



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:18 PM UTC

PDB ID : 4KI7 / pdb\_00004ki7  
Title : Design and structural analysis of aromatic inhibitors of type II dehydroquinase from Mycobacterium tuberculosis - compound 41c [3-hydroxy-5-(3-nitrophenoxy)benzoic acid]  
Authors : Dias, M.V.B.; Howard, N.G.; Blundell, T.L.; Abell, C.  
Deposited on : 2013-05-01  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

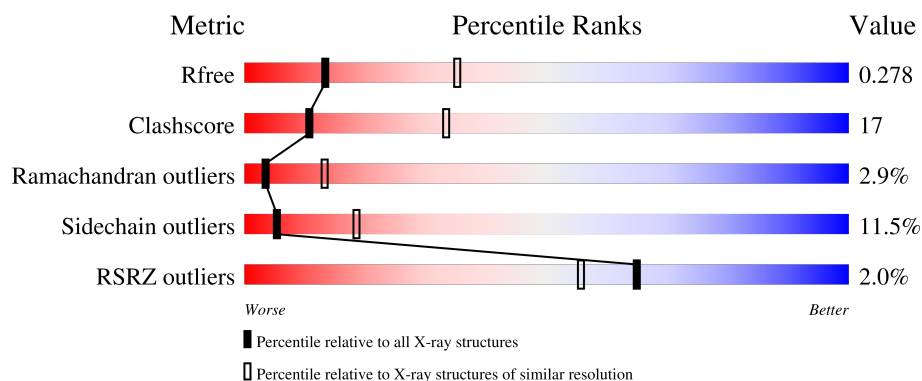
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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     | 153    | <div> <div>2%</div> <div>57% 25% 5% • 12%</div> </div> |
| 1   | B     | 153    | <div> <div>66% 24% • 8%</div> </div>                   |
| 1   | C     | 153    | <div> <div>• 64% 24% 5% 8%</div> </div>                |
| 1   | D     | 153    | <div> <div>• 59% 27% 5% • 7%</div> </div>              |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 153    |                  |
| 1   | F     | 153    |                  |
| 1   | G     | 153    |                  |
| 1   | H     | 153    |                  |
| 1   | I     | 153    |                  |
| 1   | J     | 153    |                  |
| 1   | K     | 153    |                  |
| 1   | L     | 153    |                  |
| 1   | M     | 153    |                  |
| 1   | N     | 153    |                  |
| 1   | O     | 153    |                  |
| 1   | P     | 153    |                  |
| 1   | Q     | 153    |                  |
| 1   | R     | 153    |                  |
| 1   | S     | 153    |                  |
| 1   | T     | 153    |                  |
| 1   | U     | 153    |                  |
| 1   | V     | 153    |                  |
| 1   | W     | 153    |                  |
| 1   | X     | 153    |                  |

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   | 1R2  | V     | 201 | -         | -        | X       | -                |
| 2   | 1R2  | W     | 201 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26499 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 3-dehydroquinate dehydratase.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1009  | 635 | 183 | 190 | 1 |         |         |       |
| 1   | B     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | C     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | D     | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1082  | 681 | 198 | 202 | 1 |         |         |       |
| 1   | E     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | F     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | G     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | H     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | I     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | J     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | K     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | L     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | M     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1040  | 652 | 192 | 195 | 1 |         |         |       |
| 1   | N     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | O     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | P     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Q     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1043  | 656 | 192 | 194 | 1 |         |         |       |
| 1   | R     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | S     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1057  | 665 | 192 | 199 | 1 |         |         |       |
| 1   | T     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | U     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1071  | 674 | 196 | 200 | 1 |         |         |       |
| 1   | V     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1067  | 672 | 196 | 198 | 1 |         |         |       |
| 1   | W     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1067  | 672 | 196 | 198 | 1 |         |         |       |
| 1   | X     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1150  | 725 | 208 | 215 | 2 |         |         |       |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| A     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| A     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| A     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| A     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| A     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| B     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| B     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| B     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| B     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| B     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| B     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| C     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| C     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| C     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| C     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| C     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| C     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| D     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| D     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| D     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| D     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| D     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| E     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| E     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| E     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| E     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| E     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| E     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| F     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| F     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| F     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| F     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| F     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| F     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| G     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| G     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| G     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| G     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| G     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| G     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| H     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| H     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| H     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| H     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| H     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| H     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| I     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| I     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| I     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| I     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| I     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| I     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| J     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| J     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| J     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| J     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| J     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| J     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| K     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| K     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| K     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| K     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| K     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| L     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| L     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| L     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| L     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| L     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| L     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| M     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| M     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| M     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| M     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| M     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| M     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| N     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| N     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| N     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| N     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| N     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| N     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| O     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| O     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| O     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| O     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| O     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| O     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| P     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| P     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| P     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| P     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| P     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| P     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| Q     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| Q     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| Q     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| Q     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| Q     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| Q     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| R     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| R     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| R     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| R     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| R     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |

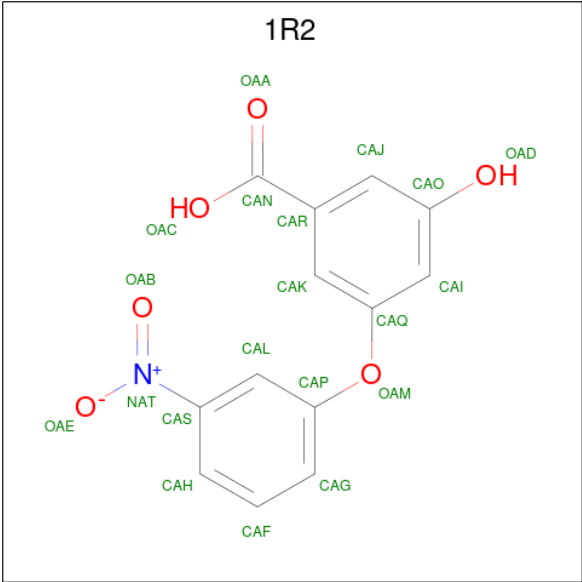
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| R     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| S     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| S     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| S     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| S     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| S     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| S     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| T     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| T     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| T     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| T     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| T     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| T     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| U     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| U     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| U     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| U     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| U     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| U     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| V     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| V     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| V     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| V     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| V     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| V     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| W     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| W     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| W     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| W     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| W     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| W     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |
| X     | -6      | LEU      | -      | expression tag | UNP P0A4Z6 |
| X     | -5      | TYR      | -      | expression tag | UNP P0A4Z6 |
| X     | -4      | PHE      | -      | expression tag | UNP P0A4Z6 |
| X     | -3      | GLN      | -      | expression tag | UNP P0A4Z6 |
| X     | -2      | SER      | -      | expression tag | UNP P0A4Z6 |
| X     | -1      | HIS      | -      | expression tag | UNP P0A4Z6 |

- Molecule 2 is 3-hydroxy-5-(3-nitrophenoxy)benzoic acid (CCD ID: 1R2) (formula:  $C_{13}H_9NO_6$ ).





| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | O     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | R     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | S     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | T     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | U     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | V     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | W     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |
| 2   | X     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 20    | 13 | 1 | 6 |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 3   | B     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 3   | C     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 3   | D     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 3   | E     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 3   | F     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 3   | G     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 3   | H     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 3   | I     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 3   | J     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 3   | K     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |

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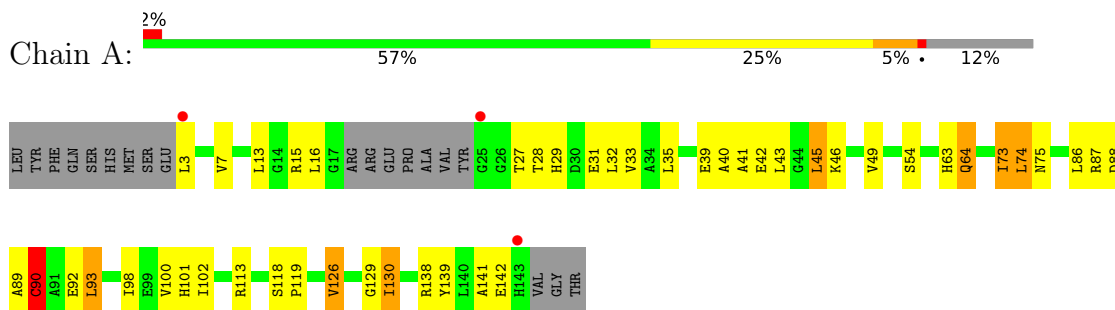
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | L     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | M     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | N     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | O     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | P     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 3   | Q     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | R     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 3   | S     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | T     | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 3   | U     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | V     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 3   | W     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | X     | 16       | Total<br>16 | O<br>16 | 0       | 0       |

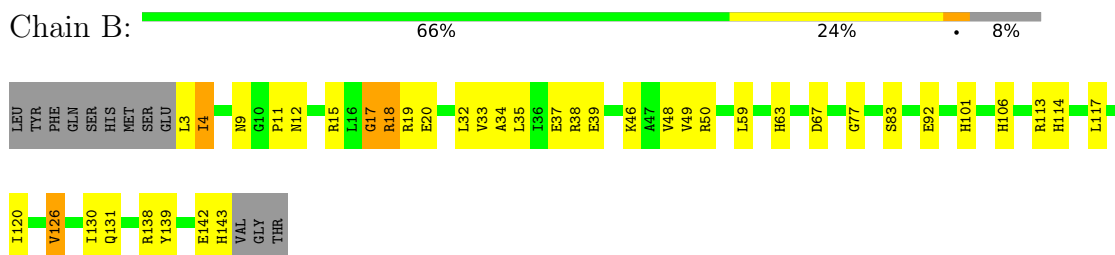
### 3 Residue-property plots [i](#)

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.

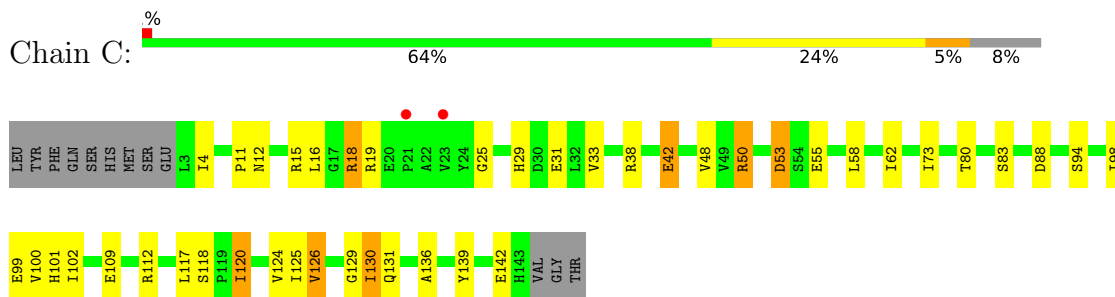
- Molecule 1: 3-dehydroquinate dehydratase



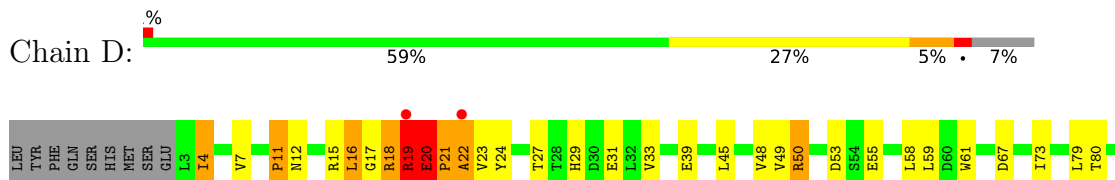
- Molecule 1: 3-dehydroquinate dehydratase

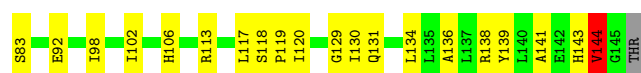


- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase

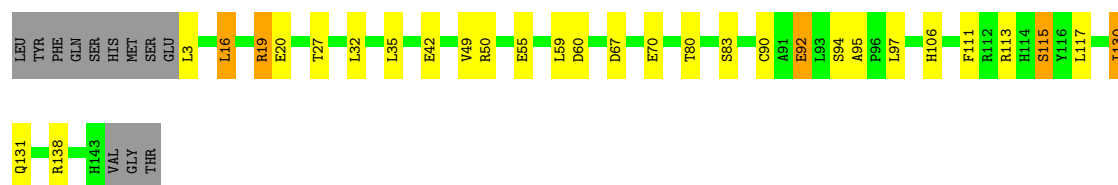




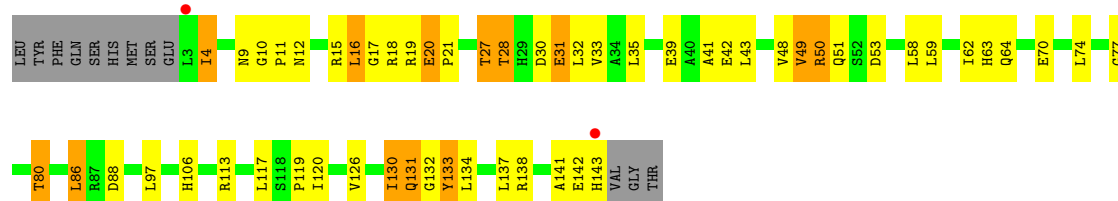
- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase

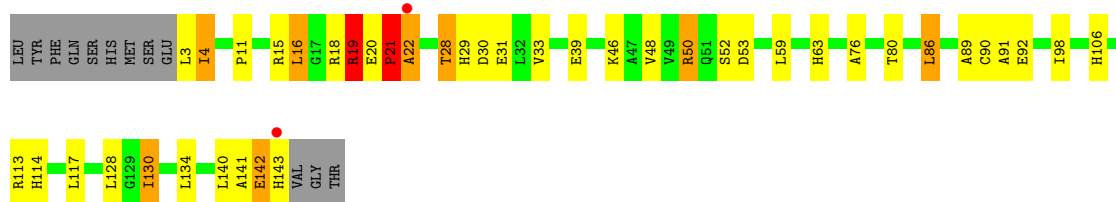


- Molecule 1: 3-dehydroquinate dehydratase

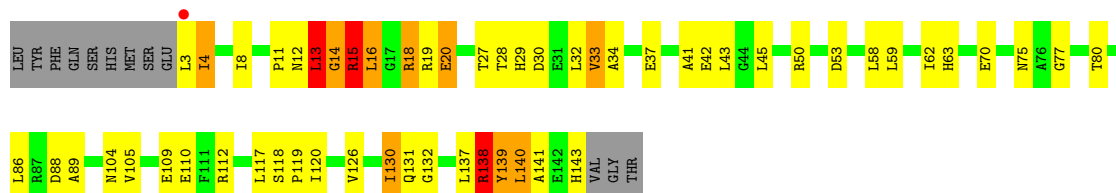




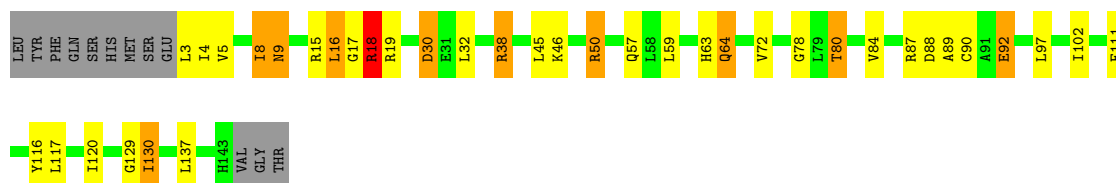
- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase



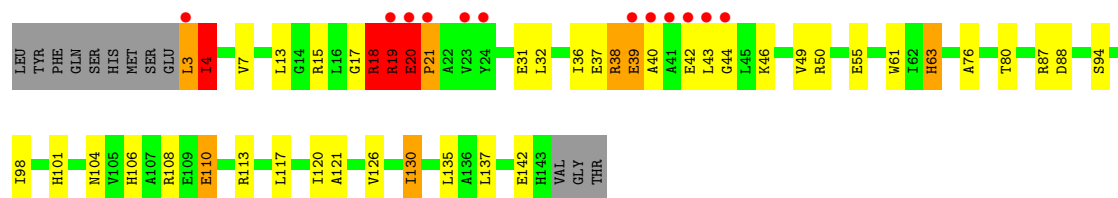
- Molecule 1: 3-dehydroquinase dehydratase



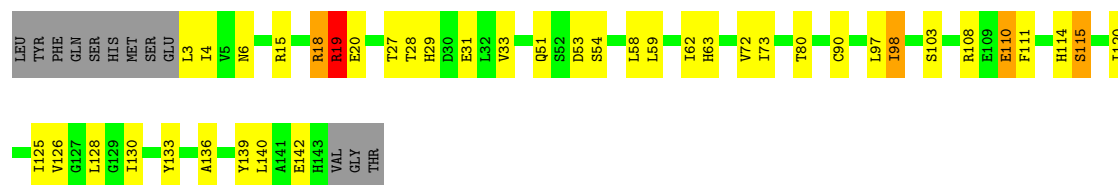
- Molecule 1: 3-dehydroquinase dehydratase



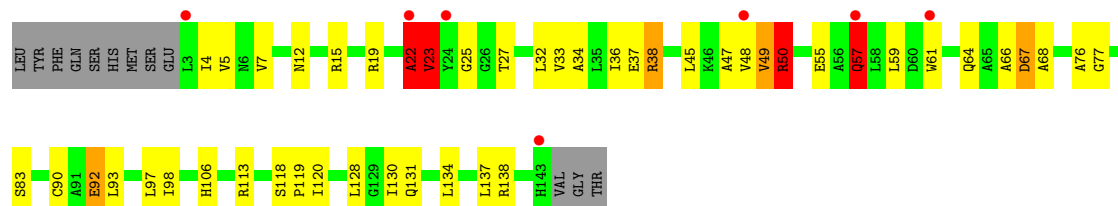
- Molecule 1: 3-dehydroquinase dehydratase



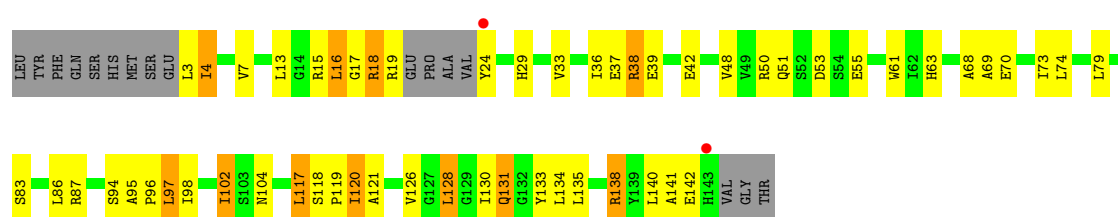
- Molecule 1: 3-dehydroquinatase dehydratase



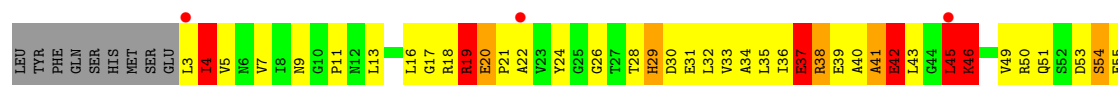
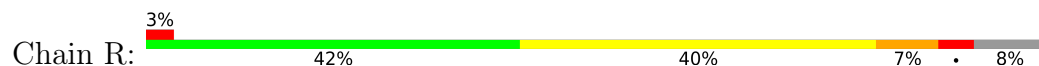
- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase

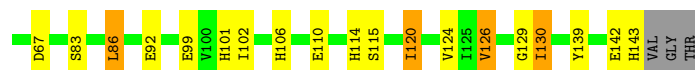
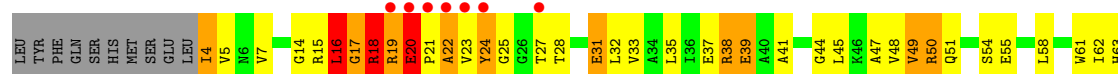


- Molecule 1: 3-dehydroquinatase dehydratase





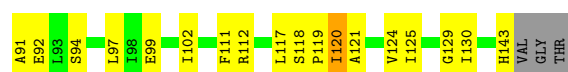
- Molecule 1: 3-dehydroquinate dehydratase



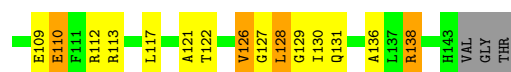
- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase



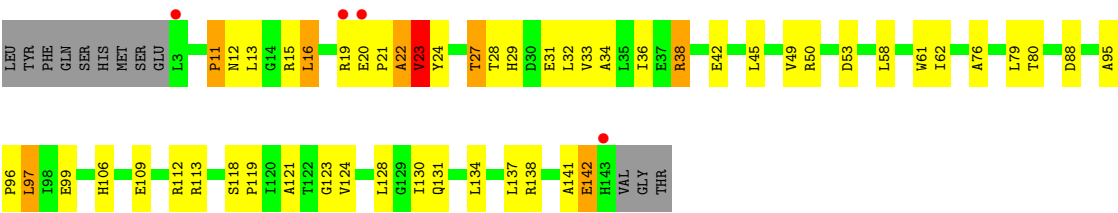
- Molecule 1: 3-dehydroquinate dehydratase



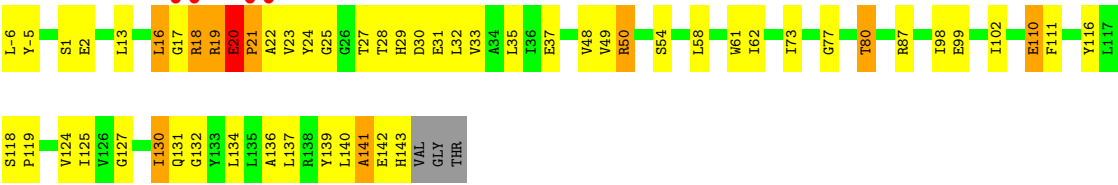
- Molecule 1: 3-dehydroquinate dehydratase







● Molecule 1: 3-dehydroquinate dehydratase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 96.74Å 139.69Å 143.81Å<br>90.00° 96.43° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 56.51 – 2.80<br>56.51 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (56.51-2.80)<br>99.7 (56.51-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.37 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.188 , 0.278<br>0.189 , 0.278                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4676 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.020                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 36.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 26499                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 24.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: 1R2

