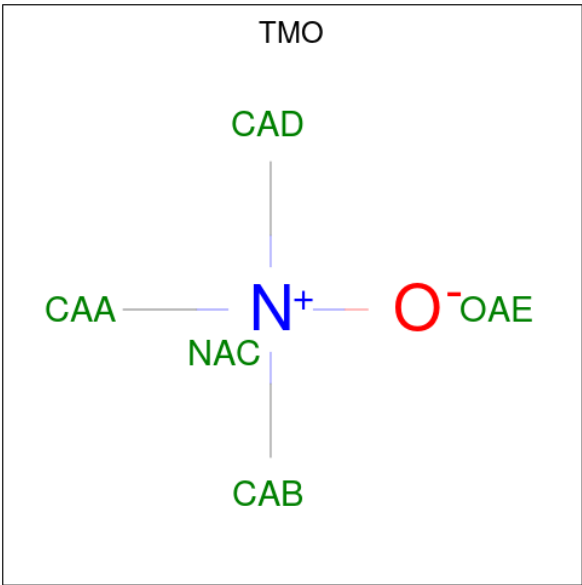
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| D     | 0       | MET      | -      | expression tag | UNP Q13394 |
| D     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| E     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| E     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| E     | 0       | MET      | -      | expression tag | UNP Q13394 |
| E     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| F     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| F     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| F     | 0       | MET      | -      | expression tag | UNP Q13394 |
| F     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| G     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| G     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| G     | 0       | MET      | -      | expression tag | UNP Q13394 |
| G     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| H     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| H     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| H     | 0       | MET      | -      | expression tag | UNP Q13394 |
| H     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| I     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| I     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| I     | 0       | MET      | -      | expression tag | UNP Q13394 |
| I     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| J     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| J     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| J     | 0       | MET      | -      | expression tag | UNP Q13394 |
| J     | 1       | ASP      | -      | expression tag | UNP Q13394 |
| C     | -2      | GLY      | -      | expression tag | UNP Q13394 |
| C     | -1      | ALA      | -      | expression tag | UNP Q13394 |
| C     | 0       | MET      | -      | expression tag | UNP Q13394 |
| C     | 1       | ASP      | -      | expression tag | UNP Q13394 |

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



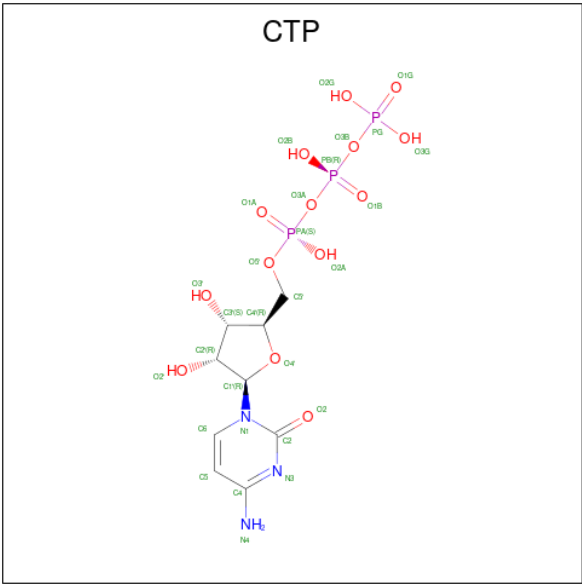
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 2   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |

- Molecule 3 is trimethylamine oxide (CCD ID: TMO) (formula:  $C_3H_9NO$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|----|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | B     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | D     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | E     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | F     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | G     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | H     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | I     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | J     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |
| 4   | C     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 29    | 9 | 3 | 14 | 3 |         |         |

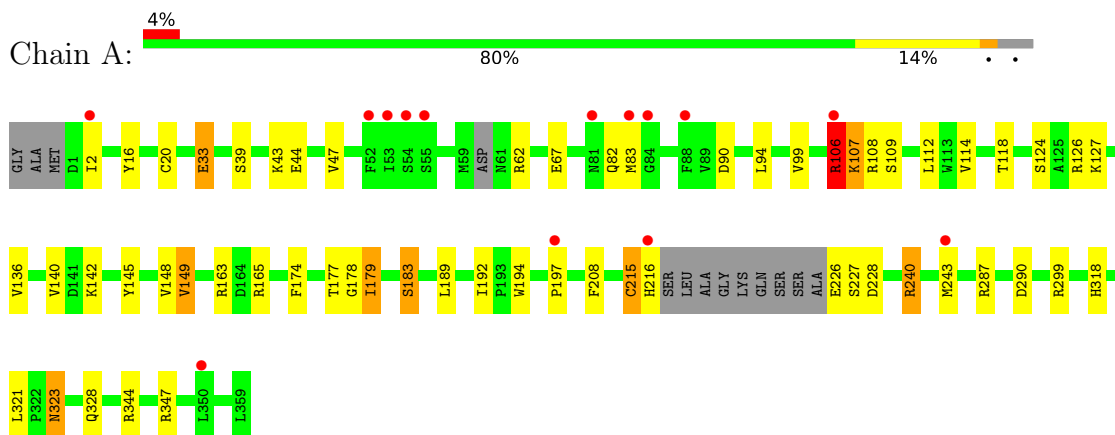
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 51       | Total | O  | 0       | 0       |
|     |       |          | 51    | 51 |         |         |
| 5   | B     | 27       | Total | O  | 0       | 0       |
|     |       |          | 27    | 27 |         |         |
| 5   | D     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 5   | E     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 5   | F     | 38       | Total | O  | 0       | 0       |
|     |       |          | 38    | 38 |         |         |
| 5   | G     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 5   | H     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 5   | I     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 5   | J     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 5   | C     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |

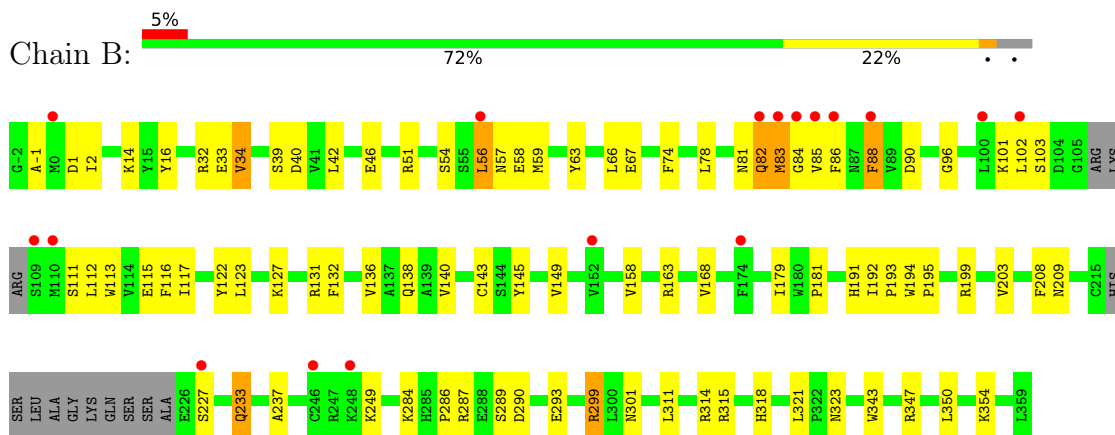
### 3 Residue-property plots [i](#)

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.

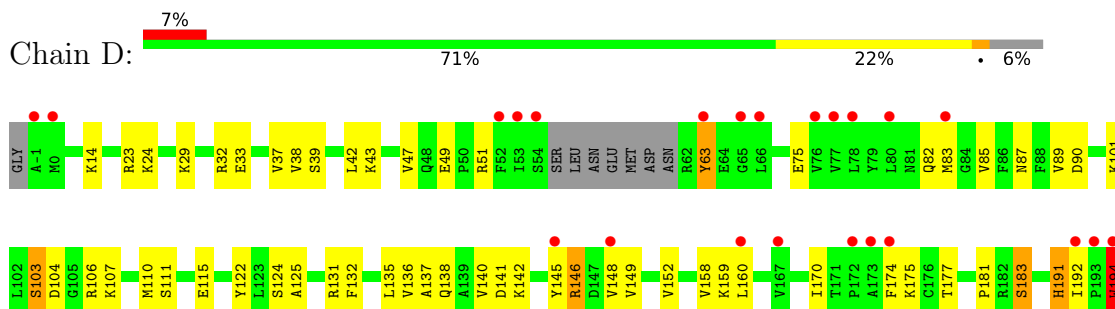
#### • Molecule 1: Protein mab-21-like 1

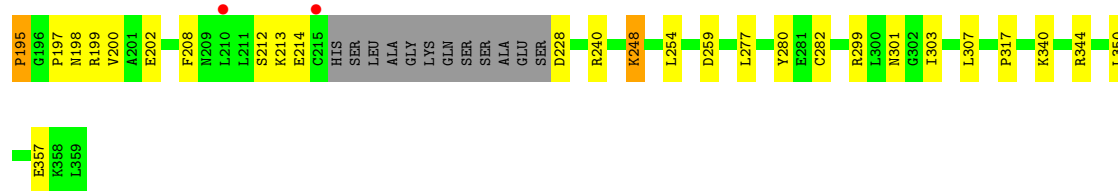


#### • Molecule 1: Protein mab-21-like 1

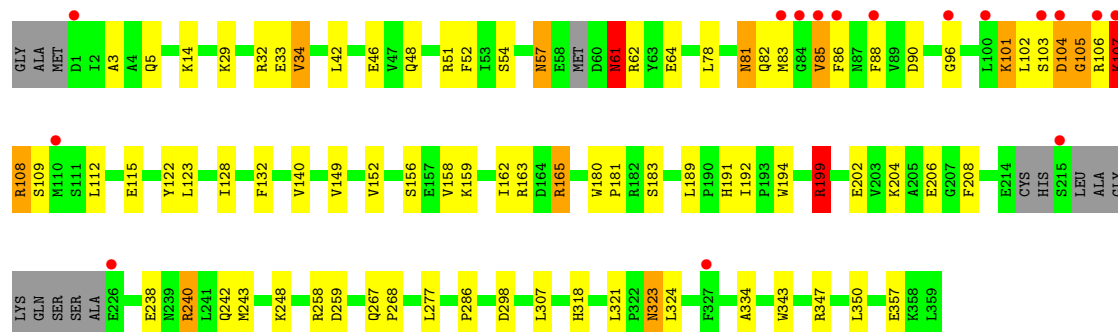
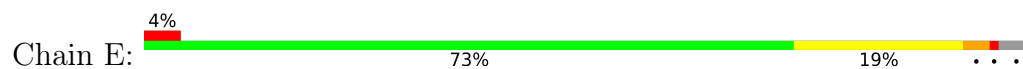


#### • Molecule 1: Protein mab-21-like 1

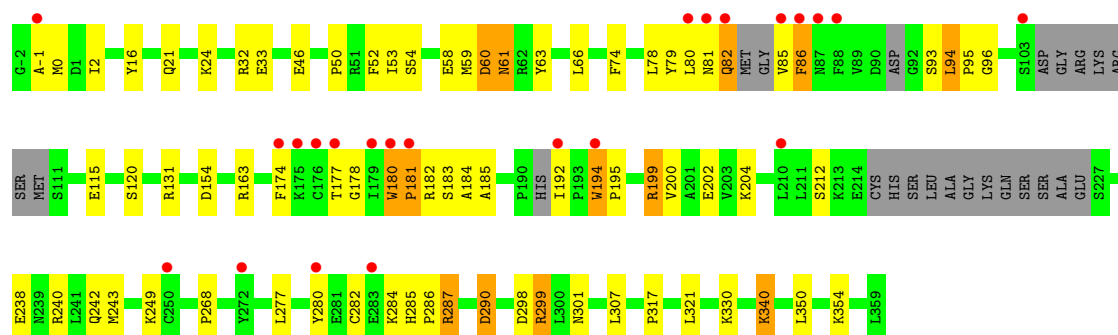




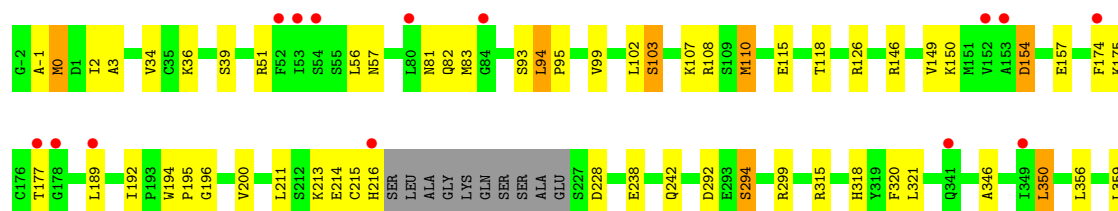
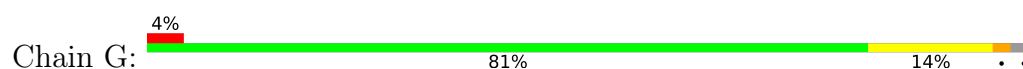
• Molecule 1: Protein mab-21-like 1



• Molecule 1: Protein mab-21-like 1

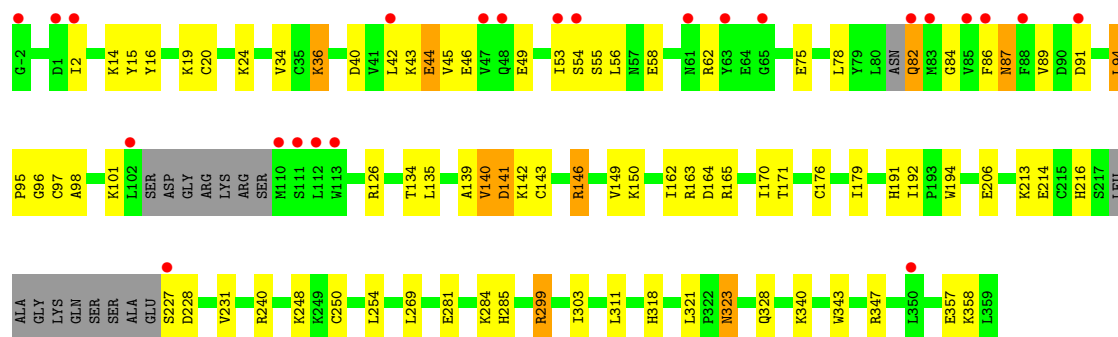


• Molecule 1: Protein mab-21-like 1

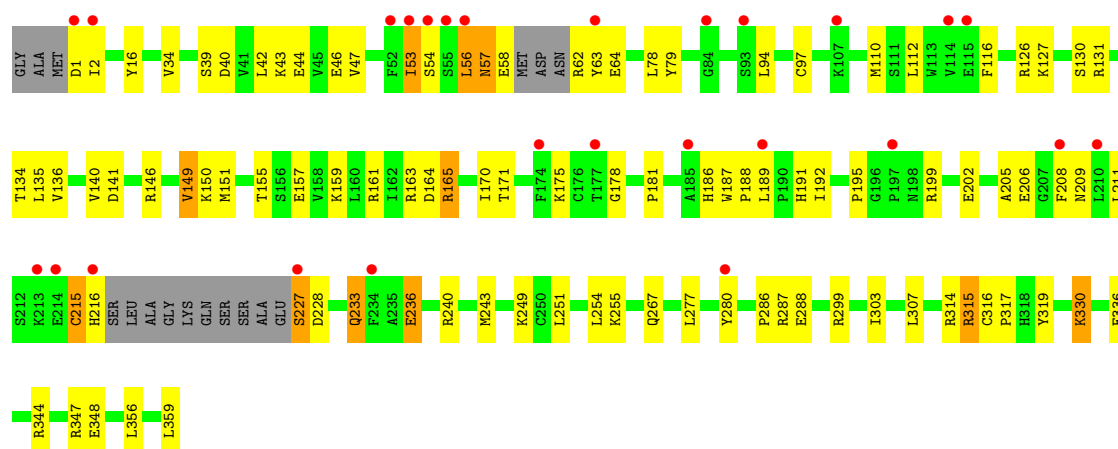


• Molecule 1: Protein mab-21-like 1

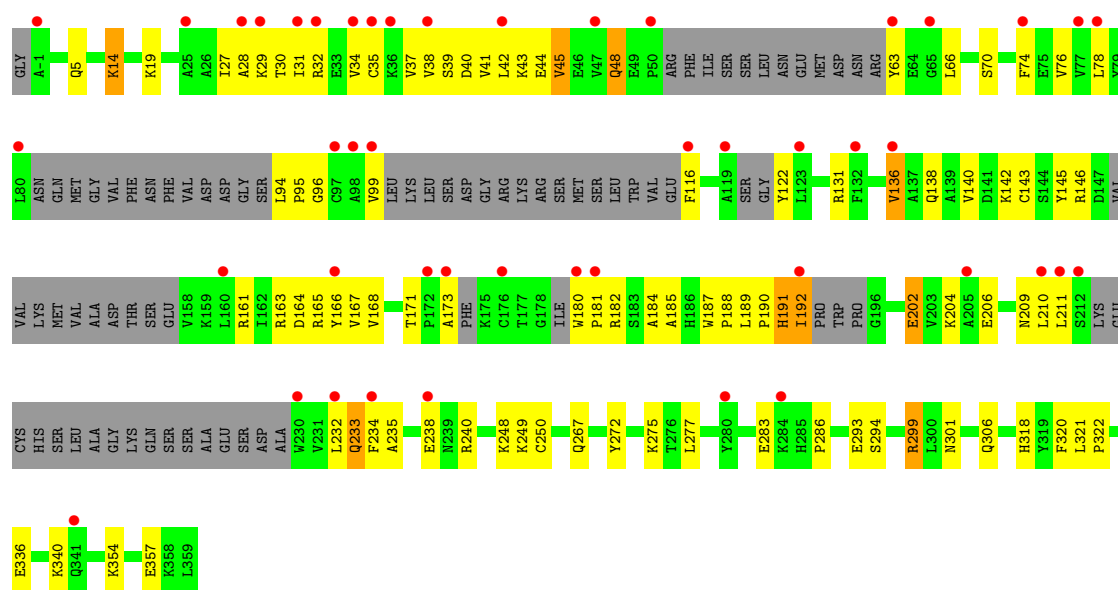




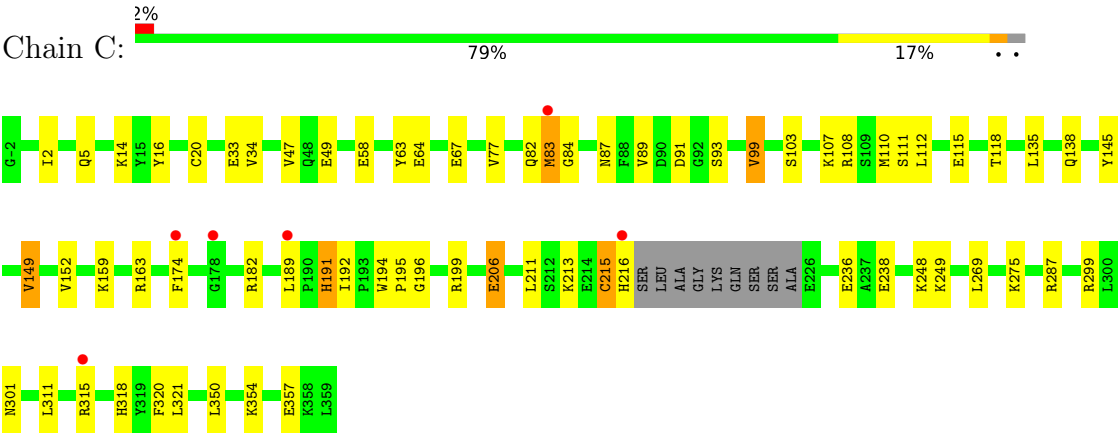
• Molecule 1: Protein mab-21-like 1



• Molecule 1: Protein mab-21-like 1



• Molecule 1: Protein mab-21-like 1



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 115.00Å 177.76Å 134.94Å<br>90.00° 97.58° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.98 – 2.55<br>49.98 – 2.55                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (49.98-2.55)<br>99.8 (49.98-2.55)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.32 (at 2.54Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.10.1_2155: ???)                                   | Depositor        |
| R, $R_{free}$                                                           | 0.199 , 0.227<br>0.207 , 0.234                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1670 reflections (0.80%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 64.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.542                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 52.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 28115                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 93.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, TMO, CTP

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     | 0.15         | 0/2886  | 0.45        | 1/3897 (0.0%)  |
| 1   | B     | 0.15         | 0/2850  | 0.41        | 0/3852         |
| 1   | C     | 0.14         | 0/2912  | 0.39        | 0/3933         |
| 1   | D     | 0.17         | 0/2807  | 0.48        | 1/3792 (0.0%)  |
| 1   | E     | 0.16         | 0/2867  | 0.46        | 5/3873 (0.1%)  |
| 1   | F     | 0.20         | 0/2775  | 0.46        | 0/3748         |
| 1   | G     | 0.13         | 0/2884  | 0.39        | 0/3897         |
| 1   | H     | 0.15         | 0/2825  | 0.42        | 0/3817         |
| 1   | I     | 0.23         | 0/2842  | 0.50        | 2/3840 (0.1%)  |
| 1   | J     | 0.18         | 0/2345  | 0.42        | 0/3159         |
| All | All   | 0.17         | 0/27993 | 0.44        | 9/37808 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 0                   | 2                   |
| 1   | J     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 107 | LYS  | N-CA-C   | 6.57  | 120.31      | 111.24   |
| 1   | D     | 194 | TRP  | CA-CB-CG | 6.51  | 125.97      | 113.60   |
| 1   | I     | 215 | CYS  | CB-CA-C  | -6.46 | 98.79       | 112.82   |
| 1   | E     | 61  | ASN  | CA-C-N   | -5.80 | 111.72      | 121.75   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 61  | ASN  | C-N-CA    | -5.80 | 111.72      | 121.75   |
| 1   | A     | 106 | ARG  | CB-CA-C   | -5.56 | 101.81      | 112.43   |
| 1   | E     | 105 | GLY  | N-CA-C    | -5.17 | 100.92      | 113.18   |
| 1   | E     | 199 | ARG  | CG-CD-NE  | -5.08 | 100.81      | 112.00   |
| 1   | I     | 319 | TYR  | OH-CZ-CE2 | -5.03 | 104.82      | 119.90   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 61  | ASN  | Peptide |
| 1   | J     | 136 | VAL  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2821  | 0        | 2860     | 51      | 0            |
| 1   | B     | 2792  | 0        | 2813     | 67      | 1            |
| 1   | C     | 2846  | 0        | 2882     | 44      | 0            |
| 1   | D     | 2749  | 0        | 2791     | 72      | 0            |
| 1   | E     | 2806  | 0        | 2839     | 62      | 0            |
| 1   | F     | 2721  | 0        | 2755     | 67      | 1            |
| 1   | G     | 2824  | 0        | 2854     | 42      | 0            |
| 1   | H     | 2767  | 0        | 2795     | 67      | 0            |
| 1   | I     | 2783  | 0        | 2817     | 79      | 0            |
| 1   | J     | 2304  | 0        | 2347     | 88      | 0            |
| 2   | A     | 13    | 0        | 5        | 1       | 0            |
| 2   | B     | 13    | 0        | 5        | 2       | 0            |
| 2   | C     | 13    | 0        | 5        | 9       | 0            |
| 2   | D     | 13    | 0        | 5        | 2       | 0            |
| 2   | E     | 13    | 0        | 5        | 0       | 0            |
| 2   | F     | 13    | 0        | 5        | 1       | 0            |
| 2   | G     | 13    | 0        | 5        | 1       | 0            |
| 2   | H     | 26    | 0        | 10       | 1       | 0            |
| 2   | I     | 13    | 0        | 5        | 2       | 0            |
| 3   | A     | 5     | 0        | 9        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | C     | 10    | 0        | 18       | 0       | 0            |
| 3   | F     | 5     | 0        | 9        | 0       | 0            |
| 4   | A     | 29    | 0        | 12       | 1       | 0            |
| 4   | B     | 29    | 0        | 12       | 0       | 0            |
| 4   | C     | 29    | 0        | 12       | 0       | 0            |
| 4   | D     | 29    | 0        | 12       | 1       | 0            |
| 4   | E     | 29    | 0        | 12       | 2       | 0            |
| 4   | F     | 29    | 0        | 12       | 1       | 0            |
| 4   | G     | 29    | 0        | 12       | 0       | 0            |
| 4   | H     | 29    | 0        | 12       | 3       | 0            |
| 4   | I     | 29    | 0        | 12       | 2       | 0            |
| 4   | J     | 29    | 0        | 12       | 0       | 0            |
| 5   | A     | 51    | 0        | 0        | 0       | 0            |
| 5   | B     | 27    | 0        | 0        | 0       | 0            |
| 5   | C     | 30    | 0        | 0        | 0       | 0            |
| 5   | D     | 21    | 0        | 0        | 0       | 0            |
| 5   | E     | 26    | 0        | 0        | 1       | 0            |
| 5   | F     | 38    | 0        | 0        | 1       | 0            |
| 5   | G     | 17    | 0        | 0        | 1       | 0            |
| 5   | H     | 18    | 0        | 0        | 4       | 0            |
| 5   | I     | 18    | 0        | 0        | 2       | 0            |
| 5   | J     | 16    | 0        | 0        | 3       | 0            |
| All | All   | 28115 | 0        | 27959    | 622     | 1            |

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 11.

