



## Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 11:17 pm BST

PDB ID : 30KH / pdb\_000030kh  
EMDB ID : EMD-57856  
Title : Structure of human Trpm4 in native lipid vesicles at 8 degrees celsius  
Authors : Schneider, D.; Ekundayo, B.; Stahlberg, H.; Abriel, H.  
Deposited on : 2026-04-30  
Resolution : 3.70 Å(reported)  
Based on initial model : 9B92

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

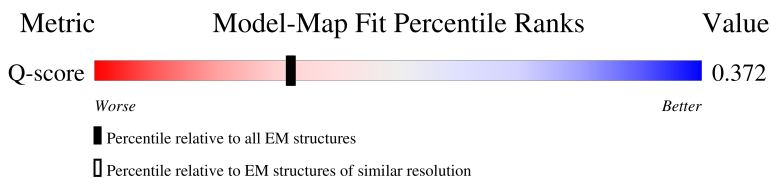
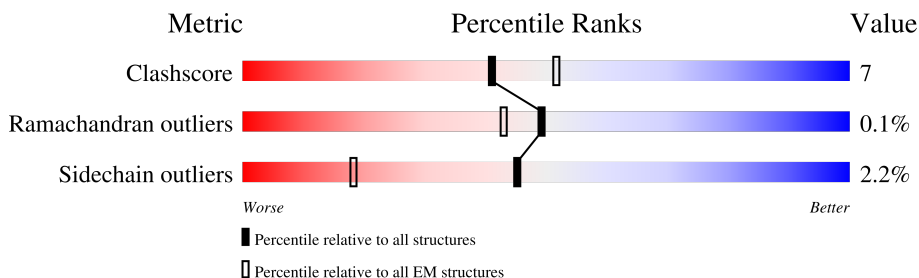
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1214   |                  |
| 1   | B     | 1214   |                  |
| 1   | C     | 1214   |                  |
| 1   | D     | 1214   |                  |

## 2 Entry composition [i](#)

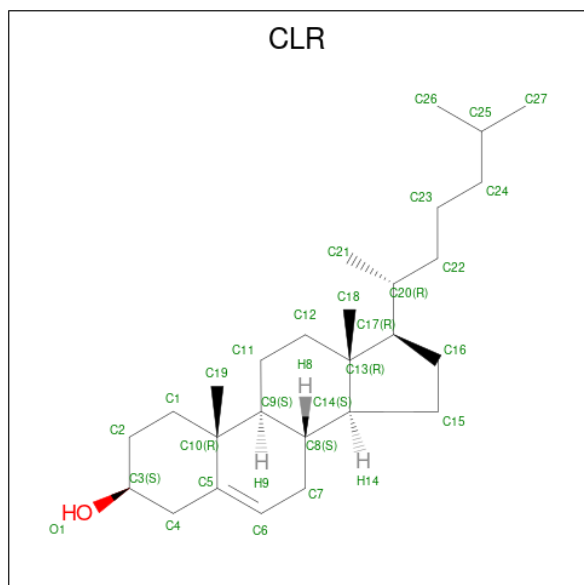
There are 2 unique types of molecules in this entry. The entry contains 61004 atoms, of which 30388 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transient receptor potential cation channel subfamily M member 4.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 1   | A     | 990      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14807 | 4851 | 7321 | 1322 | 1275 | 38 |         |       |
| 1   | B     | 990      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14807 | 4851 | 7321 | 1322 | 1275 | 38 |         |       |
| 1   | C     | 990      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14807 | 4851 | 7321 | 1322 | 1275 | 38 |         |       |
| 1   | D     | 990      | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 14807 | 4851 | 7321 | 1322 | 1275 | 38 |         |       |

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 2   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |

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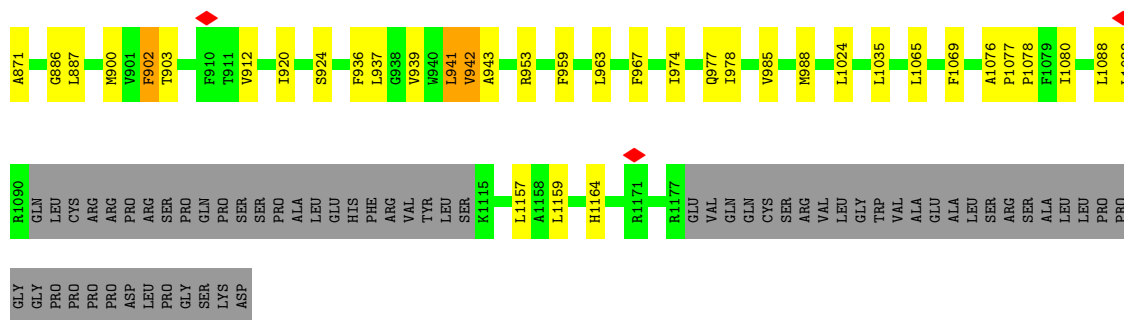
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 2   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | C     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | C     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | C     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | C     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | C     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 2   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |