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     | 0.96         | 0/1024          | 1.05        | 1/1393 (0.1%)   |
| 1   | B     | 0.94         | 1/1089 (0.1%)   | 1.09        | 3/1483 (0.2%)   |
| 1   | C     | 0.97         | 1/1089 (0.1%)   | 1.10        | 4/1483 (0.3%)   |
| 1   | D     | 1.00         | 0/1100          | 1.20        | 4/1498 (0.3%)   |
| 1   | E     | 0.94         | 1/1089 (0.1%)   | 1.10        | 5/1483 (0.3%)   |
| 1   | F     | 0.94         | 0/1089          | 1.01        | 1/1483 (0.1%)   |
| 1   | G     | 0.95         | 0/1089          | 1.16        | 3/1483 (0.2%)   |
| 1   | H     | 0.95         | 1/1089 (0.1%)   | 1.08        | 1/1483 (0.1%)   |
| 1   | I     | 0.91         | 1/1089 (0.1%)   | 1.03        | 1/1483 (0.1%)   |
| 1   | J     | 1.02         | 1/1089 (0.1%)   | 1.17        | 5/1483 (0.3%)   |
| 1   | K     | 0.96         | 0/1089          | 1.20        | 4/1483 (0.3%)   |
| 1   | L     | 1.01         | 0/1089          | 1.13        | 2/1483 (0.1%)   |
| 1   | M     | 0.89         | 0/1055          | 1.12        | 3/1433 (0.2%)   |
| 1   | N     | 0.90         | 1/1089 (0.1%)   | 1.04        | 1/1483 (0.1%)   |
| 1   | O     | 0.96         | 1/1089 (0.1%)   | 1.06        | 1/1483 (0.1%)   |
| 1   | P     | 0.95         | 0/1089          | 1.15        | 7/1483 (0.5%)   |
| 1   | Q     | 0.85         | 0/1059          | 1.06        | 3/1439 (0.2%)   |
| 1   | R     | 0.94         | 1/1089 (0.1%)   | 1.20        | 4/1483 (0.3%)   |
| 1   | S     | 0.94         | 0/1075          | 1.07        | 1/1465 (0.1%)   |
| 1   | T     | 0.93         | 0/1089          | 1.09        | 3/1483 (0.2%)   |
| 1   | U     | 0.90         | 0/1089          | 1.03        | 3/1483 (0.2%)   |
| 1   | V     | 0.93         | 0/1085          | 1.01        | 2/1478 (0.1%)   |
| 1   | W     | 0.85         | 0/1085          | 1.08        | 2/1478 (0.1%)   |
| 1   | X     | 0.92         | 1/1171 (0.1%)   | 1.00        | 0/1593          |
| All | All   | 0.94         | 10/26078 (0.0%) | 1.09        | 64/35505 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | R     | 0                   | 1                   |
| 1   | S     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | B     | 114 | HIS  | CG-CD2 | 5.51 | 1.42        | 1.35     |
| 1   | J     | 114 | HIS  | CG-CD2 | 5.40 | 1.41        | 1.35     |
| 1   | E     | 143 | HIS  | CG-CD2 | 5.29 | 1.41        | 1.35     |
| 1   | O     | 114 | HIS  | CG-CD2 | 5.24 | 1.41        | 1.35     |
| 1   | H     | 114 | HIS  | CG-CD2 | 5.23 | 1.41        | 1.35     |
| 1   | N     | 63  | HIS  | CG-CD2 | 5.18 | 1.41        | 1.35     |
| 1   | R     | 29  | HIS  | CG-CD2 | 5.18 | 1.41        | 1.35     |
| 1   | I     | 114 | HIS  | CG-CD2 | 5.13 | 1.41        | 1.35     |
| 1   | C     | 25  | GLY  | N-CA   | 5.09 | 1.49        | 1.45     |
| 1   | X     | 20  | GLU  | CA-C   | 5.05 | 1.59        | 1.52     |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | K     | 14  | GLY  | N-CA-C | -10.75 | 92.23       | 111.80   |
| 1   | L     | 8   | ILE  | N-CA-C | 9.56   | 122.52      | 112.96   |
| 1   | J     | 128 | LEU  | N-CA-C | -9.30  | 94.08       | 109.24   |
| 1   | P     | 67  | ASP  | N-CA-C | -8.51  | 98.78       | 110.35   |
| 1   | R     | 79  | LEU  | N-CA-C | -8.15  | 102.78      | 112.89   |
| 1   | S     | 24  | TYR  | N-CA-C | -7.75  | 103.95      | 113.41   |
| 1   | D     | 20  | GLU  | CA-C-N | 7.31   | 128.98      | 119.84   |
| 1   | D     | 20  | GLU  | C-N-CA | 7.31   | 128.98      | 119.84   |
| 1   | W     | 22  | ALA  | CA-C-N | 7.25   | 134.74      | 121.70   |
| 1   | W     | 22  | ALA  | C-N-CA | 7.25   | 134.74      | 121.70   |
| 1   | J     | 21  | PRO  | CA-C-N | 6.88   | 134.08      | 121.70   |
| 1   | J     | 21  | PRO  | C-N-CA | 6.88   | 134.08      | 121.70   |
| 1   | V     | 23  | VAL  | N-CA-C | -6.84  | 105.09      | 111.45   |
| 1   | J     | 20  | GLU  | CA-C-N | 6.78   | 128.31      | 119.84   |
| 1   | J     | 20  | GLU  | C-N-CA | 6.78   | 128.31      | 119.84   |
| 1   | P     | 49  | VAL  | N-CA-C | 6.73   | 117.34      | 111.56   |
| 1   | E     | 4   | ILE  | N-CA-C | 6.43   | 117.34      | 109.30   |
| 1   | C     | 42  | GLU  | N-CA-C | -6.33  | 103.19      | 113.19   |
| 1   | D     | 4   | ILE  | N-CA-C | 6.24   | 117.56      | 108.58   |
| 1   | Q     | 94  | SER  | N-CA-C | 6.22   | 118.85      | 111.33   |
| 1   | P     | 83  | SER  | N-CA-C | 6.09   | 119.07      | 107.75   |
| 1   | E     | 83  | SER  | N-CA-C | 6.03   | 118.45      | 109.59   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 83  | SER  | N-CA-C   | 5.99  | 118.05      | 108.41   |
| 1   | C     | 53  | ASP  | N-CA-C   | -5.98 | 105.64      | 113.17   |
| 1   | E     | 10  | GLY  | CA-C-N   | 5.93  | 127.25      | 119.84   |
| 1   | E     | 10  | GLY  | C-N-CA   | 5.93  | 127.25      | 119.84   |
| 1   | Q     | 117 | LEU  | N-CA-C   | 5.92  | 118.68      | 111.82   |
| 1   | T     | 73  | ILE  | N-CA-C   | -5.92 | 99.89       | 108.17   |
| 1   | K     | 15  | ARG  | N-CA-C   | 5.89  | 123.35      | 110.80   |
| 1   | G     | 10  | GLY  | CA-C-N   | 5.87  | 126.21      | 119.93   |
| 1   | G     | 10  | GLY  | C-N-CA   | 5.87  | 126.21      | 119.93   |
| 1   | L     | 137 | LEU  | N-CA-C   | -5.82 | 105.01      | 111.36   |
| 1   | T     | 131 | GLN  | N-CA-C   | -5.79 | 105.48      | 112.54   |
| 1   | T     | 83  | SER  | N-CA-C   | 5.74  | 118.93      | 107.62   |
| 1   | I     | 23  | VAL  | CB-CA-C  | -5.69 | 105.84      | 111.30   |
| 1   | F     | 83  | SER  | N-CA-C   | 5.68  | 118.32      | 107.75   |
| 1   | M     | 118 | SER  | CA-C-N   | -5.60 | 114.05      | 119.87   |
| 1   | M     | 118 | SER  | C-N-CA   | -5.60 | 114.05      | 119.87   |
| 1   | C     | 83  | SER  | N-CA-C   | 5.56  | 117.71      | 108.20   |
| 1   | E     | 6   | ASN  | N-CA-C   | 5.56  | 117.36      | 108.41   |
| 1   | R     | 45  | LEU  | N-CA-C   | 5.55  | 122.63      | 110.80   |
| 1   | K     | 138 | ARG  | CA-C-N   | 5.45  | 131.50      | 121.70   |
| 1   | K     | 138 | ARG  | C-N-CA   | 5.45  | 131.50      | 121.70   |
| 1   | O     | 4   | ILE  | N-CA-C   | 5.44  | 116.60      | 109.58   |
| 1   | Q     | 83  | SER  | N-CA-C   | 5.42  | 117.13      | 108.41   |
| 1   | U     | 83  | SER  | N-CA-C   | 5.41  | 117.55      | 108.96   |
| 1   | R     | 132 | GLY  | N-CA-C   | -5.40 | 106.24      | 112.50   |
| 1   | B     | 17  | GLY  | CA-C-N   | 5.36  | 131.34      | 121.70   |
| 1   | B     | 17  | GLY  | C-N-CA   | 5.36  | 131.34      | 121.70   |
| 1   | U     | 24  | TYR  | N-CA-C   | 5.34  | 120.15      | 113.43   |
| 1   | C     | 4   | ILE  | N-CA-C   | 5.23  | 115.49      | 108.17   |
| 1   | A     | 74  | LEU  | N-CA-C   | 5.21  | 121.90      | 110.80   |
| 1   | N     | 4   | ILE  | N-CA-C   | 5.20  | 120.16      | 109.34   |
| 1   | H     | 24  | TYR  | N-CA-C   | 5.17  | 119.28      | 112.92   |
| 1   | V     | 83  | SER  | N-CA-C   | 5.12  | 117.71      | 107.62   |
| 1   | P     | 22  | ALA  | CA-C-N   | 5.06  | 130.81      | 121.70   |
| 1   | P     | 22  | ALA  | C-N-CA   | 5.06  | 130.81      | 121.70   |
| 1   | R     | 54  | SER  | N-CA-C   | 5.04  | 120.28      | 113.72   |
| 1   | G     | 41  | ALA  | N-CA-C   | -5.04 | 105.79      | 111.28   |
| 1   | M     | 49  | VAL  | N-CA-C   | 5.03  | 115.00      | 107.51   |
| 1   | B     | 83  | SER  | N-CA-C   | 5.03  | 117.10      | 107.75   |
| 1   | P     | 57  | GLN  | CB-CG-CD | 5.03  | 121.15      | 112.60   |
| 1   | P     | 23  | VAL  | N-CA-C   | 5.02  | 125.06      | 111.00   |
| 1   | U     | 82  | THR  | N-CA-C   | 5.01  | 120.25      | 114.04   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | R     | 78  | GLY  | Peptide |
| 1   | S     | 20  | GLU  | 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     | 1009  | 0        | 1016     | 40      | 0            |
| 1   | B     | 1071  | 0        | 1079     | 35      | 0            |
| 1   | C     | 1071  | 0        | 1079     | 26      | 0            |
| 1   | D     | 1082  | 0        | 1091     | 63      | 0            |
| 1   | E     | 1071  | 0        | 1079     | 26      | 0            |
| 1   | F     | 1071  | 0        | 1079     | 19      | 0            |
| 1   | G     | 1071  | 0        | 1079     | 43      | 0            |
| 1   | H     | 1071  | 0        | 1079     | 31      | 0            |
| 1   | I     | 1071  | 0        | 1079     | 31      | 0            |
| 1   | J     | 1071  | 0        | 1079     | 35      | 0            |
| 1   | K     | 1071  | 0        | 1079     | 59      | 0            |
| 1   | L     | 1071  | 0        | 1079     | 30      | 0            |
| 1   | M     | 1040  | 0        | 1048     | 39      | 0            |
| 1   | N     | 1071  | 0        | 1079     | 35      | 0            |
| 1   | O     | 1071  | 0        | 1079     | 32      | 0            |
| 1   | P     | 1071  | 0        | 1079     | 49      | 0            |
| 1   | Q     | 1043  | 0        | 1051     | 41      | 0            |
| 1   | R     | 1071  | 0        | 1079     | 64      | 0            |
| 1   | S     | 1057  | 0        | 1057     | 59      | 0            |
| 1   | T     | 1071  | 0        | 1079     | 26      | 0            |
| 1   | U     | 1071  | 0        | 1079     | 27      | 0            |
| 1   | V     | 1067  | 0        | 1075     | 31      | 0            |
| 1   | W     | 1067  | 0        | 1075     | 49      | 0            |
| 1   | X     | 1150  | 0        | 1151     | 56      | 0            |
| 2   | A     | 20    | 0        | 8        | 1       | 0            |
| 2   | B     | 20    | 0        | 8        | 2       | 0            |
| 2   | C     | 20    | 0        | 8        | 1       | 0            |
| 2   | D     | 20    | 0        | 8        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | E     | 20    | 0        | 8        | 1       | 0            |
| 2   | F     | 20    | 0        | 7        | 1       | 0            |
| 2   | G     | 20    | 0        | 8        | 2       | 0            |
| 2   | H     | 20    | 0        | 8        | 0       | 0            |
| 2   | I     | 20    | 0        | 8        | 2       | 0            |
| 2   | J     | 20    | 0        | 8        | 0       | 0            |
| 2   | K     | 20    | 0        | 8        | 2       | 0            |
| 2   | L     | 20    | 0        | 7        | 0       | 0            |
| 2   | N     | 20    | 0        | 7        | 2       | 0            |
| 2   | O     | 20    | 0        | 8        | 1       | 0            |
| 2   | P     | 20    | 0        | 8        | 0       | 0            |
| 2   | R     | 20    | 0        | 8        | 2       | 0            |
| 2   | S     | 20    | 0        | 8        | 0       | 0            |
| 2   | T     | 20    | 0        | 8        | 5       | 0            |
| 2   | U     | 20    | 0        | 8        | 0       | 0            |
| 2   | V     | 20    | 0        | 8        | 9       | 0            |
| 2   | W     | 20    | 0        | 7        | 8       | 0            |
| 2   | X     | 20    | 0        | 7        | 3       | 0            |
| 3   | A     | 11    | 0        | 0        | 4       | 0            |
| 3   | B     | 23    | 0        | 0        | 2       | 0            |
| 3   | C     | 23    | 0        | 0        | 0       | 0            |
| 3   | D     | 18    | 0        | 0        | 0       | 0            |
| 3   | E     | 22    | 0        | 0        | 0       | 0            |
| 3   | F     | 14    | 0        | 0        | 0       | 0            |
| 3   | G     | 21    | 0        | 0        | 0       | 0            |
| 3   | H     | 21    | 0        | 0        | 1       | 0            |
| 3   | I     | 16    | 0        | 0        | 1       | 0            |
| 3   | J     | 21    | 0        | 0        | 3       | 0            |
| 3   | K     | 12    | 0        | 0        | 0       | 0            |
| 3   | L     | 15    | 0        | 0        | 1       | 0            |
| 3   | M     | 11    | 0        | 0        | 1       | 0            |
| 3   | N     | 17    | 0        | 0        | 1       | 0            |
| 3   | O     | 11    | 0        | 0        | 0       | 0            |
| 3   | P     | 21    | 0        | 0        | 2       | 0            |
| 3   | Q     | 18    | 0        | 0        | 1       | 0            |
| 3   | R     | 14    | 0        | 0        | 2       | 0            |
| 3   | S     | 11    | 0        | 0        | 2       | 0            |
| 3   | T     | 23    | 0        | 0        | 1       | 0            |
| 3   | U     | 18    | 0        | 0        | 1       | 0            |
| 3   | V     | 21    | 0        | 0        | 2       | 0            |
| 3   | W     | 10    | 0        | 0        | 1       | 0            |
| 3   | X     | 16    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 26499 | 0        | 25999    | 872     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (872) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:201:1R2:NAT  | 2:I:201:1R2:OAE  | 1.57                     | 1.36              |
| 2:V:201:1R2:OAB  | 2:V:201:1R2:NAT  | 1.61                     | 1.34              |
| 2:F:201:1R2:OAE  | 2:F:201:1R2:NAT  | 1.60                     | 1.32              |
| 2:T:201:1R2:NAT  | 2:T:201:1R2:OAB  | 1.57                     | 1.31              |
| 2:V:201:1R2:NAT  | 2:V:201:1R2:OAE  | 1.62                     | 1.30              |
| 2:W:201:1R2:OAE  | 2:W:201:1R2:NAT  | 1.62                     | 1.30              |
| 2:G:201:1R2:OAB  | 2:G:201:1R2:NAT  | 1.61                     | 1.30              |
| 1:X:142:GLU:CB   | 1:X:143:HIS:HA   | 1.62                     | 1.25              |
| 1:P:57:GLN:NE2   | 1:P:61:TRP:HE3   | 1.35                     | 1.24              |
| 1:K:138:ARG:HA   | 1:K:139:TYR:O    | 1.39                     | 1.17              |
| 1:B:17:GLY:HA3   | 1:B:18:ARG:HB2   | 1.20                     | 1.15              |
| 1:E:20:GLU:H     | 1:E:21:PRO:HD3   | 1.06                     | 1.14              |
| 1:X:21:PRO:HB2   | 1:X:22:ALA:HA    | 1.32                     | 1.12              |
| 1:H:21:PRO:HB2   | 1:H:22:ALA:CA    | 1.80                     | 1.10              |
| 1:X:142:GLU:HB3  | 1:X:143:HIS:HA   | 1.34                     | 1.09              |
| 1:S:50:ARG:HG2   | 1:S:50:ARG:HH21  | 0.96                     | 1.08              |
| 1:W:22:ALA:HB3   | 1:W:23:VAL:HB    | 1.13                     | 1.08              |
| 1:H:21:PRO:HB2   | 1:H:22:ALA:HA    | 1.19                     | 1.08              |
| 1:H:88:ASP:O     | 1:I:19:ARG:NH2   | 1.89                     | 1.05              |
| 1:S:19:ARG:O     | 1:S:20:GLU:HG2   | 1.56                     | 1.04              |
| 1:N:17:GLY:N     | 1:N:18:ARG:HB2   | 1.71                     | 1.04              |
| 1:X:17:GLY:HA3   | 1:X:18:ARG:C     | 1.80                     | 1.03              |
| 1:S:102:ILE:HG23 | 1:S:129:GLY:HA2  | 1.41                     | 1.02              |
| 1:D:21:PRO:HB3   | 1:D:23:VAL:N     | 1.75                     | 1.02              |
| 1:A:89:ALA:HB2   | 1:K:12:ASN:OD1   | 1.59                     | 1.02              |
| 1:D:18:ARG:O     | 1:D:19:ARG:HB2   | 1.57                     | 1.02              |
| 1:X:142:GLU:HB2  | 1:X:143:HIS:HA   | 1.36                     | 1.01              |
| 1:D:138:ARG:NE   | 1:I:138:ARG:HD3  | 1.77                     | 1.00              |
| 1:L:32:LEU:HD13  | 1:L:130:ILE:HG13 | 1.42                     | 1.00              |
| 1:L:50:ARG:HH11  | 1:L:50:ARG:HB2   | 1.24                     | 1.00              |
| 1:W:19:ARG:HG3   | 1:W:20:GLU:H     | 1.25                     | 1.00              |
| 1:N:17:GLY:H     | 1:N:18:ARG:HB2   | 1.22                     | 0.99              |
| 1:N:20:GLU:HB2   | 1:N:21:PRO:HA    | 1.46                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:22:ALA:CB    | 1:W:23:VAL:HB    | 1.96                     | 0.95              |
| 1:P:57:GLN:NE2   | 1:P:61:TRP:CE3   | 2.27                     | 0.94              |
| 1:E:20:GLU:N     | 1:E:21:PRO:HD3   | 1.83                     | 0.93              |
| 1:P:47:ALA:HB3   | 3:P:305:HOH:O    | 1.69                     | 0.93              |
| 1:X:17:GLY:HA3   | 1:X:18:ARG:O     | 1.65                     | 0.93              |
| 1:V:131:GLN:HE22 | 1:X:139:TYR:HA   | 1.34                     | 0.93              |
| 1:X:21:PRO:HB2   | 1:X:22:ALA:CA    | 1.98                     | 0.93              |
| 1:X:20:GLU:HB3   | 1:X:21:PRO:O     | 1.69                     | 0.92              |
| 1:B:63:HIS:HD2   | 3:B:311:HOH:O    | 1.51                     | 0.91              |
| 1:D:21:PRO:HA    | 1:D:22:ALA:HB3   | 1.53                     | 0.91              |
| 1:H:21:PRO:CB    | 1:H:22:ALA:HA    | 2.01                     | 0.90              |
| 1:L:17:GLY:HA2   | 1:L:19:ARG:N     | 1.85                     | 0.90              |
| 1:P:15:ARG:HD2   | 1:S:63:HIS:CD2   | 2.07                     | 0.90              |
| 1:X:142:GLU:CB   | 1:X:143:HIS:CA   | 2.49                     | 0.90              |
| 1:H:20:GLU:HB3   | 1:H:21:PRO:HA    | 1.54                     | 0.89              |
| 1:V:38:ARG:HG3   | 1:V:38:ARG:HH11  | 1.37                     | 0.89              |
| 1:N:20:GLU:HB2   | 1:N:21:PRO:CA    | 2.03                     | 0.89              |
| 1:G:15:ARG:O     | 1:G:16:LEU:HB3   | 1.71                     | 0.89              |
| 1:S:5:VAL:O      | 1:S:47:ALA:O     | 1.92                     | 0.88              |
| 1:W:19:ARG:HG3   | 1:W:20:GLU:N     | 1.83                     | 0.88              |
| 1:F:32:LEU:HD13  | 1:F:130:ILE:HG13 | 1.55                     | 0.88              |
| 1:K:18:ARG:HH11  | 1:K:18:ARG:HG2   | 1.36                     | 0.88              |
| 1:K:138:ARG:CA   | 1:K:139:TYR:O    | 2.20                     | 0.88              |
| 1:V:29:HIS:HB2   | 3:V:302:HOH:O    | 1.73                     | 0.88              |
| 1:G:32:LEU:HD13  | 1:G:130:ILE:HG13 | 1.56                     | 0.87              |
| 1:D:143:HIS:O    | 1:D:144:VAL:HB   | 1.75                     | 0.87              |
| 1:E:20:GLU:H     | 1:E:21:PRO:CD    | 1.87                     | 0.86              |
| 1:D:15:ARG:HD2   | 1:G:63:HIS:CD2   | 2.11                     | 0.85              |
| 1:B:17:GLY:CA    | 1:B:18:ARG:HB2   | 2.06                     | 0.85              |
| 1:S:50:ARG:HG2   | 1:S:50:ARG:NH2   | 1.75                     | 0.85              |
| 1:D:20:GLU:HB2   | 1:D:21:PRO:HD2   | 1.58                     | 0.85              |
| 1:S:86:LEU:HG    | 3:S:303:HOH:O    | 1.76                     | 0.85              |
| 1:K:14:GLY:O     | 1:K:16:LEU:N     | 2.10                     | 0.85              |
| 1:V:99:GLU:OE2   | 1:V:101:HIS:NE2  | 2.10                     | 0.85              |
| 1:I:23:VAL:HG11  | 1:I:108:ARG:NH1  | 1.92                     | 0.84              |
| 1:Q:4:ILE:HG13   | 3:Q:207:HOH:O    | 1.76                     | 0.84              |
| 1:D:21:PRO:HG3   | 1:D:23:VAL:HB    | 1.58                     | 0.84              |
| 1:G:15:ARG:O     | 1:G:16:LEU:CB    | 2.24                     | 0.84              |
| 1:I:23:VAL:HG11  | 1:I:108:ARG:HH12 | 1.40                     | 0.83              |
| 1:L:17:GLY:HA2   | 1:L:19:ARG:H     | 1.44                     | 0.83              |
| 1:R:24:TYR:HA    | 1:R:102:ILE:HD11 | 1.58                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:21:PRO:CB    | 1:X:22:ALA:HA    | 2.09                     | 0.82              |
| 2:V:201:1R2:CAG  | 2:V:201:1R2:H2   | 2.08                     | 0.82              |
| 1:C:101:HIS:HB2  | 1:C:126:VAL:HG22 | 1.60                     | 0.82              |
| 1:X:142:GLU:HB2  | 1:X:143:HIS:CA   | 2.11                     | 0.81              |
| 1:A:15:ARG:HD2   | 1:L:63:HIS:CD2   | 2.16                     | 0.81              |
| 1:E:130:ILE:O    | 1:E:131:GLN:HB3  | 1.82                     | 0.80              |
| 1:P:48:VAL:H     | 1:P:50:ARG:NH2   | 1.79                     | 0.80              |
| 1:P:57:GLN:HE22  | 1:P:61:TRP:HE3   | 0.80                     | 0.80              |
| 1:B:17:GLY:HA3   | 1:B:18:ARG:CB    | 2.09                     | 0.79              |
| 1:E:19:ARG:O     | 1:E:20:GLU:HB2   | 1.82                     | 0.79              |
| 1:J:4:ILE:HD12   | 1:J:4:ILE:H      | 1.47                     | 0.79              |
| 1:R:37:GLU:O     | 1:R:38:ARG:HB3   | 1.82                     | 0.79              |
| 1:S:50:ARG:HH21  | 1:S:50:ARG:CG    | 1.88                     | 0.79              |
| 1:J:28:THR:HG21  | 3:J:306:HOH:O    | 1.81                     | 0.78              |
| 1:K:18:ARG:HH11  | 1:K:18:ARG:CG    | 1.96                     | 0.78              |
| 1:D:20:GLU:CB    | 1:D:21:PRO:CD    | 2.60                     | 0.78              |
| 1:K:3:LEU:O      | 1:K:4:ILE:HG13   | 1.83                     | 0.78              |
| 1:W:13:LEU:HG    | 2:W:201:1R2:H8   | 1.66                     | 0.78              |
| 1:H:88:ASP:C     | 1:I:19:ARG:HH22  | 1.91                     | 0.78              |
| 1:M:32:LEU:HD13  | 1:M:130:ILE:HD12 | 1.66                     | 0.77              |
| 1:E:135:LEU:HD21 | 1:K:138:ARG:O    | 1.85                     | 0.77              |
| 1:D:18:ARG:HB2   | 1:D:18:ARG:HH21  | 1.50                     | 0.77              |
| 1:X:142:GLU:N    | 1:X:142:GLU:OE1  | 2.18                     | 0.76              |
| 1:X:141:ALA:C    | 1:X:142:GLU:OE1  | 2.27                     | 0.76              |
| 1:A:100:VAL:HG21 | 3:A:301:HOH:O    | 1.86                     | 0.76              |
| 1:N:32:LEU:O     | 1:N:36:ILE:HG13  | 1.85                     | 0.75              |
| 1:S:14:GLY:H     | 1:S:51:GLN:NE2   | 1.85                     | 0.75              |
| 1:F:80:THR:HG22  | 1:F:115:SER:HB2  | 1.65                     | 0.75              |
| 1:D:20:GLU:CB    | 1:D:21:PRO:HD2   | 2.12                     | 0.75              |
| 1:D:138:ARG:HE   | 1:I:138:ARG:HD3  | 1.49                     | 0.75              |
| 1:H:21:PRO:CB    | 1:H:22:ALA:CA    | 2.60                     | 0.74              |
| 1:R:63:HIS:ND1   | 1:S:15:ARG:HD2   | 2.02                     | 0.74              |
| 1:M:17:GLY:HA2   | 1:M:18:ARG:C     | 2.13                     | 0.74              |
| 1:D:39:GLU:HG2   | 1:D:134:LEU:HD22 | 1.70                     | 0.73              |
| 1:H:20:GLU:HB3   | 1:H:21:PRO:CA    | 2.16                     | 0.73              |
| 1:N:20:GLU:CB    | 1:N:21:PRO:HA    | 2.17                     | 0.73              |
| 1:K:58:LEU:O     | 1:K:62:ILE:HG12  | 1.90                     | 0.72              |
| 1:V:38:ARG:HH11  | 1:V:38:ARG:CG    | 2.02                     | 0.72              |
| 1:O:19:ARG:HH11  | 1:O:19:ARG:HG2   | 1.55                     | 0.72              |
| 1:B:15:ARG:O     | 1:B:18:ARG:HB3   | 1.90                     | 0.71              |
| 1:J:16:LEU:HD11  | 1:J:130:ILE:HD11 | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:37:GLU:O     | 1:S:38:ARG:HB2   | 1.91                     | 0.71              |
| 1:N:63:HIS:CD2   | 1:O:15:ARG:HD2   | 2.26                     | 0.71              |
| 1:W:19:ARG:CG    | 1:W:20:GLU:H     | 2.01                     | 0.71              |
| 1:D:21:PRO:HB3   | 1:D:23:VAL:H     | 1.55                     | 0.71              |
| 1:A:73:ILE:O     | 1:A:98:ILE:O     | 2.09                     | 0.70              |
| 1:R:130:ILE:N    | 1:R:130:ILE:HD12 | 2.07                     | 0.70              |
| 1:M:50:ARG:HB3   | 1:M:61:TRP:CZ3   | 2.26                     | 0.70              |
| 1:C:117:LEU:O    | 1:C:120:ILE:HG13 | 1.92                     | 0.69              |
| 1:B:32:LEU:HD13  | 1:B:130:ILE:HD11 | 1.74                     | 0.69              |
| 1:D:18:ARG:HH21  | 1:D:18:ARG:CB    | 2.05                     | 0.69              |
| 1:N:7:VAL:HB     | 1:N:49:VAL:HG22  | 1.74                     | 0.69              |
| 1:T:128:LEU:O    | 1:T:131:GLN:HG2  | 1.91                     | 0.69              |
| 1:N:17:GLY:CA    | 1:N:18:ARG:HB2   | 2.23                     | 0.69              |
| 2:V:201:1R2:H2   | 2:V:201:1R2:H9   | 1.75                     | 0.69              |
| 1:X:58:LEU:O     | 1:X:62:ILE:HG12  | 1.93                     | 0.69              |
| 1:B:4:ILE:HD12   | 1:B:4:ILE:H      | 1.57                     | 0.69              |
| 1:H:120:ILE:C    | 1:H:120:ILE:HD12 | 2.18                     | 0.69              |
| 1:N:120:ILE:HD12 | 1:N:120:ILE:C    | 2.18                     | 0.68              |
| 1:H:21:PRO:HB2   | 1:H:22:ALA:CB    | 2.22                     | 0.68              |
| 1:A:139:TYR:HA   | 1:G:131:GLN:OE1  | 1.94                     | 0.68              |
| 1:J:21:PRO:HB2   | 1:J:22:ALA:HB2   | 1.76                     | 0.68              |
| 1:S:129:GLY:O    | 1:S:130:ILE:HB   | 1.94                     | 0.68              |
| 1:A:101:HIS:HB2  | 1:A:126:VAL:HG22 | 1.75                     | 0.68              |
| 1:Q:117:LEU:O    | 1:Q:120:ILE:HD13 | 1.94                     | 0.68              |
| 1:R:35:LEU:O     | 1:R:39:GLU:HB2   | 1.94                     | 0.68              |
| 1:T:131:GLN:HE21 | 1:T:131:GLN:N    | 1.91                     | 0.68              |
| 1:G:20:GLU:N     | 1:G:21:PRO:CD    | 2.57                     | 0.68              |
| 1:G:20:GLU:N     | 1:G:21:PRO:HD2   | 2.08                     | 0.68              |
| 1:N:18:ARG:O     | 1:N:19:ARG:HB2   | 1.93                     | 0.68              |
| 1:W:20:GLU:O     | 1:W:23:VAL:HG12  | 1.93                     | 0.67              |
| 1:R:54:SER:O     | 1:R:56:ALA:N     | 2.24                     | 0.67              |
| 1:R:97:LEU:HD23  | 1:R:121:ALA:HA   | 1.75                     | 0.67              |
| 1:R:131:GLN:HG2  | 1:R:131:GLN:O    | 1.94                     | 0.67              |
| 1:T:131:GLN:H    | 1:T:131:GLN:NE2  | 1.92                     | 0.67              |
| 1:M:92:GLU:HG2   | 1:W:19:ARG:HD3   | 1.75                     | 0.67              |
| 1:R:3:LEU:O      | 1:R:4:ILE:HG22   | 1.95                     | 0.67              |
| 1:W:13:LEU:HG    | 2:W:201:1R2:CAF  | 2.24                     | 0.67              |
| 1:T:131:GLN:HE21 | 1:T:131:GLN:H    | 1.43                     | 0.67              |
| 1:V:109:GLU:OE1  | 1:V:112:ARG:NE   | 2.28                     | 0.66              |
| 1:H:20:GLU:CB    | 1:H:21:PRO:HA    | 2.24                     | 0.66              |
| 1:P:15:ARG:HD2   | 1:S:63:HIS:HD2   | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:88:ASP:O     | 1:O:19:ARG:NH2   | 2.28                     | 0.66              |
| 1:P:22:ALA:HA    | 1:P:23:VAL:C     | 2.21                     | 0.66              |
| 1:R:78:GLY:HA2   | 1:R:81:HIS:CD2   | 2.30                     | 0.66              |
| 1:G:4:ILE:HG13   | 1:G:70:GLU:HG2   | 1.77                     | 0.66              |
| 1:M:119:PRO:HB3  | 1:S:106:HIS:O    | 1.96                     | 0.66              |
| 1:P:130:ILE:HD11 | 3:P:303:HOH:O    | 1.93                     | 0.66              |
| 1:J:18:ARG:O     | 1:J:19:ARG:HB2   | 1.96                     | 0.66              |
| 1:M:18:ARG:NH2   | 1:M:29:HIS:H     | 1.93                     | 0.66              |
| 1:J:21:PRO:CB    | 1:J:22:ALA:HB2   | 2.25                     | 0.66              |
| 1:X:17:GLY:CA    | 1:X:18:ARG:C     | 2.61                     | 0.66              |
| 1:C:48:VAL:HG12  | 1:C:50:ARG:HD2   | 1.78                     | 0.65              |
| 1:D:48:VAL:HG12  | 1:D:50:ARG:HD2   | 1.78                     | 0.65              |
| 1:W:29:HIS:O     | 1:W:33:VAL:HG23  | 1.96                     | 0.65              |
| 1:B:138:ARG:HG2  | 3:B:306:HOH:O    | 1.94                     | 0.65              |
| 1:S:58:LEU:O     | 1:S:62:ILE:HG12  | 1.97                     | 0.65              |
| 1:N:3:LEU:C      | 1:N:4:ILE:HG13   | 2.21                     | 0.65              |
| 1:R:19:ARG:O     | 1:R:19:ARG:HG3   | 1.95                     | 0.65              |
| 1:V:19:ARG:HG3   | 1:V:19:ARG:HH11  | 1.62                     | 0.65              |
| 1:E:99:GLU:HB3   | 1:E:124:VAL:HG13 | 1.78                     | 0.65              |
| 1:H:15:ARG:HD2   | 1:J:63:HIS:CD2   | 2.31                     | 0.65              |
| 1:J:28:THR:CG2   | 3:J:306:HOH:O    | 2.43                     | 0.65              |
| 1:D:21:PRO:CG    | 1:D:23:VAL:HB    | 2.25                     | 0.65              |
| 1:N:120:ILE:HD12 | 1:N:121:ALA:N    | 2.12                     | 0.65              |
| 1:R:24:TYR:HD1   | 1:R:102:ILE:HG12 | 1.62                     | 0.65              |
| 1:O:19:ARG:HD3   | 2:O:201:1R2:OAB  | 1.97                     | 0.64              |
| 1:P:66:ALA:HB1   | 1:P:92:GLU:CG    | 2.27                     | 0.64              |
| 1:D:19:ARG:HG2   | 1:D:20:GLU:CD    | 2.22                     | 0.64              |
| 1:H:50:ARG:HD3   | 1:H:61:TRP:CD2   | 2.32                     | 0.64              |
| 1:B:32:LEU:HD13  | 1:B:130:ILE:CG1  | 2.28                     | 0.64              |
| 1:A:33:VAL:HG13  | 1:A:49:VAL:HB    | 1.79                     | 0.64              |
| 1:P:128:LEU:HD11 | 1:U:125:ILE:HD11 | 1.80                     | 0.64              |
| 1:V:99:GLU:OE2   | 1:V:101:HIS:CD2  | 2.49                     | 0.64              |
| 1:I:59:LEU:HD12  | 1:J:53:ASP:HB3   | 1.80                     | 0.64              |
| 1:K:33:VAL:HG13  | 1:K:34:ALA:N     | 2.12                     | 0.64              |
| 1:R:41:ALA:O     | 1:R:43:LEU:N     | 2.29                     | 0.64              |
| 1:M:92:GLU:CG    | 1:W:19:ARG:HD3   | 2.27                     | 0.64              |
| 1:S:15:ARG:O     | 1:S:16:LEU:O     | 2.15                     | 0.64              |
| 1:J:80:THR:HA    | 1:J:117:LEU:HD12 | 1.80                     | 0.63              |
| 1:L:32:LEU:HD13  | 1:L:130:ILE:CG1  | 2.24                     | 0.63              |
| 1:M:142:GLU:O    | 1:M:143:HIS:HB2  | 1.99                     | 0.63              |
| 1:J:4:ILE:HD12   | 1:J:4:ILE:N      | 2.11                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:92:GLU:CD    | 1:S:15:ARG:HE    | 2.07                     | 0.63              |
| 1:S:7:VAL:HB     | 1:S:49:VAL:HB    | 1.81                     | 0.63              |
| 1:O:19:ARG:NH1   | 1:O:20:GLU:OE1   | 2.32                     | 0.62              |
| 1:A:43:LEU:C     | 1:A:45:LEU:H     | 2.08                     | 0.62              |
| 1:K:33:VAL:HG13  | 1:K:34:ALA:H     | 1.63                     | 0.62              |
| 1:H:114:HIS:HA   | 3:H:311:HOH:O    | 1.98                     | 0.62              |
| 1:D:20:GLU:HB2   | 1:D:21:PRO:CD    | 2.28                     | 0.62              |
| 2:V:201:1R2:CAG  | 2:V:201:1R2:CAK  | 2.78                     | 0.61              |
| 1:K:32:LEU:HD13  | 1:K:130:ILE:HD12 | 1.82                     | 0.61              |
| 1:X:33:VAL:HG12  | 1:X:37:GLU:OE2   | 1.99                     | 0.61              |
| 1:A:63:HIS:CD2   | 1:K:15:ARG:HD2   | 2.35                     | 0.61              |
| 1:D:16:LEU:C     | 1:D:18:ARG:H     | 2.08                     | 0.61              |
| 1:E:130:ILE:O    | 1:E:131:GLN:CB   | 2.47                     | 0.61              |
| 1:K:33:VAL:CG1   | 1:K:34:ALA:H     | 2.14                     | 0.61              |
| 1:Q:140:LEU:C    | 1:Q:142:GLU:H    | 2.09                     | 0.61              |
| 1:R:38:ARG:O     | 1:R:38:ARG:HG3   | 2.01                     | 0.61              |
| 1:L:50:ARG:HH11  | 1:L:50:ARG:CB    | 2.07                     | 0.60              |
| 1:Q:38:ARG:NH1   | 1:Q:39:GLU:HG2   | 2.15                     | 0.60              |
| 1:T:32:LEU:HD13  | 1:T:130:ILE:HG12 | 1.82                     | 0.60              |
| 1:X:18:ARG:O     | 1:X:28:THR:HG22  | 2.00                     | 0.60              |
| 1:X:29:HIS:O     | 1:X:33:VAL:HG23  | 2.01                     | 0.60              |
| 1:N:13:LEU:HD23  | 2:N:201:1R2:H6   | 1.83                     | 0.60              |
| 1:R:63:HIS:CG    | 1:S:15:ARG:HD2   | 2.36                     | 0.60              |
| 1:C:38:ARG:O     | 1:C:42:GLU:HG2   | 2.02                     | 0.60              |
| 1:M:59:LEU:HD23  | 1:M:86:LEU:HD12  | 1.83                     | 0.60              |
| 1:O:73:ILE:HD11  | 1:O:140:LEU:HD12 | 1.82                     | 0.60              |
| 1:J:86:LEU:HD23  | 1:J:117:LEU:HD21 | 1.84                     | 0.59              |
| 1:R:101:HIS:HB2  | 1:R:126:VAL:HG12 | 1.83                     | 0.59              |
| 1:X:19:ARG:N     | 1:X:19:ARG:HD2   | 2.17                     | 0.59              |
| 1:C:18:ARG:O     | 1:C:19:ARG:HG3   | 2.03                     | 0.59              |
| 1:M:18:ARG:HH22  | 1:M:29:HIS:H     | 1.48                     | 0.59              |
| 1:X:33:VAL:HG13  | 1:X:49:VAL:HB    | 1.85                     | 0.59              |
| 1:P:48:VAL:N     | 1:P:50:ARG:NH2   | 2.49                     | 0.59              |
| 1:X:20:GLU:CB    | 1:X:21:PRO:HA    | 2.33                     | 0.59              |
| 1:O:28:THR:OG1   | 1:O:31:GLU:HG3   | 2.03                     | 0.59              |
| 1:V:106:HIS:HA   | 1:V:113:ARG:HG2  | 1.85                     | 0.59              |
| 1:A:63:HIS:CG    | 1:K:15:ARG:HD2   | 2.38                     | 0.58              |
| 1:B:138:ARG:HD3  | 1:F:138:ARG:HD2  | 1.83                     | 0.58              |
| 1:D:131:GLN:HE22 | 1:I:142:GLU:HG2  | 1.68                     | 0.58              |
| 1:Q:102:ILE:HD11 | 1:Q:133:TYR:HE1  | 1.68                     | 0.58              |
| 1:I:99:GLU:HB3   | 1:I:124:VAL:HG13 | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:37:GLU:O     | 1:R:37:GLU:HG2   | 2.01                     | 0.58              |
| 1:K:33:VAL:O     | 1:K:37:GLU:HG2   | 2.03                     | 0.58              |
| 1:S:102:ILE:CG2  | 1:S:129:GLY:HA2  | 2.27                     | 0.58              |
| 1:D:92:GLU:HG3   | 1:F:19:ARG:CZ    | 2.33                     | 0.58              |
| 1:K:30:ASP:O     | 1:K:33:VAL:HG12  | 2.03                     | 0.58              |
| 1:K:75:ASN:C     | 1:K:75:ASN:HD22  | 2.11                     | 0.58              |
| 1:W:106:HIS:HA   | 1:W:113:ARG:HG2  | 1.85                     | 0.58              |
| 1:J:28:THR:HG23  | 1:J:31:GLU:HG3   | 1.86                     | 0.57              |
| 1:S:19:ARG:O     | 1:S:20:GLU:CG    | 2.41                     | 0.57              |
| 1:B:139:TYR:CE1  | 1:B:143:HIS:CE1  | 2.92                     | 0.57              |
| 1:K:138:ARG:O    | 1:K:138:ARG:CG   | 2.51                     | 0.57              |
| 1:R:29:HIS:O     | 1:R:33:VAL:HG23  | 2.05                     | 0.57              |
| 1:P:130:ILE:H    | 1:P:130:ILE:HD12 | 1.70                     | 0.57              |
| 1:R:34:ALA:O     | 1:R:38:ARG:HG2   | 2.05                     | 0.57              |
| 1:O:18:ARG:HG2   | 1:O:18:ARG:HH11  | 1.69                     | 0.57              |
| 1:P:7:VAL:O      | 1:P:49:VAL:O     | 2.22                     | 0.57              |
| 1:X:20:GLU:HB2   | 1:X:21:PRO:HA    | 1.86                     | 0.57              |
| 1:B:101:HIS:HB2  | 1:B:126:VAL:HG22 | 1.86                     | 0.57              |
| 1:L:102:ILE:HG23 | 1:L:129:GLY:HA2  | 1.86                     | 0.57              |
| 1:Q:38:ARG:NH1   | 1:Q:38:ARG:HB3   | 2.19                     | 0.57              |
| 1:E:130:ILE:N    | 1:E:130:ILE:HD13 | 2.20                     | 0.57              |
| 1:C:58:LEU:O     | 1:C:62:ILE:HG12  | 2.03                     | 0.57              |
| 1:K:80:THR:HG23  | 1:K:117:LEU:HD12 | 1.87                     | 0.56              |
| 1:R:28:THR:HB    | 1:R:31:GLU:HG2   | 1.87                     | 0.56              |
| 1:U:50:ARG:NE    | 3:U:303:HOH:O    | 2.38                     | 0.56              |
| 1:L:3:LEU:HD12   | 1:L:4:ILE:H      | 1.71                     | 0.56              |
| 1:N:76:ALA:HB3   | 1:N:80:THR:OG1   | 2.05                     | 0.56              |
| 1:O:103:SER:OG   | 1:O:108:ARG:NH1  | 2.37                     | 0.56              |
| 1:L:8:ILE:O      | 1:L:9:ASN:O      | 2.22                     | 0.56              |
| 1:Q:29:HIS:CE1   | 1:Q:51:GLN:HB2   | 2.40                     | 0.56              |
| 1:X:140:LEU:C    | 1:X:142:GLU:H    | 2.13                     | 0.56              |
| 1:D:143:HIS:O    | 1:D:144:VAL:CB   | 2.52                     | 0.56              |
| 1:F:32:LEU:HD13  | 1:F:130:ILE:CG1  | 2.32                     | 0.56              |
| 2:W:201:1R2:H2   | 2:W:201:1R2:CAG  | 2.34                     | 0.56              |
| 1:J:19:ARG:HD2   | 1:J:21:PRO:HD3   | 1.87                     | 0.56              |
| 1:W:13:LEU:CG    | 2:W:201:1R2:H8   | 2.34                     | 0.56              |
| 1:D:50:ARG:HB3   | 1:D:61:TRP:CZ3   | 2.40                     | 0.56              |
| 1:W:134:LEU:HA   | 1:W:137:LEU:HD12 | 1.88                     | 0.56              |
| 1:R:103:SER:HB2  | 2:R:201:1R2:OAC  | 2.05                     | 0.56              |
| 1:T:3:LEU:HD23   | 3:T:305:HOH:O    | 2.05                     | 0.56              |
| 1:A:32:LEU:HD13  | 1:A:130:ILE:HG13 | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:32:LEU:HD13  | 1:B:130:ILE:CD1  | 2.34                     | 0.56              |
| 1:S:55:GLU:OE1   | 1:S:83:SER:OG    | 2.20                     | 0.56              |
| 1:W:99:GLU:HB3   | 1:W:124:VAL:HG22 | 1.86                     | 0.56              |
| 1:N:101:HIS:HB3  | 2:N:201:1R2:OAC  | 2.06                     | 0.56              |
| 1:Q:29:HIS:O     | 1:Q:33:VAL:HG23  | 2.06                     | 0.56              |
| 1:D:16:LEU:HD13  | 1:D:27:THR:O     | 2.06                     | 0.55              |
| 1:P:50:ARG:HD2   | 1:P:61:TRP:CZ2   | 2.41                     | 0.55              |
| 1:R:24:TYR:HE2   | 3:R:311:HOH:O    | 1.89                     | 0.55              |
| 1:W:27:THR:HG23  | 1:W:31:GLU:HB2   | 1.88                     | 0.55              |
| 1:G:16:LEU:HB2   | 2:G:201:1R2:OAE  | 2.06                     | 0.55              |
| 1:Q:4:ILE:HD13   | 1:Q:70:GLU:HG2   | 1.89                     | 0.55              |
| 1:W:20:GLU:O     | 1:W:23:VAL:CG1   | 2.54                     | 0.55              |
| 1:K:32:LEU:O     | 1:K:33:VAL:HB    | 2.06                     | 0.55              |
| 1:R:127:GLY:O    | 1:R:129:GLY:N    | 2.39                     | 0.55              |
| 1:X:140:LEU:O    | 1:X:142:GLU:N    | 2.39                     | 0.55              |
| 1:D:21:PRO:HA    | 1:D:22:ALA:CB    | 2.31                     | 0.55              |
| 1:M:102:ILE:HG23 | 1:M:129:GLY:HA2  | 1.88                     | 0.55              |
| 2:V:201:1R2:OAB  | 2:V:201:1R2:CAS  | 2.50                     | 0.55              |
| 1:C:18:ARG:C     | 1:C:19:ARG:HG3   | 2.31                     | 0.55              |
| 1:X:32:LEU:HD13  | 1:X:130:ILE:CG1  | 2.36                     | 0.55              |
| 1:I:39:GLU:HG2   | 1:I:134:LEU:HD22 | 1.88                     | 0.55              |
| 1:Q:18:ARG:O     | 1:Q:19:ARG:HG2   | 2.06                     | 0.55              |
| 1:S:18:ARG:HH21  | 1:S:18:ARG:CG    | 2.20                     | 0.55              |
| 1:D:18:ARG:HH21  | 1:D:18:ARG:CG    | 2.18                     | 0.55              |
| 1:N:142:GLU:HG3  | 1:N:142:GLU:O    | 2.06                     | 0.55              |
| 1:O:110:GLU:CD   | 1:O:110:GLU:H    | 2.15                     | 0.55              |
| 1:R:5:VAL:HG22   | 1:R:71:PRO:HG2   | 1.88                     | 0.55              |
| 1:W:95:ALA:HB3   | 3:W:309:HOH:O    | 2.07                     | 0.55              |
| 1:D:138:ARG:CD   | 1:I:138:ARG:HD3  | 2.37                     | 0.55              |
| 1:H:101:HIS:HB2  | 1:H:126:VAL:HG22 | 1.88                     | 0.55              |
| 1:R:24:TYR:CA    | 1:R:102:ILE:HD11 | 2.33                     | 0.55              |
| 1:A:39:GLU:O     | 1:A:40:ALA:C     | 2.49                     | 0.55              |
| 1:H:32:LEU:HD13  | 1:H:130:ILE:HG13 | 1.88                     | 0.54              |
| 1:M:18:ARG:NH2   | 1:M:28:THR:HB    | 2.21                     | 0.54              |
| 1:T:3:LEU:HD12   | 1:T:4:ILE:H      | 1.71                     | 0.54              |
| 1:D:16:LEU:O     | 1:D:18:ARG:N     | 2.40                     | 0.54              |
| 1:S:101:HIS:HB2  | 1:S:126:VAL:HG22 | 1.89                     | 0.54              |
| 1:L:30:ASP:OD2   | 1:L:30:ASP:N     | 2.40                     | 0.54              |
| 1:A:63:HIS:CD2   | 1:K:15:ARG:CD    | 2.90                     | 0.54              |
| 1:A:102:ILE:HG23 | 1:A:129:GLY:HA2  | 1.90                     | 0.54              |
| 1:C:29:HIS:O     | 1:C:33:VAL:HG23  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:27:THR:HB    | 1:S:31:GLU:HB2   | 1.90                     | 0.54              |
| 1:I:29:HIS:O     | 1:I:33:VAL:HG23  | 2.08                     | 0.54              |
| 1:P:66:ALA:CB    | 1:P:92:GLU:HG3   | 2.37                     | 0.54              |
| 1:F:70:GLU:O     | 1:F:95:ALA:HB3   | 2.08                     | 0.54              |
| 1:Q:128:LEU:HD13 | 1:W:123:GLY:HA3  | 1.89                     | 0.54              |
| 1:U:118:SER:HB2  | 1:U:119:PRO:HD3  | 1.88                     | 0.54              |
| 1:M:59:LEU:HD12  | 1:W:53:ASP:HB3   | 1.90                     | 0.54              |
| 1:P:67:ASP:O     | 1:P:68:ALA:HB3   | 2.08                     | 0.54              |
| 1:V:19:ARG:HG3   | 1:V:19:ARG:NH1   | 2.22                     | 0.54              |
| 1:J:4:ILE:H      | 1:J:4:ILE:CD1    | 2.19                     | 0.54              |
| 1:T:102:ILE:HG23 | 1:T:129:GLY:HA2  | 1.90                     | 0.54              |
| 1:U:59:LEU:HD22  | 1:U:89:ALA:HB2   | 1.90                     | 0.54              |
| 1:K:18:ARG:CG    | 1:K:18:ARG:NH1   | 2.61                     | 0.54              |
| 1:D:98:ILE:HD11  | 1:D:139:TYR:CD2  | 2.42                     | 0.53              |
| 1:L:50:ARG:HB2   | 1:L:50:ARG:NH1   | 2.08                     | 0.53              |
| 1:A:41:ALA:C     | 1:A:43:LEU:N     | 2.66                     | 0.53              |
| 1:C:80:THR:HG23  | 1:C:117:LEU:HD12 | 1.89                     | 0.53              |
| 1:G:132:GLY:C    | 1:G:133:TYR:O    | 2.44                     | 0.53              |
| 1:K:138:ARG:O    | 1:K:138:ARG:HG2  | 2.05                     | 0.53              |
| 1:A:64:GLN:HA    | 1:A:64:GLN:HE21  | 1.72                     | 0.53              |
| 1:S:16:LEU:O     | 1:S:17:GLY:C     | 2.49                     | 0.53              |
| 1:D:144:VAL:CG1  | 1:D:144:VAL:O    | 2.56                     | 0.53              |
| 1:R:80:THR:HA    | 1:R:117:LEU:HD12 | 1.89                     | 0.53              |
| 1:T:36:ILE:HG23  | 1:T:137:LEU:HD11 | 1.89                     | 0.53              |
| 1:G:86:LEU:O     | 1:G:86:LEU:HD12  | 2.09                     | 0.53              |
| 1:C:18:ARG:O     | 1:C:19:ARG:CG    | 2.56                     | 0.53              |
| 1:G:106:HIS:HA   | 1:G:113:ARG:HG2  | 1.91                     | 0.53              |
| 1:R:45:LEU:O     | 1:R:46:LYS:C     | 2.51                     | 0.53              |
| 1:J:29:HIS:O     | 1:J:33:VAL:HG23  | 2.09                     | 0.53              |
| 1:J:90:CYS:C     | 1:J:92:GLU:H     | 2.17                     | 0.53              |
| 1:L:80:THR:HG23  | 1:L:117:LEU:HD12 | 1.90                     | 0.53              |
| 1:P:37:GLU:O     | 1:P:38:ARG:HB3   | 2.07                     | 0.53              |
| 1:P:92:GLU:C     | 1:P:92:GLU:CD    | 2.77                     | 0.53              |
| 1:X:21:PRO:HB2   | 1:X:22:ALA:C     | 2.33                     | 0.53              |
| 1:D:7:VAL:HB     | 1:D:49:VAL:HG22  | 1.90                     | 0.52              |
| 1:D:138:ARG:CD   | 1:I:138:ARG:CD   | 2.87                     | 0.52              |
| 1:K:33:VAL:CG1   | 1:K:34:ALA:N     | 2.71                     | 0.52              |
| 1:O:63:HIS:CG    | 1:Q:15:ARG:HD3   | 2.43                     | 0.52              |
| 1:C:88:ASP:OD2   | 2:E:201:1R2:H9   | 2.10                     | 0.52              |
| 1:E:131:GLN:NE2  | 1:K:143:HIS:HE1  | 2.08                     | 0.52              |
| 1:S:17:GLY:HA3   | 1:S:28:THR:HG22  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:11:PRO:HA    | 1:G:53:ASP:OD1   | 2.10                     | 0.52              |
| 1:T:35:LEU:CD2   | 1:T:134:LEU:HD11 | 2.39                     | 0.52              |
| 1:T:52:SER:HB2   | 1:T:61:TRP:CH2   | 2.45                     | 0.52              |
| 1:D:20:GLU:HB3   | 1:D:21:PRO:CD    | 2.38                     | 0.52              |
| 1:G:35:LEU:O     | 1:G:39:GLU:HB2   | 2.09                     | 0.52              |
| 1:L:38:ARG:HD2   | 3:L:309:HOH:O    | 2.09                     | 0.52              |
| 1:R:106:HIS:HA   | 1:R:113:ARG:HG2  | 1.92                     | 0.52              |
| 1:T:86:LEU:HG    | 1:T:117:LEU:HD21 | 1.91                     | 0.52              |
| 1:P:36:ILE:HG23  | 1:P:137:LEU:HD11 | 1.90                     | 0.52              |
| 1:N:17:GLY:CA    | 1:N:18:ARG:CB    | 2.87                     | 0.52              |
| 1:R:56:ALA:HB2   | 1:S:54:SER:HB2   | 1.92                     | 0.52              |
| 1:X:20:GLU:CB    | 1:X:21:PRO:CA    | 2.87                     | 0.52              |
| 1:E:16:LEU:O     | 1:E:18:ARG:N     | 2.42                     | 0.52              |
| 1:L:87:ARG:NH1   | 1:L:116:TYR:O    | 2.42                     | 0.52              |
| 1:Q:98:ILE:HD12  | 1:W:128:LEU:HD21 | 1.91                     | 0.52              |
| 1:S:16:LEU:O     | 1:S:18:ARG:N     | 2.43                     | 0.52              |
| 1:Q:97:LEU:HD23  | 1:Q:121:ALA:HA   | 1.90                     | 0.52              |
| 1:F:80:THR:CG2   | 1:F:115:SER:HB2  | 2.39                     | 0.52              |
| 1:H:20:GLU:HG2   | 1:H:23:VAL:HB    | 1.90                     | 0.52              |
| 1:P:5:VAL:HB     | 1:P:47:ALA:HB2   | 1.92                     | 0.52              |
| 1:W:97:LEU:HD23  | 1:W:121:ALA:HA   | 1.92                     | 0.52              |
| 1:B:17:GLY:CA    | 1:B:18:ARG:CB    | 2.81                     | 0.52              |
| 1:E:99:GLU:O     | 1:E:124:VAL:HA   | 2.09                     | 0.52              |
| 1:I:124:VAL:HG12 | 1:I:126:VAL:HG23 | 1.92                     | 0.52              |
| 1:P:59:LEU:HD12  | 1:R:53:ASP:HB3   | 1.92                     | 0.52              |
| 1:X:50:ARG:NH2   | 1:X:61:TRP:CD1   | 2.78                     | 0.52              |
| 1:W:109:GLU:OE1  | 1:W:112:ARG:NE   | 2.39                     | 0.51              |
| 1:O:58:LEU:O     | 1:O:62:ILE:HG12  | 2.10                     | 0.51              |
| 1:T:35:LEU:HD23  | 1:T:134:LEU:HD11 | 1.90                     | 0.51              |
| 1:B:67:ASP:CG    | 1:C:15:ARG:HH22  | 2.18                     | 0.51              |
| 1:B:106:HIS:HA   | 1:B:113:ARG:HG2  | 1.92                     | 0.51              |
| 1:D:21:PRO:CA    | 1:D:22:ALA:HB3   | 2.35                     | 0.51              |
| 1:X:142:GLU:HB3  | 1:X:143:HIS:CA   | 2.23                     | 0.51              |
| 1:H:15:ARG:HG2   | 1:H:15:ARG:HH11  | 1.75                     | 0.51              |
| 1:M:4:ILE:N      | 1:M:4:ILE:HD12   | 2.26                     | 0.51              |
| 1:O:80:THR:HG22  | 1:O:115:SER:HB2  | 1.93                     | 0.51              |
| 1:R:28:THR:HG22  | 1:R:30:ASP:H     | 1.75                     | 0.51              |
| 1:Q:18:ARG:O     | 1:Q:18:ARG:HG3   | 2.10                     | 0.51              |
| 1:S:33:VAL:O     | 1:S:37:GLU:HG3   | 2.09                     | 0.51              |
| 1:S:86:LEU:CD2   | 3:S:303:HOH:O    | 2.59                     | 0.51              |