All (622) 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:J:187:TRP:CE3  | 1:J:204:LYS:HE3 | 1.70                     | 1.26              |
| 1:E:103:SER:O    | 1:E:106:ARG:HB2 | 1.34                     | 1.23              |
| 1:J:187:TRP:CZ3  | 1:J:204:LYS:HE3 | 1.74                     | 1.21              |
| 1:J:187:TRP:CE3  | 1:J:204:LYS:CE  | 2.34                     | 1.09              |
| 1:E:104:ASP:OD1  | 1:E:105:GLY:N   | 1.93                     | 1.02              |
| 1:J:187:TRP:HZ3  | 1:J:204:LYS:HG3 | 1.27                     | 0.99              |
| 1:D:198:ASN:HD21 | 1:J:204:LYS:HD2 | 1.29                     | 0.98              |
| 1:F:177:THR:O    | 1:I:205:ALA:HB1 | 1.64                     | 0.97              |
| 4:E:402:CTP:O2A  | 5:E:501:HOH:O   | 1.80                     | 0.97              |
| 1:F:60:ASP:O     | 1:F:61:ASN:HB2  | 1.65                     | 0.96              |
| 1:I:314:ARG:NH1  | 1:I:336:GLU:OE2 | 1.99                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:180:TRP:CD1   | 1:J:185:ALA:HA    | 2.02                     | 0.95              |
| 1:J:187:TRP:O     | 1:J:204:LYS:NZ    | 2.00                     | 0.95              |
| 1:F:32:ARG:NH1    | 1:F:58:GLU:OE1    | 2.01                     | 0.93              |
| 1:F:340:LYS:NZ    | 5:F:501:HOH:O     | 2.01                     | 0.93              |
| 1:J:187:TRP:HE3   | 1:J:204:LYS:CE    | 1.80                     | 0.92              |
| 1:H:248:LYS:NZ    | 4:H:403:CTP:O3G   | 2.04                     | 0.91              |
| 1:E:103:SER:O     | 1:E:106:ARG:CB    | 2.20                     | 0.89              |
| 1:J:31:ILE:HG23   | 1:J:32:ARG:HG2    | 1.55                     | 0.87              |
| 1:I:206:GLU:OE1   | 1:I:240:ARG:NH2   | 2.08                     | 0.86              |
| 1:J:187:TRP:HE3   | 1:J:204:LYS:HE2   | 1.39                     | 0.85              |
| 1:D:197:PRO:HG2   | 1:D:199:ARG:HE    | 1.41                     | 0.85              |
| 1:E:240:ARG:HA    | 1:E:243:MET:HE2   | 1.56                     | 0.85              |
| 1:J:187:TRP:CZ3   | 1:J:204:LYS:CE    | 2.54                     | 0.85              |
| 1:I:202:GLU:HB3   | 1:I:240:ARG:HD2   | 1.59                     | 0.85              |
| 1:I:57:ASN:O      | 1:I:62:ARG:O      | 1.96                     | 0.84              |
| 1:A:344:ARG:NH1   | 2:C:401:CIT:O3    | 2.10                     | 0.83              |
| 1:J:180:TRP:HE1   | 1:J:184:ALA:C     | 1.87                     | 0.83              |
| 1:E:61:ASN:O      | 1:E:62[A]:ARG:HG3 | 1.79                     | 0.82              |
| 1:I:155:THR:OG1   | 1:I:157:GLU:OE1   | 1.98                     | 0.80              |
| 1:J:187:TRP:HZ3   | 1:J:204:LYS:CG    | 1.94                     | 0.79              |
| 1:J:187:TRP:CZ3   | 1:J:204:LYS:HG3   | 2.16                     | 0.78              |
| 1:D:280:TYR:OH    | 1:D:317:PRO:O     | 2.00                     | 0.78              |
| 1:D:194:TRP:HZ2   | 1:D:282:CYS:HB3   | 1.49                     | 0.78              |
| 1:E:33:GLU:HG2    | 1:E:163:ARG:HH12  | 1.46                     | 0.77              |
| 1:F:180:TRP:CE3   | 1:F:180:TRP:HA    | 2.19                     | 0.77              |
| 1:I:215:CYS:O     | 1:I:216:HIS:CG    | 2.38                     | 0.76              |
| 1:H:44:GLU:OE2    | 1:H:142:LYS:HG3   | 1.84                     | 0.76              |
| 1:E:194:TRP:HB2   | 1:E:286:PRO:HB3   | 1.66                     | 0.76              |
| 1:I:151:MET:SD    | 5:I:504:HOH:O     | 2.44                     | 0.75              |
| 1:I:287:ARG:NH1   | 5:I:501:HOH:O     | 2.19                     | 0.75              |
| 1:F:180:TRP:HA    | 1:F:180:TRP:HE3   | 1.52                     | 0.75              |
| 1:G:107:LYS:NZ    | 1:G:110:MET:SD    | 2.60                     | 0.74              |
| 1:F:52:PHE:HA     | 1:F:80:LEU:HD13   | 1.68                     | 0.74              |
| 1:C:108:ARG:NH2   | 1:C:118:THR:O     | 2.21                     | 0.73              |
| 1:A:344:ARG:HH11  | 2:C:401:CIT:C5    | 2.00                     | 0.73              |
| 1:A:163:ARG:HH11  | 1:A:165:ARG:NH2   | 1.87                     | 0.73              |
| 1:A:83[B]:MET:HE2 | 1:A:112:LEU:H     | 1.55                     | 0.72              |
| 1:F:194:TRP:HB2   | 1:F:286:PRO:HB3   | 1.72                     | 0.72              |
| 1:F:280:TYR:OH    | 1:F:317:PRO:O     | 2.07                     | 0.72              |
| 1:C:14:LYS:NZ     | 1:C:357:GLU:OE1   | 2.23                     | 0.72              |
| 1:J:180:TRP:NE1   | 1:J:185:ALA:HA    | 2.04                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:192:ILE:HG22   | 1:A:194:TRP:H     | 1.56                     | 0.71              |
| 1:I:175:LYS:HG3    | 1:I:209:ASN:ND2   | 2.06                     | 0.70              |
| 1:I:175:LYS:HG3    | 1:I:209:ASN:HD21  | 1.56                     | 0.70              |
| 1:J:180:TRP:CD1    | 1:J:185:ALA:CA    | 2.74                     | 0.70              |
| 1:E:104:ASP:CG     | 1:E:105:GLY:H     | 1.97                     | 0.70              |
| 1:C:192:ILE:HG22   | 1:C:194:TRP:H     | 1.56                     | 0.70              |
| 1:I:215:CYS:O      | 1:I:216:HIS:CD2   | 2.46                     | 0.69              |
| 1:D:85:VAL:HB      | 1:D:107:LYS:HD3   | 1.74                     | 0.69              |
| 1:F:199:ARG:HA     | 1:F:202:GLU:HB2   | 1.73                     | 0.69              |
| 1:J:192:ILE:HG23   | 1:J:286:PRO:HG3   | 1.73                     | 0.69              |
| 1:F:184:ALA:HB2    | 1:F:321:LEU:HD23  | 1.75                     | 0.69              |
| 1:F:96:GLY:HA2     | 1:F:321:LEU:HD13  | 1.74                     | 0.68              |
| 1:A:62[B]:ARG:HH21 | 1:A:62[B]:ARG:HG2 | 1.58                     | 0.68              |
| 1:D:14:LYS:NZ      | 1:D:357:GLU:OE2   | 2.27                     | 0.67              |
| 1:G:150:LYS:NZ     | 5:G:501:HOH:O     | 2.25                     | 0.67              |
| 1:G:192:ILE:HG22   | 1:G:194:TRP:H     | 1.60                     | 0.67              |
| 1:E:96:GLY:HA3     | 1:E:324:LEU:HD21  | 1.77                     | 0.67              |
| 1:E:323:ASN:OD1    | 1:E:323:ASN:N     | 2.17                     | 0.67              |
| 1:F:180:TRP:HB2    | 1:F:185:ALA:HA    | 1.76                     | 0.66              |
| 1:I:63:TYR:H       | 4:I:402:CTP:HN41  | 1.44                     | 0.66              |
| 1:I:280:TYR:OH     | 1:I:317:PRO:O     | 2.13                     | 0.66              |
| 1:E:61:ASN:O       | 1:E:62[B]:ARG:HG3 | 1.95                     | 0.66              |
| 1:D:198:ASN:ND2    | 1:J:204:LYS:HD2   | 2.06                     | 0.66              |
| 1:I:267:GLN:O      | 1:I:330:LYS:NZ    | 2.28                     | 0.66              |
| 1:I:206:GLU:HB2    | 1:I:240:ARG:HH21  | 1.61                     | 0.66              |
| 1:B:112:LEU:HD12   | 1:G:83:MET:HB3    | 1.76                     | 0.66              |
| 1:A:33:GLU:OE2     | 1:A:163:ARG:NH2   | 2.29                     | 0.65              |
| 1:G:215:CYS:SG     | 1:G:216:HIS:N     | 2.62                     | 0.65              |
| 1:I:277:LEU:HD11   | 1:I:307:LEU:HD13  | 1.78                     | 0.65              |
| 1:F:54:SER:HA      | 1:F:78:LEU:HD11   | 1.78                     | 0.65              |
| 1:I:344:ARG:NH2    | 1:I:348:GLU:OE1   | 2.30                     | 0.65              |
| 1:H:299:ARG:HH11   | 1:H:299:ARG:HA    | 1.62                     | 0.65              |
| 1:C:191:HIS:CD2    | 1:C:191:HIS:H     | 2.12                     | 0.65              |
| 1:D:49:GLU:OE2     | 1:D:51:ARG:NH1    | 2.30                     | 0.65              |
| 1:G:3:ALA:HB1      | 1:I:347:ARG:HH12  | 1.62                     | 0.65              |
| 1:E:14:LYS:NZ      | 1:E:357:GLU:OE2   | 2.29                     | 0.64              |
| 1:A:106:ARG:O      | 1:A:107:LYS:HG3   | 1.97                     | 0.64              |
| 1:H:44:GLU:OE2     | 1:H:143:CYS:HA    | 1.97                     | 0.64              |
| 1:H:192:ILE:HG22   | 1:H:194:TRP:H     | 1.62                     | 0.64              |
| 1:F:32:ARG:NH1     | 1:F:63:TYR:OH     | 2.31                     | 0.64              |
| 1:F:180:TRP:CB     | 1:F:185:ALA:HA    | 2.27                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:32:ARG:HD3   | 1:J:35:CYS:SG    | 2.37                     | 0.64              |
| 1:F:81:ASN:OD1   | 1:F:82:GLN:N     | 2.31                     | 0.63              |
| 1:D:37:VAL:HG22  | 1:D:145:TYR:HD2  | 1.63                     | 0.63              |
| 1:E:86:PHE:CE2   | 1:E:123:LEU:HD22 | 2.33                     | 0.63              |
| 1:A:323:ASN:OD1  | 1:A:323:ASN:N    | 2.30                     | 0.63              |
| 1:D:194:TRP:CZ2  | 1:D:282:CYS:HB3  | 2.32                     | 0.63              |
| 2:I:401:CIT:O7   | 2:I:401:CIT:O4   | 2.17                     | 0.63              |
| 1:B:192:ILE:HG22 | 1:B:194:TRP:H    | 1.62                     | 0.63              |
| 1:J:238:GLU:HG3  | 1:J:275:LYS:NZ   | 2.13                     | 0.63              |
| 1:C:49:GLU:HG3   | 1:C:135:LEU:HD11 | 1.80                     | 0.63              |
| 1:I:136:VAL:O    | 1:I:140:VAL:HG13 | 1.99                     | 0.63              |
| 1:E:51:ARG:NH2   | 1:E:115:GLU:OE1  | 2.25                     | 0.62              |
| 1:F:301:ASN:ND2  | 1:F:350:LEU:HD21 | 2.13                     | 0.62              |
| 1:J:5:GLN:NE2    | 5:J:502:HOH:O    | 2.31                     | 0.62              |
| 1:J:48:GLN:HG2   | 1:J:138:GLN:HE22 | 1.64                     | 0.62              |
| 1:D:37:VAL:HG22  | 1:D:145:TYR:CD2  | 2.34                     | 0.62              |
| 1:J:143:CYS:O    | 1:J:146:ARG:NH2  | 2.30                     | 0.62              |
| 1:A:2:ILE:HG12   | 1:D:301:ASN:HD21 | 1.64                     | 0.62              |
| 1:G:195:PRO:HG2  | 1:G:200:VAL:HG22 | 1.82                     | 0.62              |
| 1:B:301:ASN:HD21 | 1:B:350:LEU:HD22 | 1.63                     | 0.62              |
| 1:J:187:TRP:CE3  | 1:J:204:LYS:HE2  | 2.18                     | 0.62              |
| 1:A:108:ARG:NH1  | 1:A:108:ARG:HB2  | 2.14                     | 0.62              |
| 1:I:199:ARG:NH2  | 1:I:288:GLU:OE2  | 2.33                     | 0.62              |
| 1:E:112:LEU:HD11 | 1:C:110:MET:HE3  | 1.82                     | 0.61              |
| 1:F:81:ASN:HD21  | 1:F:85:VAL:HG13  | 1.64                     | 0.61              |
| 1:A:126:ARG:HH22 | 1:A:226:GLU:HG3  | 1.65                     | 0.61              |
| 1:E:206:GLU:OE2  | 1:E:240:ARG:HD2  | 2.00                     | 0.61              |
| 1:J:63:TYR:N     | 5:J:503:HOH:O    | 2.34                     | 0.61              |
| 2:G:401:CIT:O7   | 2:G:401:CIT:O3   | 2.18                     | 0.60              |
| 1:C:82:GLN:HG2   | 1:C:84:GLY:H     | 1.64                     | 0.60              |
| 1:D:104:ASP:OD2  | 1:D:107:LYS:HE3  | 2.01                     | 0.60              |
| 1:H:149:VAL:HG23 | 1:H:162:ILE:HG12 | 1.84                     | 0.60              |
| 1:G:-1:ALA:HB2   | 1:I:1:ASP:OD2    | 2.02                     | 0.60              |
| 1:B:33:GLU:OE2   | 1:B:163:ARG:HD2  | 2.01                     | 0.60              |
| 1:E:96:GLY:HA2   | 1:E:321:LEU:HD13 | 1.83                     | 0.60              |
| 1:I:146:ARG:HH22 | 1:I:150:LYS:HA   | 1.67                     | 0.59              |
| 1:A:126:ARG:NH1  | 1:A:227:SER:O    | 2.35                     | 0.59              |
| 1:E:46:GLU:HG2   | 1:E:52:PHE:O     | 2.01                     | 0.59              |
| 1:J:181:PRO:HG2  | 1:J:232:LEU:HD13 | 1.84                     | 0.59              |
| 1:C:354:LYS:NZ   | 2:C:401:CIT:H42  | 2.17                     | 0.59              |
| 1:B:2:ILE:HG23   | 1:C:350:LEU:HD21 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:86:PHE:CZ     | 1:F:178:GLY:HA2   | 2.37                     | 0.59              |
| 1:I:140:VAL:O     | 1:I:146:ARG:HD3   | 2.02                     | 0.59              |
| 1:J:94:LEU:HD12   | 1:J:95:PRO:HD2    | 1.84                     | 0.59              |
| 1:F:115:GLU:OE2   | 1:F:131:ARG:NH2   | 2.33                     | 0.59              |
| 1:I:53:ILE:O      | 1:I:78:LEU:HD11   | 2.03                     | 0.59              |
| 1:G:0:MET:HG2     | 1:G:3:ALA:HB3     | 1.85                     | 0.59              |
| 1:D:146:ARG:NH1   | 1:D:149:VAL:O     | 2.36                     | 0.59              |
| 1:C:189:LEU:HB3   | 1:C:191:HIS:HD2   | 1.68                     | 0.59              |
| 1:H:82:GLN:N      | 1:H:82:GLN:OE1    | 2.36                     | 0.58              |
| 1:B:249:LYS:NZ    | 1:B:293:GLU:OE2   | 2.35                     | 0.58              |
| 1:C:82:GLN:HA     | 1:C:83[A]:MET:HE3 | 1.85                     | 0.58              |
| 1:A:90:ASP:OD2    | 1:A:183:SER:OG    | 2.16                     | 0.58              |
| 1:D:49:GLU:CD     | 1:D:51:ARG:HE     | 2.12                     | 0.58              |
| 1:H:54:SER:HA     | 1:H:78:LEU:HD11   | 1.85                     | 0.58              |
| 1:A:44:GLU:OE1    | 1:A:142:LYS:NZ    | 2.27                     | 0.58              |
| 1:E:101:LYS:HG3   | 1:E:122:TYR:CE1   | 2.39                     | 0.58              |
| 1:F:240:ARG:NH1   | 1:F:243:MET:SD    | 2.77                     | 0.58              |
| 1:A:215:CYS:SG    | 1:A:216:HIS:N     | 2.78                     | 0.57              |
| 1:J:14:LYS:NZ     | 1:J:357:GLU:OE1   | 2.37                     | 0.57              |
| 1:B:343:TRP:CE2   | 1:B:347:ARG:HD2   | 2.39                     | 0.57              |
| 1:B:39:SER:HA     | 1:B:56:LEU:HD22   | 1.85                     | 0.57              |
| 1:B:96:GLY:HA2    | 1:B:321:LEU:HD13  | 1.86                     | 0.57              |
| 1:D:85:VAL:HG21   | 1:D:111:SER:HB2   | 1.87                     | 0.57              |
| 1:D:248:LYS:NZ    | 1:D:248:LYS:HB3   | 2.20                     | 0.57              |
| 1:A:124:SER:OG    | 1:A:228:ASP:OD2   | 2.13                     | 0.57              |
| 1:J:32:ARG:HG3    | 1:J:63:TYR:CZ     | 2.40                     | 0.57              |
| 1:C:83[A]:MET:HE2 | 1:C:112:LEU:H     | 1.69                     | 0.57              |
| 1:C:215:CYS:O     | 1:C:216:HIS:ND1   | 2.37                     | 0.57              |
| 1:G:51:ARG:NH2    | 1:G:115:GLU:OE2   | 2.28                     | 0.57              |
| 1:C:145:TYR:O     | 1:C:149:VAL:HG23  | 2.05                     | 0.57              |
| 1:J:299:ARG:HH11  | 1:J:299:ARG:HA    | 1.70                     | 0.57              |
| 1:B:84:GLY:HA2    | 1:G:177:THR:H     | 1.70                     | 0.56              |
| 1:J:32:ARG:HG3    | 1:J:63:TYR:CE1    | 2.40                     | 0.56              |
| 1:E:54:SER:HA     | 1:E:78:LEU:HD11   | 1.87                     | 0.56              |
| 1:H:323:ASN:OD1   | 1:H:323:ASN:N     | 2.35                     | 0.56              |
| 1:F:194:TRP:CD1   | 1:F:195:PRO:HA    | 2.40                     | 0.56              |
| 1:I:150:LYS:HG3   | 1:I:161:ARG:HB3   | 1.87                     | 0.56              |
| 1:J:35:CYS:HA     | 1:J:38:VAL:HG23   | 1.85                     | 0.56              |
| 1:J:209:ASN:HB2   | 1:J:233:GLN:HG2   | 1.87                     | 0.56              |
| 1:D:131:ARG:O     | 1:D:135:LEU:HD13  | 2.05                     | 0.56              |
| 1:E:81:ASN:ND2    | 1:C:87:ASN:OD1    | 2.30                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:141:ASP:HA   | 1:H:146:ARG:CZ   | 2.36                     | 0.56              |
| 1:B:203:VAL:HG13 | 1:B:237:ALA:HB1  | 1.85                     | 0.56              |
| 1:B:354:LYS:HZ1  | 2:B:401:CIT:H41  | 1.70                     | 0.56              |
| 1:E:189:LEU:HB3  | 1:E:191:HIS:HD2  | 1.69                     | 0.56              |
| 1:H:269:LEU:HD21 | 1:H:311:LEU:HD21 | 1.87                     | 0.56              |
| 1:I:209:ASN:HB2  | 1:I:233:GLN:HG2  | 1.86                     | 0.56              |
| 1:I:146:ARG:NH2  | 1:I:149:VAL:O    | 2.39                     | 0.56              |
| 1:H:43:LYS:NZ    | 1:H:54:SER:HB3   | 2.20                     | 0.55              |
| 1:E:33:GLU:HG2   | 1:E:163:ARG:NH1  | 2.19                     | 0.55              |
| 1:F:52:PHE:HA    | 1:F:80:LEU:CD1   | 2.35                     | 0.55              |
| 1:H:163:ARG:O    | 1:H:163:ARG:HG3  | 2.05                     | 0.55              |
| 1:H:206:GLU:OE2  | 1:H:240:ARG:NH2  | 2.40                     | 0.55              |
| 1:J:28:ALA:O     | 1:J:31:ILE:HG22  | 2.06                     | 0.55              |
| 1:J:165:ARG:NH1  | 5:J:505:HOH:O    | 2.39                     | 0.55              |
| 1:J:189:LEU:HB2  | 1:J:191:HIS:CE1  | 2.42                     | 0.55              |
| 1:D:90:ASP:OD2   | 1:D:183:SER:OG   | 2.20                     | 0.55              |
| 1:A:108:ARG:HB2  | 1:A:108:ARG:HH11 | 1.71                     | 0.55              |
| 1:D:145:TYR:HB3  | 1:D:148:VAL:HG22 | 1.88                     | 0.55              |
| 1:G:3:ALA:HB1    | 1:I:347:ARG:NH1  | 2.21                     | 0.55              |
| 1:I:141:ASP:OD1  | 1:I:146:ARG:NE   | 2.40                     | 0.55              |
| 1:C:206:GLU:HG2  | 1:C:236:GLU:HB3  | 1.88                     | 0.55              |
| 1:B:299:ARG:HA   | 1:B:299:ARG:HH11 | 1.72                     | 0.55              |
| 1:F:33:GLU:OE2   | 1:F:163:ARG:HD2  | 2.06                     | 0.55              |
| 1:F:94:LEU:HG    | 1:F:95:PRO:HD2   | 1.88                     | 0.55              |
| 1:I:157:GLU:OE2  | 1:I:159:LYS:NZ   | 2.39                     | 0.55              |
| 1:J:74:PHE:HB2   | 1:J:168:VAL:HG22 | 1.87                     | 0.55              |
| 1:I:215:CYS:SG   | 1:I:216:HIS:N    | 2.66                     | 0.55              |
| 1:H:163:ARG:HE   | 1:H:165:ARG:HH12 | 1.53                     | 0.54              |
| 1:A:126:ARG:NH2  | 1:A:226:GLU:HG3  | 2.22                     | 0.54              |
| 1:H:91:ASP:O     | 1:H:94:LEU:HD11  | 2.07                     | 0.54              |
| 1:B:354:LYS:NZ   | 2:B:401:CIT:H41  | 2.21                     | 0.54              |
| 1:D:63:TYR:N     | 1:D:63:TYR:CD2   | 2.74                     | 0.54              |
| 1:B:51:ARG:NH2   | 1:B:115:GLU:OE2  | 2.40                     | 0.54              |
| 1:D:132:PHE:CD2  | 1:D:158:VAL:HG21 | 2.43                     | 0.54              |
| 1:I:189:LEU:H    | 1:I:192:ILE:HD12 | 1.73                     | 0.54              |
| 1:A:126:ARG:H    | 1:A:228:ASP:CG   | 2.16                     | 0.54              |
| 1:E:104:ASP:O    | 1:E:105:GLY:C    | 2.51                     | 0.54              |
| 2:D:401:CIT:O3   | 2:D:401:CIT:O7   | 2.18                     | 0.54              |
| 1:J:187:TRP:CZ3  | 1:J:204:LYS:CG   | 2.83                     | 0.54              |
| 1:B:57:ASN:HD22  | 1:B:59:MET:HE1   | 1.73                     | 0.53              |
| 1:E:42:LEU:O     | 1:E:46:GLU:HG3   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:181:PRO:HG2  | 1:J:232:LEU:CD1  | 2.37                     | 0.53              |
| 1:D:192:ILE:HG22 | 1:D:194:TRP:HA   | 1.89                     | 0.53              |
| 1:B:66:LEU:HD11  | 1:B:74:PHE:HB3   | 1.89                     | 0.53              |
| 1:I:146:ARG:HD2  | 1:I:146:ARG:O    | 2.08                     | 0.53              |
| 1:J:116:PHE:HZ   | 1:J:131:ARG:HD2  | 1.73                     | 0.53              |
| 1:B:102:LEU:HG   | 1:B:103:SER:O    | 2.09                     | 0.53              |
| 1:I:46:GLU:OE2   | 1:I:53:ILE:C     | 2.52                     | 0.53              |
| 1:B:86:PHE:CE1   | 1:B:123:LEU:HB2  | 2.43                     | 0.53              |
| 1:D:75:GLU:OE1   | 1:D:213:LYS:NZ   | 2.42                     | 0.53              |
| 1:G:211:LEU:HD23 | 1:G:213:LYS:HE3  | 1.91                     | 0.53              |
| 1:J:41:VAL:HA    | 1:J:143:CYS:SG   | 2.49                     | 0.53              |
| 1:F:340:LYS:NZ   | 1:F:340:LYS:HB2  | 2.24                     | 0.53              |
| 1:I:46:GLU:OE2   | 1:I:54:SER:N     | 2.42                     | 0.53              |
| 1:I:79:TYR:CE1   | 1:I:175:LYS:HE2  | 2.44                     | 0.53              |
| 1:B:111:SER:OG   | 1:B:112:LEU:N    | 2.41                     | 0.52              |
| 1:J:32:ARG:NH1   | 1:J:66:LEU:HD13  | 2.24                     | 0.52              |
| 1:B:42:LEU:O     | 1:B:46:GLU:HG3   | 2.08                     | 0.52              |
| 1:F:180:TRP:CD1  | 1:F:204:LYS:HE2  | 2.43                     | 0.52              |
| 1:H:42:LEU:HD11  | 1:H:170:ILE:HD13 | 1.92                     | 0.52              |
| 1:I:42:LEU:HD11  | 1:I:170:ILE:HD13 | 1.92                     | 0.52              |
| 2:C:401:CIT:H42  | 2:C:401:CIT:O1   | 2.08                     | 0.52              |
| 1:D:152:VAL:HB   | 1:D:159:LYS:HB2  | 1.91                     | 0.52              |
| 1:F:79:TYR:O     | 1:F:80:LEU:HG    | 2.08                     | 0.52              |
| 1:H:75:GLU:HG3   | 5:H:506:HOH:O    | 2.10                     | 0.52              |
| 1:H:140:VAL:HG13 | 1:H:146:ARG:HH21 | 1.74                     | 0.52              |
| 1:F:287:ARG:H    | 1:F:287:ARG:HD2  | 1.75                     | 0.52              |
| 1:G:-1:ALA:O     | 1:G:2:ILE:HG22   | 2.10                     | 0.52              |
| 1:H:58:GLU:H     | 1:H:58:GLU:CD    | 2.17                     | 0.52              |
| 1:H:62:ARG:NH2   | 4:H:403:CTP:O1G  | 2.42                     | 0.52              |
| 1:J:32:ARG:CZ    | 1:J:66:LEU:HD13  | 2.39                     | 0.52              |
| 1:G:102:LEU:HD21 | 1:G:108:ARG:HB2  | 1.92                     | 0.52              |
| 1:H:24:LYS:HE2   | 4:H:403:CTP:O1B  | 2.10                     | 0.52              |
| 1:H:284:LYS:HB3  | 1:H:285:HIS:HD2  | 1.74                     | 0.52              |
| 1:E:82:GLN:HE21  | 1:E:85:VAL:H     | 1.56                     | 0.52              |
| 1:D:101:LYS:HE2  | 1:D:122:TYR:CE1  | 2.45                     | 0.51              |
| 1:E:90:ASP:OD2   | 1:E:183:SER:N    | 2.38                     | 0.51              |
| 1:C:301:ASN:HD21 | 1:C:350:LEU:HD13 | 1.75                     | 0.51              |
| 1:D:198:ASN:OD1  | 1:J:204:LYS:HD3  | 2.10                     | 0.51              |
| 1:E:240:ARG:CZ   | 1:E:243:MET:HE1  | 2.41                     | 0.51              |
| 1:D:131:ARG:NH1  | 1:D:135:LEU:HD11 | 2.25                     | 0.51              |
| 1:B:-1:ALA:HA    | 1:B:2:ILE:HG22   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:195:PRO:CG   | 1:D:199:ARG:HB2  | 2.41                     | 0.51              |
| 1:F:284:LYS:HG2  | 1:F:285:HIS:CD2  | 2.45                     | 0.51              |
| 1:H:94:LEU:HD22  | 1:H:98:ALA:HA    | 1.91                     | 0.51              |
| 1:J:44:GLU:OE1   | 1:J:142:LYS:NZ   | 2.34                     | 0.51              |
| 1:A:106:ARG:C    | 1:A:107:LYS:HG3  | 2.35                     | 0.51              |
| 1:B:181:PRO:HD3  | 1:B:208:PHE:CD1  | 2.45                     | 0.51              |
| 1:E:192:ILE:HG22 | 1:E:194:TRP:H    | 1.76                     | 0.51              |
| 1:C:196:GLY:O    | 1:C:199:ARG:N    | 2.39                     | 0.51              |
| 1:C:82:GLN:HB2   | 1:C:174:PHE:CE1  | 2.46                     | 0.51              |
| 1:F:194:TRP:HB2  | 1:F:286:PRO:CB   | 2.38                     | 0.50              |
| 1:B:1:ASP:HB3    | 1:F:-1:ALA:HB2   | 1.91                     | 0.50              |
| 1:D:38:VAL:HG22  | 1:D:160:LEU:HD12 | 1.92                     | 0.50              |
| 1:D:136:VAL:HG21 | 1:D:158:VAL:HG11 | 1.93                     | 0.50              |
| 1:B:84:GLY:HA3   | 1:G:175:LYS:O    | 2.11                     | 0.50              |
| 1:B:86:PHE:CZ    | 1:B:123:LEU:HB2  | 2.45                     | 0.50              |
| 1:I:39:SER:O     | 1:I:43:LYS:HG2   | 2.12                     | 0.50              |
| 1:F:268:PRO:HA   | 1:F:330:LYS:HD2  | 1.92                     | 0.50              |
| 1:I:356:LEU:HD23 | 1:I:359:LEU:HD12 | 1.94                     | 0.50              |
| 1:D:191:HIS:HB2  | 1:D:192:ILE:HD12 | 1.93                     | 0.50              |
| 1:H:149:VAL:O    | 1:H:150:LYS:NZ   | 2.38                     | 0.50              |
| 1:A:189:LEU:HD12 | 1:A:192:ILE:HD12 | 1.94                     | 0.50              |
| 1:G:82:GLN:HB3   | 1:G:174:PHE:CE1  | 2.47                     | 0.50              |
| 1:H:44:GLU:HB2   | 1:H:139:ALA:HB1  | 1.94                     | 0.50              |
| 1:J:171:THR:HG21 | 1:J:211:LEU:HB3  | 1.93                     | 0.50              |
| 1:C:354:LYS:HZ3  | 2:C:401:CIT:H42  | 1.77                     | 0.50              |
| 1:D:277:LEU:HD23 | 1:D:280:TYR:CD2  | 2.47                     | 0.50              |
| 1:E:152:VAL:HB   | 1:E:159:LYS:HB2  | 1.93                     | 0.50              |
| 1:F:180:TRP:O    | 1:F:185:ALA:HB2  | 2.11                     | 0.50              |
| 1:F:301:ASN:HD21 | 1:F:350:LEU:HD21 | 1.76                     | 0.50              |
| 1:G:94:LEU:HD22  | 1:G:95:PRO:HD2   | 1.93                     | 0.50              |
| 1:G:238:GLU:O    | 1:G:242:GLN:HG3  | 2.12                     | 0.50              |
| 1:J:320:PHE:O    | 1:J:322:PRO:HD3  | 2.12                     | 0.50              |
| 1:H:284:LYS:HB3  | 1:H:285:HIS:CD2  | 2.47                     | 0.50              |
| 1:B:86:PHE:CE2   | 1:B:123:LEU:HD22 | 2.47                     | 0.49              |
| 1:F:194:TRP:CZ3  | 1:F:282:CYS:HB3  | 2.47                     | 0.49              |
| 1:I:131:ARG:NH1  | 1:I:135:LEU:HD11 | 2.26                     | 0.49              |
| 1:C:354:LYS:NZ   | 2:C:401:CIT:C4   | 2.76                     | 0.49              |
| 1:E:82:GLN:HE21  | 1:E:85:VAL:N     | 2.10                     | 0.49              |
| 1:F:81:ASN:HD22  | 1:F:174:PHE:HD1  | 1.59                     | 0.49              |
| 1:F:354:LYS:NZ   | 2:F:401:CIT:H42  | 2.27                     | 0.49              |
| 1:B:88:PHE:CE1   | 1:B:90:ASP:HB2   | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:145:TYR:O    | 1:D:149:VAL:HG12 | 2.13                     | 0.49              |
| 1:D:194:TRP:HE3  | 1:D:194:TRP:C    | 2.21                     | 0.49              |
| 1:F:277:LEU:HD23 | 1:F:280:TYR:CD2  | 2.48                     | 0.49              |
| 1:J:187:TRP:HZ3  | 1:J:204:LYS:CE   | 2.19                     | 0.49              |
| 1:J:96:GLY:HA2   | 1:J:321:LEU:HD13 | 1.94                     | 0.49              |
| 1:B:82:GLN:HE21  | 1:B:82:GLN:C     | 2.21                     | 0.49              |
| 1:G:196:GLY:O    | 1:G:200:VAL:HG23 | 2.13                     | 0.49              |
| 1:J:40:ASP:HB3   | 1:J:145:TYR:HE2  | 1.77                     | 0.49              |
| 1:A:145:TYR:O    | 1:A:149:VAL:HG23 | 2.13                     | 0.49              |
| 1:G:346:ALA:O    | 1:G:350:LEU:HG   | 2.13                     | 0.49              |
| 1:B:101:LYS:HE2  | 1:B:122:TYR:CE1  | 2.48                     | 0.48              |
| 1:D:124:SER:OG   | 1:D:228:ASP:OD2  | 2.15                     | 0.48              |
| 1:H:40:ASP:OD2   | 1:H:143:CYS:HB2  | 2.13                     | 0.48              |
| 1:A:2:ILE:HG12   | 1:D:301:ASN:ND2  | 2.28                     | 0.48              |
| 1:D:29:LYS:HA    | 1:D:32:ARG:CZ    | 2.43                     | 0.48              |
| 1:E:132:PHE:CD2  | 1:E:158:VAL:HG21 | 2.48                     | 0.48              |
| 1:H:281:GLU:HG3  | 1:H:303:ILE:HG12 | 1.95                     | 0.48              |
| 1:A:178:GLY:HA2  | 1:H:179:ILE:HD13 | 1.94                     | 0.48              |
| 1:F:287:ARG:HG2  | 1:F:290:ASP:H    | 1.79                     | 0.48              |
| 1:G:238:GLU:HG3  | 1:G:320:PHE:HE2  | 1.78                     | 0.48              |
| 1:B:136:VAL:O    | 1:B:140:VAL:HG13 | 2.13                     | 0.48              |
| 1:E:238:GLU:O    | 1:E:242:GLN:HG3  | 2.14                     | 0.48              |
| 1:G:82:GLN:HB3   | 1:G:174:PHE:HE1  | 1.78                     | 0.48              |
| 1:H:176:CYS:HB3  | 1:H:179:ILE:HD11 | 1.95                     | 0.48              |
| 1:I:57:ASN:OD1   | 1:I:57:ASN:N     | 2.46                     | 0.48              |
| 1:D:141:ASP:HA   | 1:D:146:ARG:HG2  | 1.95                     | 0.48              |
| 1:F:277:LEU:HD11 | 1:F:307:LEU:HD13 | 1.95                     | 0.48              |
| 1:E:123:LEU:HD11 | 1:E:128:ILE:HD11 | 1.96                     | 0.48              |
| 1:G:108:ARG:NH2  | 1:G:118:THR:O    | 2.47                     | 0.48              |
| 1:H:15:TYR:CD1   | 1:H:19:LYS:HG3   | 2.49                     | 0.48              |
| 1:I:195:PRO:HA   | 1:I:286:PRO:HB2  | 1.96                     | 0.48              |
| 1:I:206:GLU:HG2  | 1:I:236:GLU:HB2  | 1.95                     | 0.48              |
| 1:F:66:LEU:HD11  | 1:F:74:PHE:HB3   | 1.96                     | 0.47              |
| 1:I:54:SER:OG    | 1:I:56:LEU:CD2   | 2.62                     | 0.47              |
| 1:B:82:GLN:HG2   | 1:B:85:VAL:HG12  | 1.95                     | 0.47              |
| 1:F:299:ARG:HA   | 1:F:299:ARG:HD3  | 1.69                     | 0.47              |
| 1:D:301:ASN:OD1  | 1:D:350:LEU:HD11 | 2.15                     | 0.47              |
| 1:H:14:LYS:NZ    | 1:H:357:GLU:OE1  | 2.43                     | 0.47              |
| 1:B:195:PRO:HB2  | 1:B:199:ARG:HG2  | 1.96                     | 0.47              |
| 1:D:195:PRO:HD2  | 1:D:200:VAL:HG23 | 1.97                     | 0.47              |
| 1:I:94:LEU:HB3   | 1:I:97:CYS:HB2   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:39:SER:HA     | 1:J:42:LEU:HB3    | 1.95                     | 0.47              |
| 2:A:401:CIT:O3    | 2:A:401:CIT:O7    | 2.31                     | 0.47              |
| 1:H:162:ILE:C     | 1:H:164:ASP:H     | 2.22                     | 0.47              |
| 1:A:136:VAL:O     | 1:A:140:VAL:HG13  | 2.15                     | 0.47              |
| 1:A:177:THR:HG21  | 1:H:87:ASN:HD22   | 1.80                     | 0.47              |
| 1:B:58:GLU:HB2    | 1:B:63:TYR:CE2    | 2.49                     | 0.47              |
| 1:D:299:ARG:HA    | 1:D:299:ARG:HH11  | 1.78                     | 0.47              |
| 1:G:126:ARG:HD2   | 1:G:228:ASP:HB3   | 1.97                     | 0.47              |
| 1:I:171:THR:HG21  | 1:I:211:LEU:HB3   | 1.97                     | 0.47              |
| 1:I:206:GLU:CG    | 1:I:236:GLU:HB2   | 2.45                     | 0.47              |
| 1:B:40:ASP:OD2    | 1:B:143:CYS:HB2   | 2.15                     | 0.47              |
| 1:E:3:ALA:HB2     | 1:G:350:LEU:HD13  | 1.96                     | 0.47              |
| 1:E:85:VAL:O      | 1:E:102:LEU:HD12  | 2.14                     | 0.47              |
| 1:E:103:SER:O     | 1:E:106:ARG:CG    | 2.62                     | 0.47              |
| 1:F:194:TRP:CG    | 1:F:195:PRO:HA    | 2.49                     | 0.47              |
| 1:H:281:GLU:HG3   | 1:H:303:ILE:CG1   | 2.45                     | 0.47              |
| 1:C:16:TYR:CD1    | 1:C:249:LYS:HG3   | 2.49                     | 0.47              |
| 1:A:62[B]:ARG:HG2 | 1:A:62[B]:ARG:NH2 | 2.27                     | 0.47              |
| 1:A:299:ARG:HA    | 1:A:299:ARG:HD3   | 1.72                     | 0.47              |
| 1:E:33:GLU:OE2    | 1:E:163:ARG:NH1   | 2.48                     | 0.47              |
| 1:H:146:ARG:O     | 1:H:150:LYS:NZ    | 2.48                     | 0.47              |
| 1:J:189:LEU:HB3   | 1:J:190:PRO:HD2   | 1.97                     | 0.47              |
| 1:A:62[B]:ARG:NH1 | 4:A:403:CTP:H2'   | 2.29                     | 0.46              |
| 1:B:193:PRO:HG2   | 1:B:286:PRO:HG3   | 1.96                     | 0.46              |
| 1:H:140:VAL:O     | 1:H:146:ARG:NE    | 2.38                     | 0.46              |
| 1:J:37:VAL:HA     | 1:J:145:TYR:CE2   | 2.50                     | 0.46              |
| 1:J:233:GLN:HG3   | 1:J:234:PHE:N     | 2.30                     | 0.46              |
| 1:I:163:ARG:HA    | 1:I:163:ARG:HE    | 1.81                     | 0.46              |
| 1:E:199:ARG:NH1   | 1:E:202:GLU:OE1   | 2.46                     | 0.46              |
| 1:J:27:ILE:O      | 1:J:31:ILE:HB     | 2.16                     | 0.46              |
| 1:A:318:HIS:HB3   | 1:A:321:LEU:O     | 2.16                     | 0.46              |
| 1:H:91:ASP:O      | 1:H:94:LEU:CD1    | 2.64                     | 0.46              |
| 1:C:192:ILE:HG22  | 1:C:194:TRP:N     | 2.29                     | 0.46              |
| 1:D:82:GLN:HB3    | 1:D:174:PHE:CE1   | 2.50                     | 0.46              |
| 1:F:79:TYR:C      | 1:F:80:LEU:HG     | 2.41                     | 0.46              |
| 1:I:44:GLU:O      | 1:I:47:VAL:HG22   | 2.15                     | 0.46              |
| 1:J:240:ARG:HH11  | 1:J:240:ARG:HG2   | 1.80                     | 0.46              |
| 1:D:202:GLU:CD    | 1:D:240:ARG:HD2   | 2.41                     | 0.46              |
| 1:H:340:LYS:NZ    | 5:H:507:HOH:O     | 2.47                     | 0.46              |
| 1:I:315:ARG:HD2   | 1:I:317:PRO:HD3   | 1.98                     | 0.46              |
| 1:J:42:LEU:HA     | 1:J:45:VAL:HG13   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:240:ARG:HA   | 1:A:243:MET:HE2  | 1.98                     | 0.46              |
| 1:H:15:TYR:CE1   | 1:H:19:LYS:HG3   | 2.51                     | 0.46              |
| 1:E:83:MET:HE3   | 1:C:87:ASN:HA    | 1.97                     | 0.46              |
| 1:G:3:ALA:CB     | 1:I:347:ARG:HH12 | 2.28                     | 0.46              |
| 1:D:145:TYR:HB3  | 1:D:148:VAL:CG2  | 2.45                     | 0.46              |
| 1:F:24:LYS:HE2   | 4:F:403:CTP:O2B  | 2.16                     | 0.46              |
| 1:J:267:GLN:N    | 1:J:267:GLN:OE1  | 2.48                     | 0.46              |
| 1:C:189:LEU:HB3  | 1:C:191:HIS:CD2  | 2.51                     | 0.46              |
| 1:C:354:LYS:HZ3  | 2:C:401:CIT:C4   | 2.28                     | 0.46              |
| 1:A:118:THR:HG22 | 1:A:127:LYS:NZ   | 2.30                     | 0.45              |
| 1:B:101:LYS:HG2  | 1:B:102:LEU:N    | 2.31                     | 0.45              |
| 1:F:298:ASP:HB3  | 1:F:299:ARG:HH12 | 1.81                     | 0.45              |
| 1:D:107:LYS:HA   | 1:D:110:MET:HG3  | 1.98                     | 0.45              |
| 1:C:301:ASN:ND2  | 1:C:350:LEU:HD13 | 2.31                     | 0.45              |
| 1:C:33:GLU:OE2   | 1:C:163:ARG:HD2  | 2.14                     | 0.45              |
| 1:C:191:HIS:CD2  | 1:C:191:HIS:N    | 2.84                     | 0.45              |
| 1:A:108:ARG:HG2  | 1:A:114:VAL:HG23 | 1.98                     | 0.45              |
| 1:D:194:TRP:CB   | 1:D:195:PRO:HD3  | 2.47                     | 0.45              |
| 1:C:269:LEU:HD21 | 1:C:311:LEU:HD21 | 1.97                     | 0.45              |
| 1:D:42:LEU:HD11  | 1:D:170:ILE:HD13 | 1.99                     | 0.45              |
| 1:F:194:TRP:HA   | 1:F:195:PRO:HA   | 1.58                     | 0.45              |
| 1:G:149:VAL:O    | 1:G:150:LYS:HD2  | 2.16                     | 0.45              |
| 1:H:284:LYS:C    | 1:H:285:HIS:HD2  | 2.25                     | 0.45              |
| 1:C:91:ASP:OD2   | 1:C:93:SER:OG    | 2.33                     | 0.45              |
| 1:F:180:TRP:O    | 1:F:181:PRO:C    | 2.58                     | 0.45              |
| 1:C:299:ARG:HA   | 1:C:299:ARG:HD3  | 1.72                     | 0.45              |
| 1:B:1:ASP:CB     | 1:F:-1:ALA:HB2   | 2.46                     | 0.45              |
| 1:F:177:THR:OG1  | 1:I:178:GLY:CA   | 2.65                     | 0.45              |
| 1:H:43:LYS:HA    | 1:H:46:GLU:HG2   | 1.98                     | 0.45              |
| 1:I:251:LEU:HD11 | 1:I:255:LYS:HE3  | 1.98                     | 0.45              |
| 1:J:136:VAL:O    | 1:J:140:VAL:HG13 | 2.17                     | 0.45              |
| 1:B:83:MET:O     | 1:G:82:GLN:NE2   | 2.49                     | 0.45              |
| 1:I:78:LEU:HD12  | 1:I:78:LEU:HA    | 1.74                     | 0.45              |
| 1:F:195:PRO:HD2  | 1:F:200:VAL:HG22 | 1.99                     | 0.45              |
| 1:B:84:GLY:HA2   | 1:G:177:THR:OG1  | 2.16                     | 0.45              |
| 1:D:197:PRO:CG   | 1:D:199:ARG:HH11 | 2.30                     | 0.45              |
| 1:E:163:ARG:O    | 1:E:165:ARG:HG2  | 2.17                     | 0.45              |
| 1:H:163:ARG:HE   | 1:H:165:ARG:NH1  | 2.14                     | 0.45              |
| 1:B:14:LYS:HB3   | 1:B:14:LYS:HE2   | 1.84                     | 0.44              |
| 1:B:81:ASN:HD21  | 1:G:103:SER:CB   | 2.29                     | 0.44              |
| 1:B:318:HIS:HB3  | 1:B:321:LEU:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:54:SER:HB3   | 1:B:78:LEU:HD11  | 2.00                     | 0.44              |
| 1:B:116:PHE:HZ   | 1:B:131:ARG:HG2  | 1.82                     | 0.44              |
| 1:D:137:ALA:O    | 1:D:140:VAL:HG12 | 2.17                     | 0.44              |
| 1:D:194:TRP:HB3  | 1:D:195:PRO:HD3  | 1.99                     | 0.44              |
| 2:D:401:CIT:O2   | 2:D:401:CIT:H42  | 2.18                     | 0.44              |
| 1:H:213:LYS:HG3  | 1:H:231:VAL:HG21 | 1.98                     | 0.44              |
| 1:H:269:LEU:HD11 | 1:H:311:LEU:HD11 | 1.98                     | 0.44              |
| 1:J:187:TRP:HA   | 1:J:188:PRO:HA   | 1.64                     | 0.44              |
| 1:A:43:LYS:HD2   | 1:A:43:LYS:HA    | 1.66                     | 0.44              |
| 1:I:16:TYR:CD1   | 1:I:249:LYS:HG3  | 2.53                     | 0.44              |
| 1:J:19:LYS:NZ    | 1:J:357:GLU:O    | 2.37                     | 0.44              |
| 1:F:50:PRO:O     | 1:F:53:ILE:HG12  | 2.17                     | 0.44              |
| 1:H:171:THR:N    | 5:H:506:HOH:O    | 2.51                     | 0.44              |
| 1:I:215:CYS:C    | 1:I:216:HIS:CG   | 2.95                     | 0.44              |
| 1:C:238:GLU:HG3  | 1:C:320:PHE:HE2  | 1.83                     | 0.44              |
| 1:D:194:TRP:HE3  | 1:D:194:TRP:O    | 2.00                     | 0.44              |
| 1:F:180:TRP:HB3  | 1:F:185:ALA:HA   | 2.00                     | 0.44              |
| 1:F:238:GLU:O    | 1:F:242:GLN:HG3  | 2.18                     | 0.44              |
| 1:D:140:VAL:O    | 1:D:146:ARG:HG2  | 2.17                     | 0.44              |
| 1:H:96:GLY:HA2   | 1:H:321:LEU:HD13 | 1.99                     | 0.44              |
| 1:H:254:LEU:HD11 | 1:H:303:ILE:HG21 | 1.98                     | 0.44              |
| 1:J:78:LEU:O     | 1:J:173:ALA:N    | 2.42                     | 0.44              |
| 1:B:284:LYS:HE2  | 1:B:284:LYS:HB3  | 1.83                     | 0.44              |
| 1:D:146:ARG:HD3  | 1:D:146:ARG:C    | 2.43                     | 0.44              |
| 1:H:43:LYS:HZ1   | 1:H:54:SER:HB3   | 1.82                     | 0.44              |
| 1:I:141:ASP:HA   | 1:I:146:ARG:HG2  | 2.00                     | 0.44              |
| 1:A:243:MET:HE3  | 1:A:243:MET:HB2  | 1.78                     | 0.44              |
| 1:E:258:ARG:NH2  | 1:E:259:ASP:OD1  | 2.50                     | 0.44              |
| 1:J:32:ARG:NH2   | 1:J:63:TYR:HB2   | 2.33                     | 0.44              |
| 1:A:179:ILE:HG23 | 1:A:208:PHE:HE1  | 1.83                     | 0.43              |
| 1:B:323:ASN:OD1  | 1:B:323:ASN:N    | 2.42                     | 0.43              |
| 1:D:23:ARG:NH1   | 1:D:259:ASP:OD2  | 2.51                     | 0.43              |
| 1:E:140:VAL:HB   | 1:E:149:VAL:HG13 | 2.00                     | 0.43              |
| 1:G:154:ASP:OD1  | 1:G:154:ASP:C    | 2.60                     | 0.43              |
| 1:H:45:VAL:HG13  | 1:H:135:LEU:HB3  | 1.99                     | 0.43              |
| 1:J:66:LEU:HD12  | 1:J:76:VAL:HG22  | 2.00                     | 0.43              |
| 1:A:148:VAL:HB   | 1:A:163:ARG:HG2  | 1.99                     | 0.43              |
| 1:B:194:TRP:HB2  | 1:B:286:PRO:CB   | 2.48                     | 0.43              |
| 1:B:209:ASN:HB2  | 1:B:233:GLN:HG2  | 1.99                     | 0.43              |
| 1:D:87:ASN:N     | 1:D:101:LYS:O    | 2.39                     | 0.43              |
| 1:J:32:ARG:NH2   | 1:J:66:LEU:HD22  | 2.33                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:202:GLU:O     | 1:J:206:GLU:HG2  | 2.18                     | 0.43              |
| 1:C:318:HIS:HB3   | 1:C:321:LEU:O    | 2.18                     | 0.43              |
| 1:E:82:GLN:HG3    | 1:E:85:VAL:HG22  | 1.99                     | 0.43              |
| 1:E:106:ARG:HA    | 1:E:106:ARG:NE   | 2.34                     | 0.43              |
| 1:G:189:LEU:HB2   | 1:G:192:ILE:CD1  | 2.48                     | 0.43              |
| 1:I:299:ARG:HA    | 1:I:299:ARG:HD3  | 1.74                     | 0.43              |
| 1:A:287:ARG:HG3   | 1:A:290:ASP:OD2  | 2.18                     | 0.43              |
| 1:B:51:ARG:HD2    | 1:B:112:LEU:CD2  | 2.49                     | 0.43              |
| 1:B:113:TRP:O     | 1:B:117:ILE:HG13 | 2.18                     | 0.43              |
| 1:J:234:PHE:O     | 1:J:238:GLU:HG2  | 2.17                     | 0.43              |
| 1:G:299:ARG:HA    | 1:G:299:ARG:HD3  | 1.77                     | 0.43              |
| 1:I:116:PHE:CD1   | 1:I:127:LYS:HG3  | 2.53                     | 0.43              |
| 1:J:32:ARG:CZ     | 1:J:63:TYR:HB2   | 2.48                     | 0.43              |
| 1:I:126:ARG:HG3   | 1:I:228:ASP:OD1  | 2.19                     | 0.43              |
| 1:D:181:PRO:HD3   | 1:D:208:PHE:CD1  | 2.54                     | 0.43              |
| 1:E:268:PRO:HG3   | 1:E:334:ALA:HB1  | 2.00                     | 0.43              |
| 1:G:56:LEU:HD23   | 1:G:56:LEU:HA    | 1.81                     | 0.43              |
| 1:H:94:LEU:HD13   | 1:H:97:CYS:O     | 2.18                     | 0.43              |
| 1:I:40:ASP:HA     | 1:I:43:LYS:HG2   | 2.00                     | 0.43              |
| 1:I:315:ARG:CD    | 1:I:317:PRO:HD3  | 2.48                     | 0.43              |
| 1:J:336:GLU:OE2   | 1:J:340:LYS:HE2  | 2.18                     | 0.43              |
| 1:A:226:GLU:HG2   | 1:A:227:SER:N    | 2.34                     | 0.43              |
| 1:B:145:TYR:O     | 1:B:149:VAL:HG23 | 2.19                     | 0.43              |
| 1:B:287:ARG:HD3   | 1:B:289:SER:OG   | 2.19                     | 0.43              |
| 1:D:340:LYS:HE3   | 1:D:340:LYS:HB2  | 1.76                     | 0.43              |
| 1:E:62[B]:ARG:NH1 | 4:E:402:CTP:H2'  | 2.33                     | 0.43              |
| 1:H:318:HIS:HB3   | 1:H:321:LEU:O    | 2.19                     | 0.43              |
| 1:C:152:VAL:HB    | 1:C:159:LYS:HB2  | 2.01                     | 0.43              |
| 1:D:83:MET:HB2    | 1:D:85:VAL:HG13  | 2.01                     | 0.43              |
| 1:C:211:LEU:HD23  | 1:C:213:LYS:HE3  | 2.01                     | 0.42              |
| 1:A:107:LYS:HE3   | 1:A:107:LYS:HB2  | 1.44                     | 0.42              |
| 1:E:181:PRO:HD3   | 1:E:208:PHE:CD1  | 2.54                     | 0.42              |
| 1:H:358:LYS:HD3   | 1:H:358:LYS:HA   | 1.82                     | 0.42              |
| 1:I:146:ARG:NH2   | 1:I:150:LYS:HA   | 2.33                     | 0.42              |
| 1:I:315:ARG:HD3   | 1:I:316:CYS:N    | 2.34                     | 0.42              |
| 1:B:16:TYR:CD1    | 1:B:249:LYS:HG3  | 2.54                     | 0.42              |
| 1:B:132:PHE:CD2   | 1:B:158:VAL:HG21 | 2.55                     | 0.42              |
| 1:B:343:TRP:CZ2   | 1:B:347:ARG:HD2  | 2.55                     | 0.42              |
| 1:I:227:SER:HB3   | 1:I:228:ASP:H    | 1.46                     | 0.42              |
| 1:J:192:ILE:HD13  | 1:J:283:GLU:HG2  | 2.00                     | 0.42              |
| 1:J:299:ARG:HH11  | 1:J:299:ARG:CA   | 2.31                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:197:PRO:HG3  | 3:A:402:TMO:HABA | 2.01                     | 0.42              |
| 1:B:287:ARG:HB3  | 1:B:290:ASP:OD2  | 2.19                     | 0.42              |
| 1:F:194:TRP:CD2  | 1:F:195:PRO:HB3  | 2.55                     | 0.42              |
| 1:I:130:SER:O    | 1:I:134:THR:HG23 | 2.18                     | 0.42              |
| 1:C:16:TYR:HA    | 1:C:20:CYS:HB2   | 2.02                     | 0.42              |
| 1:A:44:GLU:O     | 1:A:47:VAL:HG22  | 2.18                     | 0.42              |
| 1:D:195:PRO:HD2  | 1:D:200:VAL:CG2  | 2.49                     | 0.42              |
| 1:G:356:LEU:HD23 | 1:G:359:LEU:HD12 | 2.02                     | 0.42              |
| 1:H:36:LYS:HD2   | 1:H:36:LYS:HA    | 1.74                     | 0.42              |
| 1:J:14:LYS:HZ1   | 1:J:357:GLU:CD   | 2.27                     | 0.42              |
| 1:B:301:ASN:ND2  | 1:B:350:LEU:HD22 | 2.34                     | 0.42              |
| 1:D:254:LEU:HD11 | 1:D:303:ILE:HG21 | 2.02                     | 0.42              |
| 1:E:107:LYS:O    | 1:E:108:ARG:C    | 2.61                     | 0.42              |
| 1:E:343:TRP:CZ2  | 1:E:347:ARG:HD3  | 2.55                     | 0.42              |
| 1:H:16:TYR:O     | 1:H:20:CYS:HB2   | 2.20                     | 0.42              |
| 1:H:284:LYS:HB3  | 1:H:284:LYS:HE2  | 1.97                     | 0.42              |
| 1:I:240:ARG:HA   | 1:I:243:MET:HG2  | 2.02                     | 0.42              |
| 1:J:272:TYR:OH   | 1:J:318:HIS:NE2  | 2.50                     | 0.42              |
| 1:B:195:PRO:CB   | 1:B:199:ARG:HG2  | 2.50                     | 0.42              |
| 1:G:350:LEU:HG   | 1:G:350:LEU:H    | 1.67                     | 0.42              |
| 2:C:401:CIT:O3   | 2:C:401:CIT:O7   | 2.22                     | 0.42              |
| 1:A:82:GLN:HB3   | 1:A:174:PHE:CE1  | 2.55                     | 0.42              |
| 1:E:57:ASN:OD1   | 1:E:57:ASN:N     | 2.52                     | 0.42              |
| 1:F:115:GLU:OE2  | 1:F:131:ARG:NH1  | 2.52                     | 0.42              |
| 1:H:84:GLY:C     | 1:H:86:PHE:H     | 2.27                     | 0.42              |
| 2:I:401:CIT:O1   | 2:I:401:CIT:H42  | 2.19                     | 0.42              |
| 1:J:180:TRP:HE1  | 1:J:185:ALA:N    | 2.18                     | 0.42              |
| 1:E:29:LYS:HA    | 1:E:32:ARG:NH1   | 2.35                     | 0.42              |
| 1:E:277:LEU:HD11 | 1:E:307:LEU:HD13 | 2.02                     | 0.42              |
| 1:H:45:VAL:HG13  | 1:H:135:LEU:HD23 | 2.01                     | 0.42              |
| 1:H:343:TRP:NE1  | 1:H:347:ARG:HH11 | 2.17                     | 0.42              |
| 1:I:254:LEU:HD11 | 1:I:303:ILE:HG21 | 2.02                     | 0.42              |
| 1:J:238:GLU:HG3  | 1:J:275:LYS:HZ3  | 1.83                     | 0.42              |
| 1:A:16:TYR:O     | 1:A:20:CYS:HB2   | 2.19                     | 0.41              |
| 1:B:116:PHE:HD1  | 1:B:127:LYS:HB3  | 1.84                     | 0.41              |
| 1:E:191:HIS:CD2  | 1:E:191:HIS:H    | 2.38                     | 0.41              |
| 1:H:228:ASP:OD1  | 1:H:228:ASP:O    | 2.37                     | 0.41              |
| 2:H:401:CIT:H21  | 1:J:354:LYS:NZ   | 2.35                     | 0.41              |
| 1:I:62:ARG:HG3   | 1:I:63:TYR:H     | 1.84                     | 0.41              |
| 1:D:175:LYS:HE3  | 1:D:177:THR:CG2  | 2.50                     | 0.41              |
| 1:F:287:ARG:HD3  | 1:F:290:ASP:HB2  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:164:ASP:HB3   | 1:I:165:ARG:HH11  | 1.84                     | 0.41              |
| 1:F:46:GLU:HG2    | 1:I:110:MET:SD    | 2.60                     | 0.41              |
| 1:H:46:GLU:HA     | 1:H:49:GLU:O      | 2.20                     | 0.41              |
| 1:I:189:LEU:HD13  | 1:I:191:HIS:HE1   | 1.86                     | 0.41              |
| 4:I:402:CTP:O3G   | 4:I:402:CTP:H3'   | 2.20                     | 0.41              |
| 1:C:354:LYS:HZ2   | 2:C:401:CIT:H42   | 1.86                     | 0.41              |
| 1:B:42:LEU:HD23   | 1:B:42:LEU:HA     | 1.83                     | 0.41              |
| 1:F:180:TRP:O     | 1:F:181:PRO:O     | 2.38                     | 0.41              |
| 1:G:157:GLU:OE2   | 1:G:213:LYS:HB2   | 2.19                     | 0.41              |
| 1:B:85:VAL:O      | 1:B:86:PHE:CD2    | 2.73                     | 0.41              |
| 1:D:195:PRO:HG2   | 1:D:199:ARG:HB2   | 2.00                     | 0.41              |
| 1:E:5:GLN:NE2     | 1:E:298:ASP:OD2   | 2.53                     | 0.41              |
| 1:F:16:TYR:CD1    | 1:F:249:LYS:HG3   | 2.55                     | 0.41              |
| 1:I:187:TRP:HA    | 1:I:188:PRO:HA    | 1.78                     | 0.41              |
| 1:J:191:HIS:CG    | 1:J:192:ILE:HD12  | 2.55                     | 0.41              |
| 1:J:277:LEU:HD22  | 1:J:306:GLN:HG3   | 2.02                     | 0.41              |
| 1:F:93:SER:OG     | 1:F:94:LEU:N      | 2.51                     | 0.41              |
| 1:F:340:LYS:HB2   | 1:F:340:LYS:HZ2   | 1.84                     | 0.41              |
| 1:H:95:PRO:HG2    | 1:H:216:HIS:NE2   | 2.36                     | 0.41              |
| 1:J:161:ARG:HA    | 1:J:167:VAL:HG22  | 2.01                     | 0.41              |
| 1:J:249:LYS:NZ    | 1:J:293:GLU:OE1   | 2.43                     | 0.41              |
| 1:C:83[A]:MET:HG2 | 1:C:111:SER:HA    | 2.03                     | 0.41              |
| 1:B:57:ASN:HB3    | 1:B:59:MET:HE2    | 2.01                     | 0.41              |
| 1:D:32:ARG:NH2    | 1:D:33:GLU:OE2    | 2.54                     | 0.41              |
| 1:D:197:PRO:HD2   | 1:D:199:ARG:HH11  | 1.86                     | 0.41              |
| 1:J:210:LEU:C     | 1:J:211:LEU:HD23  | 2.46                     | 0.41              |
| 1:C:89:VAL:HB     | 1:C:99:VAL:HG12   | 2.03                     | 0.41              |
| 1:A:163:ARG:O     | 1:A:165:ARG:HG3   | 2.20                     | 0.41              |
| 1:B:311:LEU:O     | 1:B:314:ARG:NH1   | 2.51                     | 0.41              |
| 1:E:90:ASP:OD1    | 1:E:183:SER:OG    | 2.33                     | 0.41              |
| 1:F:81:ASN:O      | 1:F:82:GLN:NE2    | 2.53                     | 0.41              |
| 1:G:194:TRP:CG    | 1:G:195:PRO:HA    | 2.56                     | 0.41              |
| 1:H:87:ASN:N      | 1:H:101:LYS:O     | 2.37                     | 0.41              |
| 1:H:164:ASP:OD1   | 5:H:501:HOH:O     | 2.22                     | 0.41              |
| 1:I:181:PRO:HD3   | 1:I:208:PHE:CD2   | 2.56                     | 0.41              |
| 1:J:299:ARG:HA    | 1:J:299:ARG:HD3   | 1.84                     | 0.41              |
| 1:A:82:GLN:HA     | 1:A:83[B]:MET:HE3 | 2.03                     | 0.41              |
| 1:A:347:ARG:HA    | 1:A:347:ARG:HD2   | 1.86                     | 0.41              |
| 1:B:34:VAL:HG13   | 1:B:168:VAL:HG21  | 2.03                     | 0.41              |
| 1:B:194:TRP:HB2   | 1:B:286:PRO:HB3   | 2.03                     | 0.41              |
| 1:D:24:LYS:HE2    | 4:D:402:CTP:O2B   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:125:ALA:HB1   | 1:D:212:SER:HB2  | 2.02                     | 0.41              |
| 1:D:202:GLU:OE2   | 1:D:240:ARG:HD2  | 2.21                     | 0.41              |
| 1:E:106:ARG:HA    | 1:E:106:ARG:HE   | 1.86                     | 0.41              |
| 1:E:318:HIS:HB3   | 1:E:321:LEU:O    | 2.20                     | 0.41              |
| 1:G:93:SER:O      | 1:G:94:LEU:HD23  | 2.21                     | 0.41              |
| 1:G:292:ASP:OD2   | 1:G:294:SER:OG   | 2.39                     | 0.41              |
| 1:G:318:HIS:HB3   | 1:G:321:LEU:O    | 2.20                     | 0.41              |
| 1:I:116:PHE:HD1   | 1:I:127:LYS:HG3  | 1.86                     | 0.41              |
| 1:I:186:HIS:HB2   | 1:I:189:LEU:HD21 | 2.03                     | 0.41              |
| 1:I:356:LEU:HA    | 1:I:359:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:215:CYS:O     | 1:C:216:HIS:CG   | 2.74                     | 0.41              |
| 1:B:112:LEU:HD23  | 1:B:112:LEU:O    | 2.21                     | 0.41              |
| 1:D:277:LEU:HD11  | 1:D:307:LEU:HD13 | 2.03                     | 0.41              |
| 1:H:126:ARG:HH12  | 1:H:227:SER:N    | 2.19                     | 0.41              |
| 1:C:58:GLU:HB2    | 1:C:63:TYR:CE1   | 2.56                     | 0.41              |
| 1:C:238:GLU:HB3   | 1:C:275:LYS:HE2  | 2.03                     | 0.41              |
| 1:A:83[B]:MET:HE2 | 1:A:112:LEU:N    | 2.31                     | 0.40              |
| 1:H:299:ARG:HA    | 1:H:299:ARG:HD3  | 1.63                     | 0.40              |
| 1:I:161:ARG:NH1   | 1:I:164:ASP:O    | 2.55                     | 0.40              |
| 1:J:181:PRO:O     | 1:J:185:ALA:HB2  | 2.20                     | 0.40              |
| 1:J:234:PHE:O     | 1:J:235:ALA:C    | 2.65                     | 0.40              |
| 1:E:34:VAL:HG22   | 1:E:162:ILE:HD12 | 2.03                     | 0.40              |
| 1:E:85:VAL:HG23   | 1:E:86:PHE:CG    | 2.55                     | 0.40              |
| 1:J:31:ILE:O      | 1:J:34:VAL:HG12  | 2.21                     | 0.40              |
| 1:J:180:TRP:NE1   | 1:J:185:ALA:CA   | 2.78                     | 0.40              |
| 1:C:194:TRP:CD1   | 1:C:195:PRO:HA   | 2.56                     | 0.40              |
| 1:D:103:SER:H     | 1:D:107:LYS:HD2  | 1.86                     | 0.40              |
| 1:D:132:PHE:O     | 1:D:136:VAL:HG23 | 2.21                     | 0.40              |
| 1:E:107:LYS:O     | 1:E:109:SER:N    | 2.53                     | 0.40              |
| 1:F:32:ARG:HH22   | 1:F:58:GLU:CD    | 2.30                     | 0.40              |
| 1:F:285:HIS:HA    | 1:F:287:ARG:HH21 | 1.86                     | 0.40              |
| 1:J:163:ARG:HH21  | 1:J:165:ARG:CZ   | 2.34                     | 0.40              |
| 1:A:179:ILE:HG23  | 1:A:208:PHE:CE1  | 2.57                     | 0.40              |
| 1:D:299:ARG:HA    | 1:D:299:ARG:HD3  | 1.71                     | 0.40              |
| 1:E:180:TRP:CD2   | 1:E:204:LYS:HG2  | 2.56                     | 0.40              |
| 1:J:48:GLN:HG2    | 1:J:138:GLN:NE2  | 2.33                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:B:32:ARG:NH1 | 1:F:154:ASP:OD2[2_846] | 2.13                     | 0.07              |