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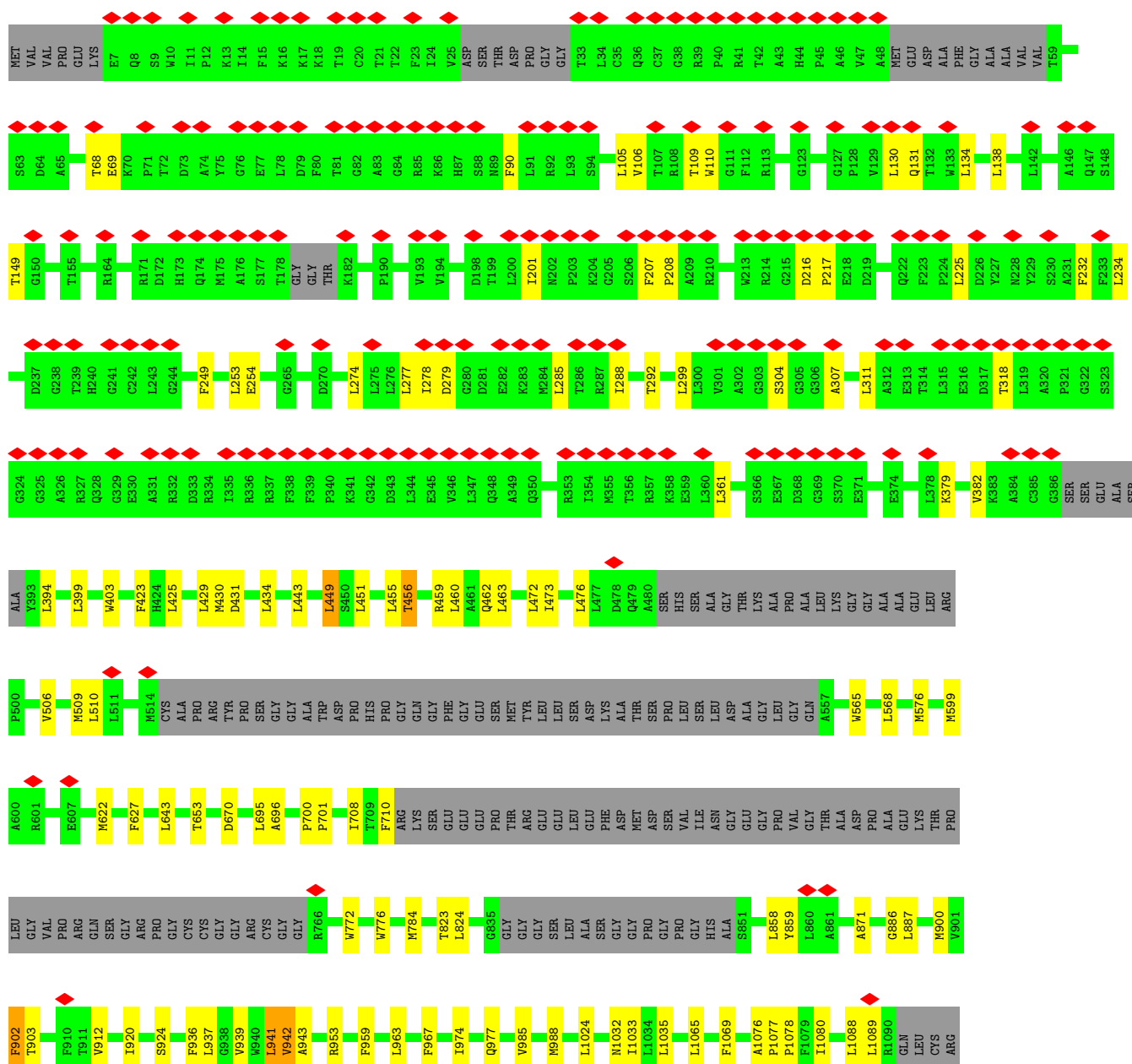
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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
|     |       |          | Total | C  | H  | O |         |
| 2   | D     | 1        | 74    | 27 | 46 | 1 | 0       |