| 1:S:142:GLU:O    | 1:S:143:HIS:HB2  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:73:ILE:HD13  | 1:V:136:ALA:HB3  | 1.93                     | 0.51              |
| 1:H:54:SER:O     | 1:H:58:LEU:HG    | 2.11                     | 0.51              |
| 1:N:50:ARG:HD3   | 1:N:61:TRP:CE2   | 2.46                     | 0.51              |
| 1:W:141:ALA:HB3  | 1:W:142:GLU:OE2  | 2.11                     | 0.51              |
| 1:B:138:ARG:HD3  | 1:F:138:ARG:CD   | 2.40                     | 0.51              |
| 1:I:63:HIS:HD2   | 3:I:305:HOH:O    | 1.94                     | 0.51              |
| 1:K:3:LEU:HG     | 1:K:4:ILE:N      | 2.25                     | 0.51              |
| 1:G:9:ASN:O      | 1:G:51:GLN:HA    | 2.11                     | 0.51              |
| 1:K:19:ARG:HD3   | 2:K:201:1R2:OAB  | 2.11                     | 0.51              |
| 1:Q:13:LEU:O     | 1:Q:16:LEU:HB2   | 2.11                     | 0.51              |
| 1:A:138:ARG:HD2  | 1:G:138:ARG:NE   | 2.26                     | 0.51              |
| 1:C:102:ILE:HG23 | 1:C:129:GLY:HA2  | 1.93                     | 0.51              |
| 1:M:58:LEU:O     | 1:M:62:ILE:HG12  | 2.11                     | 0.51              |
| 1:O:59:LEU:HD12  | 1:Q:53:ASP:HB3   | 1.93                     | 0.51              |
| 1:K:41:ALA:C     | 1:K:43:LEU:N     | 2.69                     | 0.50              |
| 1:P:34:ALA:O     | 1:P:37:GLU:O     | 2.29                     | 0.50              |
| 1:V:101:HIS:HB2  | 1:V:126:VAL:HG22 | 1.92                     | 0.50              |
| 1:B:63:HIS:CG    | 1:C:15:ARG:HD2   | 2.47                     | 0.50              |
| 1:D:67:ASP:O     | 1:M:18:ARG:HD3   | 2.11                     | 0.50              |
| 1:K:12:ASN:C     | 1:K:13:LEU:O     | 2.51                     | 0.50              |
| 1:P:118:SER:HB2  | 1:P:119:PRO:HD3  | 1.92                     | 0.50              |
| 1:H:120:ILE:C    | 1:H:120:ILE:CD1  | 2.84                     | 0.50              |
| 1:I:62:ILE:HD13  | 1:I:90:CYS:SG    | 2.51                     | 0.50              |
| 1:X:142:GLU:HB2  | 1:X:143:HIS:CB   | 2.41                     | 0.50              |
| 1:P:66:ALA:HB1   | 1:P:92:GLU:HG3   | 1.93                     | 0.50              |
| 1:P:120:ILE:HD12 | 1:P:120:ILE:O    | 2.11                     | 0.50              |
| 1:R:36:ILE:HG23  | 1:R:137:LEU:HD11 | 1.93                     | 0.50              |
| 1:R:50:ARG:HB3   | 1:R:61:TRP:CZ3   | 2.46                     | 0.50              |
| 1:S:41:ALA:O     | 1:S:44:GLY:N     | 2.39                     | 0.50              |
| 1:R:33:VAL:O     | 1:R:36:ILE:O     | 2.29                     | 0.50              |
| 1:V:97:LEU:HD23  | 1:V:121:ALA:HA   | 1.92                     | 0.50              |
| 1:W:19:ARG:CG    | 1:W:20:GLU:N     | 2.62                     | 0.50              |
| 1:K:63:HIS:CD2   | 1:L:15:ARG:HD2   | 2.46                     | 0.50              |
| 1:M:18:ARG:HB3   | 1:M:19:ARG:HE    | 1.75                     | 0.50              |
| 1:N:120:ILE:C    | 1:N:120:ILE:CD1  | 2.85                     | 0.50              |
| 1:P:37:GLU:O     | 1:P:38:ARG:CB    | 2.58                     | 0.50              |
| 1:Q:16:LEU:C     | 1:Q:18:ARG:H     | 2.19                     | 0.50              |
| 1:V:109:GLU:O    | 1:V:110:GLU:C    | 2.55                     | 0.50              |
| 1:W:16:LEU:O     | 1:W:28:THR:HA    | 2.11                     | 0.50              |
| 1:J:11:PRO:HA    | 1:J:53:ASP:OD1   | 2.12                     | 0.50              |
| 1:Q:50:ARG:HB3   | 1:Q:61:TRP:CH2   | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:89:ALA:HB2   | 1:K:12:ASN:CG    | 2.35                     | 0.50              |
| 1:G:58:LEU:O     | 1:G:62:ILE:HD12  | 2.11                     | 0.50              |
| 1:N:87:ARG:HA    | 1:N:117:LEU:HD23 | 1.93                     | 0.50              |
| 1:T:124:VAL:HG12 | 1:T:126:VAL:HG23 | 1.94                     | 0.50              |
| 1:X:20:GLU:HB3   | 1:X:21:PRO:C     | 2.37                     | 0.50              |
| 1:A:73:ILE:HG23  | 3:A:301:HOH:O    | 2.12                     | 0.49              |
| 1:A:113:ARG:NH1  | 1:G:119:PRO:HG3  | 2.27                     | 0.49              |
| 1:K:3:LEU:HG     | 1:K:4:ILE:H      | 1.77                     | 0.49              |
| 1:X:87:ARG:HD2   | 1:X:116:TYR:O    | 2.12                     | 0.49              |
| 1:N:40:ALA:O     | 1:N:44:GLY:HA2   | 2.13                     | 0.49              |
| 1:P:33:VAL:HG22  | 1:P:49:VAL:HB    | 1.94                     | 0.49              |
| 1:U:33:VAL:O     | 1:U:37:GLU:HB2   | 2.12                     | 0.49              |
| 1:E:20:GLU:N     | 1:E:21:PRO:CD    | 2.53                     | 0.49              |
| 1:J:59:LEU:HD22  | 1:J:89:ALA:HB2   | 1.93                     | 0.49              |
| 1:I:57:GLN:HE21  | 1:I:57:GLN:HA    | 1.77                     | 0.49              |
| 1:K:75:ASN:C     | 1:K:75:ASN:ND2   | 2.71                     | 0.49              |
| 1:U:24:TYR:H     | 1:U:25:GLY:HA2   | 1.77                     | 0.49              |
| 1:V:17:GLY:HA3   | 1:V:28:THR:HG22  | 1.94                     | 0.49              |
| 1:A:90:CYS:HA    | 1:A:93:LEU:HD22  | 1.94                     | 0.49              |
| 1:P:90:CYS:HB3   | 1:P:97:LEU:HD22  | 1.93                     | 0.49              |
| 1:C:98:ILE:HD11  | 1:C:139:TYR:CD2  | 2.47                     | 0.49              |
| 1:U:52:SER:HB3   | 1:U:58:LEU:CD1   | 2.43                     | 0.49              |
| 1:F:32:LEU:CD1   | 1:F:130:ILE:HG13 | 2.36                     | 0.49              |
| 1:M:18:ARG:HH22  | 1:M:29:HIS:N     | 2.10                     | 0.49              |
| 1:O:125:ILE:CG2  | 1:O:128:LEU:HD12 | 2.43                     | 0.49              |
| 1:P:134:LEU:HA   | 1:P:137:LEU:HD12 | 1.93                     | 0.49              |
| 1:R:67:ASP:OD1   | 1:S:15:ARG:NH2   | 2.46                     | 0.49              |
| 1:T:29:HIS:O     | 1:T:33:VAL:HG23  | 2.12                     | 0.49              |
| 1:T:96:PRO:HB2   | 1:T:140:LEU:HD21 | 1.93                     | 0.49              |
| 1:D:144:VAL:HA   | 1:X:-5:TYR:O     | 2.12                     | 0.49              |
| 1:M:17:GLY:HA2   | 1:M:19:ARG:N     | 2.27                     | 0.49              |
| 1:R:7:VAL:HB     | 1:R:49:VAL:HG13  | 1.93                     | 0.49              |
| 1:U:32:LEU:HD13  | 1:U:130:ILE:HD12 | 1.94                     | 0.49              |
| 1:Q:118:SER:N    | 1:Q:119:PRO:HD2  | 2.27                     | 0.49              |
| 1:R:37:GLU:O     | 1:R:38:ARG:CB    | 2.55                     | 0.49              |
| 1:N:36:ILE:HG23  | 1:N:137:LEU:HD11 | 1.95                     | 0.49              |
| 1:Q:104:ASN:HA   | 1:Q:126:VAL:HG12 | 1.94                     | 0.48              |
| 1:S:24:TYR:O     | 1:S:102:ILE:CG2  | 2.61                     | 0.48              |
| 1:T:13:LEU:HD23  | 1:T:16:LEU:CD1   | 2.43                     | 0.48              |
| 1:U:90:CYS:C     | 1:U:92:GLU:H     | 2.21                     | 0.48              |
| 1:D:11:PRO:O     | 1:D:12:ASN:HB2   | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:48:VAL:HG12  | 1:G:50:ARG:HD2   | 1.95                     | 0.48              |
| 1:I:50:ARG:NH1   | 1:I:61:TRP:CD1   | 2.81                     | 0.48              |
| 1:A:73:ILE:CG2   | 3:A:301:HOH:O    | 2.60                     | 0.48              |
| 1:K:59:LEU:HD22  | 1:K:89:ALA:HB2   | 1.94                     | 0.48              |
| 1:X:118:SER:HB2  | 1:X:119:PRO:HD3  | 1.93                     | 0.48              |
| 1:E:36:ILE:HG23  | 1:E:137:LEU:HD11 | 1.96                     | 0.48              |
| 1:F:111:PHE:CD1  | 1:F:111:PHE:C    | 2.90                     | 0.48              |
| 1:L:90:CYS:HB2   | 1:L:120:ILE:HD11 | 1.96                     | 0.48              |
| 1:F:16:LEU:HB3   | 1:F:27:THR:O     | 2.14                     | 0.48              |
| 1:G:11:PRO:O     | 1:G:12:ASN:HB2   | 2.13                     | 0.48              |
| 1:O:90:CYS:HB3   | 1:O:97:LEU:HD22  | 1.94                     | 0.48              |
| 1:P:48:VAL:HG12  | 1:P:49:VAL:H     | 1.79                     | 0.48              |
| 1:H:38:ARG:HB3   | 1:H:38:ARG:HH11  | 1.79                     | 0.48              |
| 1:R:9:ASN:O      | 1:R:51:GLN:HA    | 2.14                     | 0.48              |
| 1:S:22:ALA:O     | 1:S:25:GLY:O     | 2.31                     | 0.48              |
| 1:L:8:ILE:HD12   | 1:L:72:VAL:HG13  | 1.95                     | 0.48              |
| 1:X:77:GLY:O     | 1:X:80:THR:OG1   | 2.24                     | 0.48              |
| 1:D:55:GLU:O     | 1:D:59:LEU:HG    | 2.14                     | 0.48              |
| 1:H:20:GLU:CB    | 1:H:21:PRO:CA    | 2.90                     | 0.48              |
| 1:I:19:ARG:O     | 1:I:20:GLU:C     | 2.56                     | 0.48              |
| 1:L:8:ILE:O      | 1:L:9:ASN:C      | 2.54                     | 0.48              |
| 1:L:17:GLY:HA2   | 1:L:18:ARG:C     | 2.35                     | 0.48              |
| 1:S:32:LEU:HD13  | 1:S:130:ILE:HG12 | 1.95                     | 0.48              |
| 1:X:20:GLU:HG3   | 2:X:201:1R2:OAB  | 2.13                     | 0.48              |
| 1:B:139:TYR:HA   | 1:F:131:GLN:HE22 | 1.78                     | 0.48              |
| 1:D:18:ARG:O     | 1:D:19:ARG:CB    | 2.44                     | 0.48              |
| 1:R:4:ILE:HG23   | 1:R:70:GLU:HG2   | 1.95                     | 0.48              |
| 1:H:45:LEU:C     | 1:H:45:LEU:HD12  | 2.39                     | 0.48              |
| 1:M:32:LEU:CD1   | 1:M:130:ILE:HG23 | 2.44                     | 0.48              |
| 1:M:131:GLN:HE22 | 1:S:139:TYR:HA   | 1.79                     | 0.48              |
| 1:Q:38:ARG:HH12  | 1:Q:39:GLU:HG2   | 1.77                     | 0.48              |
| 1:R:63:HIS:ND1   | 1:S:15:ARG:CD    | 2.76                     | 0.48              |
| 1:A:64:GLN:HA    | 1:A:64:GLN:NE2   | 2.28                     | 0.47              |
| 1:E:130:ILE:H    | 1:E:130:ILE:CD1  | 2.26                     | 0.47              |
| 1:J:21:PRO:HB2   | 1:J:22:ALA:CB    | 2.43                     | 0.47              |
| 1:W:50:ARG:HD2   | 1:W:61:TRP:CE2   | 2.48                     | 0.47              |
| 1:C:11:PRO:O     | 1:C:12:ASN:HB2   | 2.14                     | 0.47              |
| 1:J:106:HIS:HA   | 1:J:113:ARG:HG2  | 1.94                     | 0.47              |
| 1:T:21:PRO:HA    | 1:T:25:GLY:O     | 2.14                     | 0.47              |
| 1:W:118:SER:HB2  | 1:W:119:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:88:ASP:HB3   | 2:K:201:1R2:H9   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:112:ARG:HD3  | 2:C:201:1R2:OAA  | 2.15                     | 0.47              |
| 1:G:133:TYR:O    | 1:G:134:LEU:HB2  | 2.14                     | 0.47              |
| 1:P:134:LEU:O    | 1:P:137:LEU:HB2  | 2.14                     | 0.47              |
| 1:R:94:SER:HA    | 3:R:302:HOH:O    | 2.14                     | 0.47              |
| 1:V:86:LEU:HD12  | 1:V:86:LEU:HA    | 1.61                     | 0.47              |
| 1:A:7:VAL:HG13   | 1:A:73:ILE:HG21  | 1.96                     | 0.47              |
| 1:B:92:GLU:OE1   | 1:C:19:ARG:HD3   | 2.15                     | 0.47              |
| 1:A:29:HIS:O     | 1:A:33:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:43:LEU:C     | 1:A:45:LEU:N     | 2.73                     | 0.47              |
| 1:A:86:LEU:O     | 1:A:90:CYS:HB2   | 2.15                     | 0.47              |
| 1:C:130:ILE:HD12 | 1:C:130:ILE:H    | 1.80                     | 0.47              |
| 1:H:15:ARG:HG2   | 1:H:15:ARG:NH1   | 2.29                     | 0.47              |
| 1:I:10:GLY:HA2   | 1:I:58:LEU:HD11  | 1.95                     | 0.47              |
| 1:J:39:GLU:HG2   | 1:J:134:LEU:HD13 | 1.95                     | 0.47              |
| 1:R:3:LEU:HD11   | 1:R:46:LYS:HD3   | 1.95                     | 0.47              |
| 1:S:99:GLU:HB3   | 1:S:124:VAL:HG22 | 1.97                     | 0.47              |
| 1:W:13:LEU:HG    | 2:W:201:1R2:CAG  | 2.45                     | 0.47              |
| 2:I:201:1R2:OAE  | 2:I:201:1R2:CAS  | 2.51                     | 0.47              |
| 1:L:64:GLN:HE21  | 1:L:64:GLN:HB3   | 1.53                     | 0.47              |
| 1:N:46:LYS:NZ    | 3:N:316:HOH:O    | 2.47                     | 0.47              |
| 1:B:48:VAL:HG12  | 1:B:50:ARG:HD2   | 1.97                     | 0.47              |
| 1:O:18:ARG:HH11  | 1:O:18:ARG:CG    | 2.28                     | 0.47              |
| 1:U:9:ASN:O      | 1:U:51:GLN:HA    | 2.14                     | 0.47              |
| 1:E:118:SER:HB2  | 1:E:119:PRO:HD3  | 1.97                     | 0.47              |
| 1:E:130:ILE:N    | 1:E:130:ILE:CD1  | 2.77                     | 0.47              |
| 1:G:16:LEU:HA    | 1:G:17:GLY:HA2   | 1.67                     | 0.47              |
| 1:G:117:LEU:O    | 1:G:120:ILE:HG13 | 2.15                     | 0.47              |
| 1:M:93:LEU:HD12  | 1:M:97:LEU:HB2   | 1.97                     | 0.47              |
| 1:V:131:GLN:HE22 | 1:X:139:TYR:CA   | 2.16                     | 0.47              |
| 1:A:41:ALA:C     | 1:A:43:LEU:H     | 2.21                     | 0.46              |
| 1:A:73:ILE:HG12  | 3:A:301:HOH:O    | 2.14                     | 0.46              |
| 1:D:39:GLU:CG    | 1:D:134:LEU:HD22 | 2.42                     | 0.46              |
| 1:F:92:GLU:HG3   | 1:G:19:ARG:HG2   | 1.96                     | 0.46              |
| 1:M:101:HIS:HB2  | 1:M:126:VAL:HG22 | 1.96                     | 0.46              |
| 1:P:32:LEU:HD13  | 1:P:130:ILE:HG23 | 1.97                     | 0.46              |
| 1:R:41:ALA:O     | 1:R:42:GLU:HG2   | 2.15                     | 0.46              |
| 1:D:118:SER:HB2  | 1:D:119:PRO:HD3  | 1.97                     | 0.46              |
| 1:N:15:ARG:HD2   | 1:Q:63:HIS:CD2   | 2.50                     | 0.46              |
| 1:O:27:THR:HG23  | 1:O:31:GLU:HB2   | 1.97                     | 0.46              |
| 1:P:57:GLN:CD    | 1:P:61:TRP:CE3   | 2.91                     | 0.46              |
| 1:P:128:LEU:CD1  | 1:U:125:ILE:HD11 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:13:LEU:CD2   | 2:W:201:1R2:H8   | 2.45                     | 0.46              |
| 1:B:11:PRO:O     | 1:B:12:ASN:HB2   | 2.14                     | 0.46              |
| 1:I:32:LEU:HD13  | 1:I:130:ILE:CG1  | 2.46                     | 0.46              |
| 1:O:120:ILE:C    | 1:O:120:ILE:HD12 | 2.40                     | 0.46              |
| 1:S:14:GLY:N     | 1:S:51:GLN:NE2   | 2.60                     | 0.46              |
| 1:G:28:THR:HG22  | 1:G:30:ASP:N     | 2.30                     | 0.46              |
| 1:B:63:HIS:CD2   | 1:C:15:ARG:HD2   | 2.51                     | 0.46              |
| 1:Q:140:LEU:O    | 1:Q:142:GLU:N    | 2.39                     | 0.46              |
| 1:V:13:LEU:HG    | 2:V:201:1R2:H9   | 1.97                     | 0.46              |
| 1:X:134:LEU:HA   | 1:X:137:LEU:HD12 | 1.98                     | 0.46              |
| 1:D:11:PRO:HD3   | 1:D:58:LEU:HD11  | 1.97                     | 0.46              |
| 1:M:88:ASP:HB2   | 1:W:12:ASN:ND2   | 2.31                     | 0.46              |
| 1:P:48:VAL:C     | 1:P:50:ARG:NE    | 2.74                     | 0.46              |
| 1:Q:38:ARG:HB3   | 1:Q:38:ARG:HH11  | 1.81                     | 0.46              |
| 1:R:127:GLY:C    | 1:R:129:GLY:H    | 2.24                     | 0.46              |
| 1:G:43:LEU:HD22  | 1:G:141:ALA:CB   | 2.45                     | 0.46              |
| 1:W:76:ALA:HB3   | 1:W:80:THR:OG1   | 2.15                     | 0.46              |
| 1:X:19:ARG:HD2   | 1:X:19:ARG:H     | 1.81                     | 0.46              |
| 1:X:99:GLU:HB3   | 1:X:124:VAL:HG13 | 1.97                     | 0.46              |
| 1:A:27:THR:HG22  | 1:A:28:THR:O     | 2.15                     | 0.46              |
| 1:D:21:PRO:HB3   | 1:D:23:VAL:CA    | 2.45                     | 0.46              |
| 1:U:59:LEU:CD2   | 1:U:89:ALA:HB2   | 2.44                     | 0.46              |
| 2:W:201:1R2:OAE  | 2:W:201:1R2:CAS  | 2.51                     | 0.46              |
| 1:D:92:GLU:HG3   | 1:F:19:ARG:NH1   | 2.30                     | 0.46              |
| 1:K:29:HIS:O     | 1:K:32:LEU:O     | 2.32                     | 0.46              |
| 1:K:120:ILE:C    | 1:K:120:ILE:HD12 | 2.40                     | 0.46              |
| 1:R:40:ALA:C     | 1:R:41:ALA:O     | 2.57                     | 0.46              |
| 1:V:54:SER:O     | 1:V:58:LEU:HG    | 2.16                     | 0.46              |
| 1:X:32:LEU:HD13  | 1:X:130:ILE:HG12 | 1.97                     | 0.46              |
| 1:J:140:LEU:C    | 1:J:142:GLU:H    | 2.23                     | 0.46              |
| 1:N:104:ASN:HA   | 1:N:126:VAL:HG12 | 1.97                     | 0.46              |
| 1:Q:128:LEU:HD12 | 1:Q:128:LEU:HA   | 1.76                     | 0.46              |
| 1:R:19:ARG:HD2   | 2:R:201:1R2:OAB  | 2.15                     | 0.46              |
| 1:X:111:PHE:CD1  | 1:X:111:PHE:C    | 2.94                     | 0.46              |
| 1:E:19:ARG:HD2   | 1:E:19:ARG:HA    | 1.62                     | 0.45              |
| 1:U:48:VAL:HG12  | 1:U:50:ARG:HD2   | 1.99                     | 0.45              |
| 1:K:41:ALA:C     | 1:K:43:LEU:H     | 2.25                     | 0.45              |
| 1:N:63:HIS:HE1   | 1:O:53:ASP:OD2   | 1.99                     | 0.45              |
| 1:B:120:ILE:HD12 | 1:B:120:ILE:C    | 2.41                     | 0.45              |
| 1:I:108:ARG:HE   | 1:I:112:ARG:CD   | 2.30                     | 0.45              |
| 1:Q:138:ARG:NH1  | 1:W:138:ARG:HD3  | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:111:PHE:CE1  | 1:U:112:ARG:HG3  | 2.51                     | 0.45              |
| 1:V:13:LEU:HG    | 2:V:201:1R2:CAG  | 2.46                     | 0.45              |
| 1:V:128:LEU:HD22 | 1:X:139:TYR:CG   | 2.51                     | 0.45              |
| 1:D:80:THR:HG23  | 1:D:117:LEU:HD12 | 1.99                     | 0.45              |
| 1:O:98:ILE:HD11  | 1:O:139:TYR:CD2  | 2.52                     | 0.45              |
| 1:R:3:LEU:O      | 1:R:4:ILE:CG2    | 2.64                     | 0.45              |
| 1:T:142:GLU:O    | 1:T:143:HIS:HB2  | 2.17                     | 0.45              |
| 1:A:27:THR:HG23  | 1:A:31:GLU:HB3   | 1.99                     | 0.45              |
| 1:K:118:SER:HB2  | 1:K:119:PRO:HD3  | 1.99                     | 0.45              |
| 1:M:87:ARG:HH12  | 1:M:119:PRO:HG2  | 1.82                     | 0.45              |
| 1:Q:18:ARG:O     | 1:Q:19:ARG:CB    | 2.65                     | 0.45              |
| 1:K:8:ILE:CG2    | 1:K:58:LEU:HD22  | 2.46                     | 0.45              |
| 1:K:104:ASN:OD1  | 1:K:104:ASN:C    | 2.59                     | 0.45              |
| 1:P:64:GLN:O     | 1:P:67:ASP:O     | 2.35                     | 0.45              |
| 1:V:128:LEU:HD22 | 1:X:139:TYR:CD1  | 2.51                     | 0.45              |
| 1:W:58:LEU:O     | 1:W:62:ILE:HG12  | 2.17                     | 0.45              |
| 1:W:88:ASP:OD2   | 2:X:201:1R2:H9   | 2.16                     | 0.45              |
| 1:X:140:LEU:C    | 1:X:142:GLU:N    | 2.75                     | 0.45              |
| 1:L:16:LEU:HD21  | 1:L:102:ILE:HD13 | 1.98                     | 0.45              |
| 1:P:92:GLU:O     | 1:P:93:LEU:C     | 2.59                     | 0.45              |
| 1:R:29:HIS:O     | 1:R:32:LEU:HB3   | 2.16                     | 0.45              |
| 1:E:35:LEU:HD21  | 1:E:134:LEU:HD11 | 1.98                     | 0.44              |
| 1:U:4:ILE:HG23   | 1:U:46:LYS:HB3   | 1.99                     | 0.44              |
| 1:E:18:ARG:O     | 1:E:19:ARG:O     | 2.34                     | 0.44              |
| 1:G:33:VAL:HG22  | 1:G:49:VAL:CG2   | 2.47                     | 0.44              |
| 1:N:20:GLU:HB2   | 1:N:21:PRO:C     | 2.41                     | 0.44              |
| 1:O:29:HIS:O     | 1:O:33:VAL:HG23  | 2.17                     | 0.44              |
| 1:U:13:LEU:O     | 1:U:16:LEU:HB2   | 2.17                     | 0.44              |
| 1:F:106:HIS:HA   | 1:F:113:ARG:HG2  | 2.00                     | 0.44              |
| 1:K:30:ASP:O     | 1:K:33:VAL:CG1   | 2.64                     | 0.44              |
| 1:R:130:ILE:N    | 1:R:130:ILE:CD1  | 2.75                     | 0.44              |
| 1:T:125:ILE:HG23 | 1:T:128:LEU:HD12 | 1.99                     | 0.44              |
| 1:X:73:ILE:HD13  | 1:X:136:ALA:HB3  | 1.98                     | 0.44              |
| 1:J:18:ARG:O     | 1:J:19:ARG:CB    | 2.64                     | 0.44              |
| 1:K:14:GLY:C     | 1:K:16:LEU:H     | 2.14                     | 0.44              |
| 1:N:32:LEU:HD13  | 1:N:130:ILE:CG1  | 2.47                     | 0.44              |
| 1:Q:4:ILE:HD12   | 1:Q:4:ILE:H      | 1.82                     | 0.44              |
| 1:R:11:PRO:HA    | 1:R:53:ASP:OD1   | 2.17                     | 0.44              |
| 1:U:117:LEU:O    | 1:U:120:ILE:HG13 | 2.17                     | 0.44              |
| 1:W:16:LEU:HD22  | 1:W:16:LEU:HA    | 1.87                     | 0.44              |
| 1:W:95:ALA:HB1   | 1:W:96:PRO:CD    | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:138:ARG:HD2  | 1:G:138:ARG:CZ   | 2.48                     | 0.44              |
| 1:B:9:ASN:HD22   | 1:B:9:ASN:HA     | 1.66                     | 0.44              |
| 1:N:106:HIS:HA   | 1:N:113:ARG:HG2  | 1.99                     | 0.44              |
| 1:R:41:ALA:C     | 1:R:43:LEU:N     | 2.75                     | 0.44              |
| 1:R:70:GLU:HA    | 1:R:71:PRO:HD2   | 1.74                     | 0.44              |
| 1:X:20:GLU:HB3   | 1:X:21:PRO:CA    | 2.47                     | 0.44              |
| 1:D:50:ARG:HB3   | 1:D:61:TRP:CH2   | 2.53                     | 0.44              |
| 1:B:19:ARG:C     | 1:B:20:GLU:HG2   | 2.42                     | 0.44              |
| 1:D:29:HIS:O     | 1:D:33:VAL:HG23  | 2.18                     | 0.44              |
| 1:I:63:HIS:HE1   | 1:J:53:ASP:OD2   | 2.01                     | 0.44              |
| 1:X:102:ILE:O    | 1:X:127:GLY:HA2  | 2.17                     | 0.44              |
| 1:X:110:GLU:HG3  | 1:X:111:PHE:N    | 2.33                     | 0.44              |
| 1:D:120:ILE:HD12 | 1:D:120:ILE:C    | 2.43                     | 0.44              |
| 1:J:28:THR:OG1   | 1:J:29:HIS:N     | 2.51                     | 0.44              |
| 1:L:59:LEU:HD22  | 1:L:89:ALA:HB2   | 2.00                     | 0.44              |
| 1:N:110:GLU:OE2  | 1:N:113:ARG:HD3  | 2.18                     | 0.44              |
| 1:N:135:LEU:HD22 | 1:R:135:LEU:HB3  | 1.98                     | 0.44              |
| 1:O:19:ARG:HG2   | 1:O:19:ARG:NH1   | 2.27                     | 0.44              |
| 1:S:31:GLU:O     | 1:S:35:LEU:HG    | 2.17                     | 0.44              |
| 2:V:201:1R2:OAB  | 2:V:201:1R2:CAH  | 2.66                     | 0.44              |
| 1:K:88:ASP:O     | 1:L:19:ARG:NH1   | 2.47                     | 0.44              |
| 1:R:118:SER:HB2  | 1:R:119:PRO:HD3  | 2.00                     | 0.44              |
| 1:S:4:ILE:HD13   | 1:S:4:ILE:C      | 2.43                     | 0.44              |
| 1:A:43:LEU:O     | 1:A:45:LEU:N     | 2.51                     | 0.43              |
| 1:G:16:LEU:HD13  | 1:G:27:THR:O     | 2.18                     | 0.43              |
| 1:S:17:GLY:H     | 1:S:28:THR:HA    | 1.83                     | 0.43              |
| 1:W:32:LEU:O     | 1:W:36:ILE:HG13  | 2.18                     | 0.43              |
| 1:K:109:GLU:OE1  | 1:K:112:ARG:NE   | 2.46                     | 0.43              |
| 1:R:131:GLN:O    | 1:R:131:GLN:CG   | 2.66                     | 0.43              |
| 1:B:33:VAL:HG12  | 1:B:37:GLU:OE2   | 2.18                     | 0.43              |
| 1:D:19:ARG:HA    | 1:D:20:GLU:HA    | 1.47                     | 0.43              |
| 1:E:7:VAL:HB     | 1:E:49:VAL:HG22  | 2.01                     | 0.43              |
| 1:Q:140:LEU:C    | 1:Q:142:GLU:N    | 2.76                     | 0.43              |
| 1:A:118:SER:HB2  | 1:A:119:PRO:HD3  | 2.00                     | 0.43              |
| 1:K:63:HIS:CD2   | 1:L:15:ARG:CD    | 3.02                     | 0.43              |
| 1:L:90:CYS:HB3   | 1:L:97:LEU:HD22  | 2.00                     | 0.43              |
| 1:N:110:GLU:OE2  | 1:N:110:GLU:HA   | 2.18                     | 0.43              |
| 1:B:34:ALA:HB1   | 1:B:38:ARG:HH21  | 1.84                     | 0.43              |
| 1:G:130:ILE:HD12 | 1:G:130:ILE:HA   | 1.79                     | 0.43              |
| 1:K:105:VAL:HG22 | 1:K:126:VAL:HG11 | 2.00                     | 0.43              |
| 1:Q:138:ARG:HE   | 1:Q:138:ARG:HB2  | 1.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:29:HIS:CE1   | 1:E:51:GLN:HB2   | 2.54                     | 0.43              |
| 1:P:92:GLU:CD    | 1:P:92:GLU:O     | 2.62                     | 0.43              |
| 1:Q:33:VAL:O     | 1:Q:37:GLU:HG3   | 2.18                     | 0.43              |
| 1:S:15:ARG:O     | 1:S:18:ARG:HB2   | 2.19                     | 0.43              |
| 1:H:16:LEU:C     | 1:H:18:ARG:H     | 2.27                     | 0.43              |
| 1:K:13:LEU:C     | 1:K:14:GLY:O     | 2.50                     | 0.43              |
| 1:M:142:GLU:O    | 1:M:143:HIS:CB   | 2.67                     | 0.43              |
| 1:P:49:VAL:O     | 1:P:50:ARG:HG2   | 2.18                     | 0.43              |
| 1:P:66:ALA:C     | 1:P:67:ASP:O     | 2.59                     | 0.43              |
| 1:P:106:HIS:HA   | 1:P:113:ARG:HG2  | 2.00                     | 0.43              |
| 1:R:17:GLY:C     | 1:R:18:ARG:O     | 2.60                     | 0.43              |
| 1:R:86:LEU:HD23  | 1:R:117:LEU:HD11 | 2.01                     | 0.43              |
| 1:U:76:ALA:O     | 1:U:77:GLY:C     | 2.60                     | 0.43              |
| 1:V:5:VAL:HG13   | 1:V:71:PRO:HB2   | 1.99                     | 0.43              |
| 1:V:19:ARG:HA    | 1:V:20:GLU:HA    | 1.73                     | 0.43              |
| 1:A:92:GLU:OE2   | 1:K:15:ARG:NE    | 2.49                     | 0.43              |
| 1:B:117:LEU:HD23 | 1:B:117:LEU:HA   | 1.70                     | 0.43              |
| 1:K:11:PRO:HA    | 1:K:53:ASP:OD1   | 2.17                     | 0.43              |
| 1:L:111:PHE:C    | 1:L:111:PHE:CD2  | 2.97                     | 0.43              |
| 1:M:55:GLU:O     | 1:M:56:ALA:C     | 2.61                     | 0.43              |
| 1:S:114:HIS:CG   | 1:S:115:SER:N    | 2.86                     | 0.43              |
| 1:T:50:ARG:HB3   | 1:T:61:TRP:CH2   | 2.54                     | 0.43              |
| 1:E:7:VAL:HG21   | 1:E:36:ILE:HG21  | 1.99                     | 0.43              |
| 1:I:80:THR:HG22  | 1:I:115:SER:HB2  | 2.00                     | 0.43              |
| 1:J:21:PRO:HB2   | 1:J:22:ALA:CA    | 2.48                     | 0.43              |
| 1:M:50:ARG:HG2   | 1:M:61:TRP:CZ2   | 2.54                     | 0.43              |
| 1:O:90:CYS:HB2   | 1:O:120:ILE:HD11 | 2.00                     | 0.43              |
| 1:A:75:ASN:OD1   | 1:A:75:ASN:C     | 2.62                     | 0.43              |
| 1:I:32:LEU:HD13  | 1:I:130:ILE:HG12 | 2.00                     | 0.43              |
| 1:R:104:ASN:OD1  | 1:R:104:ASN:C    | 2.62                     | 0.43              |
| 1:F:67:ASP:OD1   | 1:G:18:ARG:NH1   | 2.52                     | 0.42              |
| 1:L:78:GLY:C     | 1:L:80:THR:N     | 2.76                     | 0.42              |
| 1:M:16:LEU:O     | 1:M:18:ARG:NH1   | 2.52                     | 0.42              |
| 1:M:131:GLN:NE2  | 1:S:139:TYR:HA   | 2.33                     | 0.42              |
| 1:R:35:LEU:HD23  | 1:R:35:LEU:HA    | 1.76                     | 0.42              |
| 1:S:120:ILE:H    | 1:S:120:ILE:HG13 | 1.78                     | 0.42              |
| 1:V:127:GLY:C    | 1:V:129:GLY:H    | 2.27                     | 0.42              |
| 1:W:88:ASP:HB3   | 2:X:201:1R2:H8   | 2.00                     | 0.42              |
| 1:X:98:ILE:HD11  | 1:X:139:TYR:CD2  | 2.54                     | 0.42              |
| 1:C:100:VAL:HG22 | 1:C:125:ILE:HB   | 2.01                     | 0.42              |
| 1:G:20:GLU:H     | 1:G:21:PRO:HD2   | 1.81                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:27:THR:HG23  | 1:G:31:GLU:HB3   | 2.00                     | 0.42              |
| 1:J:30:ASP:HB2   | 3:J:306:HOH:O    | 2.19                     | 0.42              |
| 1:Q:96:PRO:HB2   | 1:Q:140:LEU:HD21 | 2.00                     | 0.42              |
| 1:K:104:ASN:HA   | 1:K:126:VAL:HG12 | 2.01                     | 0.42              |
| 1:M:92:GLU:HG3   | 1:W:19:ARG:HD3   | 1.99                     | 0.42              |
| 1:O:133:TYR:O    | 1:O:136:ALA:HB3  | 2.19                     | 0.42              |
| 1:P:15:ARG:HH22  | 1:S:67:ASP:CG    | 2.26                     | 0.42              |
| 1:U:74:LEU:HD23  | 1:U:117:LEU:HD13 | 2.01                     | 0.42              |
| 1:X:73:ILE:HD13  | 1:X:136:ALA:CB   | 2.49                     | 0.42              |
| 2:A:201:1R2:H9   | 1:L:88:ASP:OD2   | 2.19                     | 0.42              |
| 2:T:201:1R2:OAB  | 2:T:201:1R2:CAS  | 2.51                     | 0.42              |
| 1:F:59:LEU:HD12  | 1:G:53:ASP:HB3   | 2.01                     | 0.42              |
| 1:G:4:ILE:H      | 1:G:4:ILE:HG12   | 1.14                     | 0.42              |
| 1:H:21:PRO:HG2   | 1:H:22:ALA:HB2   | 2.02                     | 0.42              |
| 1:J:86:LEU:O     | 1:J:89:ALA:HB3   | 2.19                     | 0.42              |
| 1:K:32:LEU:CD1   | 1:K:130:ILE:HD12 | 2.49                     | 0.42              |
| 1:O:29:HIS:CE1   | 1:O:51:GLN:HB2   | 2.54                     | 0.42              |
| 1:T:63:HIS:CG    | 1:U:15:ARG:HD3   | 2.55                     | 0.42              |
| 1:H:20:GLU:HG2   | 1:H:23:VAL:CB    | 2.49                     | 0.42              |
| 1:M:32:LEU:HG    | 1:M:36:ILE:HD12  | 2.00                     | 0.42              |
| 1:O:19:ARG:HB3   | 1:O:20:GLU:H     | 1.69                     | 0.42              |
| 1:O:98:ILE:HD13  | 1:T:128:LEU:HD21 | 2.02                     | 0.42              |
| 1:Q:74:LEU:HD21  | 1:Q:86:LEU:HD11  | 2.01                     | 0.42              |
| 1:Q:87:ARG:HH12  | 1:Q:119:PRO:HG2  | 1.85                     | 0.42              |
| 1:S:24:TYR:O     | 1:S:102:ILE:HG21 | 2.20                     | 0.42              |
| 1:T:20:GLU:N     | 1:T:21:PRO:HD3   | 2.35                     | 0.42              |
| 1:F:117:LEU:HD23 | 1:F:117:LEU:HA   | 1.71                     | 0.42              |
| 1:I:67:ASP:CG    | 1:J:15:ARG:HH12  | 2.28                     | 0.42              |
| 1:J:16:LEU:O     | 1:J:28:THR:HA    | 2.19                     | 0.42              |
| 1:N:38:ARG:O     | 1:N:39:GLU:C     | 2.61                     | 0.42              |
| 1:A:7:VAL:HG13   | 1:A:73:ILE:CG2   | 2.49                     | 0.42              |
| 1:D:15:ARG:HD2   | 1:G:63:HIS:CG    | 2.53                     | 0.42              |
| 1:I:15:ARG:O     | 1:I:18:ARG:HG2   | 2.19                     | 0.42              |
| 1:M:18:ARG:CZ    | 1:M:29:HIS:H     | 2.32                     | 0.42              |
| 1:M:80:THR:HG21  | 1:M:101:HIS:CE1  | 2.55                     | 0.42              |
| 1:Q:95:ALA:HB1   | 1:Q:96:PRO:HD2   | 2.02                     | 0.42              |
| 1:Q:138:ARG:CZ   | 1:W:138:ARG:HD3  | 2.49                     | 0.42              |
| 1:S:50:ARG:HB2   | 1:S:61:TRP:CZ3   | 2.55                     | 0.42              |
| 1:V:128:LEU:CD1  | 1:X:125:ILE:HD11 | 2.50                     | 0.42              |
| 1:B:77:GLY:HA2   | 2:B:201:1R2:CAQ  | 2.50                     | 0.42              |
| 1:C:73:ILE:HD13  | 1:C:136:ALA:HB3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:15:ARG:CD    | 1:G:63:HIS:CD2   | 2.95                     | 0.42              |
| 1:O:6:ASN:HB2    | 1:O:72:VAL:HG22  | 2.02                     | 0.42              |
| 1:Q:102:ILE:HD11 | 1:Q:133:TYR:CE1  | 2.53                     | 0.42              |
| 1:S:18:ARG:CG    | 1:S:18:ARG:NH2   | 2.82                     | 0.42              |
| 1:V:138:ARG:O    | 1:V:138:ARG:HG3  | 2.20                     | 0.42              |
| 1:B:32:LEU:HD13  | 1:B:130:ILE:HG13 | 1.98                     | 0.42              |
| 1:B:33:VAL:CG1   | 1:B:37:GLU:OE2   | 2.68                     | 0.42              |
| 1:G:74:LEU:HB3   | 1:G:97:LEU:HD11  | 2.02                     | 0.42              |
| 1:Q:131:GLN:HE21 | 1:Q:135:LEU:HG   | 1.85                     | 0.42              |
| 1:S:38:ARG:HB3   | 1:S:39:GLU:H     | 1.75                     | 0.42              |
| 1:V:29:HIS:CB    | 3:V:302:HOH:O    | 2.50                     | 0.42              |
| 1:W:79:LEU:HD23  | 1:W:79:LEU:HA    | 1.92                     | 0.42              |
| 1:B:67:ASP:OD1   | 1:C:15:ARG:NH2   | 2.52                     | 0.41              |
| 1:D:102:ILE:HG23 | 1:D:129:GLY:HA2  | 2.01                     | 0.41              |
| 1:H:11:PRO:O     | 1:H:12:ASN:HB2   | 2.19                     | 0.41              |
| 1:J:28:THR:CG2   | 1:J:31:GLU:HG3   | 2.50                     | 0.41              |
| 1:P:12:ASN:O     | 1:P:15:ARG:HB2   | 2.20                     | 0.41              |
| 1:S:18:ARG:HA    | 1:S:18:ARG:HD3   | 1.68                     | 0.41              |
| 1:S:38:ARG:O     | 1:S:39:GLU:C     | 2.63                     | 0.41              |
| 1:U:97:LEU:HD23  | 1:U:121:ALA:HA   | 2.00                     | 0.41              |
| 1:U:118:SER:N    | 1:U:119:PRO:CD   | 2.83                     | 0.41              |
| 1:C:109:GLU:OE1  | 1:C:112:ARG:NE   | 2.45                     | 0.41              |
| 1:D:138:ARG:HD2  | 1:I:138:ARG:HD2  | 2.02                     | 0.41              |
| 1:K:32:LEU:O     | 1:K:33:VAL:CB    | 2.68                     | 0.41              |
| 1:P:137:LEU:O    | 1:P:138:ARG:C    | 2.62                     | 0.41              |
| 1:R:3:LEU:O      | 1:R:4:ILE:CB     | 2.68                     | 0.41              |
| 1:W:49:VAL:O     | 1:W:50:ARG:HG2   | 2.21                     | 0.41              |
| 1:D:11:PRO:HG2   | 1:D:79:LEU:HG    | 2.02                     | 0.41              |
| 1:F:90:CYS:HB3   | 1:F:97:LEU:HD22  | 2.02                     | 0.41              |
| 1:J:48:VAL:HG12  | 1:J:50:ARG:HD2   | 2.01                     | 0.41              |
| 1:M:88:ASP:O     | 1:M:91:ALA:HB3   | 2.20                     | 0.41              |
| 1:P:66:ALA:HB2   | 1:P:92:GLU:HG3   | 2.02                     | 0.41              |
| 1:S:50:ARG:NH2   | 1:S:50:ARG:CG    | 2.58                     | 0.41              |
| 1:U:51:GLN:HE21  | 1:U:51:GLN:HB3   | 1.73                     | 0.41              |
| 1:K:75:ASN:ND2   | 1:K:77:GLY:H     | 2.18                     | 0.41              |
| 1:H:36:ILE:HG23  | 1:H:137:LEU:HD11 | 2.03                     | 0.41              |
| 1:L:89:ALA:O     | 1:L:92:GLU:HG3   | 2.20                     | 0.41              |
| 1:P:49:VAL:C     | 1:P:50:ARG:HG2   | 2.46                     | 0.41              |
| 1:Q:7:VAL:HG11   | 1:Q:36:ILE:HD13  | 2.03                     | 0.41              |
| 2:T:201:1R2:H8   | 1:V:88:ASP:HB3   | 2.03                     | 0.41              |
| 2:T:201:1R2:CAF  | 1:V:88:ASP:HB3   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:20:GLU:HA    | 1:W:21:PRO:HD3   | 1.96                     | 0.41              |
| 1:A:89:ALA:CB    | 1:K:12:ASN:OD1   | 2.47                     | 0.41              |
| 1:H:21:PRO:HB2   | 1:H:22:ALA:HB2   | 2.00                     | 0.41              |
| 1:J:76:ALA:HB3   | 1:J:80:THR:OG1   | 2.20                     | 0.41              |
| 1:O:125:ILE:HG23 | 1:O:128:LEU:HD12 | 2.03                     | 0.41              |
| 1:T:15:ARG:HD3   | 1:V:63:HIS:CG    | 2.56                     | 0.41              |
| 1:B:59:LEU:HD12  | 1:C:53:ASP:HB3   | 2.02                     | 0.41              |
| 1:D:106:HIS:HA   | 1:D:113:ARG:HG2  | 2.02                     | 0.41              |
| 1:D:144:VAL:O    | 1:D:144:VAL:HG13 | 2.21                     | 0.41              |
| 1:G:133:TYR:O    | 1:G:134:LEU:CB   | 2.68                     | 0.41              |
| 1:I:76:ALA:HB1   | 1:I:79:LEU:HB2   | 2.03                     | 0.41              |
| 1:W:38:ARG:CZ    | 1:W:38:ARG:HB3   | 2.51                     | 0.41              |
| 1:D:53:ASP:HB3   | 1:G:59:LEU:HD12  | 2.03                     | 0.41              |
| 1:D:138:ARG:HD2  | 1:I:138:ARG:CD   | 2.50                     | 0.41              |
| 1:G:15:ARG:O     | 1:G:16:LEU:HB2   | 2.13                     | 0.41              |
| 1:U:99:GLU:HB3   | 1:U:124:VAL:HG22 | 2.03                     | 0.41              |
| 1:C:99:GLU:HB3   | 1:C:124:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:73:ILE:HD13  | 1:D:136:ALA:HB3  | 2.03                     | 0.41              |
| 1:K:59:LEU:HD21  | 1:K:86:LEU:HA    | 2.02                     | 0.41              |
| 1:M:63:HIS:HB3   | 1:W:15:ARG:NH1   | 2.35                     | 0.41              |
| 1:M:89:ALA:O     | 1:M:92:GLU:HB2   | 2.21                     | 0.41              |
| 1:R:24:TYR:C     | 1:R:102:ILE:HD11 | 2.46                     | 0.41              |
| 1:S:4:ILE:HD13   | 1:S:5:VAL:N      | 2.35                     | 0.41              |
| 1:S:38:ARG:O     | 1:S:41:ALA:N     | 2.54                     | 0.41              |
| 1:U:57:GLN:NE2   | 1:U:61:TRP:CE2   | 2.89                     | 0.41              |
| 1:U:102:ILE:HG23 | 1:U:129:GLY:HA2  | 2.02                     | 0.41              |
| 1:U:130:ILE:HD13 | 1:U:130:ILE:HA   | 1.84                     | 0.41              |
| 1:W:34:ALA:O     | 1:W:38:ARG:HB2   | 2.21                     | 0.41              |
| 1:A:27:THR:HG23  | 1:A:31:GLU:CB    | 2.51                     | 0.41              |
| 1:E:135:LEU:CD2  | 1:K:138:ARG:O    | 2.64                     | 0.41              |
| 1:H:140:LEU:C    | 1:H:142:GLU:H    | 2.29                     | 0.41              |
| 1:R:28:THR:HG22  | 1:R:30:ASP:N     | 2.35                     | 0.41              |
| 1:W:23:VAL:HG13  | 1:W:24:TYR:CD2   | 2.55                     | 0.41              |
| 1:X:16:LEU:HD12  | 1:X:27:THR:O     | 2.20                     | 0.41              |
| 1:X:131:GLN:O    | 1:X:132:GLY:C    | 2.63                     | 0.41              |
| 2:B:201:1R2:H9   | 1:E:88:ASP:OD2   | 2.22                     | 0.40              |
| 1:D:21:PRO:CB    | 1:D:24:TYR:H     | 2.34                     | 0.40              |
| 1:D:45:LEU:HD11  | 1:D:141:ALA:HB2  | 2.02                     | 0.40              |
| 2:D:201:1R2:H9   | 1:G:88:ASP:OD2   | 2.20                     | 0.40              |
| 1:E:5:VAL:HG21   | 1:E:45:LEU:HD13  | 2.03                     | 0.40              |
| 1:G:77:GLY:O     | 1:G:80:THR:HB    | 2.21                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:97:LEU:HD23 | 1:I:121:ALA:HA   | 2.02                     | 0.40              |
| 1:J:19:ARG:HE   | 1:J:19:ARG:HB3   | 1.59                     | 0.40              |
| 1:M:20:GLU:HA   | 3:M:205:HOH:O    | 2.21                     | 0.40              |
| 1:M:80:THR:HG23 | 1:M:117:LEU:HD12 | 2.03                     | 0.40              |
| 1:P:76:ALA:O    | 1:P:77:GLY:C     | 2.64                     | 0.40              |
| 2:T:201:1R2:OAB | 2:T:201:1R2:CAH  | 2.69                     | 0.40              |
| 1:X:48:VAL:HG12 | 1:X:50:ARG:HD3   | 2.04                     | 0.40              |
| 1:B:49:VAL:O    | 1:B:50:ARG:HG3   | 2.22                     | 0.40              |
| 1:D:27:THR:HG23 | 1:D:31:GLU:HB3   | 2.03                     | 0.40              |
| 1:O:19:ARG:NH1  | 1:O:19:ARG:CG    | 2.84                     | 0.40              |
| 1:T:48:VAL:HG12 | 1:T:50:ARG:HD2   | 2.04                     | 0.40              |
| 1:Q:68:ALA:O    | 1:Q:69:ALA:C     | 2.64                     | 0.40              |
| 1:R:99:GLU:OE2  | 1:R:101:HIS:NE2  | 2.51                     | 0.40              |
| 1:S:31:GLU:H    | 1:S:31:GLU:HG2   | 1.75                     | 0.40              |
| 1:K:19:ARG:O    | 1:K:20:GLU:C     | 2.64                     | 0.40              |
| 1:O:111:PHE:CD1 | 1:O:111:PHE:C    | 2.98                     | 0.40              |
| 1:K:41:ALA:O    | 1:K:43:LEU:N     | 2.55                     | 0.40              |
| 1:P:48:VAL:O    | 1:P:50:ARG:NH2   | 2.54                     | 0.40              |
| 1:W:11:PRO:O    | 1:W:12:ASN:HB2   | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 130/153 (85%) | 116 (89%) | 10 (8%) | 4 (3%)   | 3           | 12  |
| 1   | B     | 139/153 (91%) | 130 (94%) | 8 (6%)  | 1 (1%)   | 18          | 47  |
| 1   | C     | 139/153 (91%) | 134 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 1   | D     | 141/153 (92%) | 131 (93%) | 4 (3%)  | 6 (4%)   | 2           | 7   |
| 1   | E     | 139/153 (91%) | 127 (91%) | 6 (4%)  | 6 (4%)   | 2           | 7   |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | F     | 139/153 (91%)   | 133 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | G     | 139/153 (91%)   | 125 (90%)  | 12 (9%)  | 2 (1%)   | 9           | 30  |
| 1   | H     | 139/153 (91%)   | 129 (93%)  | 6 (4%)   | 4 (3%)   | 3           | 13  |
| 1   | I     | 139/153 (91%)   | 132 (95%)  | 6 (4%)   | 1 (1%)   | 18          | 47  |
| 1   | J     | 139/153 (91%)   | 129 (93%)  | 5 (4%)   | 5 (4%)   | 2           | 10  |
| 1   | K     | 139/153 (91%)   | 118 (85%)  | 12 (9%)  | 9 (6%)   | 1           | 3   |
| 1   | L     | 139/153 (91%)   | 128 (92%)  | 8 (6%)   | 3 (2%)   | 5           | 19  |
| 1   | M     | 133/153 (87%)   | 124 (93%)  | 8 (6%)   | 1 (1%)   | 16          | 44  |
| 1   | N     | 139/153 (91%)   | 117 (84%)  | 14 (10%) | 8 (6%)   | 1           | 4   |
| 1   | O     | 139/153 (91%)   | 134 (96%)  | 4 (3%)   | 1 (1%)   | 18          | 47  |
| 1   | P     | 139/153 (91%)   | 112 (81%)  | 21 (15%) | 6 (4%)   | 2           | 7   |
| 1   | Q     | 133/153 (87%)   | 123 (92%)  | 8 (6%)   | 2 (2%)   | 8           | 28  |
| 1   | R     | 139/153 (91%)   | 110 (79%)  | 14 (10%) | 15 (11%) | 0           | 1   |
| 1   | S     | 138/153 (90%)   | 116 (84%)  | 11 (8%)  | 11 (8%)  | 1           | 1   |
| 1   | T     | 139/153 (91%)   | 131 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 1   | U     | 139/153 (91%)   | 126 (91%)  | 10 (7%)  | 3 (2%)   | 5           | 19  |
| 1   | V     | 139/153 (91%)   | 125 (90%)  | 12 (9%)  | 2 (1%)   | 9           | 30  |
| 1   | W     | 139/153 (91%)   | 124 (89%)  | 14 (10%) | 1 (1%)   | 18          | 47  |
| 1   | X     | 148/153 (97%)   | 135 (91%)  | 8 (5%)   | 5 (3%)   | 3           | 11  |
| All | All   | 3325/3672 (91%) | 3009 (90%) | 220 (7%) | 96 (3%)  | 3           | 13  |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | LEU  |
| 1   | A     | 90  | CYS  |
| 1   | D     | 19  | ARG  |
| 1   | D     | 20  | GLU  |
| 1   | D     | 21  | PRO  |
| 1   | D     | 22  | ALA  |
| 1   | D     | 144 | VAL  |
| 1   | E     | 18  | ARG  |
| 1   | E     | 19  | ARG  |
| 1   | E     | 20  | GLU  |
| 1   | H     | 21  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 21  | PRO  |
| 1   | J     | 22  | ALA  |
| 1   | K     | 15  | ARG  |
| 1   | K     | 33  | VAL  |
| 1   | K     | 139 | TYR  |
| 1   | L     | 9   | ASN  |
| 1   | L     | 16  | LEU  |
| 1   | N     | 18  | ARG  |
| 1   | N     | 19  | ARG  |
| 1   | P     | 19  | ARG  |
| 1   | P     | 23  | VAL  |
| 1   | P     | 50  | ARG  |
| 1   | Q     | 141 | ALA  |
| 1   | R     | 4   | ILE  |
| 1   | R     | 19  | ARG  |
| 1   | R     | 21  | PRO  |
| 1   | R     | 22  | ALA  |
| 1   | R     | 41  | ALA  |
| 1   | S     | 16  | LEU  |
| 1   | S     | 18  | ARG  |
| 1   | S     | 20  | GLU  |
| 1   | S     | 21  | PRO  |
| 1   | S     | 38  | ARG  |
| 1   | W     | 23  | VAL  |
| 1   | X     | 20  | GLU  |
| 1   | X     | 21  | PRO  |
| 1   | X     | 141 | ALA  |
| 1   | B     | 18  | ARG  |
| 1   | E     | 17  | GLY  |
| 1   | H     | 20  | GLU  |
| 1   | H     | 141 | ALA  |
| 1   | J     | 19  | ARG  |
| 1   | K     | 4   | ILE  |
| 1   | K     | 141 | ALA  |
| 1   | N     | 4   | ILE  |
| 1   | N     | 39  | GLU  |
| 1   | N     | 42  | GLU  |
| 1   | P     | 38  | ARG  |
| 1   | R     | 46  | LYS  |
| 1   | R     | 70  | GLU  |
| 1   | S     | 17  | GLY  |
| 1   | S     | 22  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 18  | ARG  |
| 1   | X     | 25  | GLY  |
| 1   | A     | 141 | ALA  |
| 1   | E     | 131 | GLN  |
| 1   | G     | 16  | LEU  |
| 1   | H     | 23  | VAL  |
| 1   | J     | 91  | ALA  |
| 1   | J     | 141 | ALA  |
| 1   | K     | 42  | GLU  |
| 1   | K     | 140 | LEU  |
| 1   | L     | 18  | ARG  |
| 1   | N     | 38  | ARG  |
| 1   | R     | 26  | GLY  |
| 1   | R     | 42  | GLU  |
| 1   | R     | 45  | LEU  |
| 1   | R     | 55  | GLU  |
| 1   | R     | 128 | LEU  |
| 1   | S     | 19  | ARG  |
| 1   | V     | 110 | GLU  |
| 1   | V     | 128 | LEU  |
| 1   | E     | 16  | LEU  |
| 1   | K     | 13  | LEU  |
| 1   | O     | 19  | ARG  |
| 1   | P     | 22  | ALA  |
| 1   | R     | 69  | ALA  |
| 1   | S     | 23  | VAL  |
| 1   | G     | 133 | TYR  |
| 1   | R     | 37  | GLU  |
| 1   | U     | 21  | PRO  |
| 1   | U     | 91  | ALA  |
| 1   | A     | 42  | GLU  |
| 1   | K     | 132 | GLY  |
| 1   | M     | 26  | GLY  |
| 1   | R     | 20  | GLU  |
| 1   | D     | 17  | GLY  |
| 1   | I     | 20  | GLU  |
| 1   | Q     | 17  | GLY  |
| 1   | S     | 130 | ILE  |
| 1   | U     | 25  | GLY  |
| 1   | N     | 20  | GLU  |
| 1   | S     | 48  | VAL  |
| 1   | P     | 25  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 21  | 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     | 104/121 (86%) | 89 (86%)  | 15 (14%) | 3           | 11 |
| 1   | B     | 110/121 (91%) | 102 (93%) | 8 (7%)   | 13          | 38 |
| 1   | C     | 110/121 (91%) | 98 (89%)  | 12 (11%) | 6           | 21 |
| 1   | D     | 111/121 (92%) | 103 (93%) | 8 (7%)   | 13          | 39 |
| 1   | E     | 110/121 (91%) | 98 (89%)  | 12 (11%) | 6           | 21 |
| 1   | F     | 110/121 (91%) | 96 (87%)  | 14 (13%) | 4           | 15 |
| 1   | G     | 110/121 (91%) | 93 (84%)  | 17 (16%) | 2           | 9  |
| 1   | H     | 110/121 (91%) | 102 (93%) | 8 (7%)   | 13          | 38 |
| 1   | I     | 110/121 (91%) | 101 (92%) | 9 (8%)   | 10          | 33 |
| 1   | J     | 110/121 (91%) | 97 (88%)  | 13 (12%) | 5           | 17 |
| 1   | K     | 110/121 (91%) | 95 (86%)  | 15 (14%) | 3           | 13 |
| 1   | L     | 110/121 (91%) | 97 (88%)  | 13 (12%) | 5           | 17 |
| 1   | M     | 107/121 (88%) | 97 (91%)  | 10 (9%)  | 8           | 27 |
| 1   | N     | 110/121 (91%) | 96 (87%)  | 14 (13%) | 4           | 15 |
| 1   | O     | 110/121 (91%) | 100 (91%) | 10 (9%)  | 9           | 28 |
| 1   | P     | 110/121 (91%) | 100 (91%) | 10 (9%)  | 9           | 28 |
| 1   | Q     | 107/121 (88%) | 88 (82%)  | 19 (18%) | 2           | 6  |
| 1   | R     | 110/121 (91%) | 96 (87%)  | 14 (13%) | 4           | 15 |
| 1   | S     | 108/121 (89%) | 95 (88%)  | 13 (12%) | 5           | 17 |
| 1   | T     | 110/121 (91%) | 97 (88%)  | 13 (12%) | 5           | 17 |
| 1   | U     | 110/121 (91%) | 98 (89%)  | 12 (11%) | 6           | 21 |
| 1   | V     | 109/121 (90%) | 92 (84%)  | 17 (16%) | 2           | 9  |
| 1   | W     | 109/121 (90%) | 98 (90%)  | 11 (10%) | 7           | 23 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | X     | 119/121 (98%)   | 103 (87%)  | 16 (13%)  | 4           | 13 |
| All | All   | 2634/2904 (91%) | 2331 (88%) | 303 (12%) | 5           | 18 |