## 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     | 345/362 (95%)   | 337 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 1   | B     | 343/362 (95%)   | 333 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 1   | C     | 351/362 (97%)   | 344 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 1   | D     | 336/362 (93%)   | 320 (95%)  | 15 (4%) | 1 (0%)   | 36          | 45  |
| 1   | E     | 343/362 (95%)   | 333 (97%)  | 8 (2%)  | 2 (1%)   | 21          | 29  |
| 1   | F     | 327/362 (90%)   | 310 (95%)  | 15 (5%) | 2 (1%)   | 21          | 29  |
| 1   | G     | 348/362 (96%)   | 339 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 1   | H     | 337/362 (93%)   | 326 (97%)  | 11 (3%) | 0        | 100         | 100 |
| 1   | I     | 340/362 (94%)   | 335 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | J     | 266/362 (74%)   | 255 (96%)  | 11 (4%) | 0        | 100         | 100 |
| All | All   | 3336/3620 (92%) | 3232 (97%) | 99 (3%) | 5 (0%)   | 43          | 61  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 195 | PRO  |
| 1   | E     | 108 | ARG  |
| 1   | E     | 104 | ASP  |
| 1   | F     | 61  | ASN  |
| 1   | F     | 181 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 311/317 (98%)   | 296 (95%)  | 15 (5%)  | 23          | 35 |
| 1   | B     | 307/317 (97%)   | 294 (96%)  | 13 (4%)  | 26          | 40 |
| 1   | C     | 313/317 (99%)   | 291 (93%)  | 22 (7%)  | 14          | 19 |
| 1   | D     | 301/317 (95%)   | 284 (94%)  | 17 (6%)  | 19          | 29 |
| 1   | E     | 309/317 (98%)   | 292 (94%)  | 17 (6%)  | 19          | 29 |
| 1   | F     | 299/317 (94%)   | 279 (93%)  | 20 (7%)  | 15          | 21 |
| 1   | G     | 310/317 (98%)   | 294 (95%)  | 16 (5%)  | 21          | 32 |
| 1   | H     | 304/317 (96%)   | 283 (93%)  | 21 (7%)  | 14          | 20 |
| 1   | I     | 306/317 (96%)   | 291 (95%)  | 15 (5%)  | 22          | 34 |
| 1   | J     | 251/317 (79%)   | 230 (92%)  | 21 (8%)  | 10          | 14 |
| All | All   | 3011/3170 (95%) | 2834 (94%) | 177 (6%) | 18          | 27 |

All (177) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | GLU  |
| 1   | A     | 39  | SER  |
| 1   | A     | 67  | GLU  |
| 1   | A     | 94  | LEU  |
| 1   | A     | 99  | VAL  |
| 1   | A     | 106 | ARG  |
| 1   | A     | 107 | LYS  |
| 1   | A     | 109 | SER  |
| 1   | A     | 149 | VAL  |
| 1   | A     | 179 | ILE  |
| 1   | A     | 183 | SER  |
| 1   | A     | 215 | CYS  |
| 1   | A     | 240 | ARG  |
| 1   | A     | 323 | ASN  |
| 1   | A     | 328 | GLN  |
| 1   | B     | 34  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 56  | LEU  |
| 1   | B     | 67  | GLU  |
| 1   | B     | 82  | GLN  |
| 1   | B     | 83  | MET  |
| 1   | B     | 88  | PHE  |
| 1   | B     | 138 | GLN  |
| 1   | B     | 179 | ILE  |
| 1   | B     | 191 | HIS  |
| 1   | B     | 227 | SER  |
| 1   | B     | 233 | GLN  |
| 1   | B     | 299 | ARG  |
| 1   | B     | 315 | ARG  |
| 1   | D     | 39  | SER  |
| 1   | D     | 43  | LYS  |
| 1   | D     | 47  | VAL  |
| 1   | D     | 63  | TYR  |
| 1   | D     | 89  | VAL  |
| 1   | D     | 103 | SER  |
| 1   | D     | 106 | ARG  |
| 1   | D     | 115 | GLU  |
| 1   | D     | 138 | GLN  |
| 1   | D     | 142 | LYS  |
| 1   | D     | 146 | ARG  |
| 1   | D     | 183 | SER  |
| 1   | D     | 191 | HIS  |
| 1   | D     | 194 | TRP  |
| 1   | D     | 214 | GLU  |
| 1   | D     | 248 | LYS  |
| 1   | D     | 344 | ARG  |
| 1   | E     | 34  | VAL  |
| 1   | E     | 48  | GLN  |
| 1   | E     | 57  | ASN  |
| 1   | E     | 64  | GLU  |
| 1   | E     | 81  | ASN  |
| 1   | E     | 85  | VAL  |
| 1   | E     | 88  | PHE  |
| 1   | E     | 101 | LYS  |
| 1   | E     | 107 | LYS  |
| 1   | E     | 156 | SER  |
| 1   | E     | 165 | ARG  |
| 1   | E     | 199 | ARG  |
| 1   | E     | 240 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 248 | LYS  |
| 1   | E     | 267 | GLN  |
| 1   | E     | 323 | ASN  |
| 1   | E     | 350 | LEU  |
| 1   | F     | 0   | MET  |
| 1   | F     | 2   | ILE  |
| 1   | F     | 21  | GLN  |
| 1   | F     | 59  | MET  |
| 1   | F     | 60  | ASP  |
| 1   | F     | 82  | GLN  |
| 1   | F     | 86  | PHE  |
| 1   | F     | 94  | LEU  |
| 1   | F     | 120 | SER  |
| 1   | F     | 180 | TRP  |
| 1   | F     | 182 | ARG  |
| 1   | F     | 183 | SER  |
| 1   | F     | 192 | ILE  |
| 1   | F     | 194 | TRP  |
| 1   | F     | 199 | ARG  |
| 1   | F     | 212 | SER  |
| 1   | F     | 287 | ARG  |
| 1   | F     | 290 | ASP  |
| 1   | F     | 299 | ARG  |
| 1   | F     | 340 | LYS  |
| 1   | G     | 0   | MET  |
| 1   | G     | 34  | VAL  |
| 1   | G     | 36  | LYS  |
| 1   | G     | 39  | SER  |
| 1   | G     | 57  | ASN  |
| 1   | G     | 81  | ASN  |
| 1   | G     | 94  | LEU  |
| 1   | G     | 99  | VAL  |
| 1   | G     | 103 | SER  |
| 1   | G     | 110 | MET  |
| 1   | G     | 146 | ARG  |
| 1   | G     | 154 | ASP  |
| 1   | G     | 214 | GLU  |
| 1   | G     | 294 | SER  |
| 1   | G     | 315 | ARG  |
| 1   | G     | 350 | LEU  |
| 1   | H     | 2   | ILE  |
| 1   | H     | 34  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 36  | LYS  |
| 1   | H     | 44  | GLU  |
| 1   | H     | 53  | ILE  |
| 1   | H     | 55  | SER  |
| 1   | H     | 56  | LEU  |
| 1   | H     | 82  | GLN  |
| 1   | H     | 87  | ASN  |
| 1   | H     | 89  | VAL  |
| 1   | H     | 94  | LEU  |
| 1   | H     | 134 | THR  |
| 1   | H     | 140 | VAL  |
| 1   | H     | 141 | ASP  |
| 1   | H     | 146 | ARG  |
| 1   | H     | 191 | HIS  |
| 1   | H     | 214 | GLU  |
| 1   | H     | 250 | CYS  |
| 1   | H     | 299 | ARG  |
| 1   | H     | 323 | ASN  |
| 1   | H     | 328 | GLN  |
| 1   | I     | 2   | ILE  |
| 1   | I     | 34  | VAL  |
| 1   | I     | 53  | ILE  |
| 1   | I     | 56  | LEU  |
| 1   | I     | 57  | ASN  |
| 1   | I     | 58  | GLU  |
| 1   | I     | 64  | GLU  |
| 1   | I     | 112 | LEU  |
| 1   | I     | 149 | VAL  |
| 1   | I     | 165 | ARG  |
| 1   | I     | 227 | SER  |
| 1   | I     | 233 | GLN  |
| 1   | I     | 236 | GLU  |
| 1   | I     | 315 | ARG  |
| 1   | I     | 330 | LYS  |
| 1   | J     | 14  | LYS  |
| 1   | J     | 29  | LYS  |
| 1   | J     | 30  | THR  |
| 1   | J     | 43  | LYS  |
| 1   | J     | 45  | VAL  |
| 1   | J     | 48  | GLN  |
| 1   | J     | 70  | SER  |
| 1   | J     | 99  | VAL  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | J     | 122   | TYR  |
| 1   | J     | 164   | ASP  |
| 1   | J     | 166   | TYR  |
| 1   | J     | 182   | ARG  |
| 1   | J     | 191   | HIS  |
| 1   | J     | 192   | ILE  |
| 1   | J     | 202   | GLU  |
| 1   | J     | 233   | GLN  |
| 1   | J     | 248   | LYS  |
| 1   | J     | 250   | CYS  |
| 1   | J     | 294   | SER  |
| 1   | J     | 299   | ARG  |
| 1   | J     | 301   | ASN  |
| 1   | C     | 2     | ILE  |
| 1   | C     | 5     | GLN  |
| 1   | C     | 34    | VAL  |
| 1   | C     | 47    | VAL  |
| 1   | C     | 64    | GLU  |
| 1   | C     | 67    | GLU  |
| 1   | C     | 77    | VAL  |
| 1   | C     | 83[A] | MET  |
| 1   | C     | 83[B] | MET  |
| 1   | C     | 99    | VAL  |
| 1   | C     | 103   | SER  |
| 1   | C     | 107   | LYS  |
| 1   | C     | 115   | GLU  |
| 1   | C     | 138   | GLN  |
| 1   | C     | 149   | VAL  |
| 1   | C     | 182   | ARG  |
| 1   | C     | 191   | HIS  |
| 1   | C     | 206   | GLU  |
| 1   | C     | 215   | CYS  |
| 1   | C     | 248   | LYS  |
| 1   | C     | 287   | ARG  |
| 1   | C     | 315   | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | GLN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 133 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 198 | ASN  |
| 1   | A     | 301 | ASN  |
| 1   | A     | 328 | GLN  |
| 1   | B     | 57  | ASN  |
| 1   | B     | 81  | ASN  |
| 1   | B     | 82  | GLN  |
| 1   | B     | 301 | ASN  |
| 1   | D     | 81  | ASN  |
| 1   | D     | 82  | GLN  |
| 1   | D     | 186 | HIS  |
| 1   | D     | 209 | ASN  |
| 1   | D     | 233 | GLN  |
| 1   | D     | 267 | GLN  |
| 1   | D     | 285 | HIS  |
| 1   | E     | 48  | GLN  |
| 1   | E     | 82  | GLN  |
| 1   | E     | 191 | HIS  |
| 1   | E     | 261 | HIS  |
| 1   | E     | 271 | ASN  |
| 1   | E     | 306 | GLN  |
| 1   | F     | 5   | GLN  |
| 1   | F     | 21  | GLN  |
| 1   | F     | 82  | GLN  |
| 1   | F     | 209 | ASN  |
| 1   | F     | 233 | GLN  |
| 1   | G     | 82  | GLN  |
| 1   | G     | 191 | HIS  |
| 1   | G     | 198 | ASN  |
| 1   | H     | 21  | GLN  |
| 1   | H     | 82  | GLN  |
| 1   | H     | 87  | ASN  |
| 1   | H     | 186 | HIS  |
| 1   | H     | 216 | HIS  |
| 1   | H     | 242 | GLN  |
| 1   | H     | 328 | GLN  |
| 1   | I     | 11  | HIS  |
| 1   | I     | 191 | HIS  |
| 1   | I     | 271 | ASN  |
| 1   | J     | 21  | GLN  |
| 1   | J     | 138 | GLN  |
| 1   | C     | 48  | GLN  |
| 1   | C     | 191 | HIS  |