All (303) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LEU  |
| 1   | A     | 13  | LEU  |
| 1   | A     | 16  | LEU  |
| 1   | A     | 35  | LEU  |
| 1   | A     | 45  | LEU  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 54  | SER  |
| 1   | A     | 64  | GLN  |
| 1   | A     | 73  | ILE  |
| 1   | A     | 87  | ARG  |
| 1   | A     | 90  | CYS  |
| 1   | A     | 93  | LEU  |
| 1   | A     | 126 | VAL  |
| 1   | A     | 130 | ILE  |
| 1   | A     | 142 | GLU  |
| 1   | B     | 3   | LEU  |
| 1   | B     | 4   | ILE  |
| 1   | B     | 35  | LEU  |
| 1   | B     | 39  | GLU  |
| 1   | B     | 46  | LYS  |
| 1   | B     | 126 | VAL  |
| 1   | B     | 131 | GLN  |
| 1   | B     | 142 | GLU  |
| 1   | C     | 16  | LEU  |
| 1   | C     | 18  | ARG  |
| 1   | C     | 31  | GLU  |
| 1   | C     | 50  | ARG  |
| 1   | C     | 55  | GLU  |
| 1   | C     | 94  | SER  |
| 1   | C     | 118 | SER  |
| 1   | C     | 120 | ILE  |
| 1   | C     | 126 | VAL  |
| 1   | C     | 130 | ILE  |
| 1   | C     | 131 | GLN  |
| 1   | C     | 142 | GLU  |
| 1   | D     | 4   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 11  | PRO  |
| 1   | D     | 16  | LEU  |
| 1   | D     | 18  | ARG  |
| 1   | D     | 19  | ARG  |
| 1   | D     | 50  | ARG  |
| 1   | D     | 130 | ILE  |
| 1   | D     | 144 | VAL  |
| 1   | E     | 3   | LEU  |
| 1   | E     | 11  | PRO  |
| 1   | E     | 19  | ARG  |
| 1   | E     | 35  | LEU  |
| 1   | E     | 39  | GLU  |
| 1   | E     | 42  | GLU  |
| 1   | E     | 46  | LYS  |
| 1   | E     | 50  | ARG  |
| 1   | E     | 55  | GLU  |
| 1   | E     | 59  | LEU  |
| 1   | E     | 130 | ILE  |
| 1   | E     | 143 | HIS  |
| 1   | F     | 3   | LEU  |
| 1   | F     | 16  | LEU  |
| 1   | F     | 19  | ARG  |
| 1   | F     | 20  | GLU  |
| 1   | F     | 35  | LEU  |
| 1   | F     | 42  | GLU  |
| 1   | F     | 49  | VAL  |
| 1   | F     | 50  | ARG  |
| 1   | F     | 55  | GLU  |
| 1   | F     | 60  | ASP  |
| 1   | F     | 92  | GLU  |
| 1   | F     | 94  | SER  |
| 1   | F     | 115 | SER  |
| 1   | F     | 130 | ILE  |
| 1   | G     | 4   | ILE  |
| 1   | G     | 20  | GLU  |
| 1   | G     | 27  | THR  |
| 1   | G     | 28  | THR  |
| 1   | G     | 31  | GLU  |
| 1   | G     | 42  | GLU  |
| 1   | G     | 49  | VAL  |
| 1   | G     | 50  | ARG  |
| 1   | G     | 64  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 80  | THR  |
| 1   | G     | 86  | LEU  |
| 1   | G     | 126 | VAL  |
| 1   | G     | 130 | ILE  |
| 1   | G     | 131 | GLN  |
| 1   | G     | 137 | LEU  |
| 1   | G     | 142 | GLU  |
| 1   | G     | 143 | HIS  |
| 1   | H     | 19  | ARG  |
| 1   | H     | 20  | GLU  |
| 1   | H     | 23  | VAL  |
| 1   | H     | 42  | GLU  |
| 1   | H     | 45  | LEU  |
| 1   | H     | 50  | ARG  |
| 1   | H     | 130 | ILE  |
| 1   | H     | 143 | HIS  |
| 1   | I     | 16  | LEU  |
| 1   | I     | 35  | LEU  |
| 1   | I     | 42  | GLU  |
| 1   | I     | 48  | VAL  |
| 1   | I     | 57  | GLN  |
| 1   | I     | 99  | GLU  |
| 1   | I     | 115 | SER  |
| 1   | I     | 120 | ILE  |
| 1   | I     | 130 | ILE  |
| 1   | J     | 3   | LEU  |
| 1   | J     | 4   | ILE  |
| 1   | J     | 16  | LEU  |
| 1   | J     | 19  | ARG  |
| 1   | J     | 28  | THR  |
| 1   | J     | 46  | LYS  |
| 1   | J     | 50  | ARG  |
| 1   | J     | 52  | SER  |
| 1   | J     | 86  | LEU  |
| 1   | J     | 98  | ILE  |
| 1   | J     | 130 | ILE  |
| 1   | J     | 142 | GLU  |
| 1   | J     | 143 | HIS  |
| 1   | K     | 13  | LEU  |
| 1   | K     | 16  | LEU  |
| 1   | K     | 18  | ARG  |
| 1   | K     | 20  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 27  | THR  |
| 1   | K     | 28  | THR  |
| 1   | K     | 45  | LEU  |
| 1   | K     | 50  | ARG  |
| 1   | K     | 70  | GLU  |
| 1   | K     | 110 | GLU  |
| 1   | K     | 130 | ILE  |
| 1   | K     | 131 | GLN  |
| 1   | K     | 137 | LEU  |
| 1   | K     | 138 | ARG  |
| 1   | K     | 140 | LEU  |
| 1   | L     | 5   | VAL  |
| 1   | L     | 18  | ARG  |
| 1   | L     | 30  | ASP  |
| 1   | L     | 38  | ARG  |
| 1   | L     | 45  | LEU  |
| 1   | L     | 46  | LYS  |
| 1   | L     | 50  | ARG  |
| 1   | L     | 57  | GLN  |
| 1   | L     | 64  | GLN  |
| 1   | L     | 80  | THR  |
| 1   | L     | 84  | VAL  |
| 1   | L     | 92  | GLU  |
| 1   | L     | 130 | ILE  |
| 1   | M     | 3   | LEU  |
| 1   | M     | 8   | ILE  |
| 1   | M     | 16  | LEU  |
| 1   | M     | 27  | THR  |
| 1   | M     | 31  | GLU  |
| 1   | M     | 35  | LEU  |
| 1   | M     | 36  | ILE  |
| 1   | M     | 80  | THR  |
| 1   | M     | 99  | GLU  |
| 1   | M     | 126 | VAL  |
| 1   | N     | 3   | LEU  |
| 1   | N     | 4   | ILE  |
| 1   | N     | 18  | ARG  |
| 1   | N     | 19  | ARG  |
| 1   | N     | 20  | GLU  |
| 1   | N     | 31  | GLU  |
| 1   | N     | 37  | GLU  |
| 1   | N     | 43  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 55  | GLU  |
| 1   | N     | 94  | SER  |
| 1   | N     | 98  | ILE  |
| 1   | N     | 108 | ARG  |
| 1   | N     | 110 | GLU  |
| 1   | N     | 130 | ILE  |
| 1   | O     | 3   | LEU  |
| 1   | O     | 18  | ARG  |
| 1   | O     | 19  | ARG  |
| 1   | O     | 54  | SER  |
| 1   | O     | 98  | ILE  |
| 1   | O     | 110 | GLU  |
| 1   | O     | 115 | SER  |
| 1   | O     | 126 | VAL  |
| 1   | O     | 130 | ILE  |
| 1   | O     | 142 | GLU  |
| 1   | P     | 4   | ILE  |
| 1   | P     | 23  | VAL  |
| 1   | P     | 27  | THR  |
| 1   | P     | 45  | LEU  |
| 1   | P     | 50  | ARG  |
| 1   | P     | 55  | GLU  |
| 1   | P     | 57  | GLN  |
| 1   | P     | 92  | GLU  |
| 1   | P     | 98  | ILE  |
| 1   | P     | 131 | GLN  |
| 1   | Q     | 3   | LEU  |
| 1   | Q     | 4   | ILE  |
| 1   | Q     | 16  | LEU  |
| 1   | Q     | 18  | ARG  |
| 1   | Q     | 24  | TYR  |
| 1   | Q     | 38  | ARG  |
| 1   | Q     | 42  | GLU  |
| 1   | Q     | 48  | VAL  |
| 1   | Q     | 55  | GLU  |
| 1   | Q     | 73  | ILE  |
| 1   | Q     | 79  | LEU  |
| 1   | Q     | 97  | LEU  |
| 1   | Q     | 102 | ILE  |
| 1   | Q     | 120 | ILE  |
| 1   | Q     | 128 | LEU  |
| 1   | Q     | 130 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 131 | GLN  |
| 1   | Q     | 134 | LEU  |
| 1   | Q     | 138 | ARG  |
| 1   | R     | 4   | ILE  |
| 1   | R     | 13  | LEU  |
| 1   | R     | 16  | LEU  |
| 1   | R     | 19  | ARG  |
| 1   | R     | 20  | GLU  |
| 1   | R     | 37  | GLU  |
| 1   | R     | 38  | ARG  |
| 1   | R     | 42  | GLU  |
| 1   | R     | 46  | LYS  |
| 1   | R     | 59  | LEU  |
| 1   | R     | 80  | THR  |
| 1   | R     | 98  | ILE  |
| 1   | R     | 102 | ILE  |
| 1   | R     | 130 | ILE  |
| 1   | S     | 4   | ILE  |
| 1   | S     | 16  | LEU  |
| 1   | S     | 18  | ARG  |
| 1   | S     | 31  | GLU  |
| 1   | S     | 39  | GLU  |
| 1   | S     | 45  | LEU  |
| 1   | S     | 49  | VAL  |
| 1   | S     | 50  | ARG  |
| 1   | S     | 86  | LEU  |
| 1   | S     | 92  | GLU  |
| 1   | S     | 110 | GLU  |
| 1   | S     | 120 | ILE  |
| 1   | S     | 126 | VAL  |
| 1   | T     | 13  | LEU  |
| 1   | T     | 16  | LEU  |
| 1   | T     | 20  | GLU  |
| 1   | T     | 35  | LEU  |
| 1   | T     | 42  | GLU  |
| 1   | T     | 46  | LYS  |
| 1   | T     | 50  | ARG  |
| 1   | T     | 54  | SER  |
| 1   | T     | 59  | LEU  |
| 1   | T     | 62  | ILE  |
| 1   | T     | 130 | ILE  |
| 1   | T     | 131 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 142 | GLU  |
| 1   | U     | 3   | LEU  |
| 1   | U     | 4   | ILE  |
| 1   | U     | 11  | PRO  |
| 1   | U     | 16  | LEU  |
| 1   | U     | 19  | ARG  |
| 1   | U     | 20  | GLU  |
| 1   | U     | 35  | LEU  |
| 1   | U     | 46  | LYS  |
| 1   | U     | 50  | ARG  |
| 1   | U     | 94  | SER  |
| 1   | U     | 120 | ILE  |
| 1   | U     | 143 | HIS  |
| 1   | V     | 13  | LEU  |
| 1   | V     | 16  | LEU  |
| 1   | V     | 18  | ARG  |
| 1   | V     | 19  | ARG  |
| 1   | V     | 35  | LEU  |
| 1   | V     | 38  | ARG  |
| 1   | V     | 46  | LYS  |
| 1   | V     | 48  | VAL  |
| 1   | V     | 50  | ARG  |
| 1   | V     | 97  | LEU  |
| 1   | V     | 98  | ILE  |
| 1   | V     | 99  | GLU  |
| 1   | V     | 117 | LEU  |
| 1   | V     | 122 | THR  |
| 1   | V     | 126 | VAL  |
| 1   | V     | 130 | ILE  |
| 1   | V     | 138 | ARG  |
| 1   | W     | 11  | PRO  |
| 1   | W     | 16  | LEU  |
| 1   | W     | 23  | VAL  |
| 1   | W     | 27  | THR  |
| 1   | W     | 38  | ARG  |
| 1   | W     | 42  | GLU  |
| 1   | W     | 45  | LEU  |
| 1   | W     | 97  | LEU  |
| 1   | W     | 130 | ILE  |
| 1   | W     | 131 | GLN  |
| 1   | W     | 142 | GLU  |
| 1   | X     | -6  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 1   | SER  |
| 1   | X     | 2   | GLU  |
| 1   | X     | 13  | LEU  |
| 1   | X     | 16  | LEU  |
| 1   | X     | 19  | ARG  |
| 1   | X     | 23  | VAL  |
| 1   | X     | 24  | TYR  |
| 1   | X     | 30  | ASP  |
| 1   | X     | 31  | GLU  |
| 1   | X     | 35  | LEU  |
| 1   | X     | 50  | ARG  |
| 1   | X     | 54  | SER  |
| 1   | X     | 80  | THR  |
| 1   | X     | 110 | GLU  |
| 1   | X     | 130 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ASN  |
| 1   | A     | 64  | GLN  |
| 1   | B     | 9   | ASN  |
| 1   | B     | 63  | HIS  |
| 1   | C     | 63  | HIS  |
| 1   | C     | 114 | HIS  |
| 1   | C     | 131 | GLN  |
| 1   | D     | 57  | GLN  |
| 1   | D     | 131 | GLN  |
| 1   | D     | 143 | HIS  |
| 1   | F     | 131 | GLN  |
| 1   | H     | 114 | HIS  |
| 1   | H     | 131 | GLN  |
| 1   | I     | 51  | GLN  |
| 1   | I     | 57  | GLN  |
| 1   | I     | 63  | HIS  |
| 1   | I     | 101 | HIS  |
| 1   | K     | 9   | ASN  |
| 1   | K     | 29  | HIS  |
| 1   | K     | 63  | HIS  |
| 1   | K     | 75  | ASN  |
| 1   | K     | 143 | HIS  |
| 1   | L     | 12  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 57  | GLN  |
| 1   | L     | 63  | HIS  |
| 1   | L     | 64  | GLN  |
| 1   | M     | 114 | HIS  |
| 1   | M     | 131 | GLN  |
| 1   | N     | 63  | HIS  |
| 1   | O     | 6   | ASN  |
| 1   | O     | 114 | HIS  |
| 1   | O     | 131 | GLN  |
| 1   | P     | 51  | GLN  |
| 1   | Q     | 81  | HIS  |
| 1   | R     | 6   | ASN  |
| 1   | R     | 131 | GLN  |
| 1   | S     | 6   | ASN  |
| 1   | S     | 12  | ASN  |
| 1   | S     | 51  | GLN  |
| 1   | S     | 63  | HIS  |
| 1   | S     | 64  | GLN  |
| 1   | T     | 131 | GLN  |
| 1   | U     | 51  | GLN  |
| 1   | V     | 63  | HIS  |
| 1   | V     | 131 | GLN  |
| 1   | W     | 9   | ASN  |
| 1   | W     | 12  | ASN  |
| 1   | W     | 63  | HIS  |
| 1   | X     | 6   | ASN  |
| 1   | X     | 9   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