### 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 ⓘ

24 ligands are modelled in this entry.

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 |
| 4   | CTP  | G     | 402 | -    | 29,30,30     | 1.00 | 1 (3%)   | 43,47,47    | 0.84 | 0        |
| 2   | CIT  | H     | 402 | -    | 12,12,12     | 1.08 | 0        | 17,17,17    | 1.47 | 2 (11%)  |
| 4   | CTP  | F     | 403 | -    | 29,30,30     | 1.05 | 2 (6%)   | 43,47,47    | 0.87 | 1 (2%)   |
| 4   | CTP  | B     | 402 | -    | 29,30,30     | 1.03 | 1 (3%)   | 43,47,47    | 0.86 | 1 (2%)   |
| 3   | TMO  | A     | 402 | -    | 4,4,4        | 1.89 | 3 (75%)  | 6,6,6       | 0.24 | 0        |
| 4   | CTP  | H     | 403 | -    | 29,30,30     | 1.00 | 0        | 43,47,47    | 0.92 | 1 (2%)   |
| 4   | CTP  | C     | 404 | -    | 29,30,30     | 1.02 | 1 (3%)   | 43,47,47    | 0.85 | 0        |
| 4   | CTP  | J     | 401 | -    | 29,30,30     | 1.09 | 3 (10%)  | 43,47,47    | 1.01 | 2 (4%)   |
| 2   | CIT  | G     | 401 | -    | 12,12,12     | 1.07 | 0        | 17,17,17    | 1.50 | 1 (5%)   |
| 2   | CIT  | F     | 401 | -    | 12,12,12     | 1.06 | 0        | 17,17,17    | 1.76 | 5 (29%)  |
| 2   | CIT  | C     | 401 | -    | 12,12,12     | 1.21 | 1 (8%)   | 17,17,17    | 1.21 | 1 (5%)   |
| 4   | CTP  | A     | 403 | -    | 29,30,30     | 1.00 | 1 (3%)   | 43,47,47    | 0.91 | 2 (4%)   |
| 2   | CIT  | A     | 401 | -    | 12,12,12     | 1.05 | 0        | 17,17,17    | 1.52 | 1 (5%)   |
| 4   | CTP  | D     | 402 | -    | 29,30,30     | 1.03 | 0        | 43,47,47    | 0.89 | 1 (2%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | CIT  | D     | 401 | -    | 12,12,12     | 1.05 | 0        | 17,17,17    | 1.55 | 3 (17%)  |
| 2   | CIT  | H     | 401 | -    | 12,12,12     | 1.03 | 0        | 17,17,17    | 1.51 | 2 (11%)  |
| 2   | CIT  | E     | 401 | -    | 12,12,12     | 1.08 | 0        | 17,17,17    | 1.47 | 3 (17%)  |
| 3   | TMO  | F     | 402 | -    | 4,4,4        | 1.86 | 1 (25%)  | 6,6,6       | 0.23 | 0        |
| 2   | CIT  | I     | 401 | -    | 12,12,12     | 1.05 | 0        | 17,17,17    | 1.59 | 4 (23%)  |
| 3   | TMO  | C     | 403 | -    | 4,4,4        | 1.87 | 2 (50%)  | 6,6,6       | 0.22 | 0        |
| 2   | CIT  | B     | 401 | -    | 12,12,12     | 1.05 | 0        | 17,17,17    | 1.55 | 2 (11%)  |
| 3   | TMO  | C     | 402 | -    | 4,4,4        | 1.91 | 2 (50%)  | 6,6,6       | 0.22 | 0        |
| 4   | CTP  | E     | 402 | -    | 29,30,30     | 0.98 | 0        | 43,47,47    | 0.88 | 1 (2%)   |
| 4   | CTP  | I     | 402 | -    | 29,30,30     | 1.09 | 3 (10%)  | 43,47,47    | 0.99 | 1 (2%)   |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 4   | CTP  | G     | 402 | -    | -       | 7/22/38/38  | 0/2/2/2 |
| 2   | CIT  | H     | 402 | -    | -       | 8/16/16/16  | -       |
| 4   | CTP  | F     | 403 | -    | -       | 8/22/38/38  | 0/2/2/2 |
| 4   | CTP  | B     | 402 | -    | -       | 6/22/38/38  | 0/2/2/2 |
| 4   | CTP  | H     | 403 | -    | -       | 6/22/38/38  | 0/2/2/2 |
| 4   | CTP  | C     | 404 | -    | -       | 3/22/38/38  | 0/2/2/2 |
| 4   | CTP  | J     | 401 | -    | -       | 4/22/38/38  | 0/2/2/2 |
| 2   | CIT  | G     | 401 | -    | -       | 8/16/16/16  | -       |
| 2   | CIT  | F     | 401 | -    | -       | 14/16/16/16 | -       |
| 2   | CIT  | C     | 401 | -    | -       | 8/16/16/16  | -       |
| 4   | CTP  | A     | 403 | -    | -       | 1/22/38/38  | 0/2/2/2 |
| 2   | CIT  | A     | 401 | -    | -       | 4/16/16/16  | -       |
| 4   | CTP  | D     | 402 | -    | -       | 6/22/38/38  | 0/2/2/2 |
| 2   | CIT  | D     | 401 | -    | -       | 10/16/16/16 | -       |
| 2   | CIT  | H     | 401 | -    | -       | 7/16/16/16  | -       |
| 2   | CIT  | E     | 401 | -    | -       | 5/16/16/16  | -       |
| 2   | CIT  | I     | 401 | -    | -       | 8/16/16/16  | -       |
| 2   | CIT  | B     | 401 | -    | -       | 4/16/16/16  | -       |
| 4   | CTP  | E     | 402 | -    | -       | 4/22/38/38  | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 4   | CTP  | I     | 402 | -    | -       | 10/22/38/38 | 0/2/2/2 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | I     | 402 | CTP  | PA-O3A  | 2.46  | 1.62        | 1.59     |
| 4   | J     | 401 | CTP  | PB-O3A  | 2.42  | 1.62        | 1.59     |
| 2   | C     | 401 | CIT  | C3-C6   | -2.29 | 1.51        | 1.53     |
| 4   | J     | 401 | CTP  | PA-O3A  | 2.27  | 1.61        | 1.59     |
| 4   | C     | 404 | CTP  | PA-O3A  | 2.18  | 1.61        | 1.59     |
| 4   | A     | 403 | CTP  | PA-O3A  | 2.16  | 1.61        | 1.59     |
| 4   | F     | 403 | CTP  | PB-O3B  | 2.13  | 1.61        | 1.59     |
| 4   | B     | 402 | CTP  | PA-O3A  | 2.13  | 1.61        | 1.59     |
| 3   | C     | 402 | TMO  | CAA-NAC | -2.11 | 1.45        | 1.48     |
| 4   | I     | 402 | CTP  | PB-O3B  | 2.10  | 1.61        | 1.59     |
| 3   | A     | 402 | TMO  | CAA-NAC | -2.07 | 1.45        | 1.48     |
| 3   | C     | 402 | TMO  | CAB-NAC | -2.06 | 1.45        | 1.48     |
| 4   | I     | 402 | CTP  | PB-O3A  | 2.03  | 1.61        | 1.59     |
| 3   | C     | 403 | TMO  | CAB-NAC | -2.02 | 1.45        | 1.48     |
| 3   | C     | 403 | TMO  | CAA-NAC | -2.02 | 1.45        | 1.48     |
| 4   | G     | 402 | CTP  | C4-N3   | 2.02  | 1.38        | 1.34     |
| 3   | F     | 402 | TMO  | CAD-NAC | -2.01 | 1.45        | 1.48     |
| 4   | F     | 403 | CTP  | PB-O3A  | 2.01  | 1.61        | 1.59     |
| 3   | A     | 402 | TMO  | CAB-NAC | -2.01 | 1.45        | 1.48     |
| 3   | A     | 402 | TMO  | CAD-NAC | -2.00 | 1.45        | 1.48     |
| 4   | J     | 401 | CTP  | C4-N3   | 2.00  | 1.38        | 1.34     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | B     | 401 | CIT  | O6-C6-C3 | 4.02 | 120.86      | 113.14   |
| 2   | A     | 401 | CIT  | O6-C6-C3 | 3.93 | 120.69      | 113.14   |
| 2   | E     | 401 | CIT  | O6-C6-C3 | 3.90 | 120.62      | 113.14   |
| 2   | I     | 401 | CIT  | O6-C6-C3 | 3.80 | 120.42      | 113.14   |
| 2   | F     | 401 | CIT  | O6-C6-C3 | 3.62 | 120.08      | 113.14   |
| 2   | G     | 401 | CIT  | O6-C6-C3 | 3.58 | 120.02      | 113.14   |
| 2   | H     | 402 | CIT  | O6-C6-C3 | 3.54 | 119.93      | 113.14   |
| 2   | D     | 401 | CIT  | O6-C6-C3 | 3.50 | 119.86      | 113.14   |
| 2   | H     | 401 | CIT  | O6-C6-C3 | 3.29 | 119.44      | 113.14   |
| 2   | F     | 401 | CIT  | O2-C1-C2 | 3.06 | 124.04      | 114.35   |
| 2   | C     | 401 | CIT  | O6-C6-C3 | 2.90 | 118.71      | 113.14   |
| 2   | D     | 401 | CIT  | O2-C1-C2 | 2.44 | 122.09      | 114.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | F     | 403 | CTP  | C3'-C2'-C1' | 2.42  | 106.04      | 101.46   |
| 4   | H     | 403 | CTP  | C3'-C2'-C1' | 2.39  | 105.98      | 101.46   |
| 4   | B     | 402 | CTP  | C3'-C2'-C1' | 2.39  | 105.98      | 101.46   |
| 2   | F     | 401 | CIT  | O4-C5-C4    | 2.32  | 121.71      | 114.35   |
| 4   | D     | 402 | CTP  | C3'-C2'-C1' | 2.31  | 105.83      | 101.46   |
| 2   | F     | 401 | CIT  | O2-C1-O1    | -2.30 | 117.42      | 123.33   |
| 2   | I     | 401 | CIT  | C4-C3-C2    | 2.25  | 115.09      | 109.31   |
| 4   | A     | 403 | CTP  | O2A-PA-O3A  | 2.24  | 113.32      | 107.27   |
| 4   | E     | 402 | CTP  | C3'-C2'-C1' | 2.20  | 105.63      | 101.46   |
| 4   | J     | 401 | CTP  | C3'-C2'-C1' | 2.17  | 105.57      | 101.46   |
| 2   | E     | 401 | CIT  | O4-C5-C4    | 2.15  | 121.16      | 114.35   |
| 2   | H     | 401 | CIT  | O2-C1-O1    | -2.14 | 117.82      | 123.33   |
| 4   | I     | 402 | CTP  | C3'-C2'-C1' | 2.14  | 105.51      | 101.46   |
| 2   | F     | 401 | CIT  | C3-C2-C1    | 2.13  | 119.75      | 113.92   |
| 2   | I     | 401 | CIT  | O2-C1-O1    | -2.12 | 117.89      | 123.33   |
| 2   | D     | 401 | CIT  | O2-C1-O1    | -2.10 | 117.94      | 123.33   |
| 2   | I     | 401 | CIT  | O4-C5-C4    | 2.09  | 120.97      | 114.35   |
| 2   | E     | 401 | CIT  | O2-C1-O1    | -2.08 | 117.97      | 123.33   |
| 4   | A     | 403 | CTP  | C3'-C2'-C1' | 2.08  | 105.40      | 101.46   |
| 2   | B     | 401 | CIT  | O2-C1-C2    | 2.08  | 120.93      | 114.35   |
| 2   | H     | 402 | CIT  | O4-C5-C4    | 2.06  | 120.88      | 114.35   |
| 4   | J     | 401 | CTP  | O3G-PG-O3B  | 2.00  | 111.36      | 104.64   |

There are no chirality outliers.