22 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$ |
| 2   | 1R2  | T     | 201 | -    | 21,21,21     | 4.82 | 5 (23%)     | 27,29,29    | 2.13 | 9 (33%)     |
| 2   | 1R2  | P     | 201 | -    | 21,21,21     | 2.32 | 3 (14%)     | 27,29,29    | 1.50 | 5 (18%)     |
| 2   | 1R2  | I     | 201 | -    | 21,21,21     | 3.20 | 4 (19%)     | 27,29,29    | 1.67 | 5 (18%)     |
| 2   | 1R2  | A     | 201 | -    | 21,21,21     | 3.58 | 3 (14%)     | 27,29,29    | 1.59 | 6 (22%)     |
| 2   | 1R2  | V     | 201 | -    | 21,21,21     | 5.28 | 4 (19%)     | 27,29,29    | 1.99 | 6 (22%)     |
| 2   | 1R2  | U     | 201 | -    | 21,21,21     | 4.11 | 3 (14%)     | 27,29,29    | 1.22 | 4 (14%)     |
| 2   | 1R2  | D     | 201 | -    | 21,21,21     | 2.99 | 4 (19%)     | 27,29,29    | 1.34 | 2 (7%)      |
| 2   | 1R2  | G     | 201 | -    | 21,21,21     | 5.22 | 3 (14%)     | 27,29,29    | 1.90 | 4 (14%)     |
| 2   | 1R2  | J     | 201 | -    | 21,21,21     | 2.85 | 4 (19%)     | 27,29,29    | 1.58 | 5 (18%)     |
| 2   | 1R2  | O     | 201 | -    | 21,21,21     | 2.75 | 4 (19%)     | 27,29,29    | 1.82 | 4 (14%)     |
| 2   | 1R2  | K     | 201 | -    | 21,21,21     | 3.32 | 3 (14%)     | 27,29,29    | 1.72 | 7 (25%)     |
| 2   | 1R2  | C     | 201 | -    | 21,21,21     | 3.39 | 4 (19%)     | 27,29,29    | 1.67 | 4 (14%)     |
| 2   | 1R2  | N     | 201 | -    | 21,21,21     | 3.71 | 3 (14%)     | 27,29,29    | 1.69 | 2 (7%)      |
| 2   | 1R2  | L     | 201 | -    | 21,21,21     | 4.58 | 5 (23%)     | 27,29,29    | 1.52 | 3 (11%)     |
| 2   | 1R2  | S     | 201 | -    | 21,21,21     | 3.48 | 4 (19%)     | 27,29,29    | 1.47 | 7 (25%)     |
| 2   | 1R2  | R     | 201 | -    | 21,21,21     | 3.36 | 5 (23%)     | 27,29,29    | 1.80 | 4 (14%)     |
| 2   | 1R2  | F     | 201 | -    | 21,21,21     | 4.15 | 4 (19%)     | 27,29,29    | 1.95 | 4 (14%)     |
| 2   | 1R2  | X     | 201 | -    | 21,21,21     | 2.27 | 3 (14%)     | 27,29,29    | 1.86 | 5 (18%)     |
| 2   | 1R2  | E     | 201 | -    | 21,21,21     | 2.93 | 3 (14%)     | 27,29,29    | 1.49 | 4 (14%)     |
| 2   | 1R2  | B     | 201 | -    | 21,21,21     | 2.75 | 4 (19%)     | 27,29,29    | 1.80 | 6 (22%)     |
| 2   | 1R2  | H     | 201 | -    | 21,21,21     | 2.88 | 3 (14%)     | 27,29,29    | 1.56 | 4 (14%)     |
| 2   | 1R2  | W     | 201 | -    | 21,21,21     | 3.80 | 4 (19%)     | 27,29,29    | 1.74 | 5 (18%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 1R2  | T     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | P     | 201 | -    | -       | 6/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | I     | 201 | -    | -       | 0/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | A     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | V     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | U     | 201 | -    | -       | 6/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | D     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | G     | 201 | -    | -       | 6/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | J     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | O     | 201 | -    | -       | 2/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | K     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | C     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | N     | 201 | -    | -       | 0/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | L     | 201 | -    | -       | 0/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | S     | 201 | -    | -       | 6/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | R     | 201 | -    | -       | 0/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | F     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | X     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | E     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | B     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | H     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |
| 2   | 1R2  | W     | 201 | -    | -       | 4/10/12/12 | 0/2/2/2 |