All (131) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | A     | 401 | CIT  | C2-C3-C4-C5 |
| 2   | B     | 401 | CIT  | O7-C3-C6-O5 |
| 2   | B     | 401 | CIT  | O7-C3-C6-O6 |
| 2   | B     | 401 | CIT  | C4-C3-C6-O5 |
| 2   | B     | 401 | CIT  | C4-C3-C6-O6 |
| 2   | D     | 401 | CIT  | O7-C3-C4-C5 |
| 2   | D     | 401 | CIT  | C6-C3-C4-C5 |
| 2   | D     | 401 | CIT  | C2-C3-C6-O5 |
| 2   | D     | 401 | CIT  | C2-C3-C6-O6 |
| 2   | D     | 401 | CIT  | O7-C3-C6-O5 |
| 2   | D     | 401 | CIT  | O7-C3-C6-O6 |
| 2   | E     | 401 | CIT  | O7-C3-C6-O5 |
| 2   | E     | 401 | CIT  | O7-C3-C6-O6 |
| 2   | E     | 401 | CIT  | C4-C3-C6-O5 |
| 2   | E     | 401 | CIT  | C4-C3-C6-O6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | G     | 401 | CIT  | O7-C3-C4-C5     |
| 2   | G     | 401 | CIT  | C6-C3-C4-C5     |
| 2   | G     | 401 | CIT  | O7-C3-C6-O5     |
| 2   | G     | 401 | CIT  | O7-C3-C6-O6     |
| 2   | G     | 401 | CIT  | C4-C3-C6-O5     |
| 2   | G     | 401 | CIT  | C4-C3-C6-O6     |
| 2   | H     | 401 | CIT  | C2-C3-C6-O5     |
| 2   | H     | 401 | CIT  | C2-C3-C6-O6     |
| 2   | H     | 401 | CIT  | O7-C3-C6-O5     |
| 2   | H     | 401 | CIT  | O7-C3-C6-O6     |
| 2   | I     | 401 | CIT  | C1-C2-C3-C4     |
| 2   | I     | 401 | CIT  | C1-C2-C3-C6     |
| 2   | I     | 401 | CIT  | C2-C3-C4-C5     |
| 2   | I     | 401 | CIT  | O7-C3-C4-C5     |
| 2   | I     | 401 | CIT  | C6-C3-C4-C5     |
| 2   | C     | 401 | CIT  | O7-C3-C6-O5     |
| 2   | C     | 401 | CIT  | O7-C3-C6-O6     |
| 2   | C     | 401 | CIT  | C4-C3-C6-O5     |
| 2   | C     | 401 | CIT  | C4-C3-C6-O6     |
| 4   | B     | 402 | CTP  | C5'-O5'-PA-O2A  |
| 4   | D     | 402 | CTP  | O4'-C4'-C5'-O5' |
| 4   | D     | 402 | CTP  | C5'-O5'-PA-O1A  |
| 4   | D     | 402 | CTP  | C5'-O5'-PA-O2A  |
| 4   | E     | 402 | CTP  | C5'-O5'-PA-O1A  |
| 4   | E     | 402 | CTP  | C5'-O5'-PA-O3A  |
| 4   | F     | 403 | CTP  | C5'-O5'-PA-O2A  |
| 4   | G     | 402 | CTP  | O4'-C4'-C5'-O5' |
| 4   | G     | 402 | CTP  | C5'-O5'-PA-O2A  |
| 4   | G     | 402 | CTP  | C5'-O5'-PA-O3A  |
| 4   | H     | 403 | CTP  | O4'-C4'-C5'-O5' |
| 4   | H     | 403 | CTP  | C5'-O5'-PA-O1A  |
| 4   | H     | 403 | CTP  | C5'-O5'-PA-O2A  |
| 4   | H     | 403 | CTP  | C5'-O5'-PA-O3A  |
| 4   | I     | 402 | CTP  | O4'-C4'-C5'-O5' |
| 4   | I     | 402 | CTP  | C5'-O5'-PA-O1A  |
| 4   | I     | 402 | CTP  | C5'-O5'-PA-O2A  |
| 4   | I     | 402 | CTP  | C5'-O5'-PA-O3A  |
| 4   | I     | 402 | CTP  | PB-O3B-PG-O2G   |
| 4   | D     | 402 | CTP  | C3'-C4'-C5'-O5' |
| 4   | G     | 402 | CTP  | C3'-C4'-C5'-O5' |
| 4   | I     | 402 | CTP  | C3'-C4'-C5'-O5' |
| 4   | C     | 404 | CTP  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 401 | CIT  | C6-C3-C4-C5     |
| 2   | D     | 401 | CIT  | C2-C3-C4-C5     |
| 2   | G     | 401 | CIT  | C2-C3-C4-C5     |
| 4   | B     | 402 | CTP  | O4'-C4'-C5'-O5' |
| 4   | J     | 401 | CTP  | O4'-C4'-C5'-O5' |
| 2   | F     | 401 | CIT  | C1-C2-C3-O7     |
| 2   | I     | 401 | CIT  | C1-C2-C3-O7     |
| 4   | H     | 403 | CTP  | C3'-C4'-C5'-O5' |
| 2   | F     | 401 | CIT  | C1-C2-C3-C6     |
| 4   | C     | 404 | CTP  | C3'-C4'-C5'-O5' |
| 2   | A     | 401 | CIT  | O7-C3-C4-C5     |
| 2   | D     | 401 | CIT  | C1-C2-C3-C6     |
| 2   | F     | 401 | CIT  | C6-C3-C4-C5     |
| 2   | H     | 402 | CIT  | O7-C3-C4-C5     |
| 4   | F     | 403 | CTP  | O4'-C4'-C5'-O5' |
| 4   | B     | 402 | CTP  | C3'-C4'-C5'-O5' |
| 4   | J     | 401 | CTP  | C3'-C4'-C5'-O5' |
| 2   | D     | 401 | CIT  | C1-C2-C3-C4     |
| 2   | H     | 401 | CIT  | C1-C2-C3-O7     |
| 2   | H     | 402 | CIT  | C2-C3-C4-C5     |
| 2   | H     | 402 | CIT  | C6-C3-C4-C5     |
| 4   | G     | 402 | CTP  | PB-O3A-PA-O5'   |
| 2   | F     | 401 | CIT  | C1-C2-C3-C4     |
| 4   | F     | 403 | CTP  | PB-O3B-PG-O1G   |
| 4   | E     | 402 | CTP  | PB-O3B-PG-O2G   |
| 4   | I     | 402 | CTP  | PA-O3A-PB-O2B   |
| 2   | F     | 401 | CIT  | C2-C3-C6-O6     |
| 2   | F     | 401 | CIT  | C4-C3-C6-O6     |
| 2   | D     | 401 | CIT  | C1-C2-C3-O7     |
| 2   | C     | 401 | CIT  | C6-C3-C4-C5     |
| 4   | A     | 403 | CTP  | C5'-O5'-PA-O1A  |
| 4   | B     | 402 | CTP  | C5'-O5'-PA-O1A  |
| 4   | B     | 402 | CTP  | C5'-O5'-PA-O3A  |
| 4   | D     | 402 | CTP  | C5'-O5'-PA-O3A  |
| 4   | F     | 403 | CTP  | C5'-O5'-PA-O1A  |
| 4   | F     | 403 | CTP  | C5'-O5'-PA-O3A  |
| 2   | F     | 401 | CIT  | C2-C3-C4-C5     |
| 2   | C     | 401 | CIT  | O7-C3-C4-C5     |
| 2   | F     | 401 | CIT  | O7-C3-C6-O6     |
| 4   | F     | 403 | CTP  | C3'-C4'-C5'-O5' |
| 2   | F     | 401 | CIT  | C2-C3-C6-O5     |
| 2   | H     | 402 | CIT  | C2-C3-C6-O5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | H     | 402 | CIT  | C2-C3-C6-O6     |
| 4   | E     | 402 | CTP  | O4'-C4'-C5'-O5' |
| 4   | D     | 402 | CTP  | PB-O3A-PA-O1A   |
| 2   | H     | 402 | CIT  | C4-C3-C6-O5     |
| 2   | H     | 402 | CIT  | C4-C3-C6-O6     |
| 2   | C     | 401 | CIT  | C2-C3-C6-O6     |
| 2   | A     | 401 | CIT  | C1-C2-C3-C4     |
| 2   | H     | 402 | CIT  | C1-C2-C3-O7     |
| 2   | C     | 401 | CIT  | C2-C3-C4-C5     |
| 4   | F     | 403 | CTP  | PB-O3B-PG-O2G   |
| 4   | F     | 403 | CTP  | PB-O3B-PG-O3G   |
| 4   | I     | 402 | CTP  | PB-O3B-PG-O3G   |
| 2   | E     | 401 | CIT  | C1-C2-C3-O7     |
| 2   | G     | 401 | CIT  | C1-C2-C3-C4     |
| 4   | G     | 402 | CTP  | PG-O3B-PB-O1B   |
| 4   | G     | 402 | CTP  | PG-O3B-PB-O2B   |
| 4   | I     | 402 | CTP  | PA-O3A-PB-O1B   |
| 2   | F     | 401 | CIT  | O7-C3-C6-O5     |
| 2   | F     | 401 | CIT  | C3-C4-C5-O4     |
| 2   | I     | 401 | CIT  | C3-C4-C5-O3     |
| 2   | F     | 401 | CIT  | C4-C3-C6-O5     |
| 2   | F     | 401 | CIT  | C3-C4-C5-O3     |
| 4   | J     | 401 | CTP  | PG-O3B-PB-O3A   |
| 4   | H     | 403 | CTP  | PB-O3B-PG-O1G   |
| 4   | I     | 402 | CTP  | PB-O3B-PG-O1G   |
| 2   | H     | 401 | CIT  | C3-C4-C5-O3     |
| 2   | F     | 401 | CIT  | O1-C1-C2-C3     |
| 2   | I     | 401 | CIT  | C3-C4-C5-O4     |
| 4   | B     | 402 | CTP  | PB-O3A-PA-O2A   |
| 4   | J     | 401 | CTP  | PG-O3B-PB-O1B   |
| 4   | C     | 404 | CTP  | PG-O3B-PB-O2B   |
| 2   | H     | 401 | CIT  | C3-C4-C5-O4     |

There are no ring outliers.

15 monomers are involved in 30 short contacts:

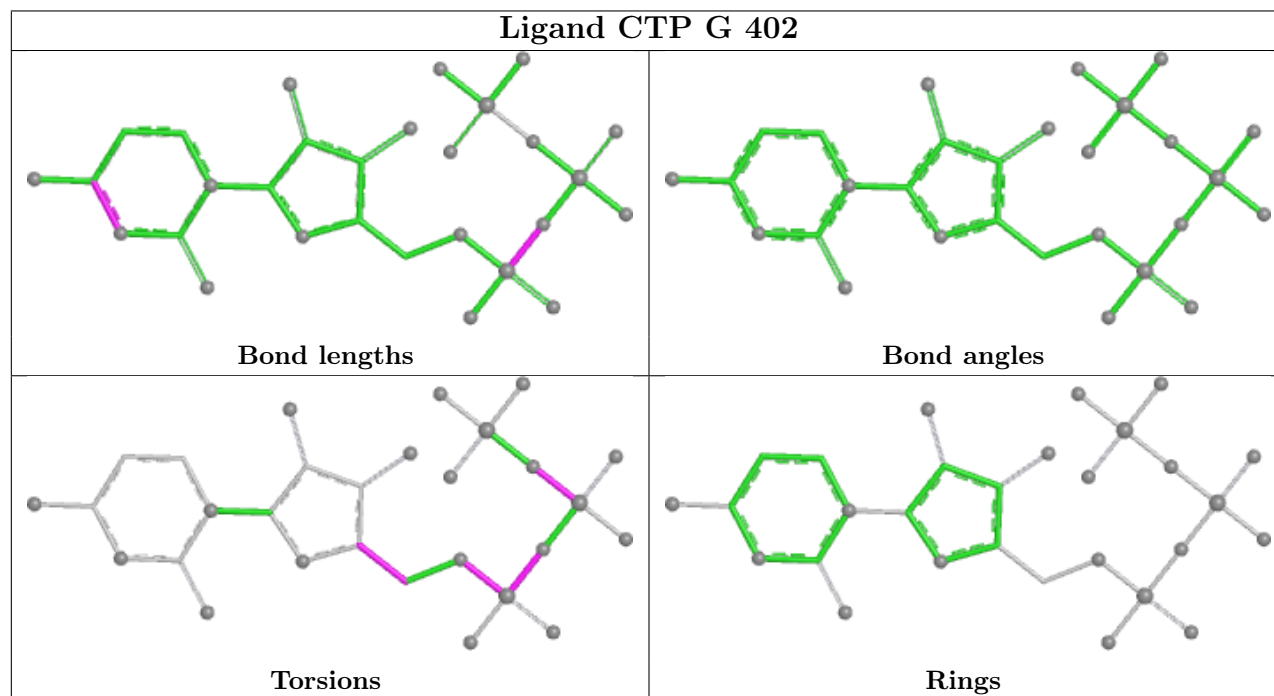
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | F     | 403 | CTP  | 1       | 0            |
| 3   | A     | 402 | TMO  | 1       | 0            |
| 4   | H     | 403 | CTP  | 3       | 0            |
| 2   | G     | 401 | CIT  | 1       | 0            |
| 2   | F     | 401 | CIT  | 1       | 0            |

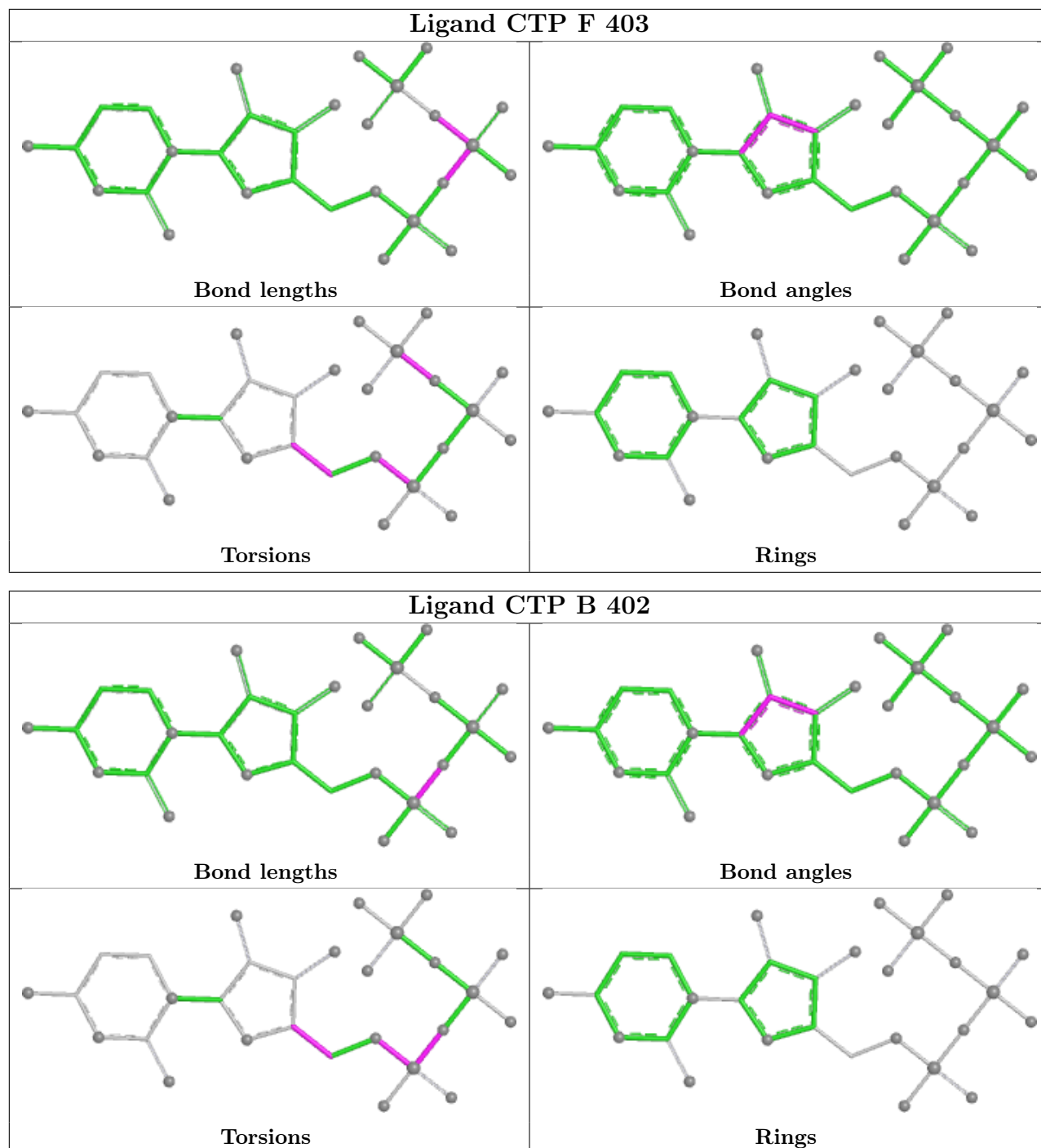
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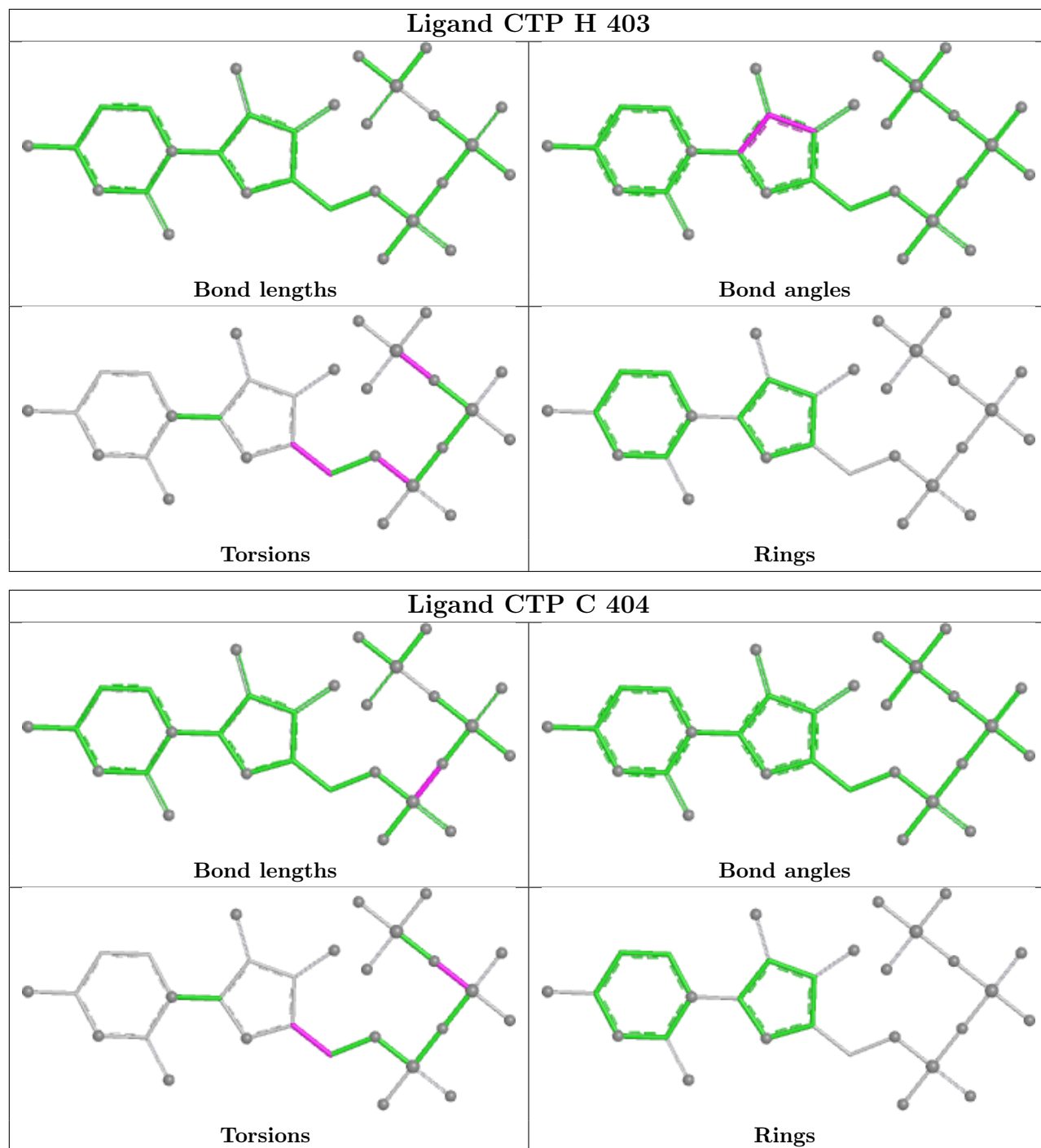
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 401 | CIT  | 9       | 0            |
| 4   | A     | 403 | CTP  | 1       | 0            |
| 2   | A     | 401 | CIT  | 1       | 0            |
| 4   | D     | 402 | CTP  | 1       | 0            |
| 2   | D     | 401 | CIT  | 2       | 0            |
| 2   | H     | 401 | CIT  | 1       | 0            |
| 2   | I     | 401 | CIT  | 2       | 0            |
| 2   | B     | 401 | CIT  | 2       | 0            |
| 4   | E     | 402 | CTP  | 2       | 0            |
| 4   | I     | 402 | CTP  | 2       | 0            |

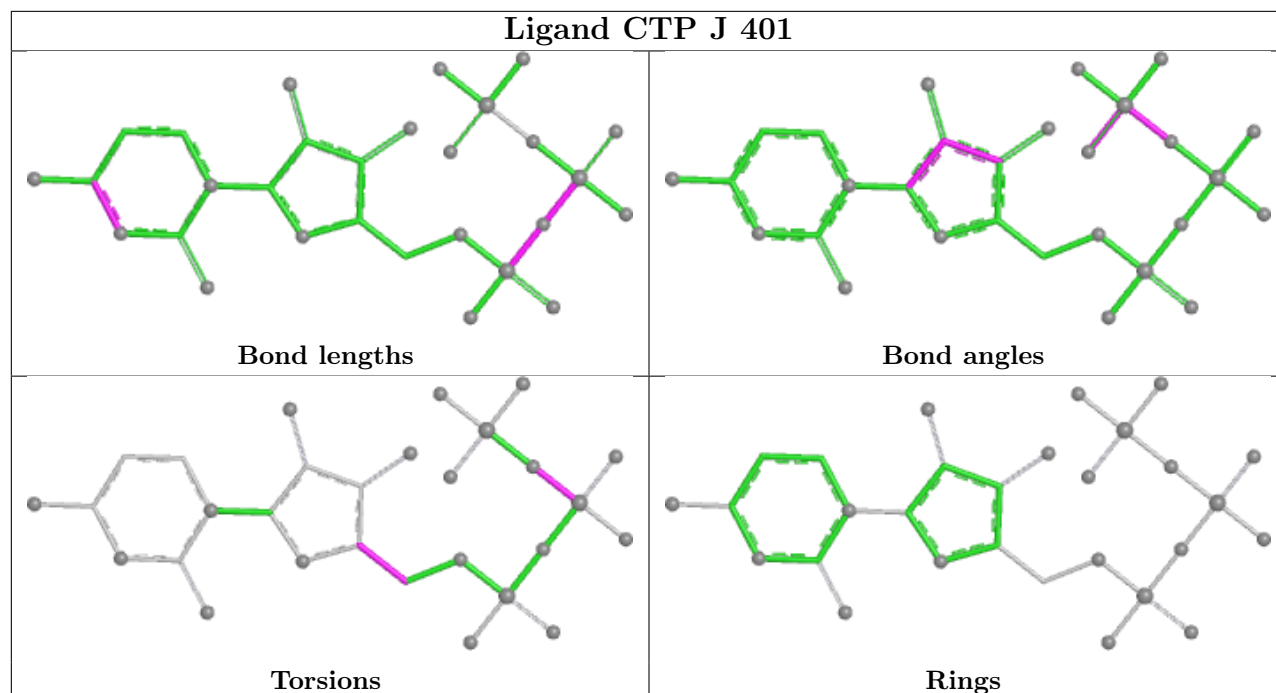
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