All (82) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 201 | 1R2  | OAB-NAT | 22.58 | 1.61        | 1.22     |
| 2   | V     | 201 | 1R2  | OAB-NAT | 22.43 | 1.61        | 1.22     |
| 2   | T     | 201 | 1R2  | OAB-NAT | 20.35 | 1.57        | 1.22     |
| 2   | L     | 201 | 1R2  | OAB-NAT | 19.22 | 1.55        | 1.22     |
| 2   | F     | 201 | 1R2  | OAB-NAT | 17.37 | 1.52        | 1.22     |
| 2   | U     | 201 | 1R2  | OAB-NAT | 17.29 | 1.52        | 1.22     |
| 2   | N     | 201 | 1R2  | OAB-NAT | 15.25 | 1.49        | 1.22     |
| 2   | W     | 201 | 1R2  | OAB-NAT | 15.10 | 1.48        | 1.22     |
| 2   | A     | 201 | 1R2  | OAB-NAT | 14.37 | 1.47        | 1.22     |
| 2   | S     | 201 | 1R2  | OAB-NAT | 14.01 | 1.46        | 1.22     |
| 2   | R     | 201 | 1R2  | OAB-NAT | 12.99 | 1.45        | 1.22     |
| 2   | C     | 201 | 1R2  | OAB-NAT | 12.99 | 1.45        | 1.22     |
| 2   | K     | 201 | 1R2  | OAB-NAT | 12.99 | 1.45        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | I     | 201 | 1R2  | OAB-NAT | 12.09 | 1.43        | 1.22     |
| 2   | H     | 201 | 1R2  | OAB-NAT | 10.85 | 1.41        | 1.22     |
| 2   | E     | 201 | 1R2  | OAB-NAT | 10.65 | 1.41        | 1.22     |
| 2   | D     | 201 | 1R2  | OAB-NAT | 10.40 | 1.40        | 1.22     |
| 2   | J     | 201 | 1R2  | OAB-NAT | 10.03 | 1.40        | 1.22     |
| 2   | O     | 201 | 1R2  | OAB-NAT | 9.89  | 1.39        | 1.22     |
| 2   | B     | 201 | 1R2  | OAB-NAT | 9.79  | 1.39        | 1.22     |
| 2   | X     | 201 | 1R2  | OAB-NAT | 7.50  | 1.35        | 1.22     |
| 2   | P     | 201 | 1R2  | OAB-NAT | 6.97  | 1.34        | 1.22     |
| 2   | L     | 201 | 1R2  | CAR-CAN | -5.56 | 1.37        | 1.49     |
| 2   | P     | 201 | 1R2  | CAR-CAN | -5.31 | 1.38        | 1.49     |
| 2   | E     | 201 | 1R2  | CAR-CAN | -5.20 | 1.38        | 1.49     |
| 2   | D     | 201 | 1R2  | CAR-CAN | -5.19 | 1.38        | 1.49     |
| 2   | C     | 201 | 1R2  | CAS-NAT | -5.10 | 1.33        | 1.45     |
| 2   | W     | 201 | 1R2  | CAS-NAT | -5.06 | 1.33        | 1.45     |
| 2   | R     | 201 | 1R2  | CAR-CAN | -5.05 | 1.38        | 1.49     |
| 2   | A     | 201 | 1R2  | CAS-NAT | -5.02 | 1.33        | 1.45     |
| 2   | V     | 201 | 1R2  | CAS-NAT | -4.95 | 1.33        | 1.45     |
| 2   | C     | 201 | 1R2  | CAR-CAN | -4.93 | 1.39        | 1.49     |
| 2   | B     | 201 | 1R2  | CAS-NAT | -4.93 | 1.33        | 1.45     |
| 2   | T     | 201 | 1R2  | CAS-NAT | -4.88 | 1.33        | 1.45     |
| 2   | D     | 201 | 1R2  | CAS-NAT | -4.87 | 1.33        | 1.45     |
| 2   | J     | 201 | 1R2  | CAR-CAN | -4.79 | 1.39        | 1.49     |
| 2   | G     | 201 | 1R2  | CAS-NAT | -4.69 | 1.34        | 1.45     |
| 2   | T     | 201 | 1R2  | CAR-CAN | -4.67 | 1.39        | 1.49     |
| 2   | O     | 201 | 1R2  | CAR-CAN | -4.66 | 1.39        | 1.49     |
| 2   | A     | 201 | 1R2  | CAR-CAN | -4.66 | 1.39        | 1.49     |
| 2   | J     | 201 | 1R2  | CAS-NAT | -4.65 | 1.34        | 1.45     |
| 2   | U     | 201 | 1R2  | CAS-NAT | -4.55 | 1.34        | 1.45     |
| 2   | H     | 201 | 1R2  | CAS-NAT | -4.49 | 1.34        | 1.45     |
| 2   | P     | 201 | 1R2  | CAS-NAT | -4.48 | 1.34        | 1.45     |
| 2   | K     | 201 | 1R2  | CAR-CAN | -4.44 | 1.40        | 1.49     |
| 2   | K     | 201 | 1R2  | CAS-NAT | -4.41 | 1.34        | 1.45     |
| 2   | V     | 201 | 1R2  | CAR-CAN | -4.40 | 1.40        | 1.49     |
| 2   | W     | 201 | 1R2  | CAR-CAN | -4.39 | 1.40        | 1.49     |
| 2   | E     | 201 | 1R2  | CAS-NAT | -4.35 | 1.34        | 1.45     |
| 2   | H     | 201 | 1R2  | CAR-CAN | -4.33 | 1.40        | 1.49     |
| 2   | G     | 201 | 1R2  | CAR-CAN | -4.31 | 1.40        | 1.49     |
| 2   | I     | 201 | 1R2  | CAS-NAT | -4.28 | 1.35        | 1.45     |
| 2   | N     | 201 | 1R2  | CAR-CAN | -4.22 | 1.40        | 1.49     |
| 2   | X     | 201 | 1R2  | CAR-CAN | -4.21 | 1.40        | 1.49     |
| 2   | V     | 201 | 1R2  | OAE-NAT | 4.10  | 1.62        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | W     | 201 | 1R2  | OAE-NAT | 4.10  | 1.62        | 1.35     |
| 2   | S     | 201 | 1R2  | CAS-NAT | -4.09 | 1.35        | 1.45     |
| 2   | R     | 201 | 1R2  | CAS-NAT | -4.08 | 1.35        | 1.45     |
| 2   | N     | 201 | 1R2  | CAS-NAT | -4.06 | 1.35        | 1.45     |
| 2   | X     | 201 | 1R2  | CAS-NAT | -4.03 | 1.35        | 1.45     |
| 2   | L     | 201 | 1R2  | CAS-NAT | -4.02 | 1.35        | 1.45     |
| 2   | U     | 201 | 1R2  | CAR-CAN | -3.91 | 1.41        | 1.49     |
| 2   | O     | 201 | 1R2  | CAS-NAT | -3.90 | 1.35        | 1.45     |
| 2   | F     | 201 | 1R2  | OAE-NAT | 3.85  | 1.60        | 1.35     |
| 2   | S     | 201 | 1R2  | CAR-CAN | -3.84 | 1.41        | 1.49     |
| 2   | I     | 201 | 1R2  | CAR-CAN | -3.78 | 1.41        | 1.49     |
| 2   | B     | 201 | 1R2  | CAR-CAN | -3.61 | 1.41        | 1.49     |
| 2   | F     | 201 | 1R2  | CAR-CAN | -3.60 | 1.41        | 1.49     |
| 2   | F     | 201 | 1R2  | CAS-NAT | -3.41 | 1.37        | 1.45     |
| 2   | I     | 201 | 1R2  | OAE-NAT | 3.32  | 1.57        | 1.35     |
| 2   | D     | 201 | 1R2  | OAE-NAT | 3.01  | 1.55        | 1.35     |
| 2   | C     | 201 | 1R2  | OAE-NAT | 2.89  | 1.54        | 1.35     |
| 2   | L     | 201 | 1R2  | OAE-NAT | 2.78  | 1.53        | 1.35     |
| 2   | T     | 201 | 1R2  | CAI-CAQ | 2.73  | 1.43        | 1.39     |
| 2   | T     | 201 | 1R2  | CAI-CAO | 2.61  | 1.43        | 1.39     |
| 2   | O     | 201 | 1R2  | CAI-CAQ | 2.48  | 1.43        | 1.39     |
| 2   | L     | 201 | 1R2  | CAI-CAQ | 2.43  | 1.43        | 1.39     |
| 2   | S     | 201 | 1R2  | OAE-NAT | 2.36  | 1.50        | 1.35     |
| 2   | R     | 201 | 1R2  | CAI-CAO | 2.28  | 1.42        | 1.39     |
| 2   | B     | 201 | 1R2  | CAK-CAQ | 2.26  | 1.42        | 1.39     |
| 2   | R     | 201 | 1R2  | CAL-CAP | 2.25  | 1.42        | 1.39     |
| 2   | J     | 201 | 1R2  | CAI-CAO | 2.15  | 1.42        | 1.39     |

All (105) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | X     | 201 | 1R2  | CAL-CAS-NAT | 6.57  | 124.40      | 118.74   |
| 2   | O     | 201 | 1R2  | CAL-CAS-NAT | 6.13  | 124.02      | 118.74   |
| 2   | G     | 201 | 1R2  | CAL-CAS-NAT | 5.99  | 123.90      | 118.74   |
| 2   | R     | 201 | 1R2  | CAL-CAS-NAT | 5.93  | 123.85      | 118.74   |
| 2   | F     | 201 | 1R2  | CAL-CAS-NAT | 5.80  | 123.73      | 118.74   |
| 2   | V     | 201 | 1R2  | CAL-CAS-NAT | 5.53  | 123.50      | 118.74   |
| 2   | C     | 201 | 1R2  | CAP-OAM-CAQ | -5.50 | 106.22      | 118.78   |
| 2   | B     | 201 | 1R2  | CAP-OAM-CAQ | -5.47 | 106.29      | 118.78   |
| 2   | W     | 201 | 1R2  | CAL-CAS-NAT | 5.39  | 123.38      | 118.74   |
| 2   | T     | 201 | 1R2  | CAH-CAS-NAT | -5.16 | 114.83      | 119.34   |
| 2   | I     | 201 | 1R2  | CAL-CAS-NAT | 5.08  | 123.11      | 118.74   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | T     | 201 | 1R2  | CAL-CAS-NAT | 5.07  | 123.10      | 118.74   |
| 2   | N     | 201 | 1R2  | CAL-CAS-NAT | 5.05  | 123.08      | 118.74   |
| 2   | F     | 201 | 1R2  | CAP-OAM-CAQ | -4.91 | 107.55      | 118.78   |
| 2   | G     | 201 | 1R2  | CAH-CAS-NAT | -4.83 | 115.12      | 119.34   |
| 2   | H     | 201 | 1R2  | CAL-CAS-NAT | 4.76  | 122.83      | 118.74   |
| 2   | E     | 201 | 1R2  | CAL-CAS-NAT | 4.60  | 122.70      | 118.74   |
| 2   | V     | 201 | 1R2  | CAH-CAS-NAT | -4.47 | 115.44      | 119.34   |
| 2   | K     | 201 | 1R2  | CAL-CAS-NAT | 4.31  | 122.45      | 118.74   |
| 2   | P     | 201 | 1R2  | CAP-OAM-CAQ | -4.29 | 108.98      | 118.78   |
| 2   | J     | 201 | 1R2  | CAL-CAS-NAT | 4.12  | 122.29      | 118.74   |
| 2   | W     | 201 | 1R2  | CAH-CAS-NAT | -4.10 | 115.76      | 119.34   |
| 2   | A     | 201 | 1R2  | CAL-CAS-NAT | 3.87  | 122.07      | 118.74   |
| 2   | X     | 201 | 1R2  | CAH-CAS-NAT | -3.87 | 115.96      | 119.34   |
| 2   | D     | 201 | 1R2  | CAP-OAM-CAQ | -3.63 | 110.50      | 118.78   |
| 2   | V     | 201 | 1R2  | CAP-OAM-CAQ | -3.60 | 110.56      | 118.78   |
| 2   | N     | 201 | 1R2  | CAP-OAM-CAQ | -3.57 | 110.63      | 118.78   |
| 2   | S     | 201 | 1R2  | CAR-CAK-CAQ | 3.47  | 123.15      | 119.56   |
| 2   | B     | 201 | 1R2  | CAR-CAK-CAQ | 3.44  | 123.11      | 119.56   |
| 2   | A     | 201 | 1R2  | CAP-OAM-CAQ | -3.42 | 110.96      | 118.78   |
| 2   | C     | 201 | 1R2  | CAL-CAS-NAT | 3.30  | 121.58      | 118.74   |
| 2   | R     | 201 | 1R2  | CAH-CAS-NAT | -3.23 | 116.51      | 119.34   |
| 2   | L     | 201 | 1R2  | CAQ-CAI-CAO | 3.22  | 121.77      | 118.61   |
| 2   | K     | 201 | 1R2  | CAG-CAP-CAL | -3.15 | 116.26      | 120.50   |
| 2   | J     | 201 | 1R2  | CAP-OAM-CAQ | -3.11 | 111.67      | 118.78   |
| 2   | L     | 201 | 1R2  | CAJ-CAR-CAK | 3.10  | 123.28      | 119.65   |
| 2   | T     | 201 | 1R2  | CAQ-CAI-CAO | 3.08  | 121.63      | 118.61   |
| 2   | T     | 201 | 1R2  | CAF-CAG-CAP | 2.97  | 123.47      | 118.98   |
| 2   | T     | 201 | 1R2  | CAP-OAM-CAQ | -2.97 | 111.99      | 118.78   |
| 2   | O     | 201 | 1R2  | CAP-OAM-CAQ | -2.95 | 112.03      | 118.78   |
| 2   | C     | 201 | 1R2  | CAQ-CAI-CAO | 2.95  | 121.51      | 118.61   |
| 2   | O     | 201 | 1R2  | CAQ-CAI-CAO | 2.94  | 121.50      | 118.61   |
| 2   | L     | 201 | 1R2  | CAP-OAM-CAQ | -2.93 | 112.09      | 118.78   |
| 2   | T     | 201 | 1R2  | CAI-CAQ-CAK | -2.86 | 116.64      | 120.98   |
| 2   | K     | 201 | 1R2  | CAH-CAS-NAT | -2.83 | 116.86      | 119.34   |
| 2   | W     | 201 | 1R2  | CAP-OAM-CAQ | -2.82 | 112.33      | 118.78   |
| 2   | I     | 201 | 1R2  | CAH-CAS-NAT | -2.82 | 116.88      | 119.34   |
| 2   | A     | 201 | 1R2  | CAH-CAS-NAT | -2.76 | 116.93      | 119.34   |
| 2   | K     | 201 | 1R2  | CAF-CAG-CAP | 2.76  | 123.14      | 118.98   |
| 2   | S     | 201 | 1R2  | CAG-CAP-CAL | -2.75 | 116.80      | 120.50   |
| 2   | F     | 201 | 1R2  | CAR-CAK-CAQ | 2.73  | 122.38      | 119.56   |
| 2   | K     | 201 | 1R2  | CAP-OAM-CAQ | -2.69 | 112.64      | 118.78   |
| 2   | B     | 201 | 1R2  | CAL-CAS-NAT | 2.66  | 121.03      | 118.74   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | O     | 201 | 1R2  | CAH-CAS-NAT | -2.63 | 117.05      | 119.34   |
| 2   | P     | 201 | 1R2  | CAL-CAS-NAT | 2.60  | 120.98      | 118.74   |
| 2   | S     | 201 | 1R2  | CAI-CAQ-CAK | -2.59 | 117.04      | 120.98   |
| 2   | G     | 201 | 1R2  | CAG-CAP-CAL | -2.59 | 117.02      | 120.50   |
| 2   | K     | 201 | 1R2  | CAR-CAK-CAQ | 2.57  | 122.21      | 119.56   |
| 2   | U     | 201 | 1R2  | CAR-CAK-CAQ | 2.56  | 122.20      | 119.56   |
| 2   | W     | 201 | 1R2  | CAR-CAK-CAQ | 2.53  | 122.18      | 119.56   |
| 2   | B     | 201 | 1R2  | CAI-CAQ-CAK | -2.53 | 117.15      | 120.98   |
| 2   | U     | 201 | 1R2  | CAL-CAS-NAT | 2.47  | 120.86      | 118.74   |
| 2   | P     | 201 | 1R2  | CAQ-CAI-CAO | 2.46  | 121.03      | 118.61   |
| 2   | T     | 201 | 1R2  | CAG-CAP-CAL | -2.43 | 117.24      | 120.50   |
| 2   | E     | 201 | 1R2  | CAQ-CAI-CAO | 2.42  | 120.99      | 118.61   |
| 2   | D     | 201 | 1R2  | CAF-CAG-CAP | 2.40  | 122.60      | 118.98   |
| 2   | J     | 201 | 1R2  | CAQ-CAI-CAO | 2.35  | 120.92      | 118.61   |
| 2   | H     | 201 | 1R2  | OAC-CAN-CAR | 2.34  | 120.85      | 114.84   |
| 2   | C     | 201 | 1R2  | CAK-CAR-CAN | -2.33 | 115.79      | 119.96   |
| 2   | R     | 201 | 1R2  | CAG-CAP-CAL | -2.33 | 117.37      | 120.50   |
| 2   | I     | 201 | 1R2  | CAQ-CAI-CAO | 2.33  | 120.90      | 118.61   |
| 2   | V     | 201 | 1R2  | CAR-CAK-CAQ | 2.31  | 121.94      | 119.56   |
| 2   | A     | 201 | 1R2  | CAR-CAK-CAQ | 2.30  | 121.94      | 119.56   |
| 2   | S     | 201 | 1R2  | CAF-CAG-CAP | 2.30  | 122.45      | 118.98   |
| 2   | B     | 201 | 1R2  | CAF-CAG-CAP | 2.29  | 122.44      | 118.98   |
| 2   | E     | 201 | 1R2  | CAF-CAG-CAP | 2.26  | 122.40      | 118.98   |
| 2   | I     | 201 | 1R2  | CAR-CAK-CAQ | 2.26  | 121.89      | 119.56   |
| 2   | S     | 201 | 1R2  | CAS-CAL-CAP | 2.25  | 121.66      | 119.00   |
| 2   | G     | 201 | 1R2  | CAF-CAG-CAP | 2.23  | 122.35      | 118.98   |
| 2   | T     | 201 | 1R2  | CAR-CAK-CAQ | 2.23  | 121.86      | 119.56   |
| 2   | I     | 201 | 1R2  | CAR-CAJ-CAO | 2.22  | 121.72      | 119.70   |
| 2   | H     | 201 | 1R2  | CAH-CAS-NAT | -2.20 | 117.42      | 119.34   |
| 2   | U     | 201 | 1R2  | OAC-CAN-CAR | 2.17  | 120.41      | 114.84   |
| 2   | A     | 201 | 1R2  | CAF-CAG-CAP | 2.16  | 122.25      | 118.98   |
| 2   | X     | 201 | 1R2  | OAC-CAN-CAR | 2.16  | 120.38      | 114.84   |
| 2   | E     | 201 | 1R2  | CAH-CAS-NAT | -2.16 | 117.45      | 119.34   |
| 2   | B     | 201 | 1R2  | CAH-CAS-NAT | -2.15 | 117.46      | 119.34   |
| 2   | V     | 201 | 1R2  | CAG-CAP-CAL | -2.14 | 117.62      | 120.50   |
| 2   | R     | 201 | 1R2  | CAF-CAG-CAP | 2.13  | 122.20      | 118.98   |
| 2   | H     | 201 | 1R2  | CAQ-CAI-CAO | 2.13  | 120.70      | 118.61   |
| 2   | S     | 201 | 1R2  | CAQ-CAI-CAO | 2.12  | 120.69      | 118.61   |
| 2   | S     | 201 | 1R2  | OAC-CAN-OAA | -2.11 | 118.83      | 123.35   |
| 2   | X     | 201 | 1R2  | OAC-CAN-OAA | -2.09 | 118.87      | 123.35   |
| 2   | U     | 201 | 1R2  | CAQ-CAI-CAO | 2.08  | 120.66      | 118.61   |
| 2   | F     | 201 | 1R2  | OAC-CAN-CAR | 2.07  | 120.14      | 114.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 201 | 1R2  | CAQ-CAI-CAO | 2.06  | 120.64      | 118.61   |
| 2   | J     | 201 | 1R2  | CAH-CAS-NAT | -2.06 | 117.54      | 119.34   |
| 2   | J     | 201 | 1R2  | OAC-CAN-CAR | 2.06  | 120.12      | 114.84   |
| 2   | X     | 201 | 1R2  | CAR-CAK-CAQ | 2.05  | 121.68      | 119.56   |
| 2   | P     | 201 | 1R2  | CAG-CAP-CAL | -2.05 | 117.75      | 120.50   |
| 2   | T     | 201 | 1R2  | OAM-CAP-CAL | 2.05  | 125.58      | 119.16   |
| 2   | V     | 201 | 1R2  | CAF-CAG-CAP | 2.04  | 122.06      | 118.98   |
| 2   | W     | 201 | 1R2  | CAI-CAQ-CAK | -2.02 | 117.91      | 120.98   |
| 2   | K     | 201 | 1R2  | CAQ-CAI-CAO | 2.02  | 120.59      | 118.61   |
| 2   | P     | 201 | 1R2  | CAI-CAQ-CAK | -2.00 | 117.94      | 120.98   |

There are no chirality outliers.

All (78) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | P     | 201 | 1R2  | CAL-CAS-NAT-OAB |
| 2   | P     | 201 | 1R2  | CAH-CAS-NAT-OAB |
| 2   | S     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | S     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | S     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | X     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | X     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | X     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | W     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | W     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | W     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | S     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | H     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | X     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | E     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | H     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | E     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | W     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | E     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | P     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | H     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | H     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | E     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | P     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | T     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | K     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | T     | 201 | 1R2  | OAA-CAN-CAR-CAK |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | P     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | P     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | K     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | T     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | A     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | K     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | A     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | B     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | T     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | V     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | K     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | A     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | U     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | B     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | U     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | U     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | B     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | U     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | V     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | B     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | G     | 201 | 1R2  | CAL-CAS-NAT-OAB |
| 2   | G     | 201 | 1R2  | CAH-CAS-NAT-OAB |
| 2   | U     | 201 | 1R2  | CAL-CAS-NAT-OAB |
| 2   | U     | 201 | 1R2  | CAH-CAS-NAT-OAB |
| 2   | V     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | J     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | D     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | G     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | C     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | D     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | C     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | J     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | G     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | V     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | G     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | D     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | G     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | C     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | C     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | D     | 201 | 1R2  | OAC-CAN-CAR-CAJ |
| 2   | J     | 201 | 1R2  | OAA-CAN-CAR-CAK |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | S     | 201 | 1R2  | CAL-CAS-NAT-OAB |
| 2   | J     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | F     | 201 | 1R2  | OAA-CAN-CAR-CAK |
| 2   | S     | 201 | 1R2  | CAH-CAS-NAT-OAB |
| 2   | F     | 201 | 1R2  | OAA-CAN-CAR-CAJ |
| 2   | O     | 201 | 1R2  | CAL-CAS-NAT-OAB |
| 2   | O     | 201 | 1R2  | CAH-CAS-NAT-OAB |
| 2   | F     | 201 | 1R2  | OAC-CAN-CAR-CAK |
| 2   | F     | 201 | 1R2  | OAC-CAN-CAR-CAJ |

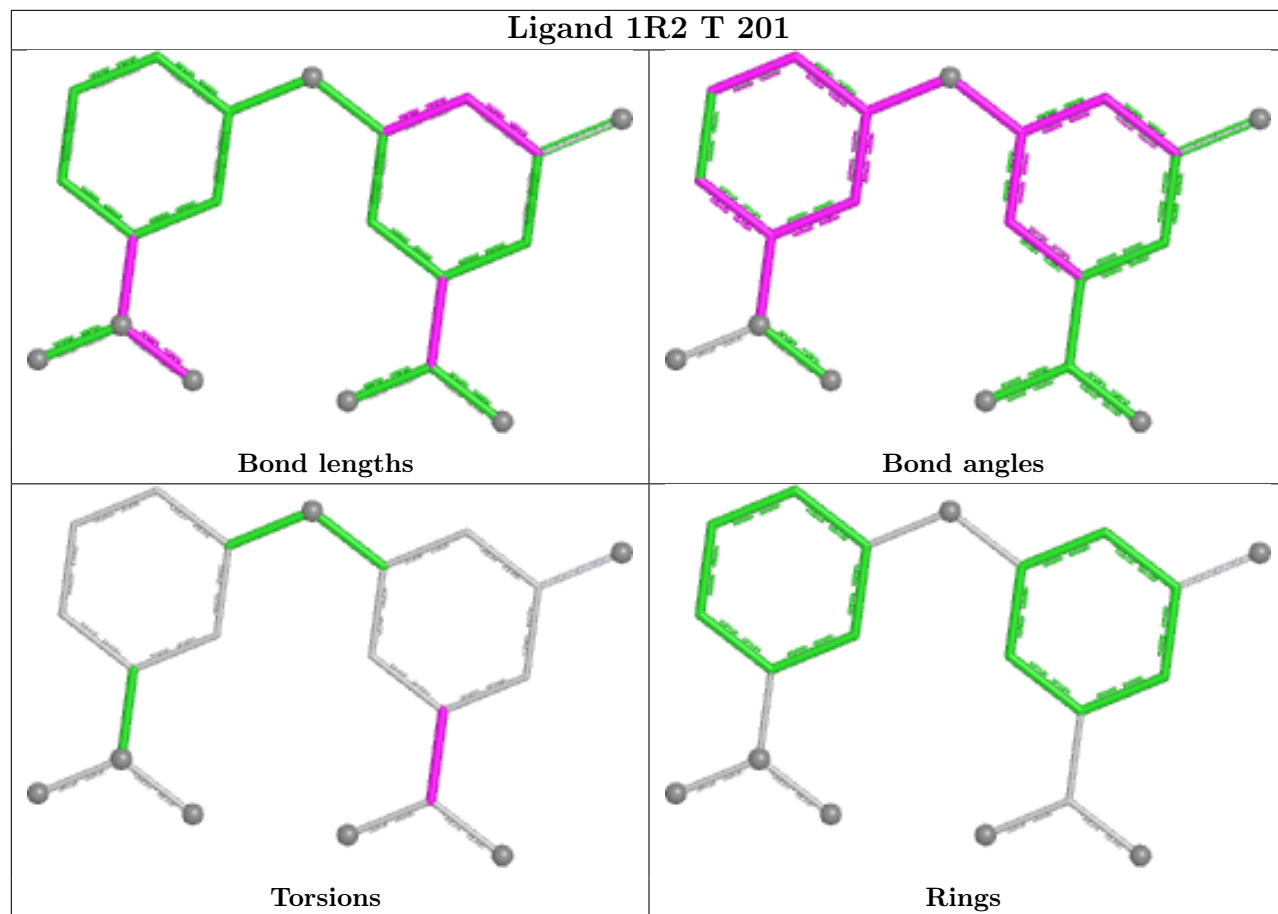
There are no ring outliers.

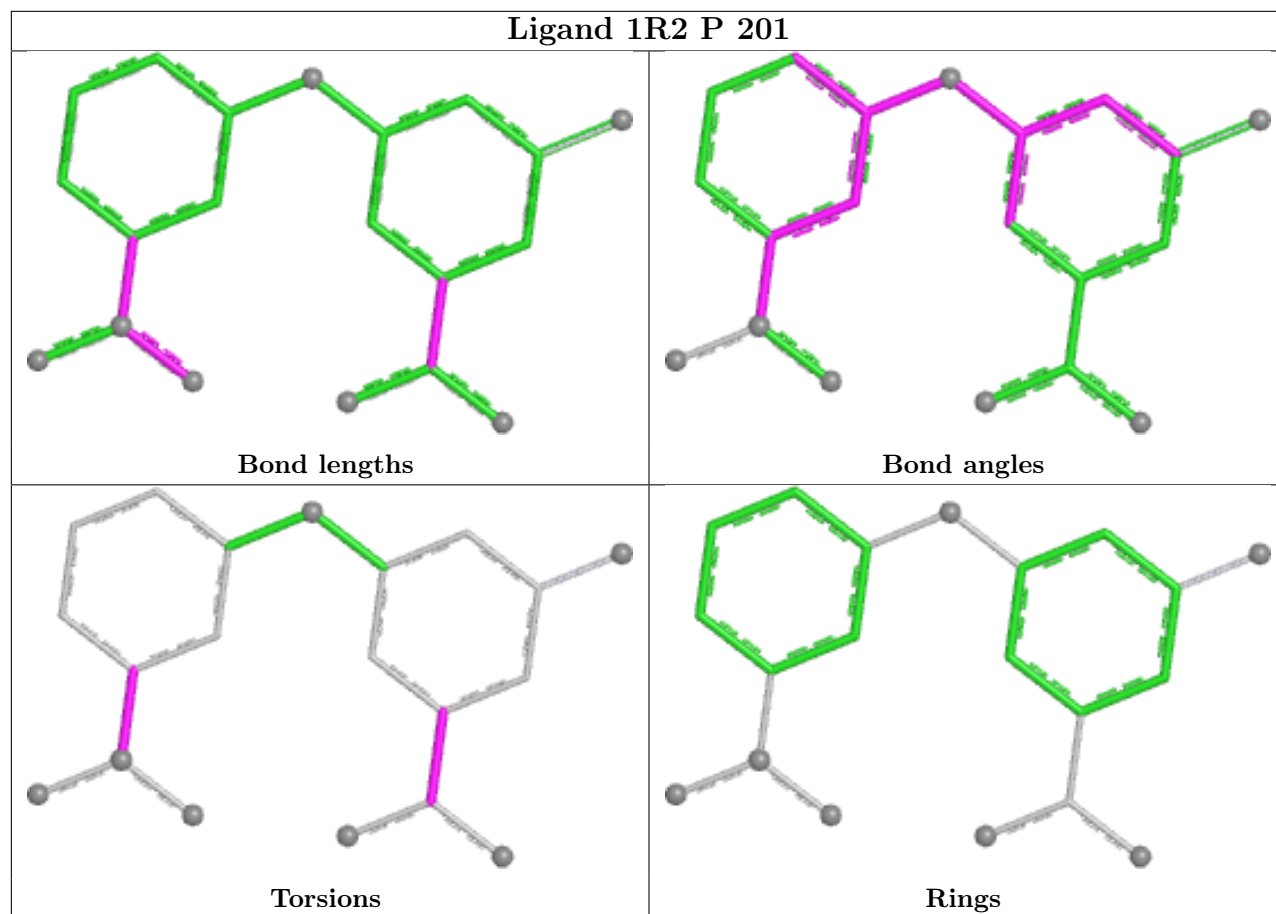
16 monomers are involved in 43 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | T     | 201 | 1R2  | 5       | 0            |
| 2   | I     | 201 | 1R2  | 2       | 0            |
| 2   | A     | 201 | 1R2  | 1       | 0            |
| 2   | V     | 201 | 1R2  | 9       | 0            |
| 2   | D     | 201 | 1R2  | 1       | 0            |
| 2   | G     | 201 | 1R2  | 2       | 0            |
| 2   | O     | 201 | 1R2  | 1       | 0            |
| 2   | K     | 201 | 1R2  | 2       | 0            |
| 2   | C     | 201 | 1R2  | 1       | 0            |
| 2   | N     | 201 | 1R2  | 2       | 0            |
| 2   | R     | 201 | 1R2  | 2       | 0            |
| 2   | F     | 201 | 1R2  | 1       | 0            |
| 2   | X     | 201 | 1R2  | 3       | 0            |
| 2   | E     | 201 | 1R2  | 1       | 0            |
| 2   | B     | 201 | 1R2  | 2       | 0            |
| 2   | W     | 201 | 1R2  | 8       | 0            |

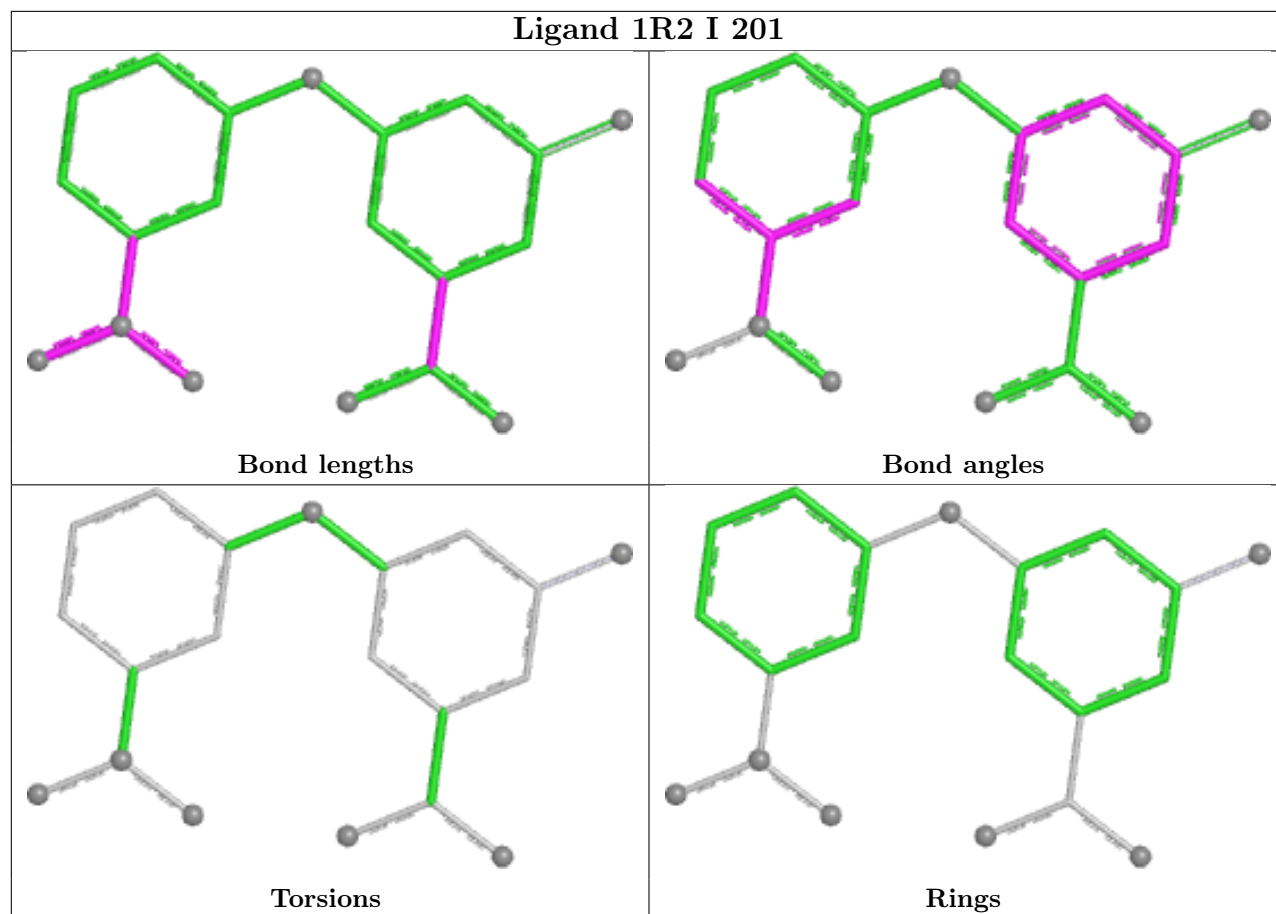
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

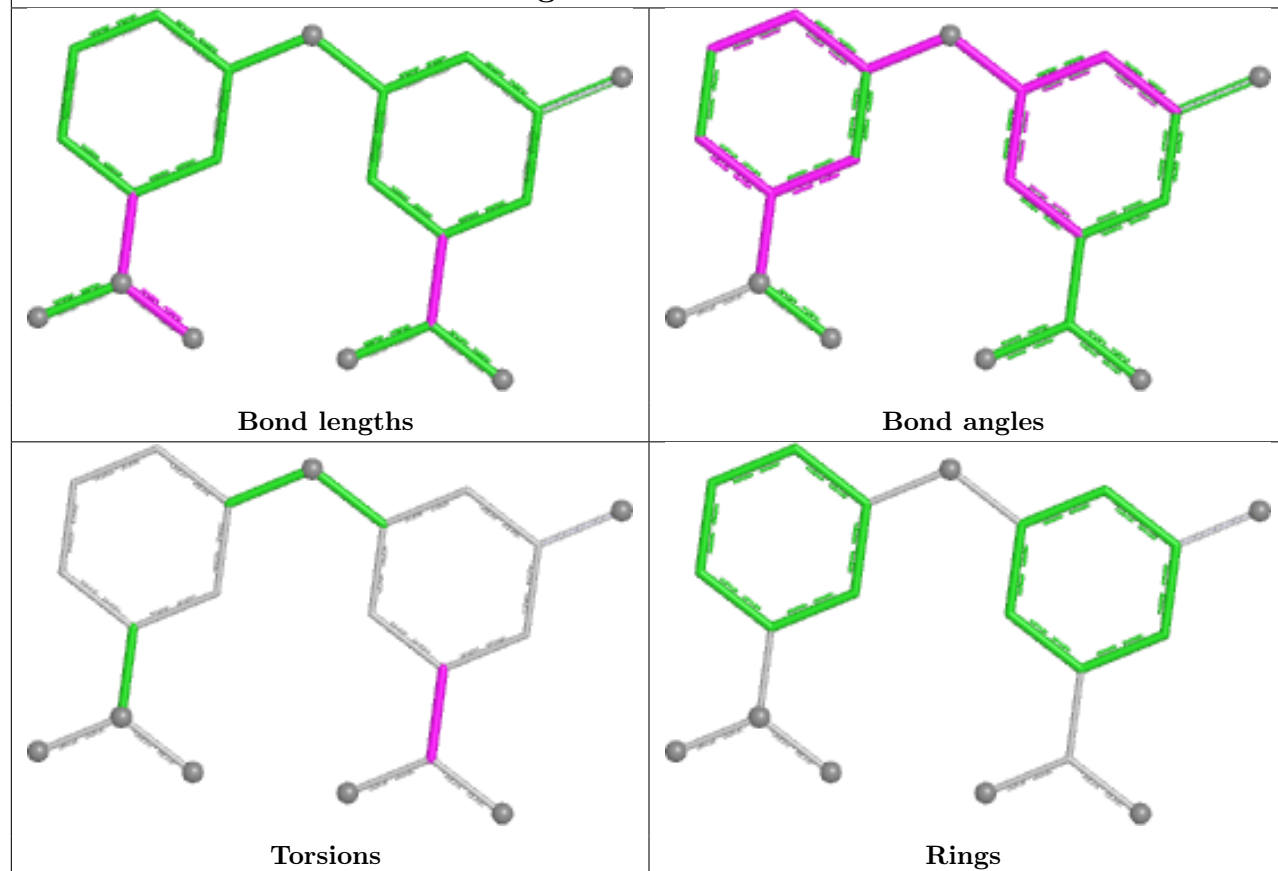




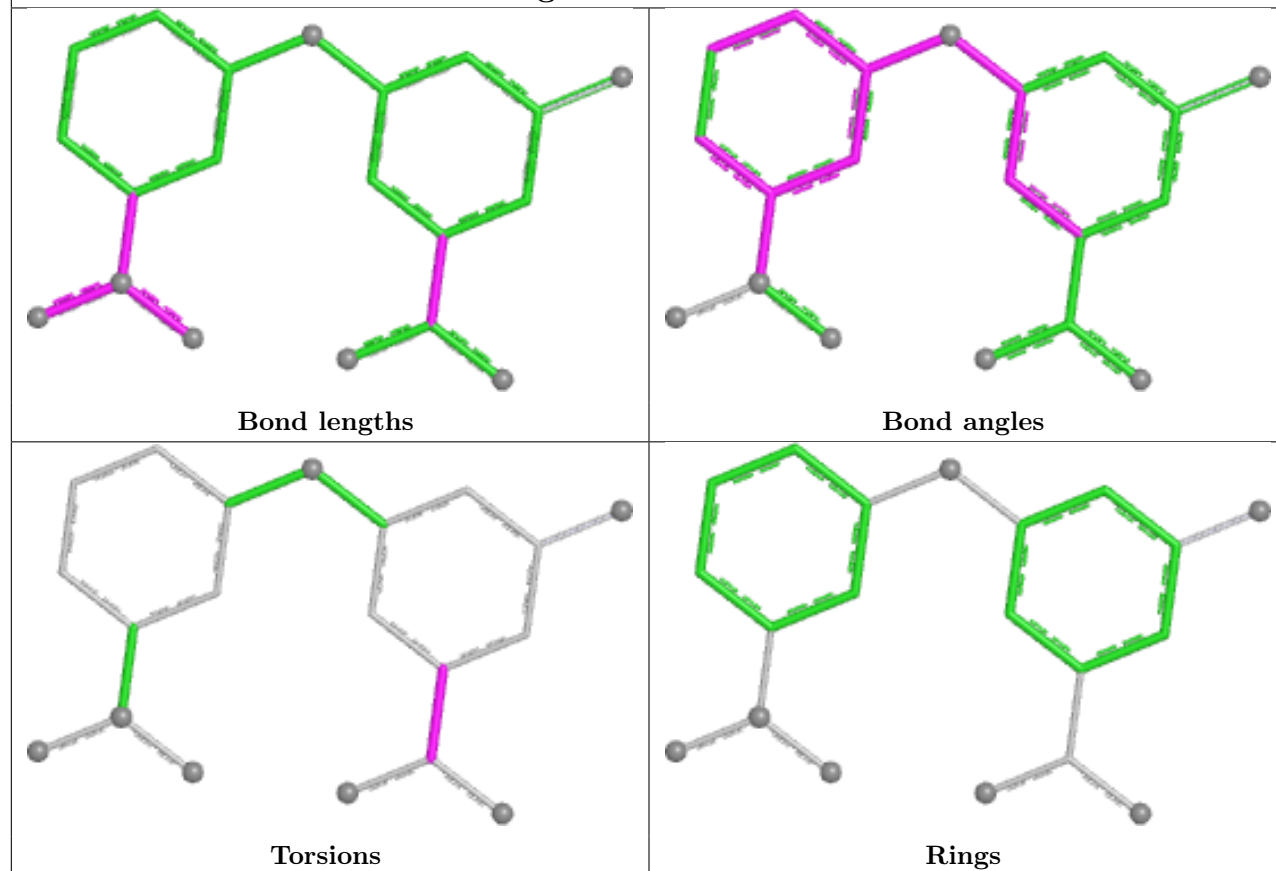
## Ligand 1R2 I 201



## Ligand 1R2 A 201

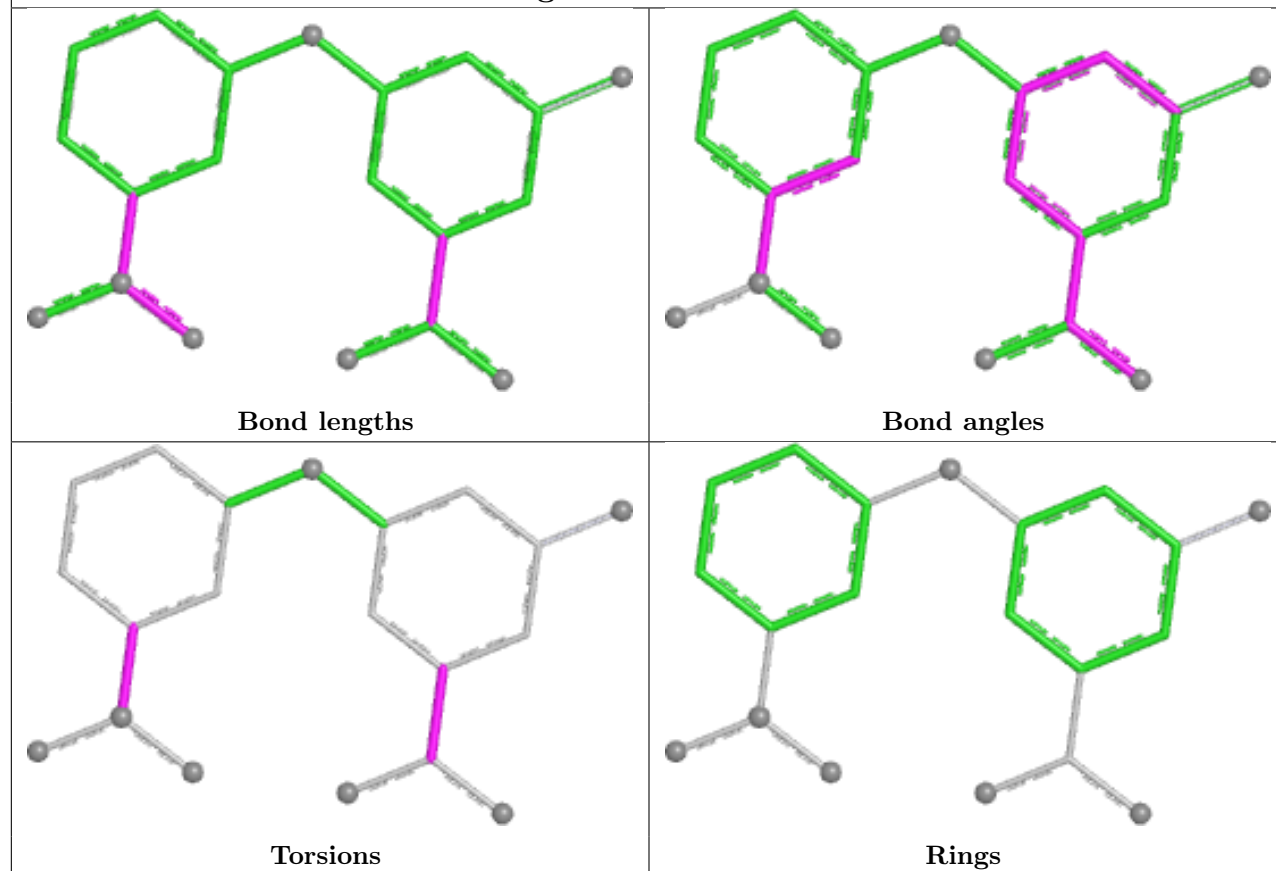


## Ligand 1R2 V 201

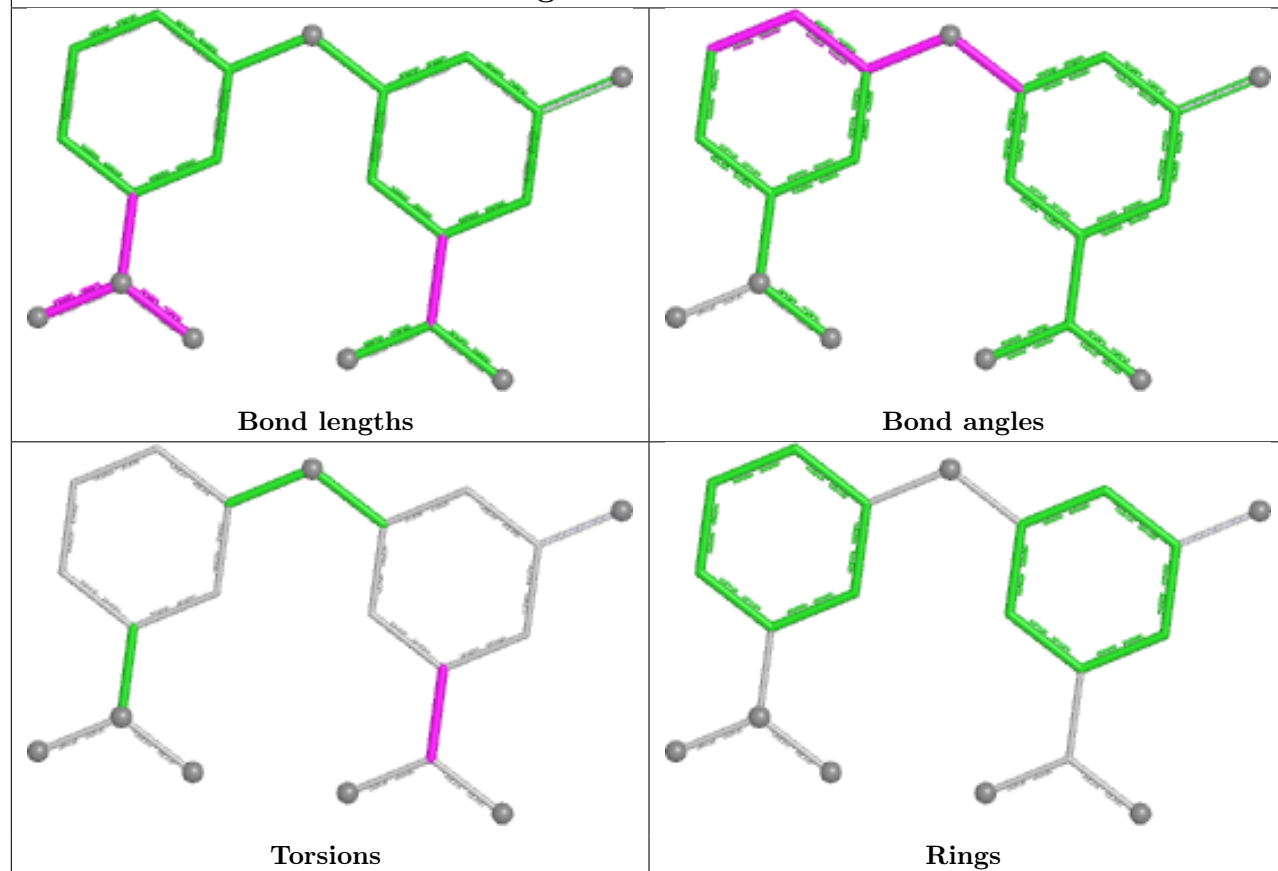




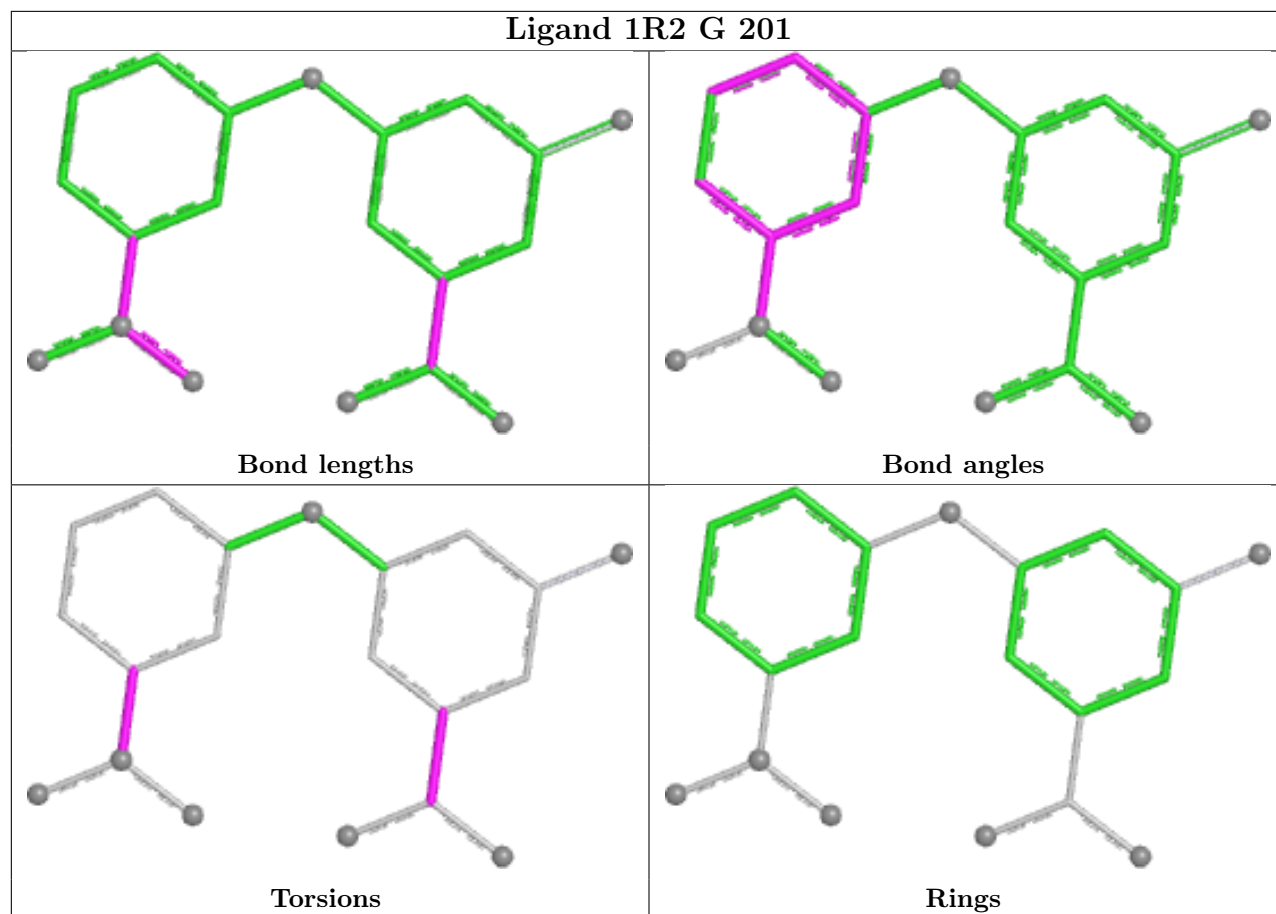
## Ligand 1R2 U 201

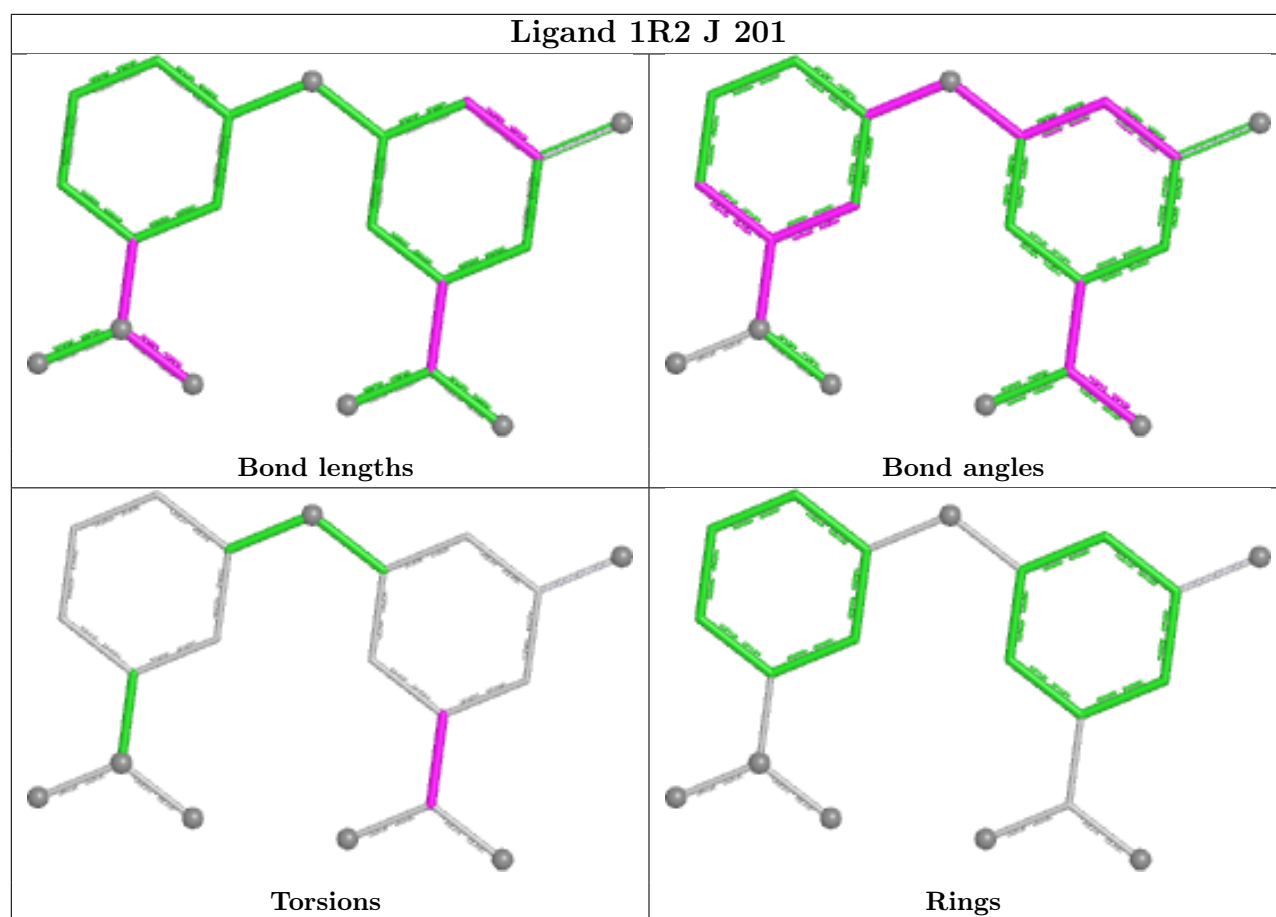


## Ligand 1R2 D 201

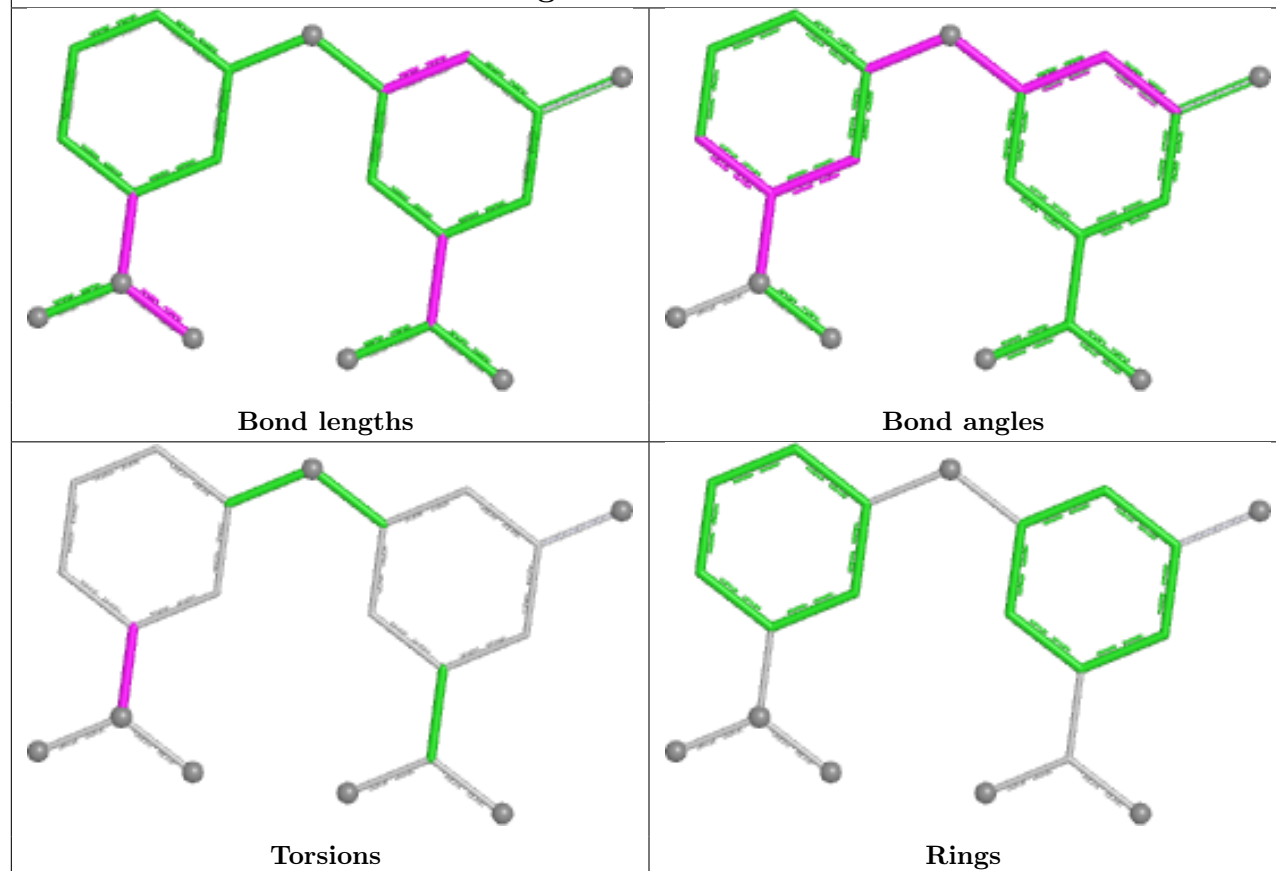


## Ligand 1R2 G 201

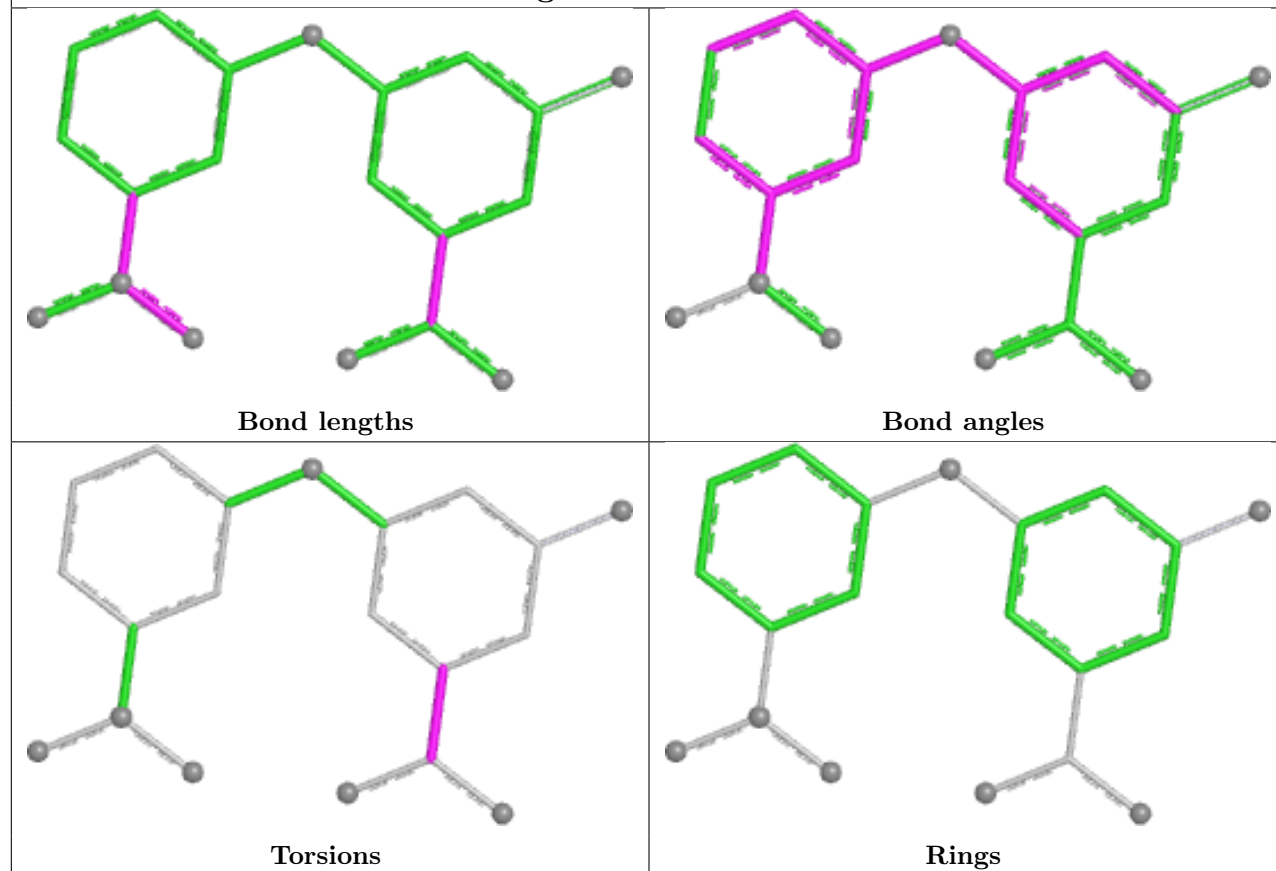




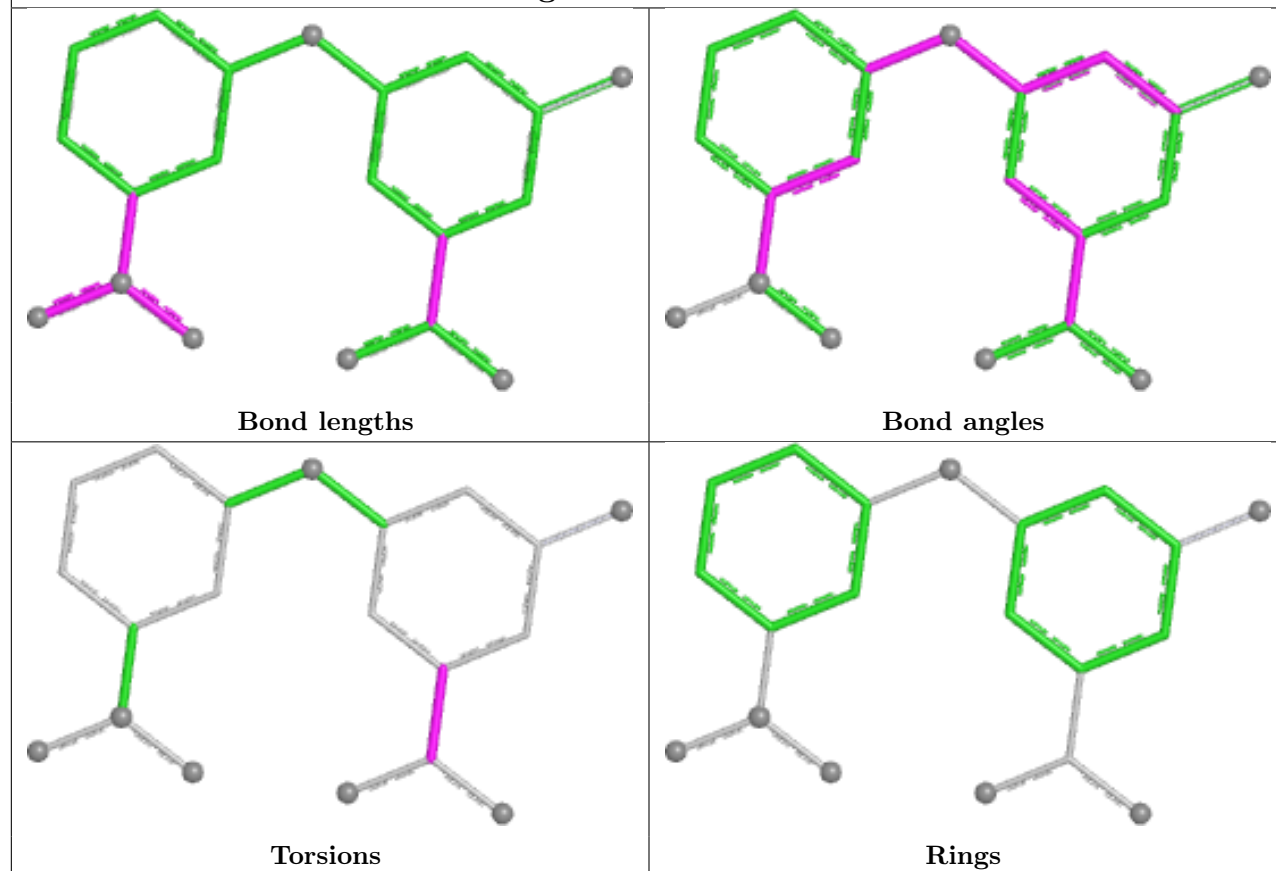
## Ligand 1R2 O 201



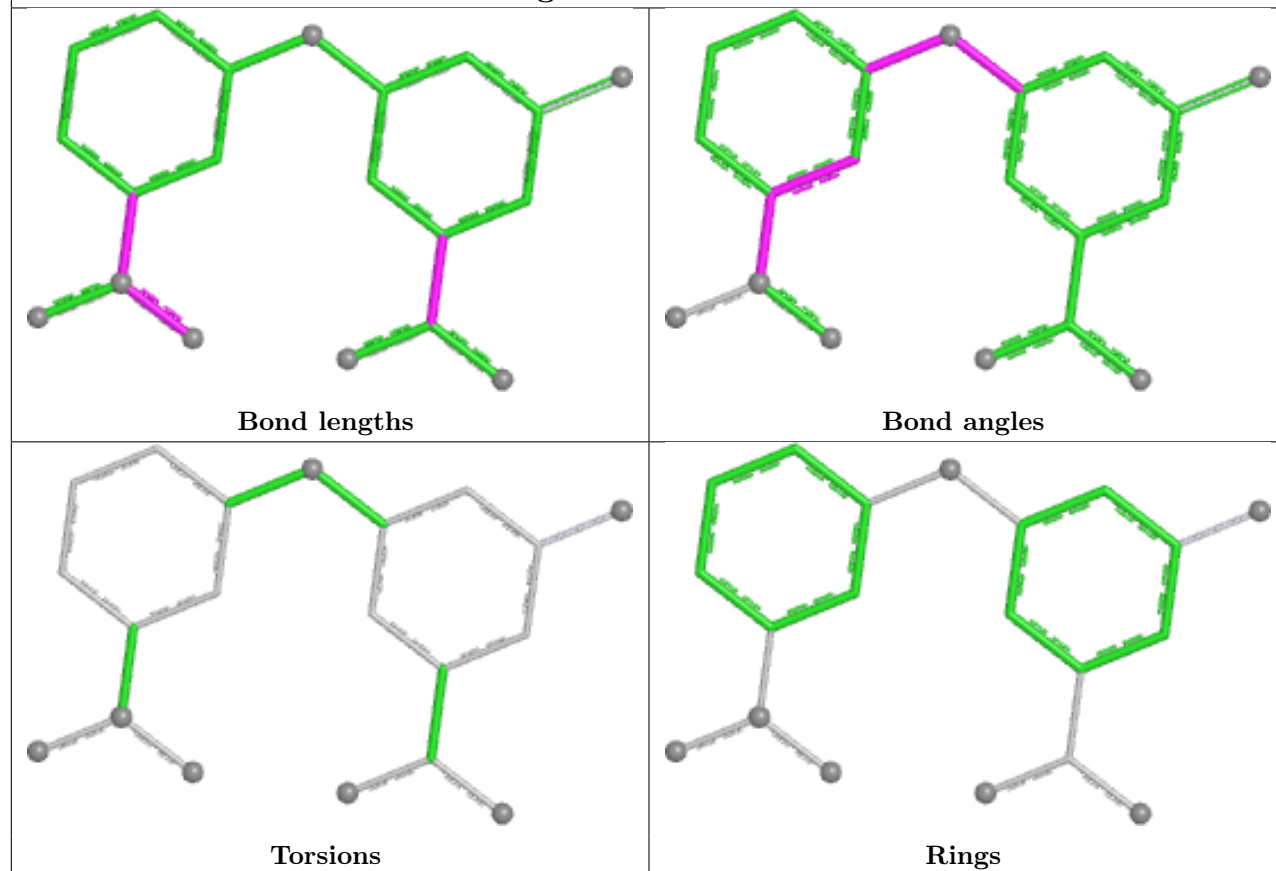
## Ligand 1R2 K 201



## Ligand 1R2 C 201

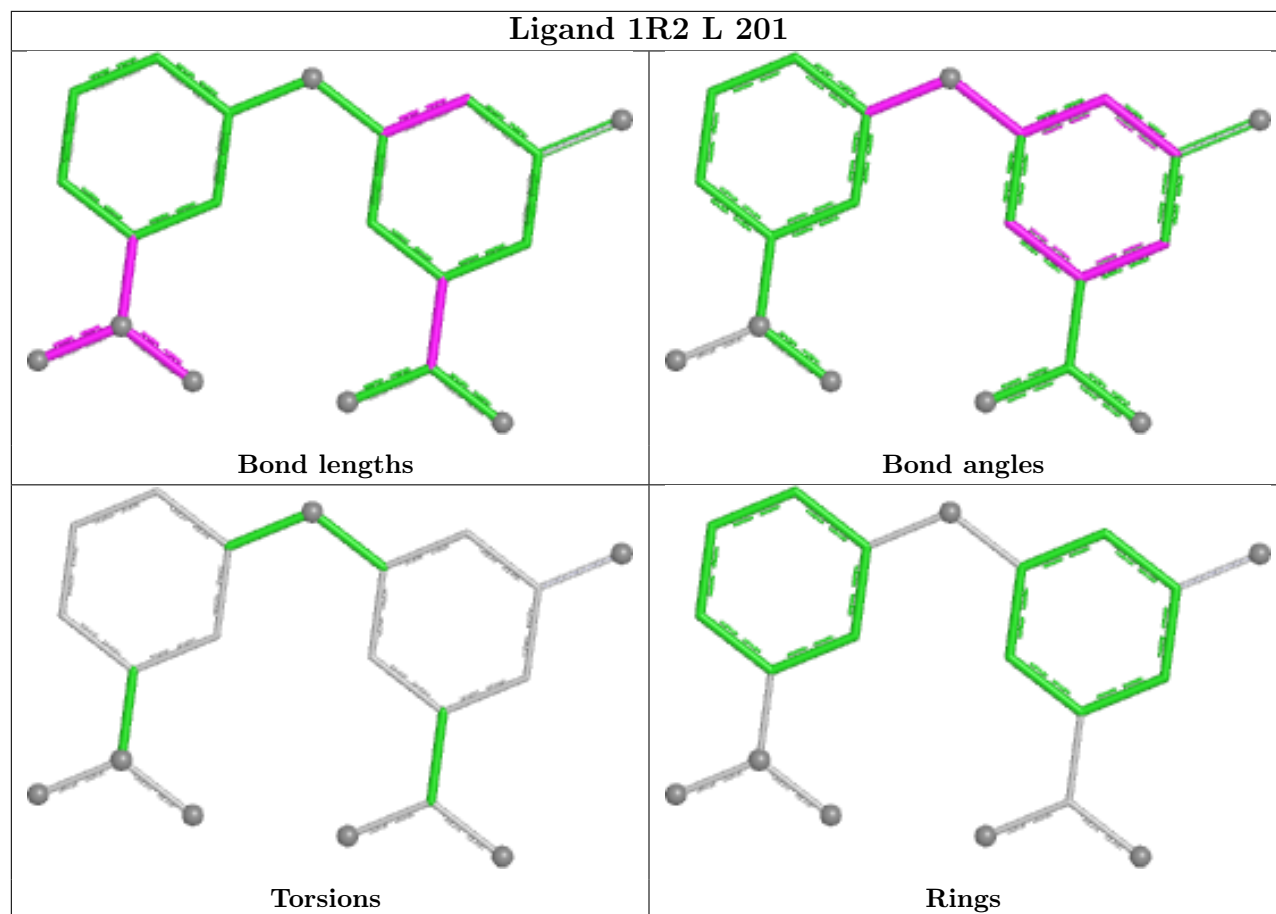


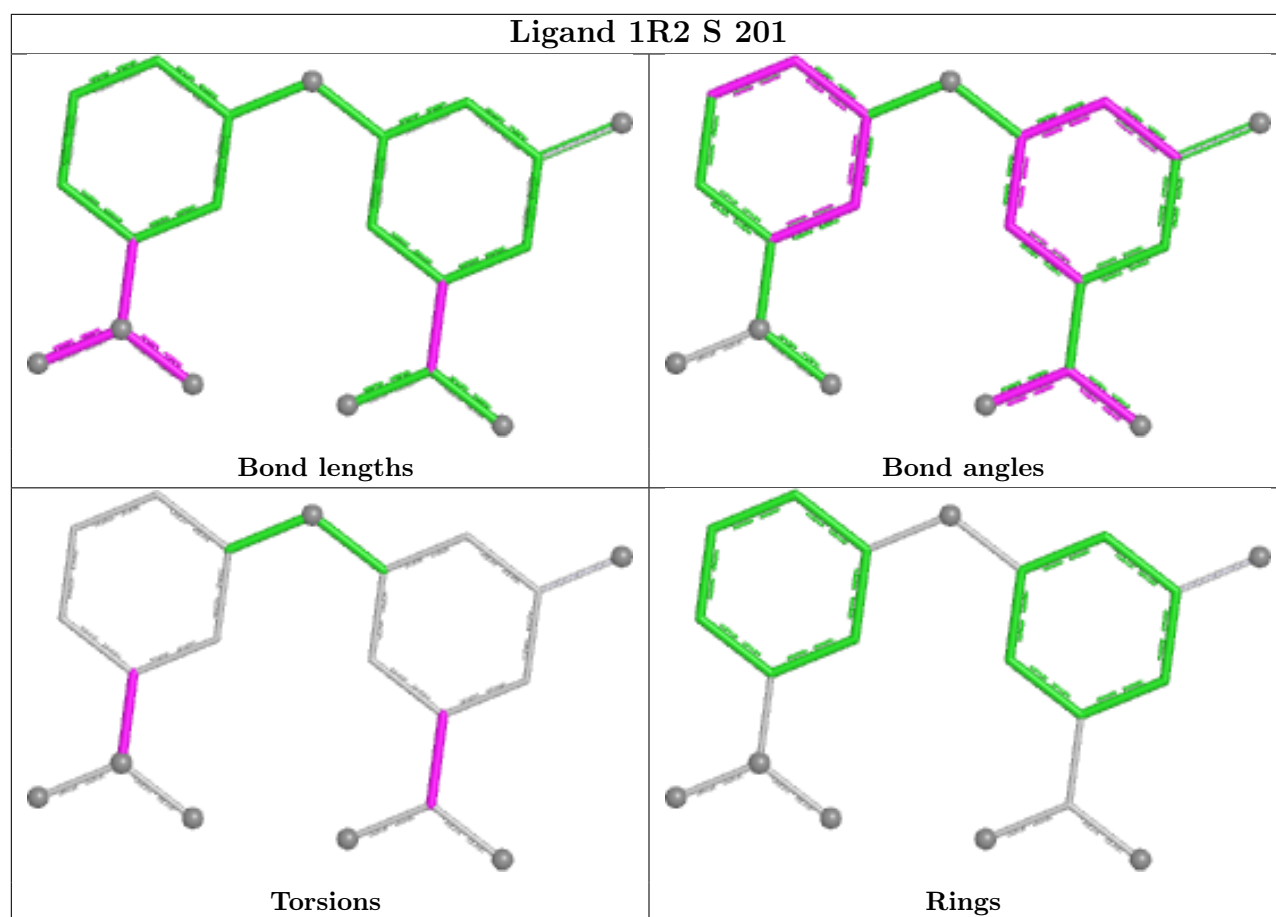
## Ligand 1R2 N 201



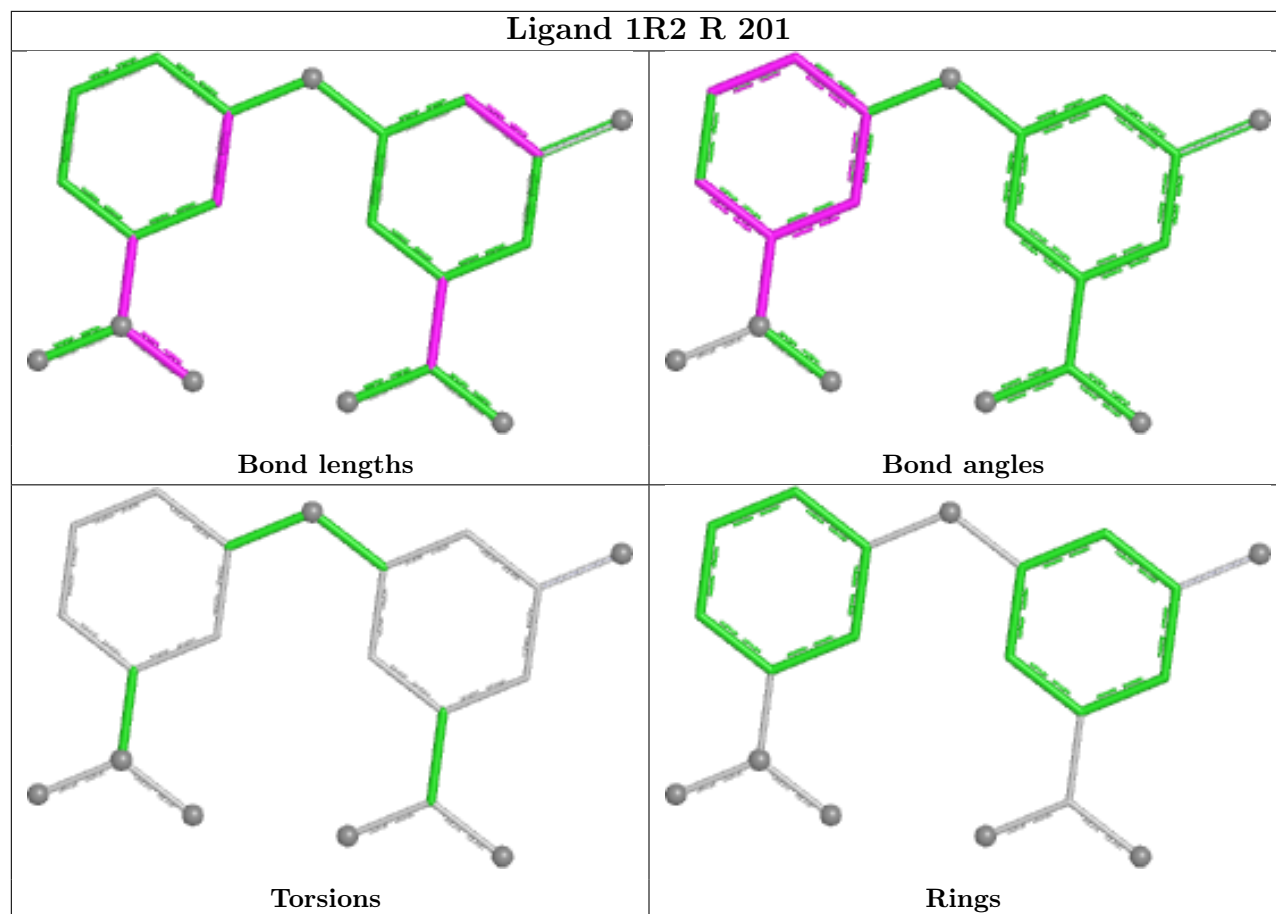


## Ligand 1R2 L 201

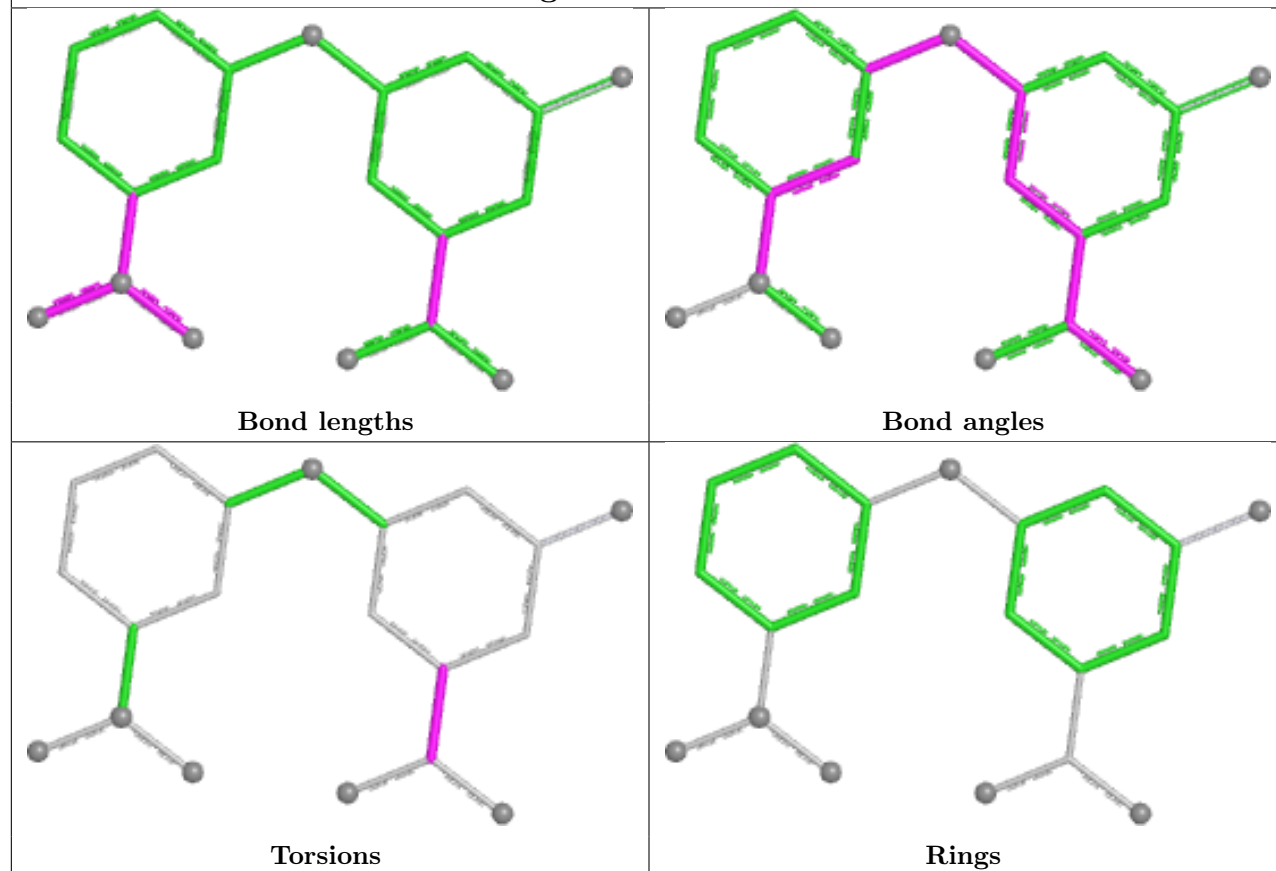




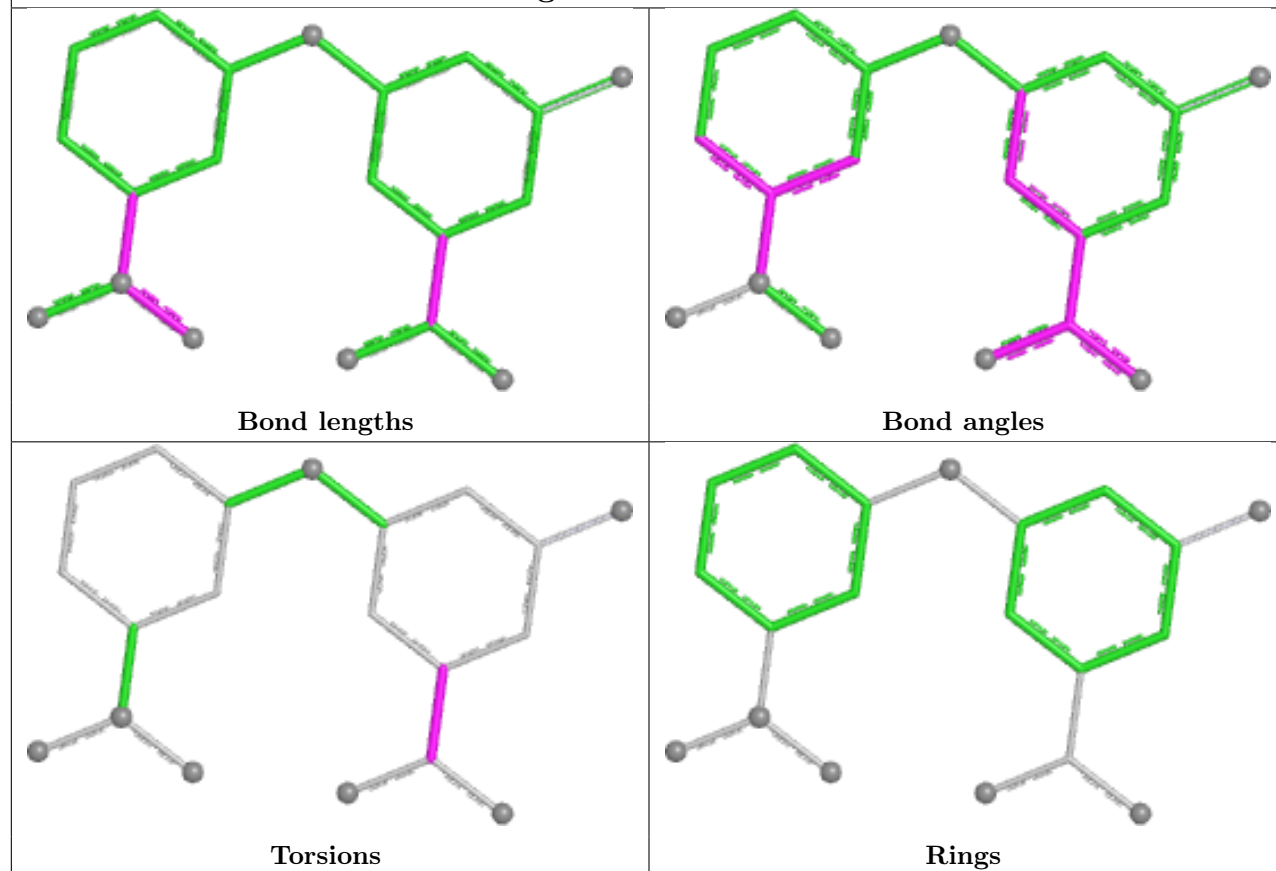
## Ligand 1R2 R 201



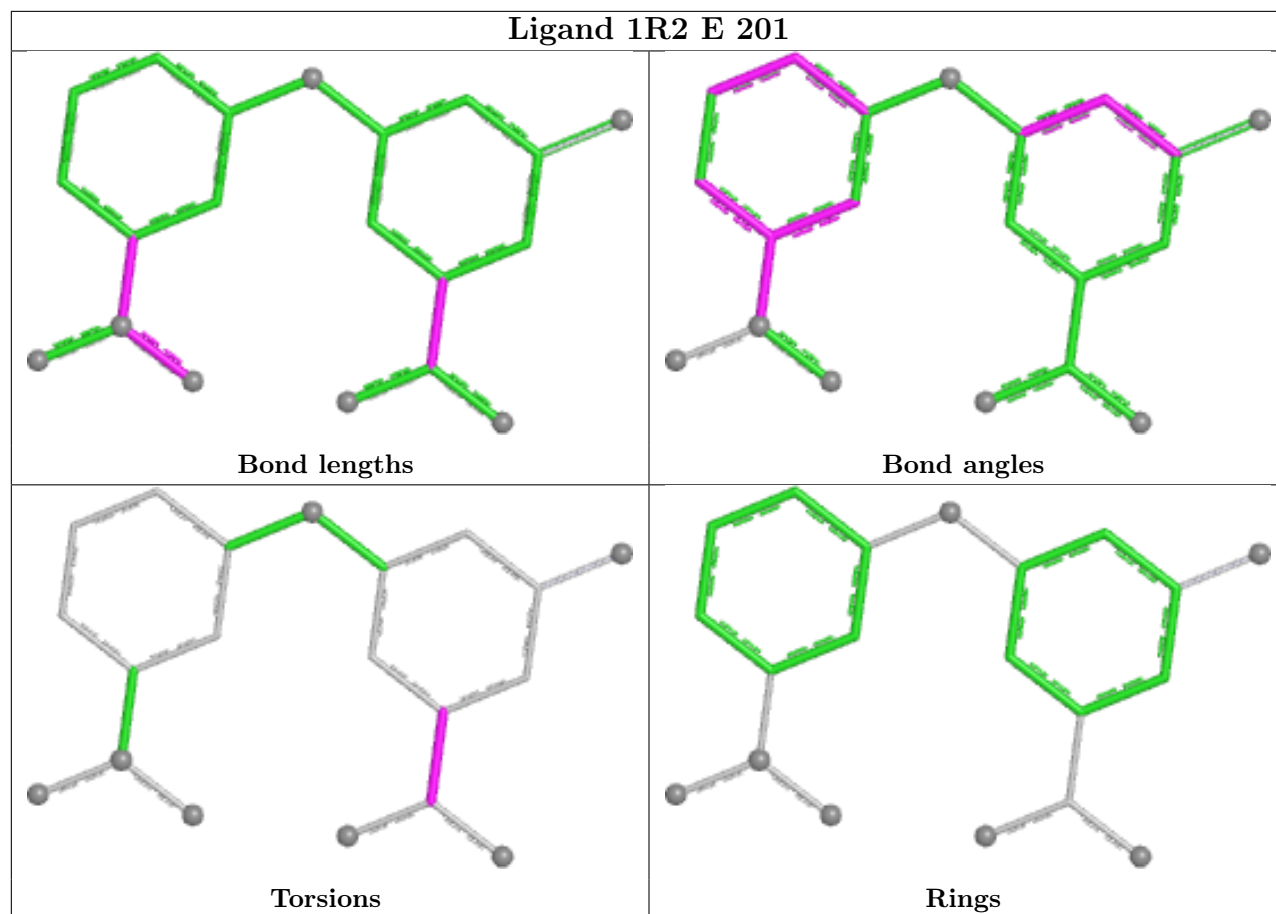
## Ligand 1R2 F 201



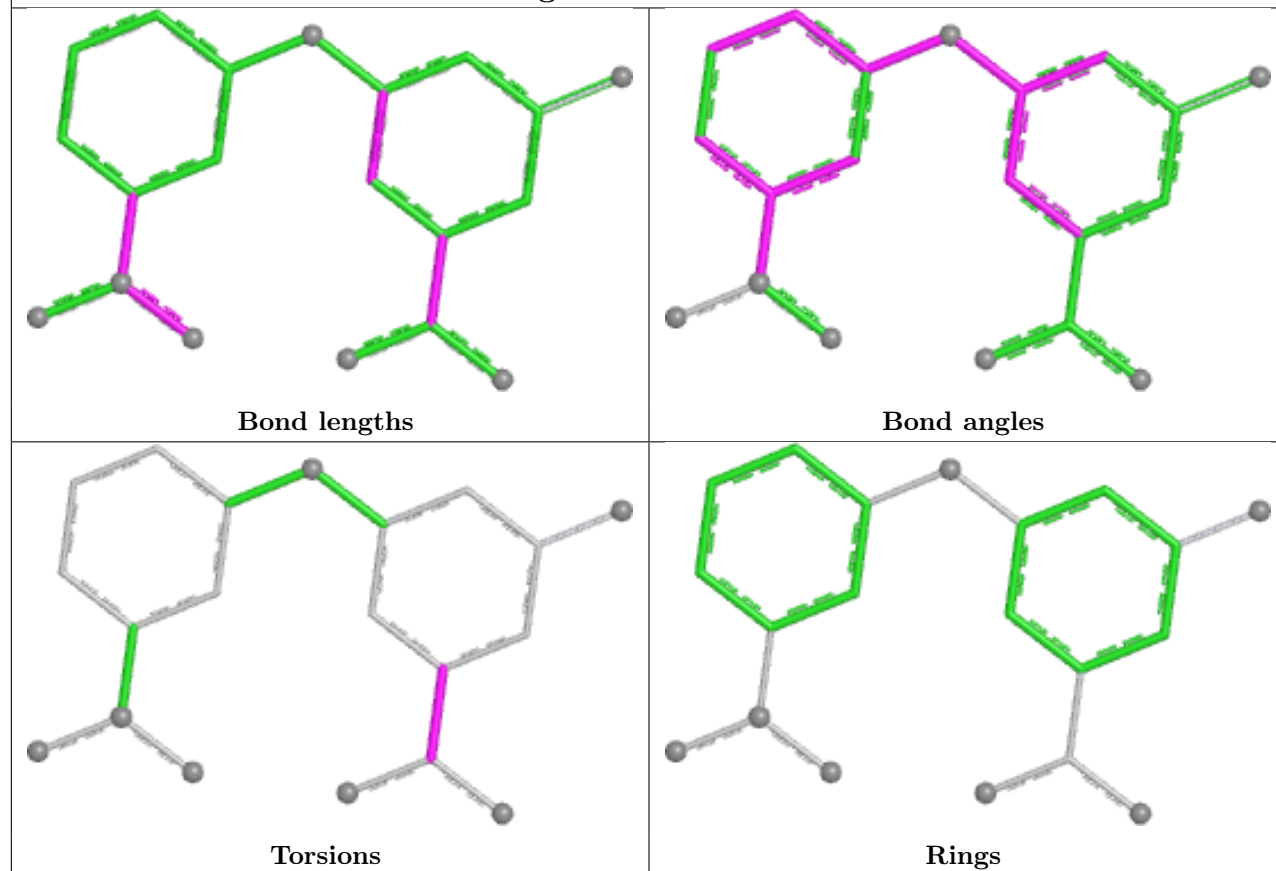
## Ligand 1R2 X 201



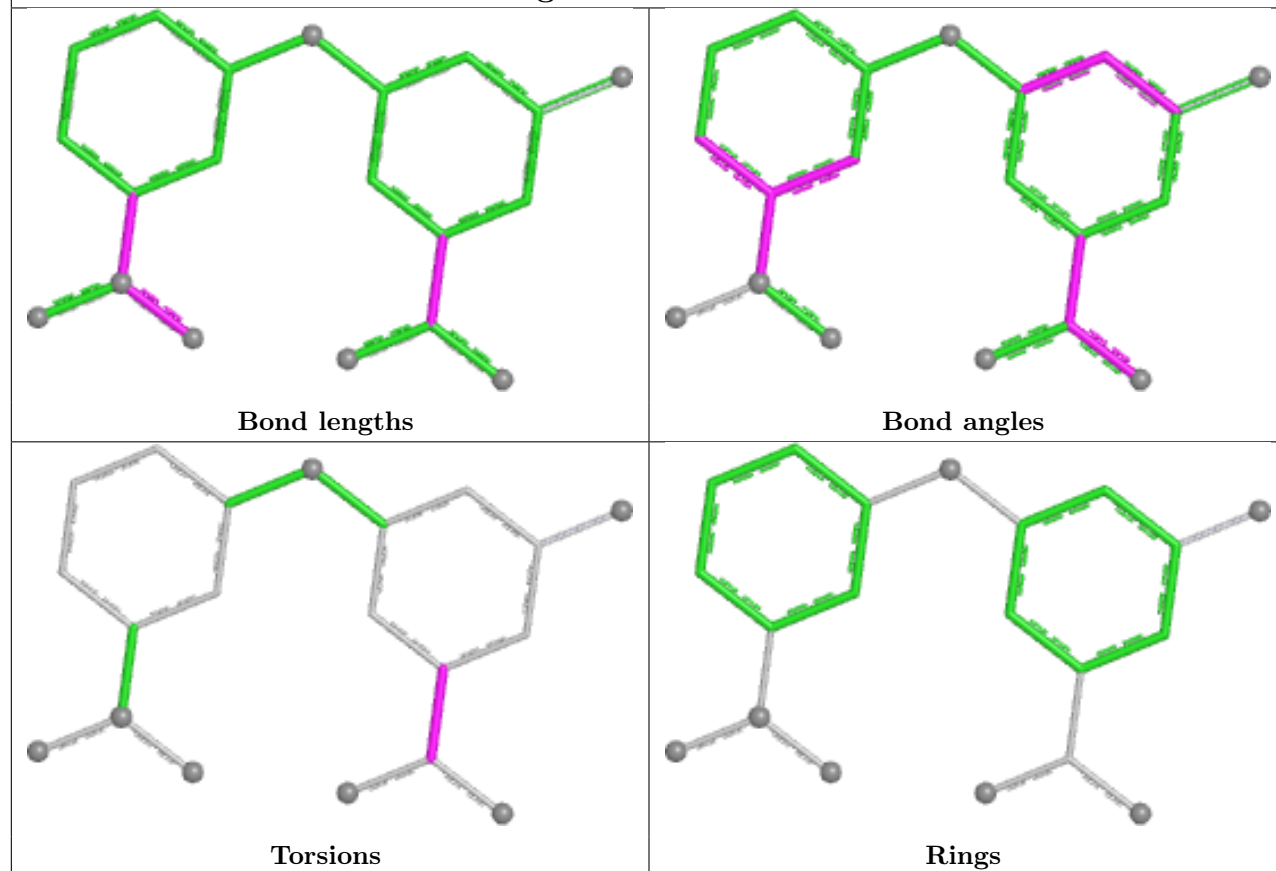
## Ligand 1R2 E 201



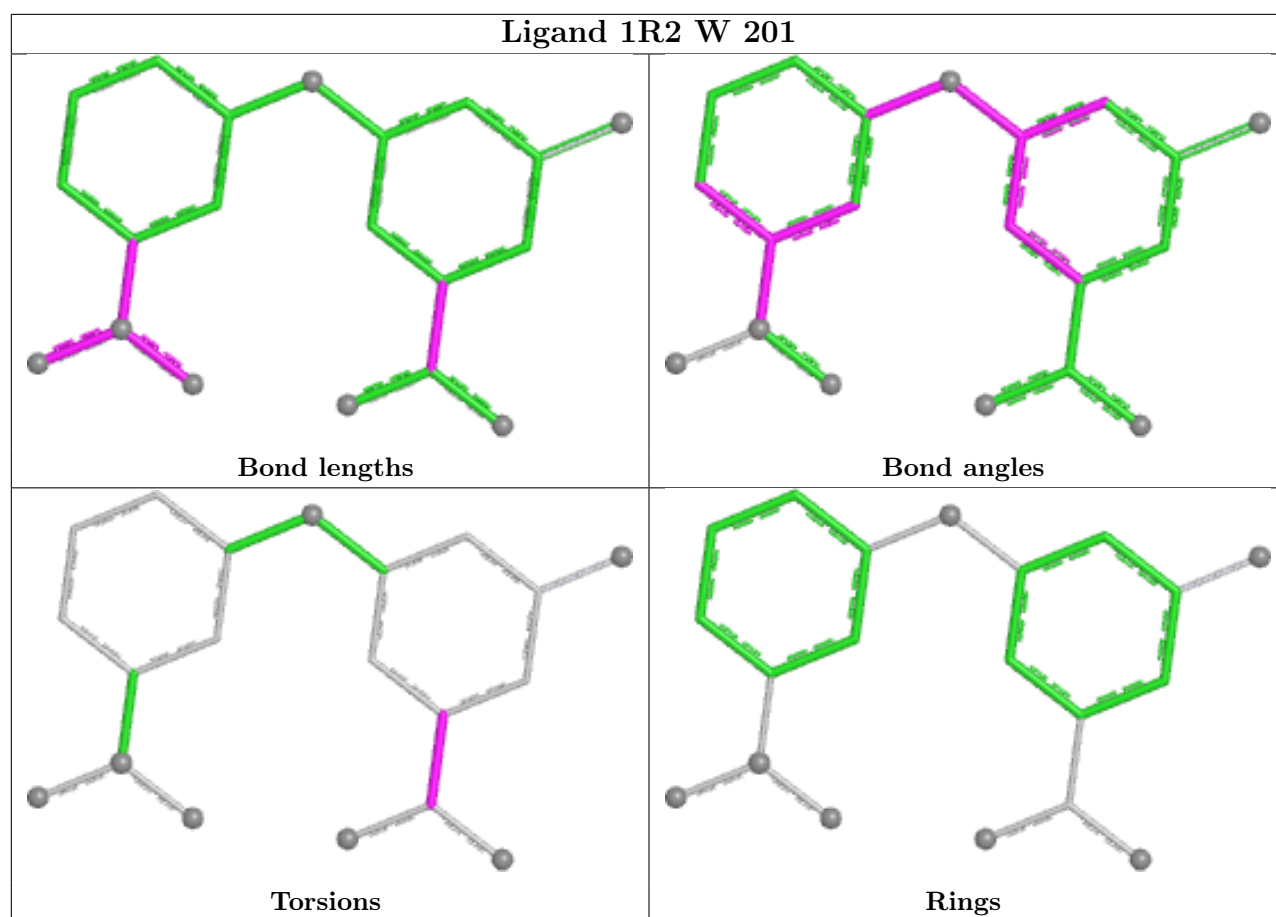
## Ligand 1R2 B 201



## Ligand 1R2 H 201







## 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     | 134/153 (87%) | -0.34  | 3 (2%) 62 52  | 11, 17, 42, 66        | 0      |
| 1   | B     | 141/153 (92%) | -0.48  | 0 100 100     | 9, 16, 35, 51         | 0      |
| 1   | C     | 141/153 (92%) | -0.37  | 2 (1%) 73 64  | 9, 17, 42, 67         | 0      |
| 1   | D     | 143/153 (93%) | -0.47  | 2 (1%) 73 64  | 8, 13, 34, 57         | 0      |
| 1   | E     | 141/153 (92%) | -0.30  | 2 (1%) 73 64  | 10, 18, 50, 76        | 0      |
| 1   | F     | 141/153 (92%) | -0.39  | 0 100 100     | 7, 16, 45, 58         | 0      |
| 1   | G     | 141/153 (92%) | -0.39  | 2 (1%) 73 64  | 10, 15, 39, 50        | 1 (0%) |
| 1   | H     | 141/153 (92%) | -0.50  | 4 (2%) 55 45  | 7, 15, 46, 66         | 0      |
| 1   | I     | 141/153 (92%) | -0.48  | 0 100 100     | 10, 16, 36, 52        | 0      |
| 1   | J     | 141/153 (92%) | -0.44  | 2 (1%) 73 64  | 9, 14, 41, 61         | 0      |
| 1   | K     | 141/153 (92%) | -0.31  | 1 (0%) 84 77  | 10, 18, 44, 62        | 0      |
| 1   | L     | 141/153 (92%) | -0.39  | 0 100 100     | 7, 17, 34, 43         | 0      |
| 1   | M     | 137/153 (89%) | -0.14  | 3 (2%) 62 52  | 16, 25, 49, 78        | 0      |
| 1   | N     | 141/153 (92%) | 0.11   | 12 (8%) 16 12 | 17, 26, 76, 110       | 0      |
| 1   | O     | 141/153 (92%) | -0.46  | 0 100 100     | 9, 18, 37, 51         | 0      |
| 1   | P     | 141/153 (92%) | -0.02  | 7 (4%) 34 26  | 14, 25, 62, 69        | 0      |
| 1   | Q     | 137/153 (89%) | -0.07  | 2 (1%) 72 63  | 19, 30, 53, 78        | 0      |
| 1   | R     | 141/153 (92%) | 0.01   | 5 (3%) 47 38  | 17, 26, 55, 68        | 0      |
| 1   | S     | 140/153 (91%) | -0.08  | 7 (5%) 34 26  | 16, 26, 62, 80        | 1 (0%) |
| 1   | T     | 141/153 (92%) | -0.39  | 0 100 100     | 9, 16, 42, 67         | 0      |
| 1   | U     | 141/153 (92%) | -0.21  | 3 (2%) 63 54  | 15, 23, 49, 82        | 0      |
| 1   | V     | 141/153 (92%) | -0.24  | 3 (2%) 63 54  | 12, 20, 50, 82        | 0      |
| 1   | W     | 141/153 (92%) | 0.06   | 4 (2%) 55 45  | 19, 30, 60, 78        | 0      |
| 1   | X     | 150/153 (98%) | -0.18  | 4 (2%) 56 46  | 11, 22, 65, 76        | 0      |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| All | All   | 3379/3672 (92%) | -0.27  | 68 (2%) 65 56 | 7, 20, 51, 110        | 2 (0%) |

All (68) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 41  | ALA  | 5.4  |
| 1   | N     | 43  | LEU  | 4.7  |
| 1   | N     | 40  | ALA  | 4.5  |
| 1   | U     | 21  | PRO  | 4.1  |
| 1   | M     | 20  | GLU  | 4.0  |
| 1   | S     | 21  | PRO  | 3.9  |
| 1   | N     | 44  | GLY  | 3.7  |
| 1   | Q     | 143 | HIS  | 3.4  |
| 1   | S     | 23  | VAL  | 3.4  |
| 1   | J     | 143 | HIS  | 3.2  |
| 1   | P     | 61  | TRP  | 3.1  |
| 1   | Q     | 24  | TYR  | 3.1  |
| 1   | M     | 25  | GLY  | 3.1  |
| 1   | N     | 21  | PRO  | 3.1  |
| 1   | X     | 21  | PRO  | 3.0  |
| 1   | W     | 20  | GLU  | 3.0  |
| 1   | S     | 27  | THR  | 3.0  |
| 1   | K     | 3   | LEU  | 2.9  |
| 1   | E     | 22  | ALA  | 2.9  |
| 1   | V     | 22  | ALA  | 2.9  |
| 1   | A     | 143 | HIS  | 2.9  |
| 1   | R     | 3   | LEU  | 2.9  |
| 1   | S     | 24  | TYR  | 2.9  |
| 1   | X     | 17  | GLY  | 2.9  |
| 1   | R     | 69  | ALA  | 2.9  |
| 1   | N     | 23  | VAL  | 2.9  |
| 1   | X     | 22  | ALA  | 2.8  |
| 1   | G     | 3   | LEU  | 2.8  |
| 1   | P     | 48  | VAL  | 2.7  |
| 1   | W     | 3   | LEU  | 2.7  |
| 1   | C     | 23  | VAL  | 2.7  |
| 1   | N     | 19  | ARG  | 2.7  |
| 1   | A     | 3   | LEU  | 2.7  |
| 1   | N     | 3   | LEU  | 2.6  |
| 1   | H     | 22  | ALA  | 2.6  |
| 1   | H     | 143 | HIS  | 2.6  |
| 1   | S     | 20  | GLU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 19  | ARG  | 2.6  |
| 1   | W     | 19  | ARG  | 2.5  |
| 1   | D     | 19  | ARG  | 2.5  |
| 1   | P     | 57  | GLN  | 2.5  |
| 1   | M     | 17  | GLY  | 2.4  |
| 1   | P     | 22  | ALA  | 2.4  |
| 1   | A     | 25  | GLY  | 2.4  |
| 1   | N     | 20  | GLU  | 2.4  |
| 1   | N     | 39  | GLU  | 2.4  |
| 1   | S     | 22  | ALA  | 2.3  |
| 1   | G     | 143 | HIS  | 2.3  |
| 1   | P     | 24  | TYR  | 2.3  |
| 1   | P     | 3   | LEU  | 2.3  |
| 1   | P     | 143 | HIS  | 2.2  |
| 1   | W     | 143 | HIS  | 2.2  |
| 1   | N     | 24  | TYR  | 2.2  |
| 1   | U     | 3   | LEU  | 2.2  |
| 1   | S     | 19  | ARG  | 2.2  |
| 1   | R     | 22  | ALA  | 2.2  |
| 1   | H     | 25  | GLY  | 2.1  |
| 1   | D     | 22  | ALA  | 2.1  |
| 1   | J     | 22  | ALA  | 2.1  |
| 1   | X     | 18  | ARG  | 2.1  |
| 1   | R     | 143 | HIS  | 2.1  |
| 1   | V     | 3   | LEU  | 2.1  |
| 1   | E     | 23  | VAL  | 2.0  |
| 1   | R     | 45  | LEU  | 2.0  |
| 1   | U     | 22  | ALA  | 2.0  |
| 1   | N     | 42  | GLU  | 2.0  |
| 1   | H     | 23  | VAL  | 2.0  |
| 1   | C     | 21  | PRO  | 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 ⓘ

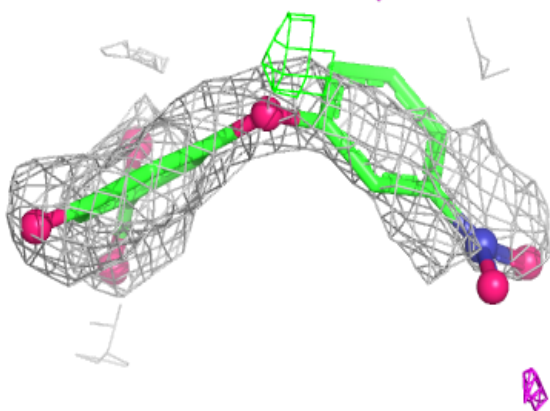
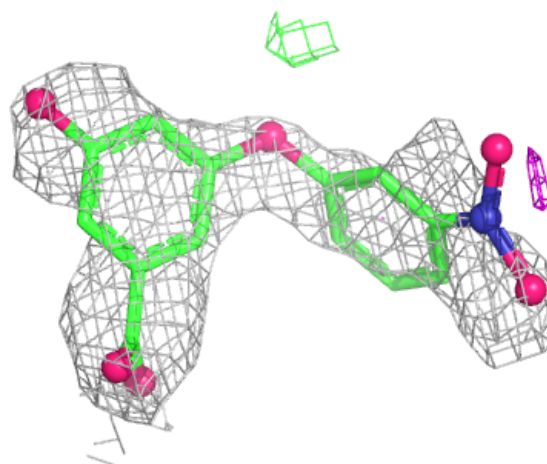
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | 1R2  | W     | 201 | 20/20 | 0.81 | 0.18 | 61,72,87,87                | 0     |
| 2   | 1R2  | S     | 201 | 20/20 | 0.83 | 0.17 | 55,65,70,71                | 0     |
| 2   | 1R2  | T     | 201 | 20/20 | 0.84 | 0.15 | 30,39,46,48                | 0     |
| 2   | 1R2  | V     | 201 | 20/20 | 0.85 | 0.14 | 31,42,52,53                | 0     |
| 2   | 1R2  | P     | 201 | 20/20 | 0.85 | 0.14 | 44,52,55,60                | 0     |
| 2   | 1R2  | X     | 201 | 20/20 | 0.87 | 0.14 | 43,54,65,65                | 0     |
| 2   | 1R2  | R     | 201 | 20/20 | 0.88 | 0.13 | 34,43,48,50                | 0     |
| 2   | 1R2  | E     | 201 | 20/20 | 0.88 | 0.14 | 41,45,60,64                | 0     |
| 2   | 1R2  | H     | 201 | 20/20 | 0.89 | 0.12 | 34,45,54,55                | 0     |
| 2   | 1R2  | N     | 201 | 20/20 | 0.89 | 0.12 | 37,49,63,64                | 0     |
| 2   | 1R2  | A     | 201 | 20/20 | 0.89 | 0.13 | 43,49,54,60                | 0     |
| 2   | 1R2  | L     | 201 | 20/20 | 0.90 | 0.12 | 25,30,40,45                | 0     |
| 2   | 1R2  | I     | 201 | 20/20 | 0.90 | 0.12 | 23,33,45,45                | 0     |
| 2   | 1R2  | U     | 201 | 20/20 | 0.90 | 0.11 | 33,40,49,51                | 0     |
| 2   | 1R2  | G     | 201 | 20/20 | 0.91 | 0.11 | 23,32,37,37                | 0     |
| 2   | 1R2  | K     | 201 | 20/20 | 0.91 | 0.11 | 28,36,47,54                | 0     |
| 2   | 1R2  | C     | 201 | 20/20 | 0.91 | 0.11 | 35,38,41,42                | 0     |
| 2   | 1R2  | O     | 201 | 20/20 | 0.92 | 0.09 | 26,32,34,36                | 0     |
| 2   | 1R2  | J     | 201 | 20/20 | 0.92 | 0.10 | 28,33,38,38                | 0     |
| 2   | 1R2  | D     | 201 | 20/20 | 0.92 | 0.11 | 24,27,33,34                | 0     |
| 2   | 1R2  | F     | 201 | 20/20 | 0.93 | 0.09 | 27,31,35,35                | 0     |
| 2   | 1R2  | B     | 201 | 20/20 | 0.94 | 0.09 | 20,24,25,26                | 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.