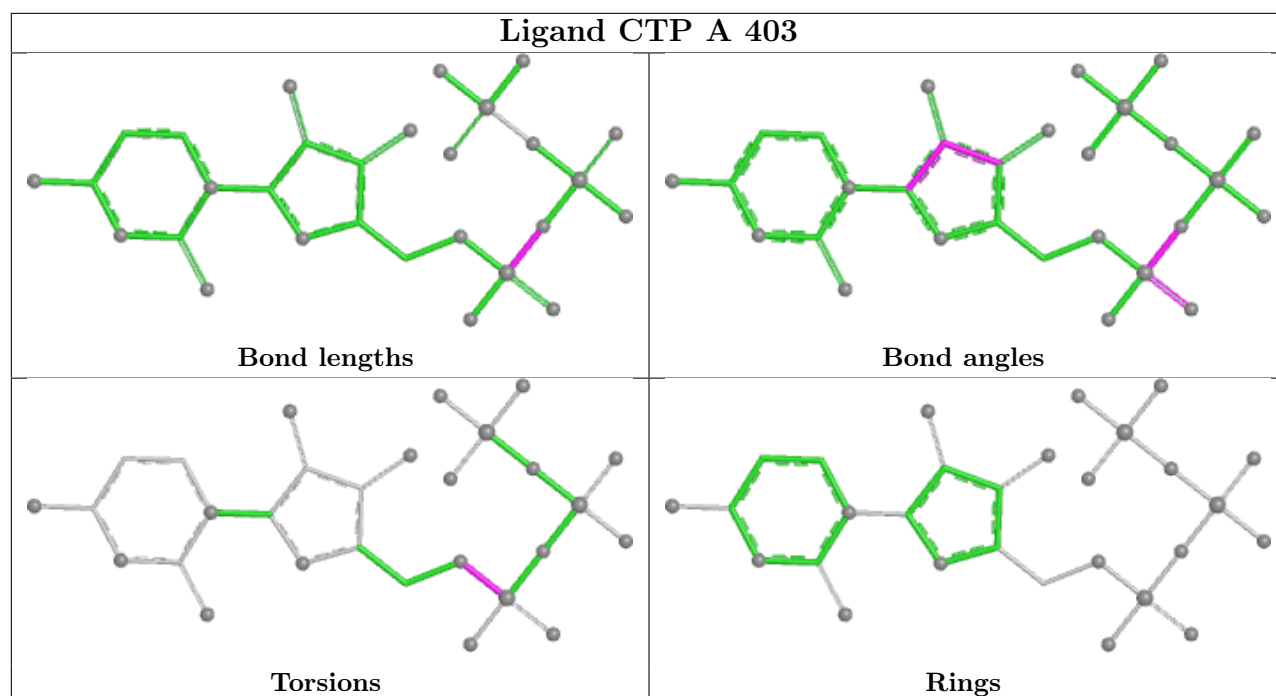


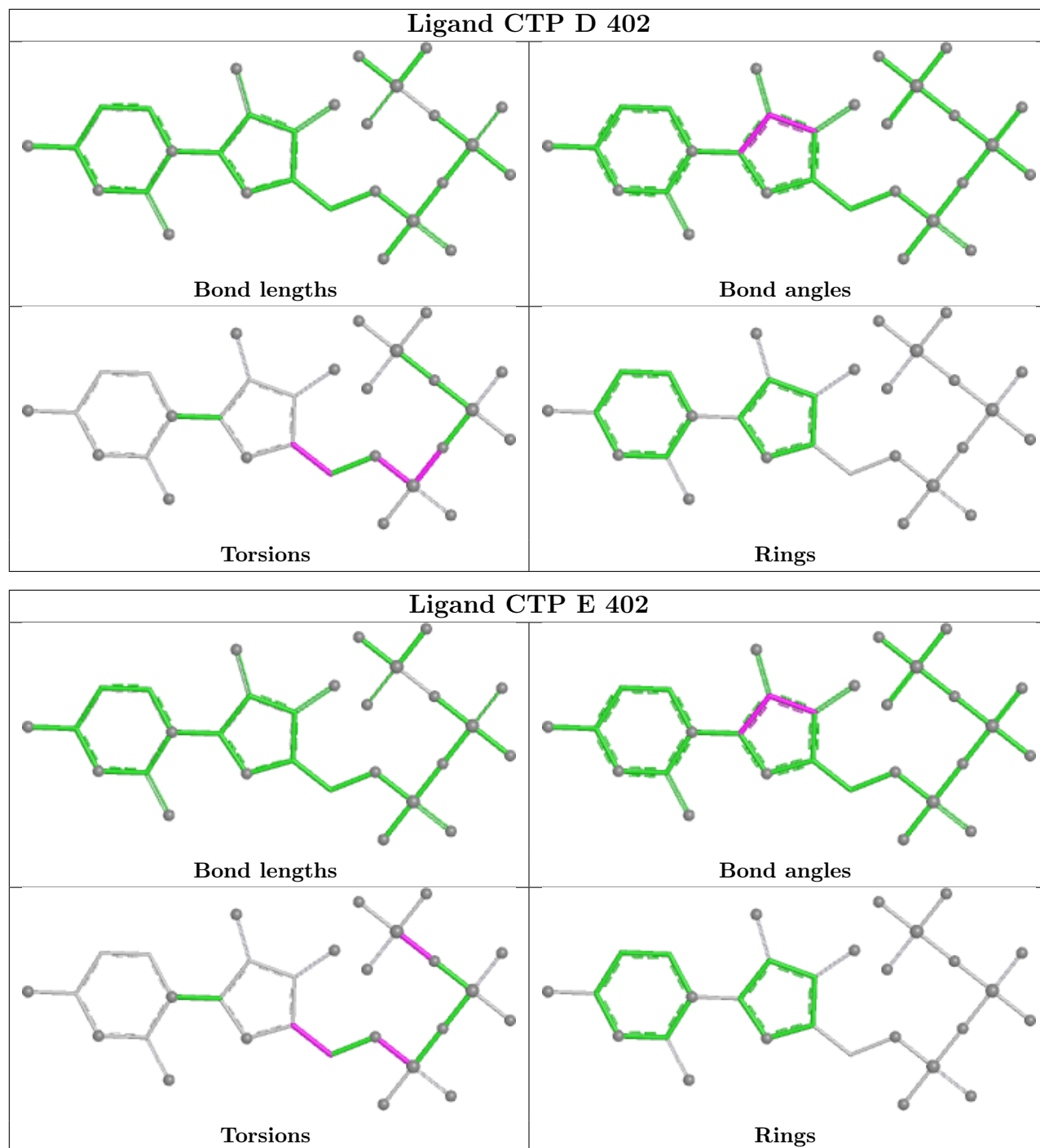


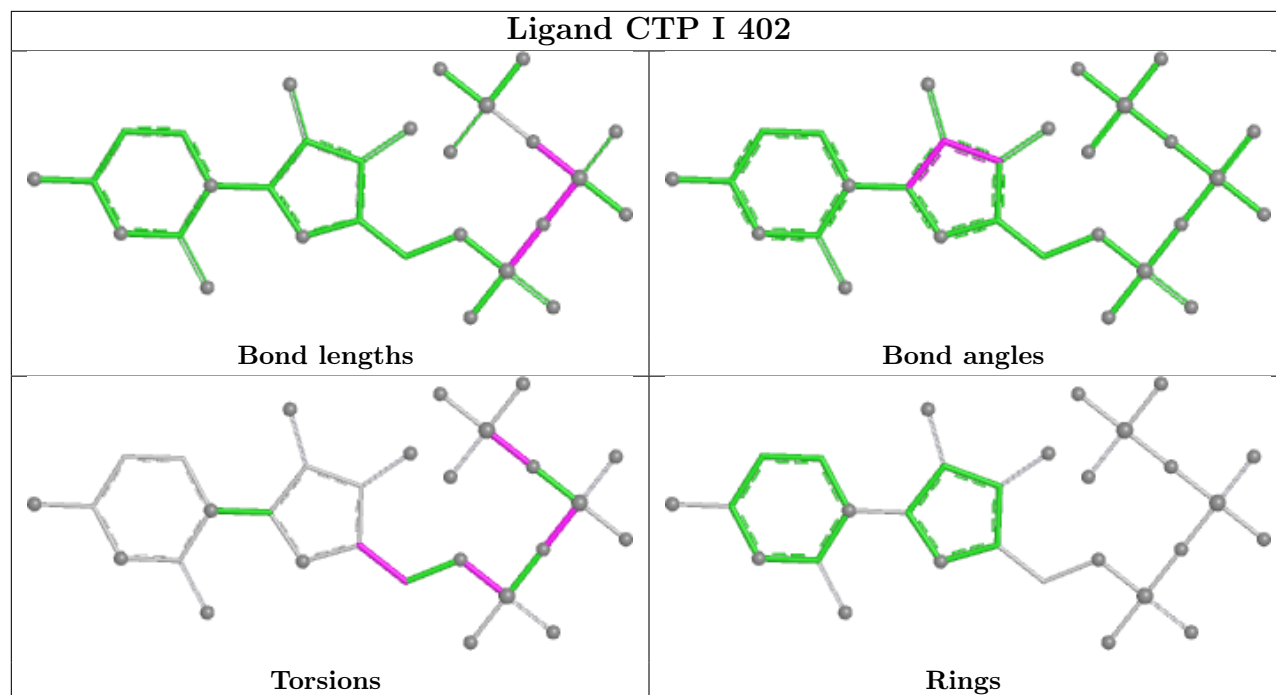
## Ligand CTP J 401



## Ligand CTP A 403







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|--------|
| 1   | A     | 349/362 (96%)   | 0.21   | 14 (4%)  | 42 | 43 | 44, 73, 123, 176      | 2 (0%) |
| 1   | B     | 349/362 (96%)   | 0.30   | 17 (4%)  | 35 | 34 | 49, 78, 134, 170      | 0      |
| 1   | C     | 353/362 (97%)   | 0.14   | 6 (1%)   | 69 | 69 | 47, 71, 125, 183      | 2 (0%) |
| 1   | D     | 342/362 (94%)   | 0.50   | 25 (7%)  | 21 | 20 | 41, 102, 170, 202     | 0      |
| 1   | E     | 348/362 (96%)   | 0.30   | 16 (4%)  | 37 | 38 | 48, 79, 134, 195      | 1 (0%) |
| 1   | F     | 339/362 (93%)   | 0.42   | 23 (6%)  | 23 | 22 | 42, 84, 143, 184      | 0      |
| 1   | G     | 352/362 (97%)   | 0.33   | 14 (3%)  | 42 | 43 | 47, 84, 132, 186      | 0      |
| 1   | H     | 345/362 (95%)   | 0.53   | 24 (6%)  | 22 | 21 | 43, 95, 163, 194      | 0      |
| 1   | I     | 346/362 (95%)   | 0.63   | 26 (7%)  | 20 | 19 | 55, 101, 148, 203     | 0      |
| 1   | J     | 286/362 (79%)   | 0.94   | 46 (16%) | 4  | 4  | 49, 114, 182, 215     | 0      |
| All | All   | 3409/3620 (94%) | 0.42   | 211 (6%) | 26 | 26 | 41, 85, 157, 215      | 5 (0%) |

All (211) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | J     | 35    | CYS  | 9.0  |
| 1   | J     | 31    | ILE  | 7.6  |
| 1   | J     | 166   | TYR  | 6.5  |
| 1   | J     | 38    | VAL  | 5.9  |
| 1   | J     | 32    | ARG  | 5.7  |
| 1   | J     | 29    | LYS  | 5.7  |
| 1   | B     | 110   | MET  | 5.5  |
| 1   | J     | 132   | PHE  | 5.2  |
| 1   | A     | 83[A] | MET  | 5.1  |
| 1   | J     | 210   | LEU  | 5.0  |
| 1   | H     | 83    | MET  | 5.0  |
| 1   | F     | 80    | LEU  | 4.9  |
| 1   | H     | 53    | ILE  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 176 | CYS  | 4.9  |
| 1   | H     | 110 | MET  | 4.6  |
| 1   | B     | 85  | VAL  | 4.6  |
| 1   | D     | 173 | ALA  | 4.5  |
| 1   | F     | 180 | TRP  | 4.4  |
| 1   | J     | 28  | ALA  | 4.4  |
| 1   | D     | 63  | TYR  | 4.4  |
| 1   | D     | 215 | CYS  | 4.4  |
| 1   | B     | 86  | PHE  | 4.3  |
| 1   | H     | 85  | VAL  | 4.3  |
| 1   | E     | 83  | MET  | 4.2  |
| 1   | B     | 102 | LEU  | 4.1  |
| 1   | D     | 76  | VAL  | 4.1  |
| 1   | H     | 102 | LEU  | 4.0  |
| 1   | H     | 113 | TRP  | 4.0  |
| 1   | D     | 80  | LEU  | 3.9  |
| 1   | J     | 119 | ALA  | 3.9  |
| 1   | B     | 56  | LEU  | 3.9  |
| 1   | D     | 194 | TRP  | 3.8  |
| 1   | F     | 85  | VAL  | 3.8  |
| 1   | H     | 112 | LEU  | 3.8  |
| 1   | I     | 1   | ASP  | 3.8  |
| 1   | B     | 83  | MET  | 3.8  |
| 1   | H     | 88  | PHE  | 3.7  |
| 1   | J     | 77  | VAL  | 3.7  |
| 1   | J     | 180 | TRP  | 3.7  |
| 1   | D     | 174 | PHE  | 3.6  |
| 1   | D     | 54  | SER  | 3.6  |
| 1   | B     | 84  | GLY  | 3.6  |
| 1   | J     | 232 | LEU  | 3.6  |
| 1   | G     | 174 | PHE  | 3.6  |
| 1   | E     | 106 | ARG  | 3.5  |
| 1   | I     | 185 | ALA  | 3.4  |
| 1   | H     | 47  | VAL  | 3.4  |
| 1   | J     | 34  | VAL  | 3.4  |
| 1   | D     | 83  | MET  | 3.3  |
| 1   | A     | 54  | SER  | 3.3  |
| 1   | B     | 88  | PHE  | 3.3  |
| 1   | I     | 52  | PHE  | 3.3  |
| 1   | F     | 87  | ASN  | 3.3  |
| 1   | E     | 85  | VAL  | 3.3  |
| 1   | F     | -1  | ALA  | 3.3  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | F     | 88    | PHE  | 3.3  |
| 1   | E     | 103   | SER  | 3.2  |
| 1   | F     | 177   | THR  | 3.2  |
| 1   | D     | 160   | LEU  | 3.2  |
| 1   | D     | 172   | PRO  | 3.2  |
| 1   | I     | 216   | HIS  | 3.1  |
| 1   | D     | 167   | VAL  | 3.1  |
| 1   | I     | 2     | ILE  | 3.1  |
| 1   | I     | 213   | LYS  | 3.0  |
| 1   | I     | 115   | GLU  | 3.0  |
| 1   | D     | 52    | PHE  | 3.0  |
| 1   | C     | 315   | ARG  | 3.0  |
| 1   | J     | 25    | ALA  | 3.0  |
| 1   | F     | 174   | PHE  | 3.0  |
| 1   | G     | 178   | GLY  | 3.0  |
| 1   | D     | 192   | ILE  | 3.0  |
| 1   | C     | 83[A] | MET  | 3.0  |
| 1   | J     | 98    | ALA  | 3.0  |
| 1   | F     | 283   | GLU  | 2.9  |
| 1   | I     | 107   | LYS  | 2.9  |
| 1   | G     | 153   | ALA  | 2.9  |
| 1   | E     | 88    | PHE  | 2.9  |
| 1   | F     | 103   | SER  | 2.9  |
| 1   | E     | 215   | SER  | 2.9  |
| 1   | D     | 77    | VAL  | 2.9  |
| 1   | G     | 216   | HIS  | 2.9  |
| 1   | D     | -1    | ALA  | 2.9  |
| 1   | A     | 84    | GLY  | 2.9  |
| 1   | D     | 193   | PRO  | 2.8  |
| 1   | I     | 177   | THR  | 2.8  |
| 1   | H     | 48    | GLN  | 2.8  |
| 1   | F     | 280   | TYR  | 2.8  |
| 1   | J     | 192   | ILE  | 2.8  |
| 1   | E     | 226   | GLU  | 2.8  |
| 1   | J     | 212   | SER  | 2.8  |
| 1   | J     | 181   | PRO  | 2.8  |
| 1   | H     | 350   | LEU  | 2.8  |
| 1   | A     | 81    | ASN  | 2.8  |
| 1   | F     | 250   | CYS  | 2.8  |
| 1   | G     | 84    | GLY  | 2.7  |
| 1   | J     | -1    | ALA  | 2.7  |
| 1   | F     | 82    | GLN  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 55  | SER  | 2.7  |
| 1   | G     | 152 | VAL  | 2.7  |
| 1   | B     | 248 | LYS  | 2.7  |
| 1   | I     | 54  | SER  | 2.7  |
| 1   | H     | 91  | ASP  | 2.7  |
| 1   | J     | 65  | GLY  | 2.7  |
| 1   | J     | 116 | PHE  | 2.7  |
| 1   | F     | 81  | ASN  | 2.7  |
| 1   | H     | 42  | LEU  | 2.6  |
| 1   | E     | 96  | GLY  | 2.6  |
| 1   | A     | 2   | ILE  | 2.6  |
| 1   | I     | 197 | PRO  | 2.6  |
| 1   | G     | 177 | THR  | 2.6  |
| 1   | D     | 0   | MET  | 2.6  |
| 1   | G     | 189 | LEU  | 2.6  |
| 1   | J     | 123 | LEU  | 2.6  |
| 1   | J     | 136 | VAL  | 2.6  |
| 1   | I     | 53  | ILE  | 2.6  |
| 1   | A     | 350 | LEU  | 2.6  |
| 1   | H     | 227 | SER  | 2.6  |
| 1   | J     | 172 | PRO  | 2.5  |
| 1   | F     | 192 | ILE  | 2.5  |
| 1   | F     | 210 | LEU  | 2.5  |
| 1   | I     | 210 | LEU  | 2.5  |
| 1   | J     | 238 | GLU  | 2.5  |
| 1   | F     | 86  | PHE  | 2.5  |
| 1   | I     | 174 | PHE  | 2.5  |
| 1   | J     | 80  | LEU  | 2.5  |
| 1   | F     | 175 | LYS  | 2.5  |
| 1   | I     | 227 | SER  | 2.5  |
| 1   | H     | 2   | ILE  | 2.5  |
| 1   | E     | 100 | LEU  | 2.5  |
| 1   | J     | 74  | PHE  | 2.5  |
| 1   | C     | 216 | HIS  | 2.5  |
| 1   | E     | 84  | GLY  | 2.4  |
| 1   | G     | 341 | GLN  | 2.4  |
| 1   | B     | 174 | PHE  | 2.4  |
| 1   | J     | 97  | CYS  | 2.4  |
| 1   | D     | 148 | VAL  | 2.4  |
| 1   | F     | 194 | TRP  | 2.4  |
| 1   | J     | 230 | TRP  | 2.4  |
| 1   | F     | 176 | CYS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 189 | LEU  | 2.4  |
| 1   | D     | 145 | TYR  | 2.4  |
| 1   | D     | 53  | ILE  | 2.4  |
| 1   | J     | 63  | TYR  | 2.4  |
| 1   | J     | 280 | TYR  | 2.4  |
| 1   | E     | 107 | LYS  | 2.4  |
| 1   | C     | 178 | GLY  | 2.3  |
| 1   | E     | 104 | ASP  | 2.3  |
| 1   | C     | 189 | LEU  | 2.3  |
| 1   | A     | 88  | PHE  | 2.3  |
| 1   | H     | 86  | PHE  | 2.3  |
| 1   | J     | 36  | LYS  | 2.3  |
| 1   | F     | 181 | PRO  | 2.3  |
| 1   | E     | 1   | ASP  | 2.3  |
| 1   | J     | 234 | PHE  | 2.3  |
| 1   | A     | 197 | PRO  | 2.3  |
| 1   | H     | -2  | GLY  | 2.3  |
| 1   | I     | 55  | SER  | 2.3  |
| 1   | H     | 1   | ASP  | 2.3  |
| 1   | J     | 50  | PRO  | 2.3  |
| 1   | H     | 63  | TYR  | 2.3  |
| 1   | I     | 280 | TYR  | 2.3  |
| 1   | A     | 216 | HIS  | 2.2  |
| 1   | D     | 65  | GLY  | 2.2  |
| 1   | J     | 341 | GLN  | 2.2  |
| 1   | G     | 349 | ILE  | 2.2  |
| 1   | J     | 211 | LEU  | 2.2  |
| 1   | A     | 52  | PHE  | 2.2  |
| 1   | E     | 327 | PHE  | 2.2  |
| 1   | I     | 63  | TYR  | 2.2  |
| 1   | B     | 100 | LEU  | 2.2  |
| 1   | J     | 42  | LEU  | 2.2  |
| 1   | J     | 78  | LEU  | 2.2  |
| 1   | I     | 93  | SER  | 2.2  |
| 1   | J     | 99  | VAL  | 2.2  |
| 1   | G     | 80  | LEU  | 2.2  |
| 1   | A     | 53  | ILE  | 2.2  |
| 1   | F     | 179 | ILE  | 2.2  |
| 1   | H     | 54  | SER  | 2.2  |
| 1   | I     | 234 | PHE  | 2.2  |
| 1   | B     | 152 | VAL  | 2.2  |
| 1   | H     | 61  | ASN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 0   | MET  | 2.2  |
| 1   | B     | 246 | CYS  | 2.2  |
| 1   | I     | 56  | LEU  | 2.2  |
| 1   | I     | 214 | GLU  | 2.2  |
| 1   | G     | 52  | PHE  | 2.2  |
| 1   | J     | 284 | LYS  | 2.2  |
| 1   | D     | 210 | LEU  | 2.1  |
| 1   | I     | 84  | GLY  | 2.1  |
| 1   | G     | 53  | ILE  | 2.1  |
| 1   | B     | 109 | SER  | 2.1  |
| 1   | I     | 114 | VAL  | 2.1  |
| 1   | A     | 243 | MET  | 2.1  |
| 1   | H     | 82  | GLN  | 2.1  |
| 1   | J     | 205 | ALA  | 2.1  |
| 1   | B     | 227 | SER  | 2.1  |
| 1   | H     | 111 | SER  | 2.1  |
| 1   | I     | 208 | PHE  | 2.1  |
| 1   | A     | 106 | ARG  | 2.1  |
| 1   | H     | 65  | GLY  | 2.1  |
| 1   | C     | 174 | PHE  | 2.0  |
| 1   | J     | 173 | ALA  | 2.0  |
| 1   | D     | 66  | LEU  | 2.0  |
| 1   | D     | 78  | LEU  | 2.0  |
| 1   | E     | 110 | MET  | 2.0  |
| 1   | B     | 82  | GLN  | 2.0  |
| 1   | E     | 86  | PHE  | 2.0  |
| 1   | J     | 47  | VAL  | 2.0  |
| 1   | J     | 160 | LEU  | 2.0  |
| 1   | F     | 272 | TYR  | 2.0  |
| 1   | G     | 54  | SER  | 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 ⓘ

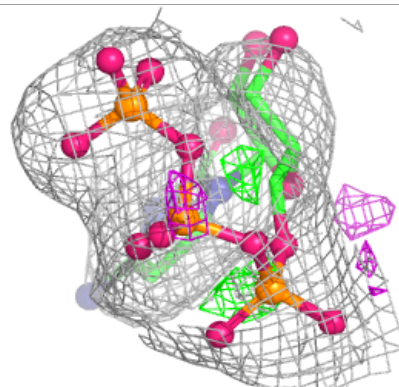
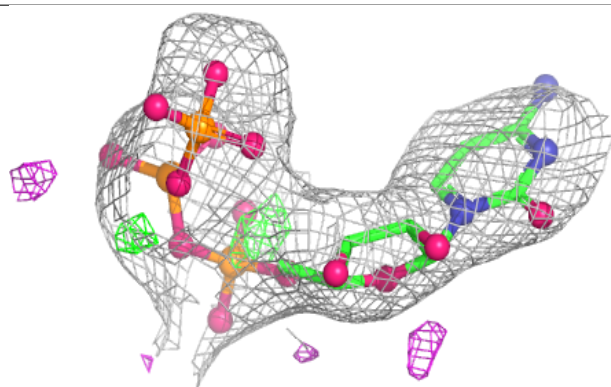
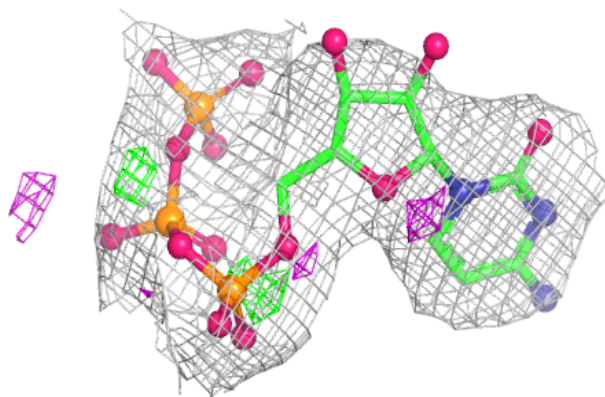
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | TMO  | C     | 403 | 5/5   | 0.74 | 0.25 | 130,130,132,137            | 0     |
| 2   | CIT  | G     | 401 | 13/13 | 0.77 | 0.12 | 107,119,134,139            | 0     |
| 3   | TMO  | A     | 402 | 5/5   | 0.82 | 0.16 | 109,112,113,115            | 0     |
| 2   | CIT  | H     | 402 | 13/13 | 0.82 | 0.10 | 106,115,124,128            | 0     |
| 2   | CIT  | D     | 401 | 13/13 | 0.84 | 0.11 | 78,109,137,142             | 0     |
| 2   | CIT  | C     | 401 | 13/13 | 0.84 | 0.11 | 86,104,126,130             | 0     |
| 2   | CIT  | A     | 401 | 13/13 | 0.85 | 0.11 | 88,115,146,147             | 0     |
| 2   | CIT  | H     | 401 | 13/13 | 0.85 | 0.08 | 93,123,140,142             | 0     |
| 4   | CTP  | I     | 402 | 29/29 | 0.85 | 0.13 | 117,146,189,197            | 0     |
| 2   | CIT  | B     | 401 | 13/13 | 0.86 | 0.10 | 84,94,123,129              | 0     |
| 2   | CIT  | I     | 401 | 13/13 | 0.86 | 0.09 | 104,112,141,144            | 0     |
| 2   | CIT  | F     | 401 | 13/13 | 0.87 | 0.09 | 94,115,131,134             | 0     |
| 3   | TMO  | F     | 402 | 5/5   | 0.88 | 0.20 | 109,113,116,116            | 0     |
| 3   | TMO  | C     | 402 | 5/5   | 0.89 | 0.16 | 97,103,104,109             | 0     |
| 4   | CTP  | J     | 401 | 29/29 | 0.90 | 0.11 | 91,126,136,157             | 0     |
| 2   | CIT  | E     | 401 | 13/13 | 0.92 | 0.09 | 87,100,110,117             | 0     |
| 4   | CTP  | D     | 402 | 29/29 | 0.92 | 0.10 | 82,117,129,130             | 0     |
| 4   | CTP  | H     | 403 | 29/29 | 0.94 | 0.10 | 82,124,129,130             | 0     |
| 4   | CTP  | G     | 402 | 29/29 | 0.95 | 0.09 | 74,94,110,114              | 0     |
| 4   | CTP  | E     | 402 | 29/29 | 0.95 | 0.09 | 60,78,89,108               | 0     |
| 4   | CTP  | C     | 404 | 29/29 | 0.95 | 0.09 | 52,75,92,99                | 0     |
| 4   | CTP  | F     | 403 | 29/29 | 0.96 | 0.07 | 55,68,82,94                | 0     |
| 4   | CTP  | B     | 402 | 29/29 | 0.96 | 0.08 | 55,77,94,119               | 0     |
| 4   | CTP  | A     | 403 | 29/29 | 0.97 | 0.06 | 45,64,83,85                | 0     |