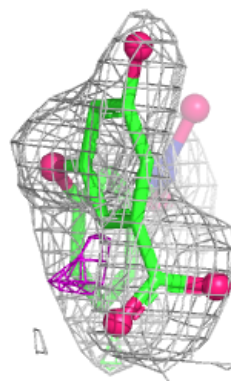
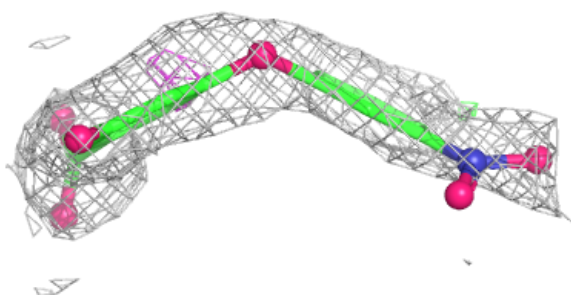
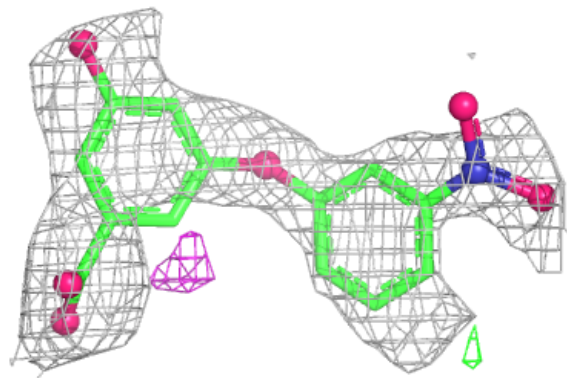
**Electron density around 1R2 W 201:**

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

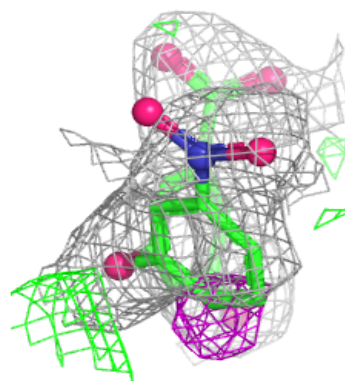
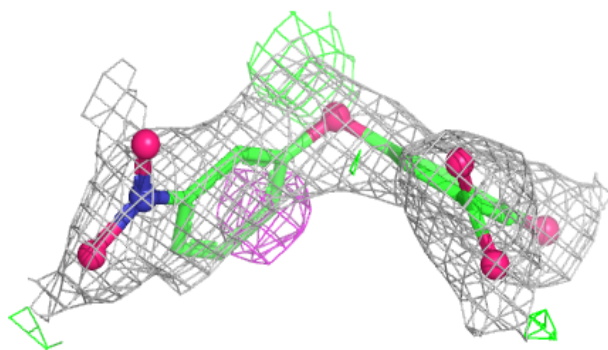
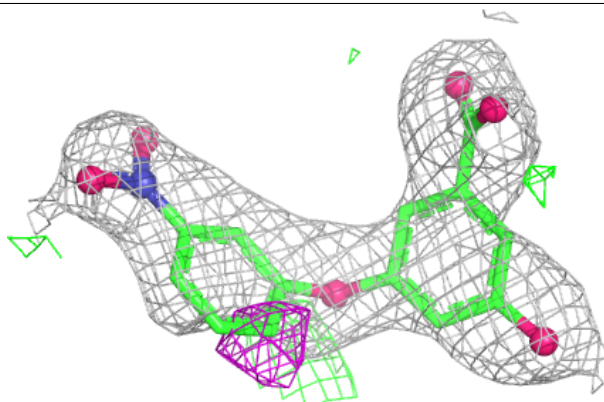


**Electron density around 1R2 S 201:**

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

**Electron density around 1R2 T 201:**

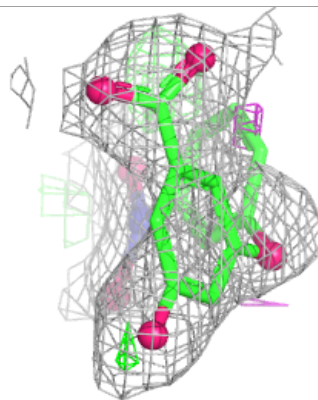
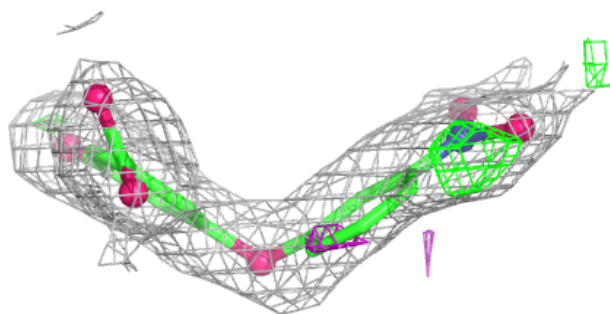
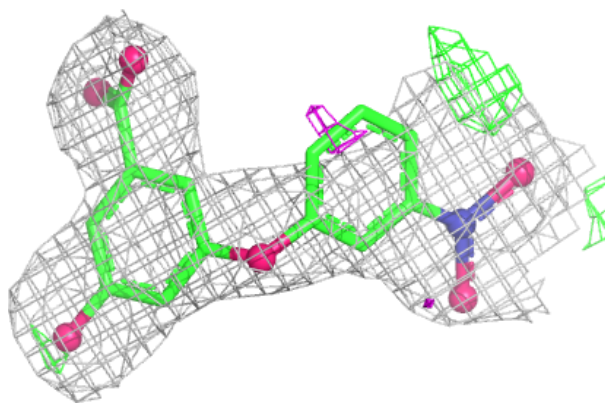
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



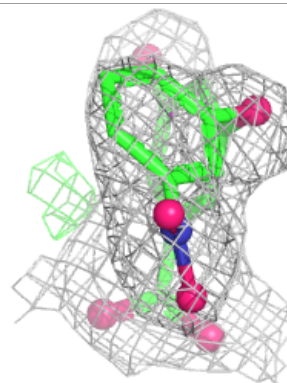
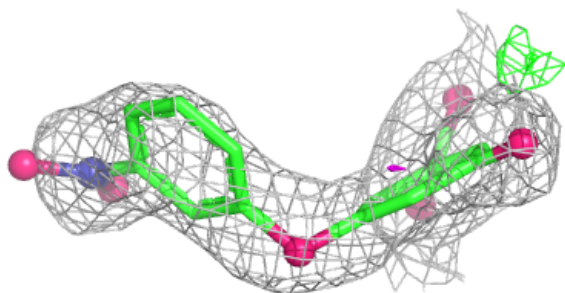
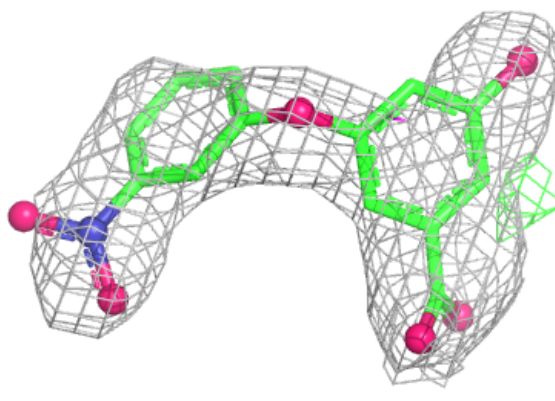


**Electron density around 1R2 V 201:**

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

**Electron density around 1R2 P 201:**

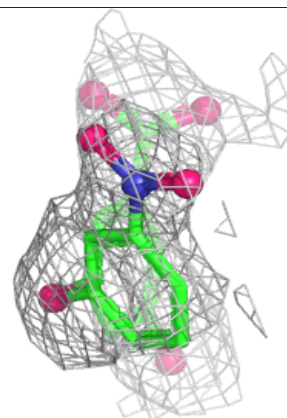
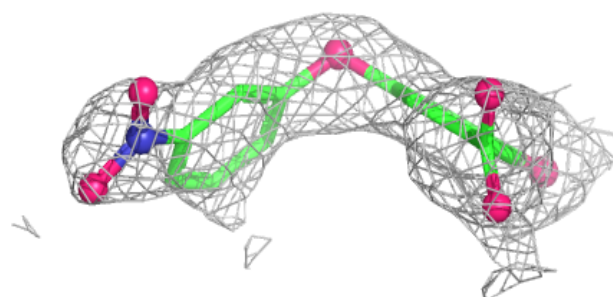
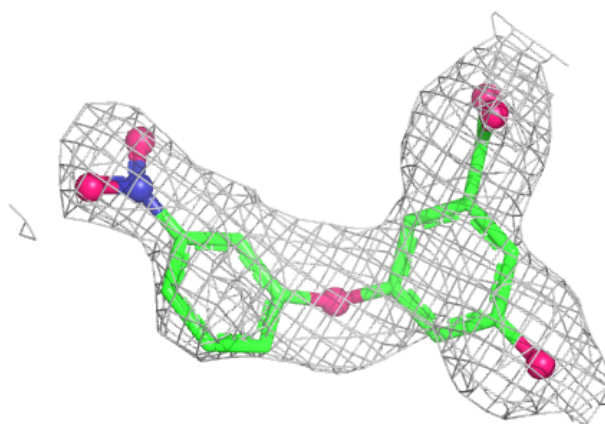
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



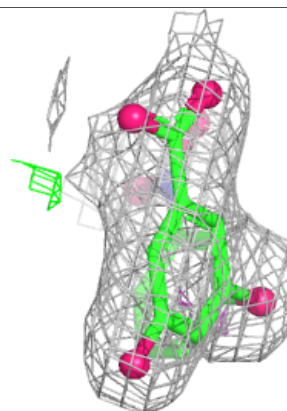
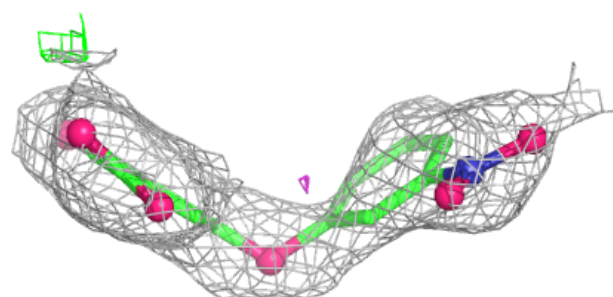
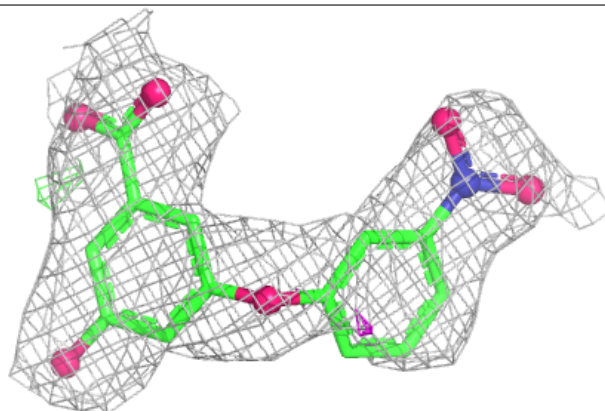


**Electron density around 1R2 X 201:**

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

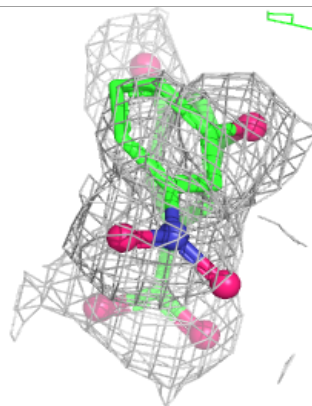
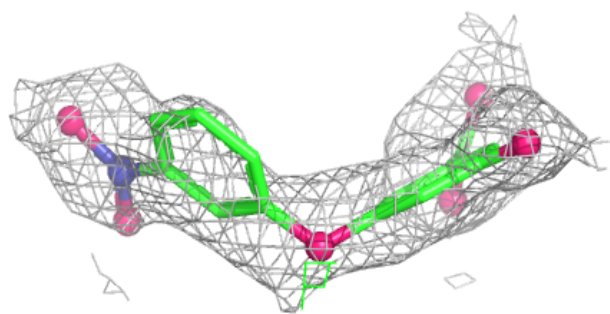
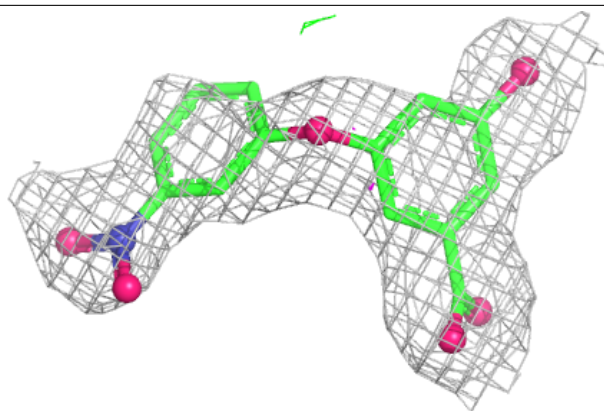
**Electron density around 1R2 R 201:**

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

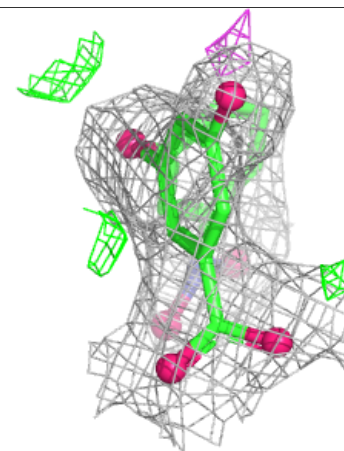
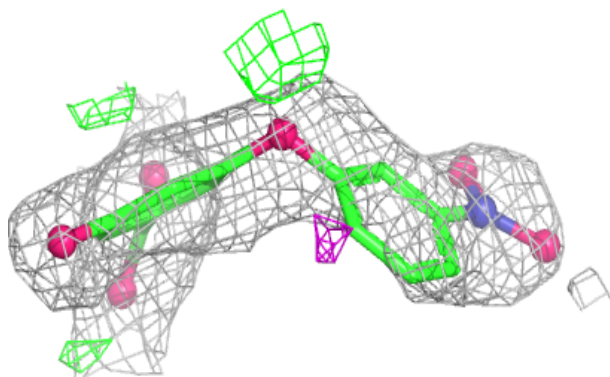
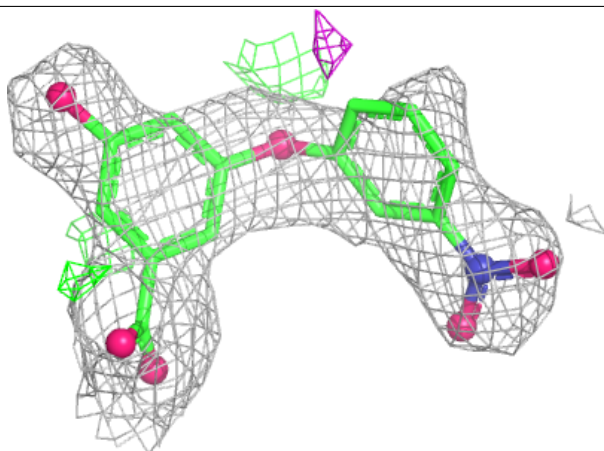


**Electron density around 1R2 E 201:**

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and green (positive)

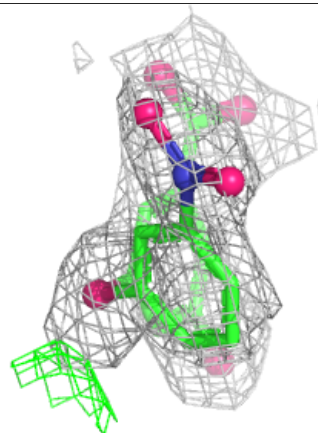
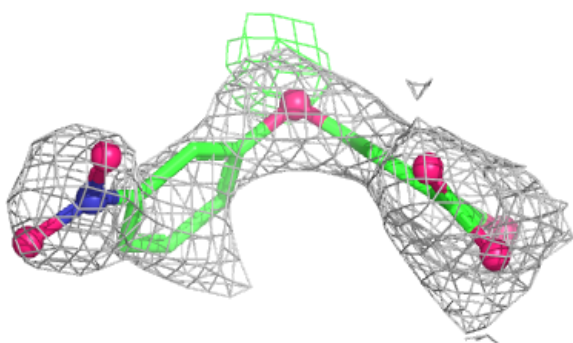
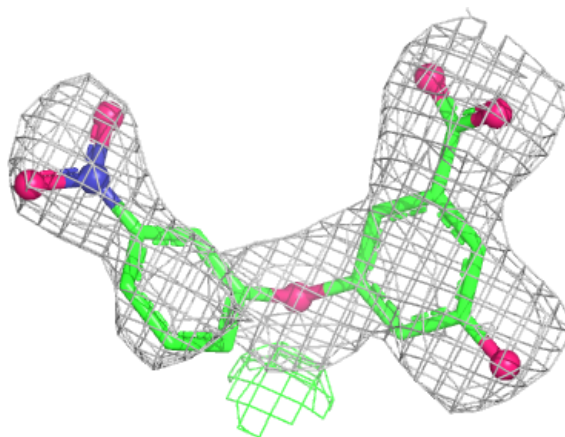
**Electron density around 1R2 H 201:**

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and green (positive)



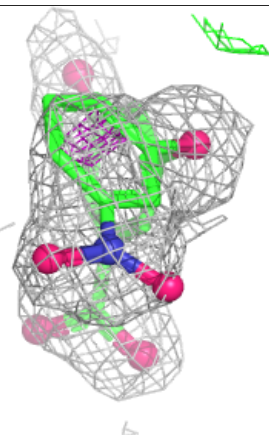
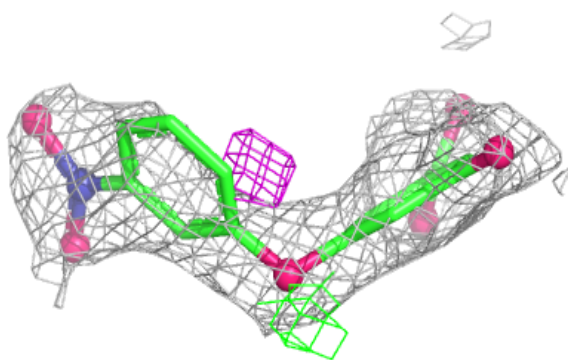
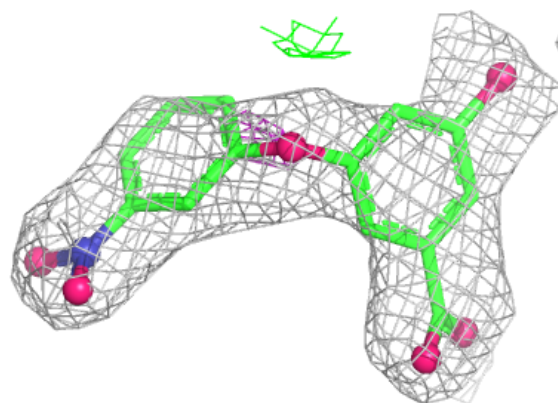
**Electron density around 1R2 N 201:**

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



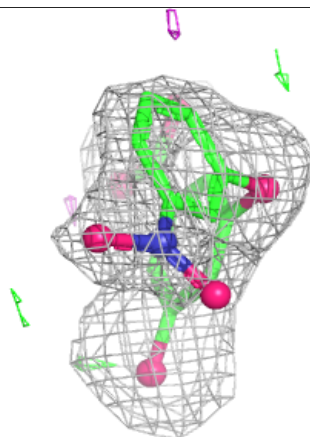
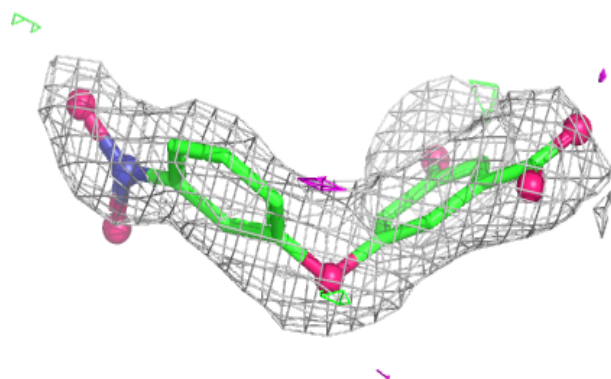
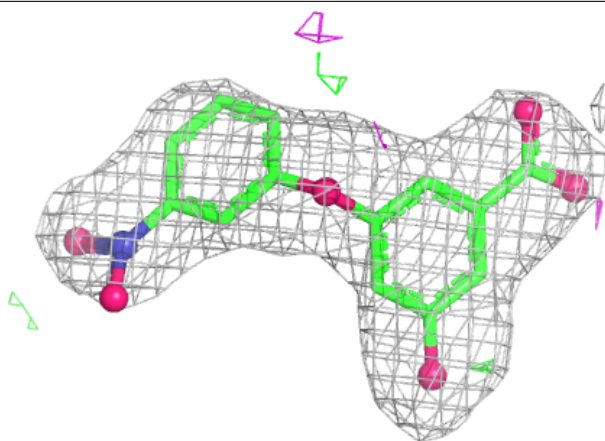
**Electron density around 1R2 A 201:**

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



**Electron density around 1R2 L 201:**

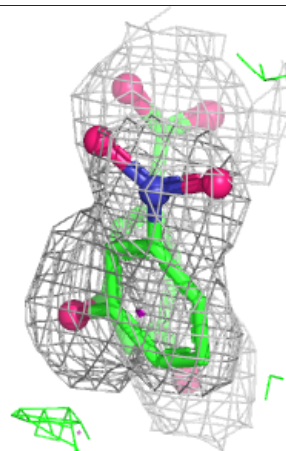
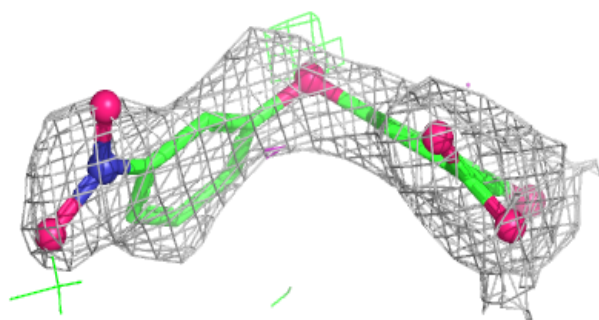
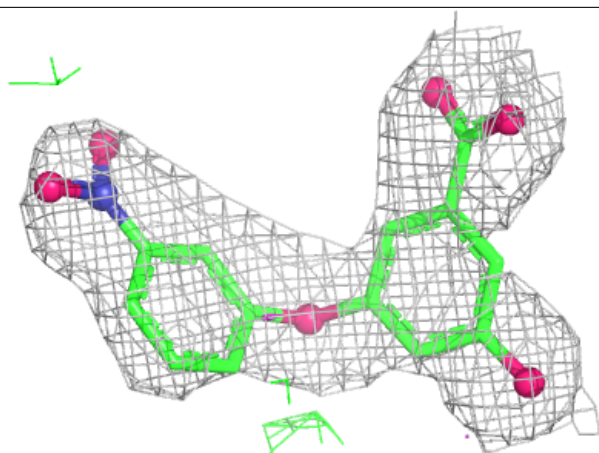
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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





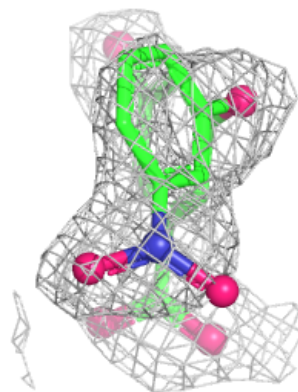
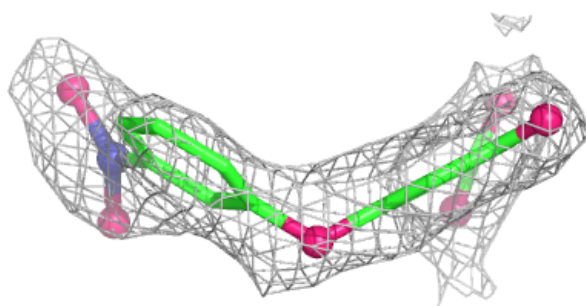
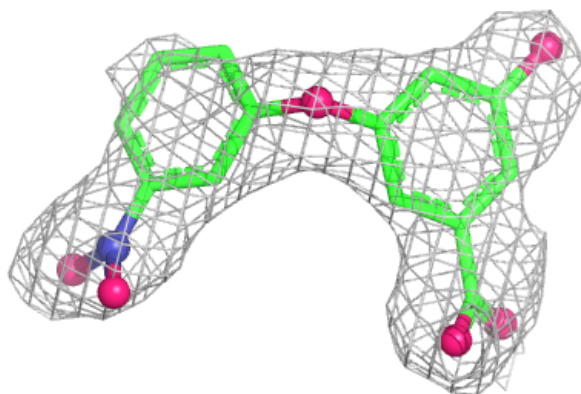
**Electron density around 1R2 I 201:**

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



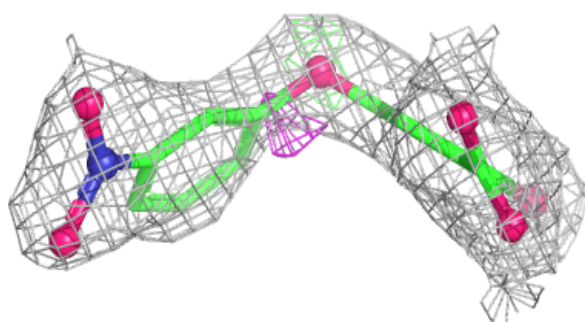
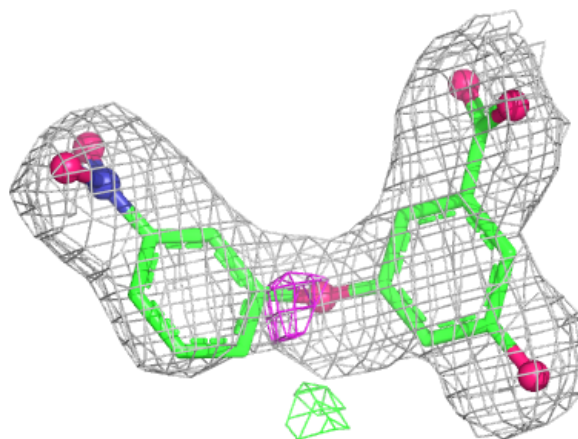
**Electron density around 1R2 U 201:**

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



**Electron density around 1R2 G 201:**

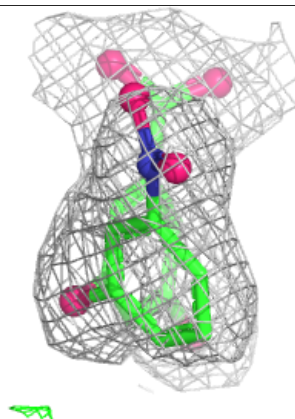
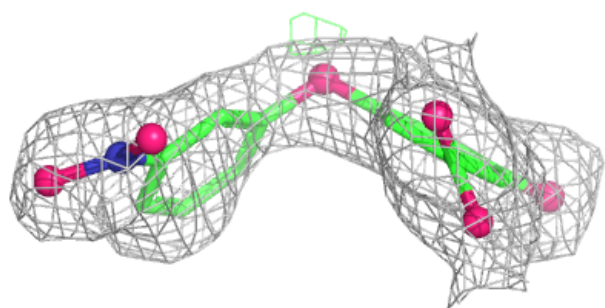
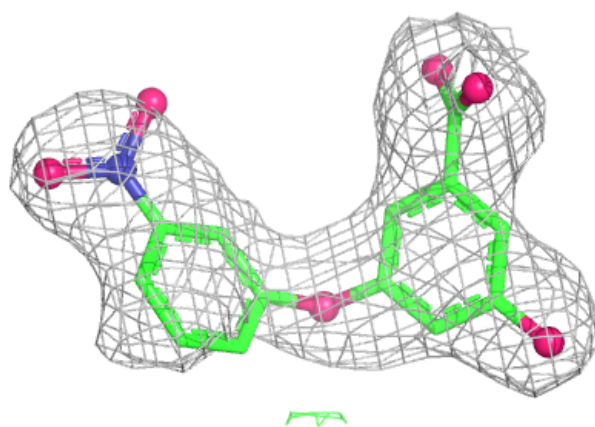
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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



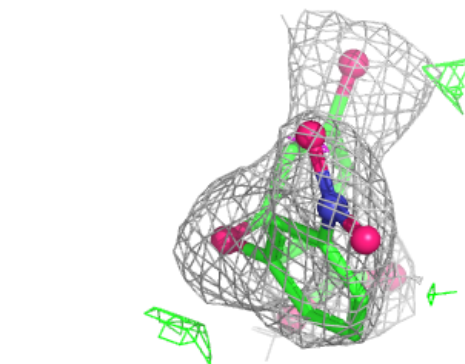
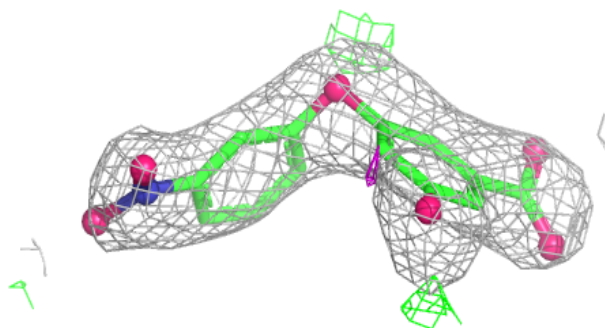
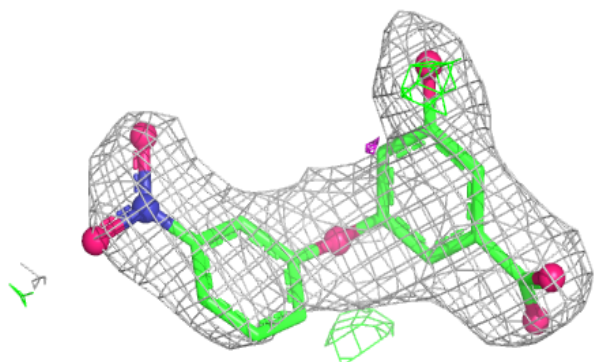


**Electron density around 1R2 K 201:**

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

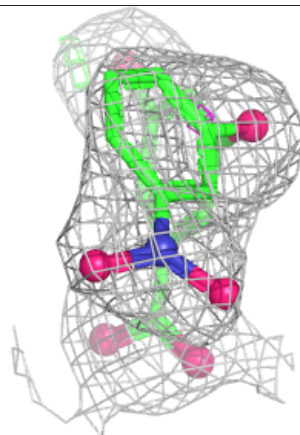
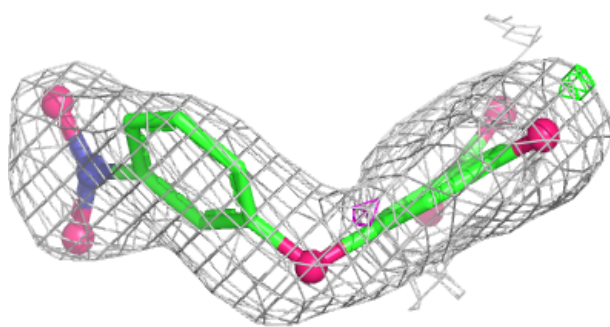
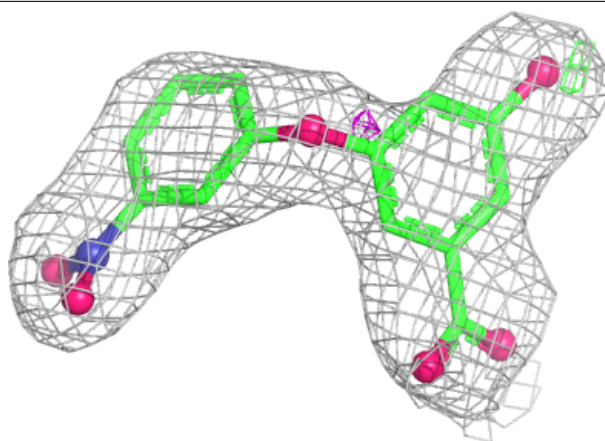
**Electron density around 1R2 C 201:**

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and green (positive)



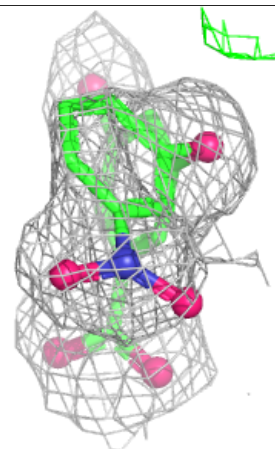
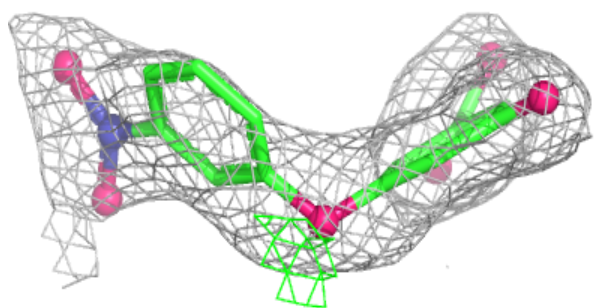
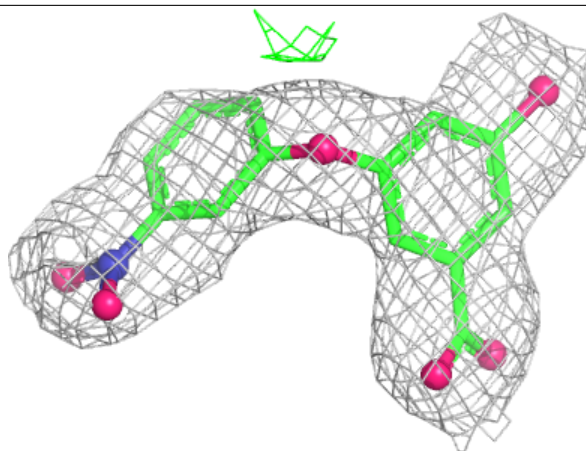
**Electron density around 1R2 O 201:**

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



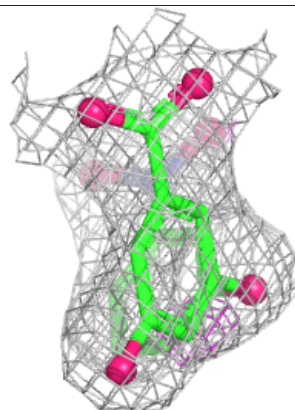
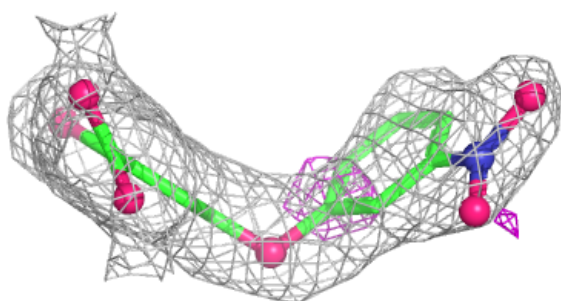
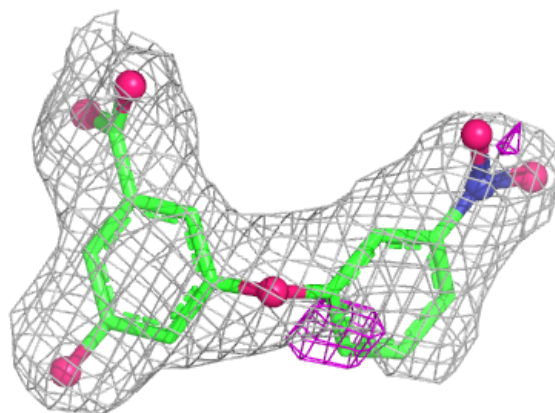
**Electron density around 1R2 J 201:**

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and green (positive)



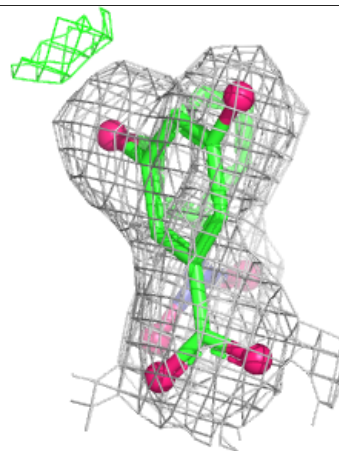
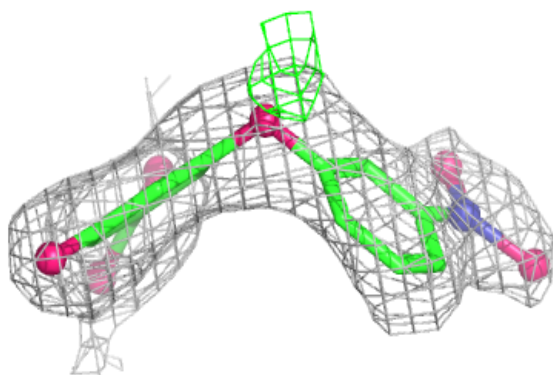
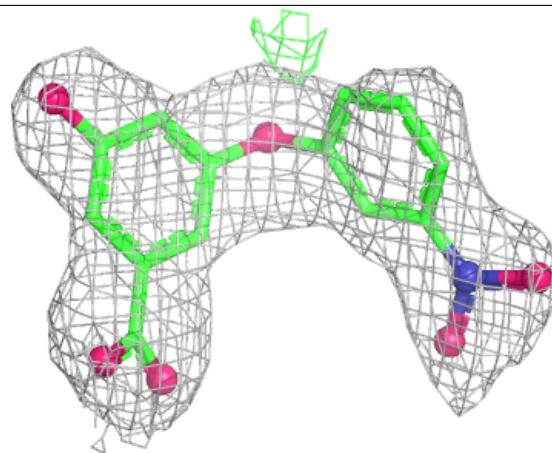
**Electron density around 1R2 D 201:**

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



**Electron density around 1R2 F 201:**

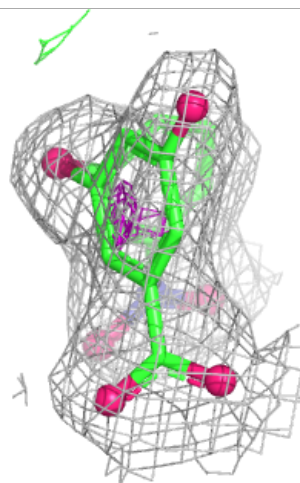
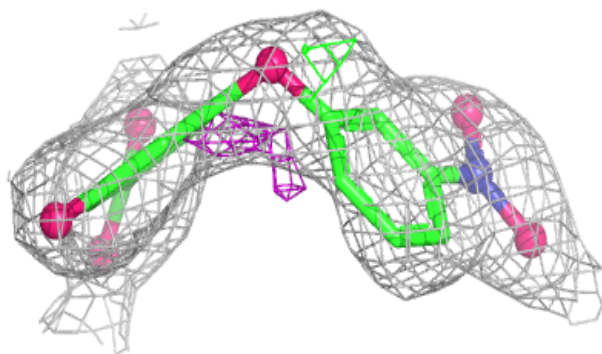
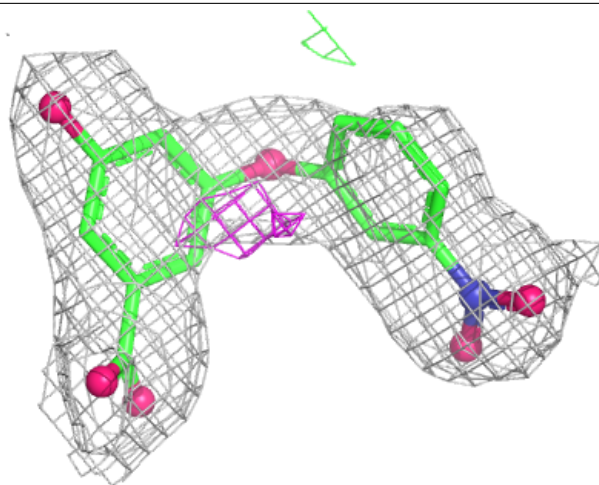
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 1R2 B 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.