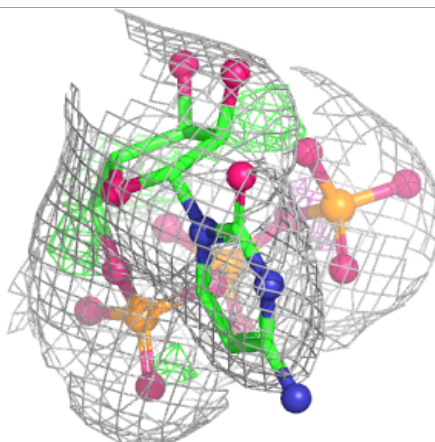
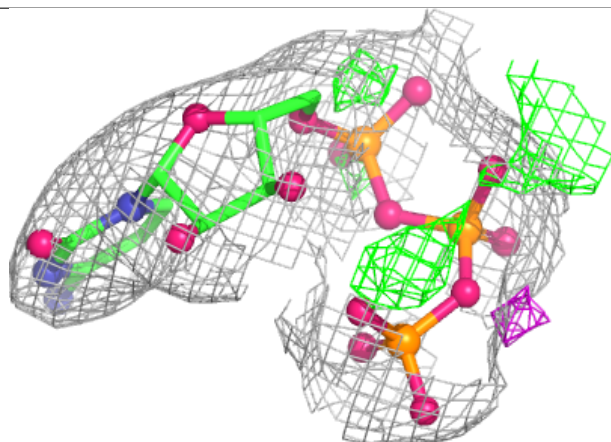
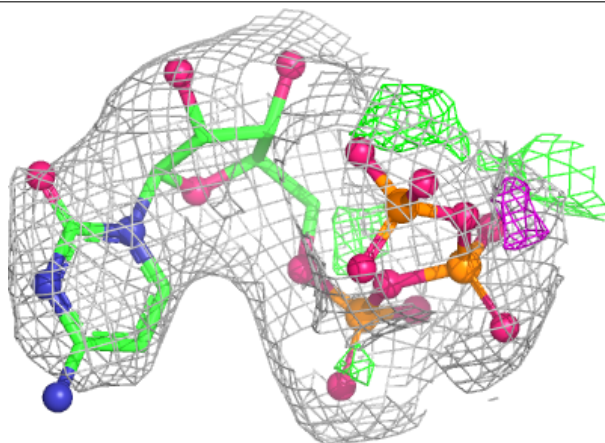
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CTP I 402:**

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

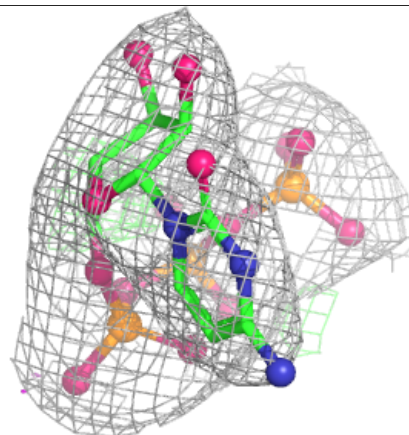
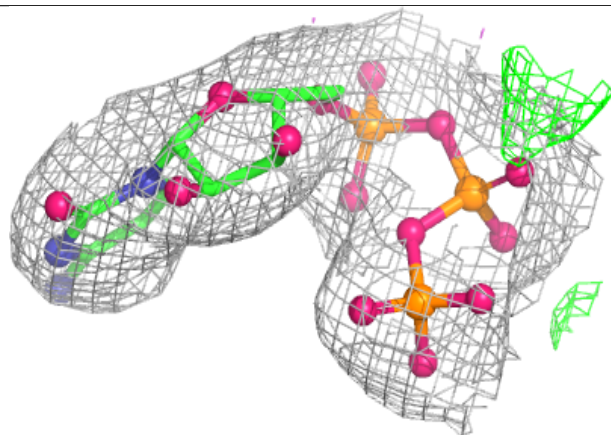
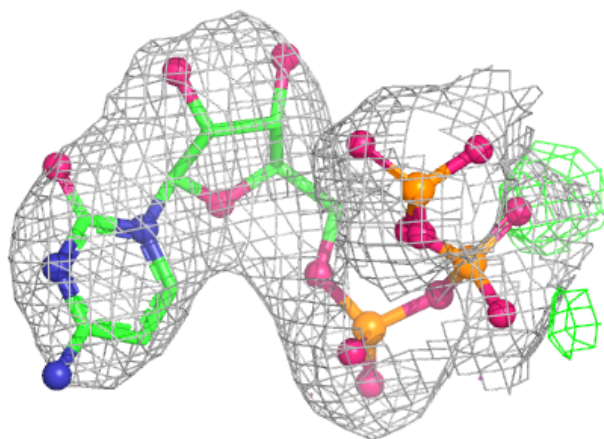
**Electron density around CTP J 401:**

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



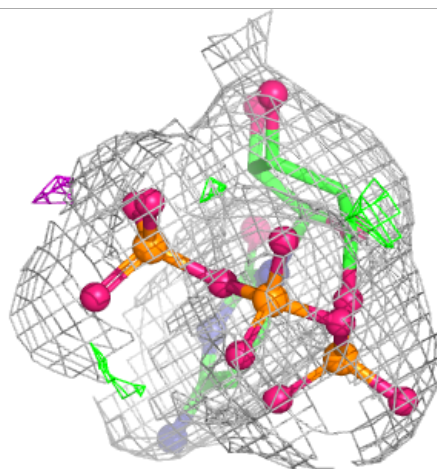
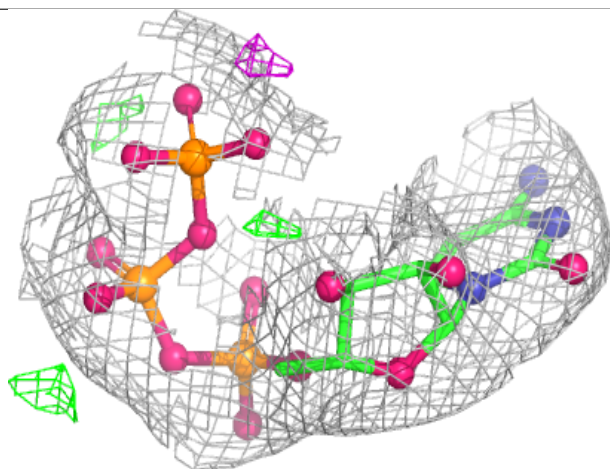
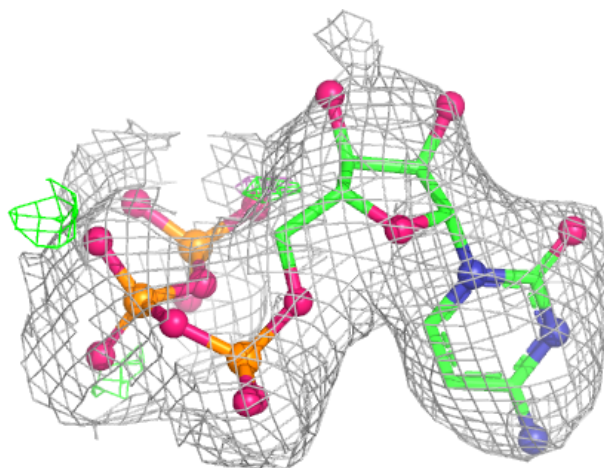
**Electron density around CTP D 402:**

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



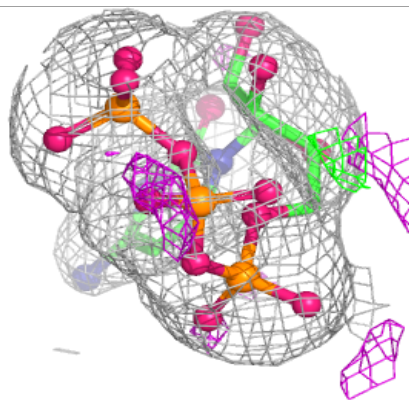
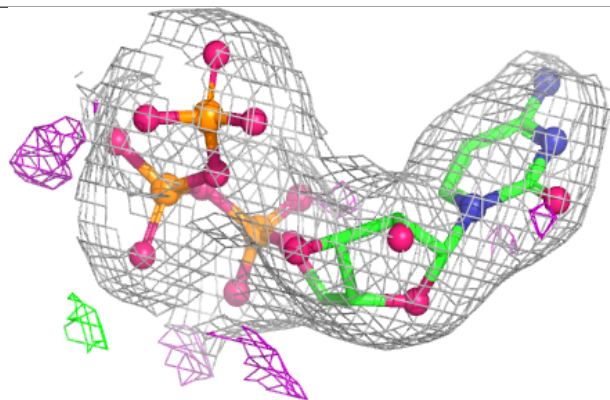
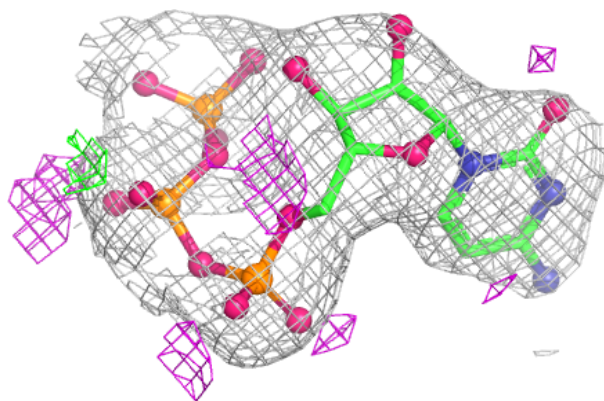
**Electron density around CTP H 403:**

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

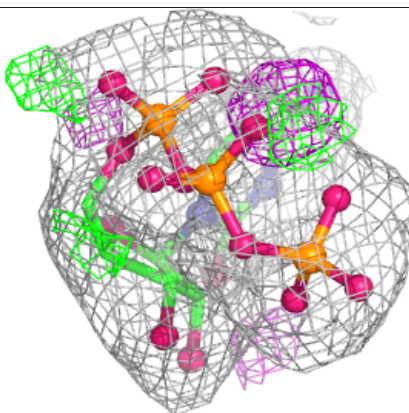
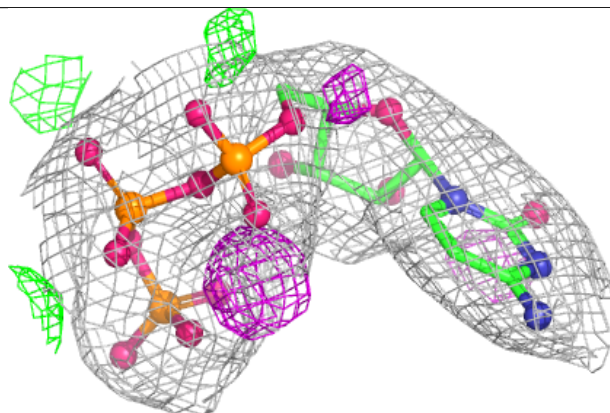
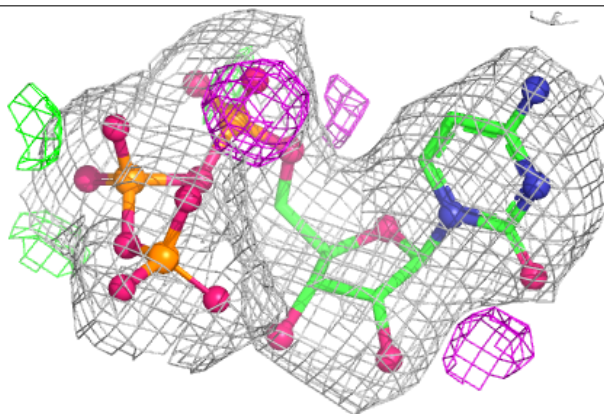


**Electron density around CTP G 402:**

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

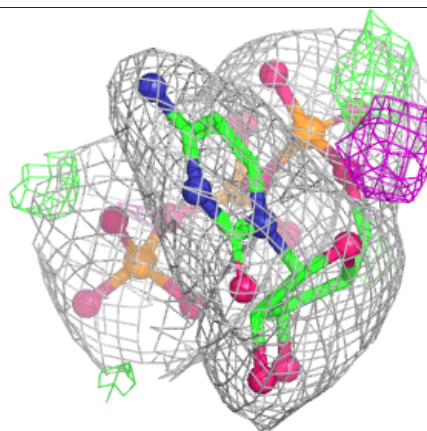
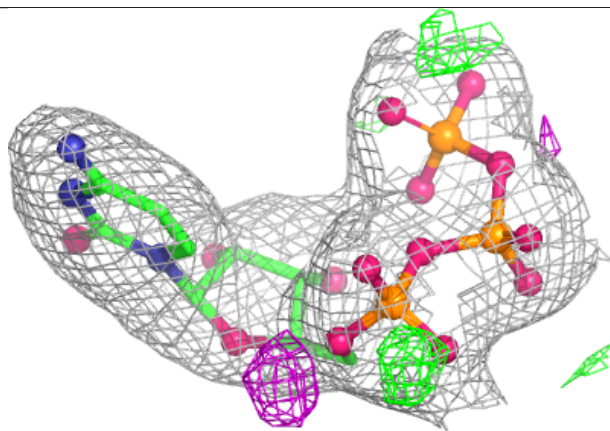
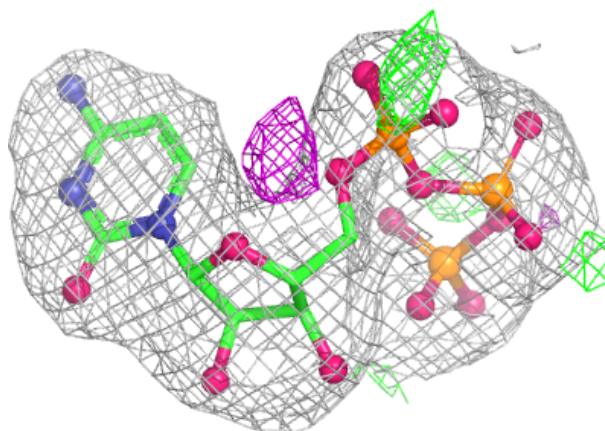
**Electron density around CTP E 402:**

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



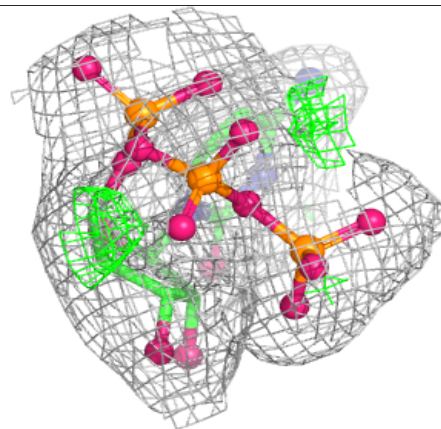
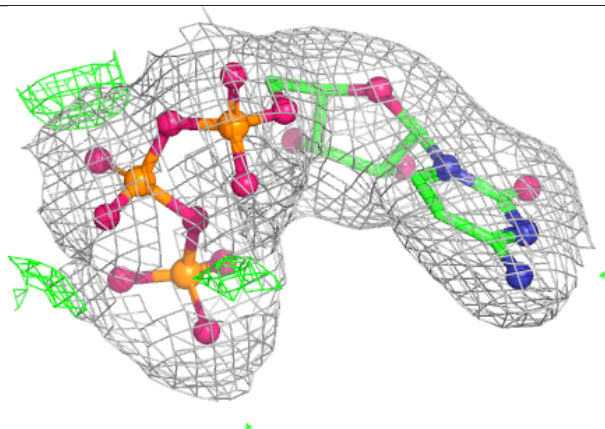
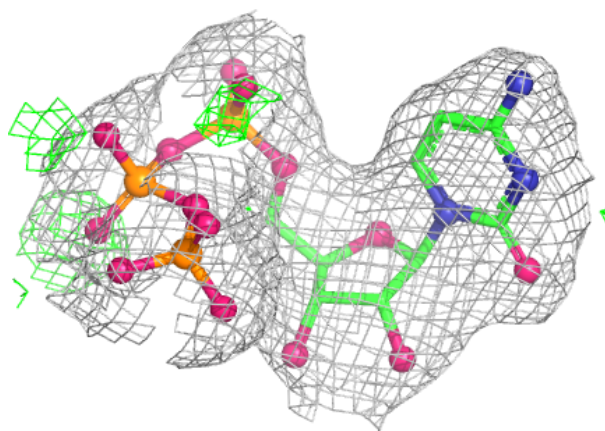
**Electron density around CTP C 404:**

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

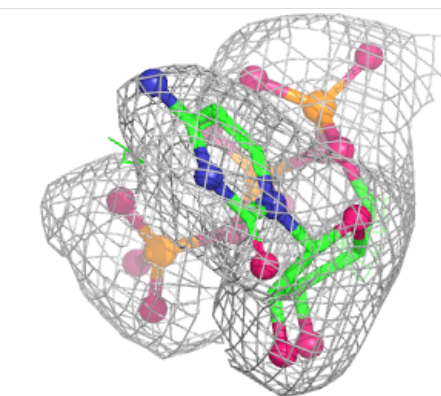
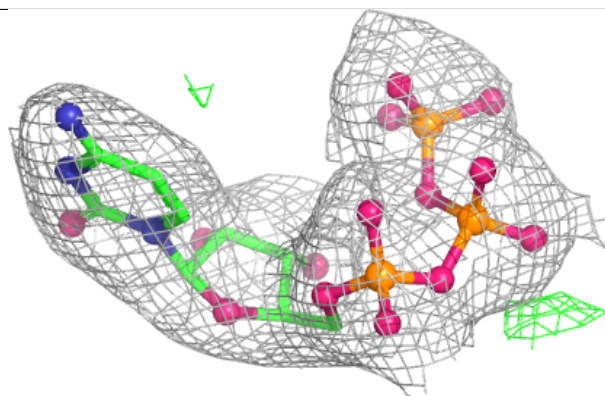
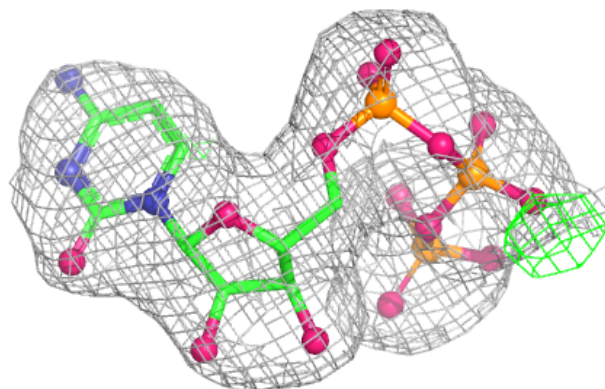


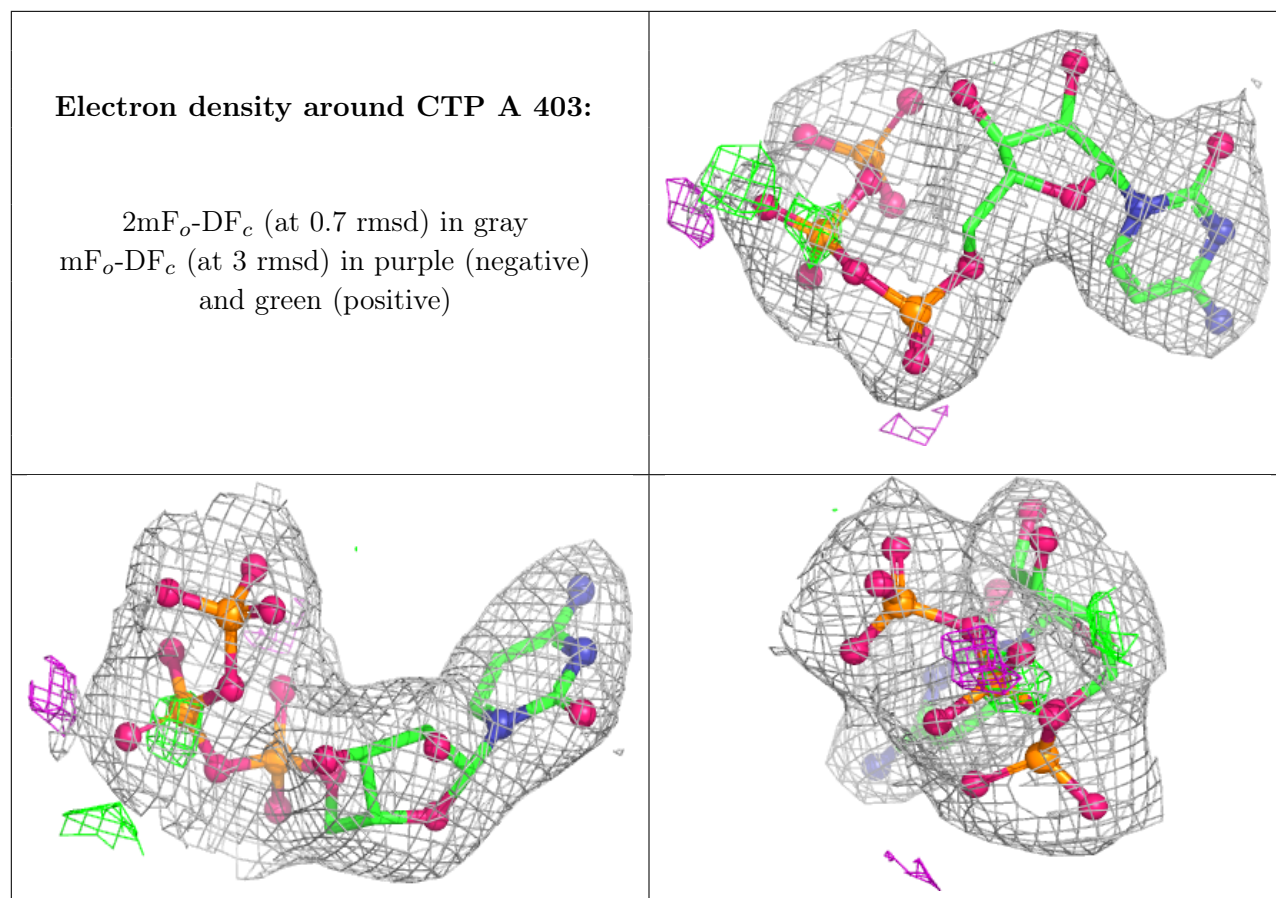
**Electron density around CTP F 403:**

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

**Electron density around CTP B 402:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.