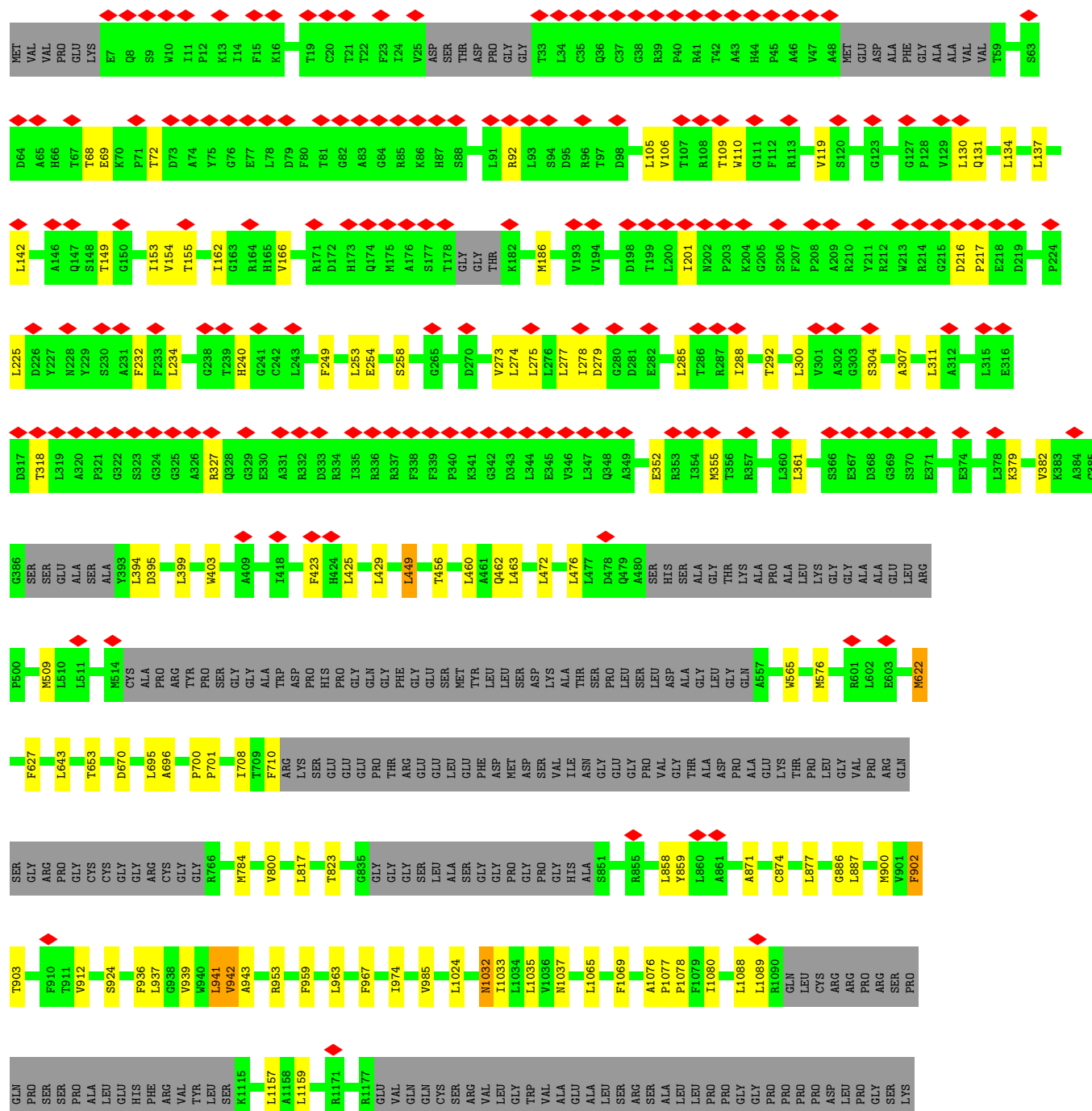


- Molecule 1: Transient receptor potential cation channel subfamily M member 4





- Molecule 1: Transient receptor potential cation channel subfamily M member 4





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 131852                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50.0                                    | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.532                                   | Depositor |
| Minimum map value                    | -0.382                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.012                                   | Depositor |
| Recommended contour level            | 0.06                                    | Depositor |
| Map size (Å)                         | 365.19998, 365.19998, 365.19998         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.9129999, 0.9129999, 0.9129999         | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CLR

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     | 0.11         | 0/7658      | 0.26        | 0/10420     |
| 1   | B     | 0.11         | 0/7658      | 0.26        | 0/10420     |
| 1   | C     | 0.12         | 0/7658      | 0.27        | 0/10420     |
| 1   | D     | 0.12         | 0/7658      | 0.27        | 0/10420     |
| All | All   | 0.12         | 0/30632     | 0.27        | 0/41680     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 7486  | 7321     | 7323     | 107     | 0            |
| 1   | B     | 7486  | 7321     | 7323     | 106     | 0            |
| 1   | C     | 7486  | 7321     | 7323     | 106     | 0            |
| 1   | D     | 7486  | 7321     | 7323     | 108     | 0            |
| 2   | A     | 168   | 276      | 270      | 10      | 0            |
| 2   | B     | 196   | 322      | 315      | 12      | 0            |
| 2   | C     | 140   | 230      | 225      | 7       | 0            |
| 2   | D     | 168   | 276      | 270      | 8       | 0            |
| All | All   | 30616 | 30388    | 30372    | 422     | 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 7.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:394:LEU:HD11  | 1:C:399:LEU:HD21  | 1.54                     | 0.87              |
| 1:B:568:LEU:HD12  | 1:B:599:MET:HE1   | 1.65                     | 0.78              |
| 1:B:900:MET:HE3   | 1:B:900:MET:HA    | 1.67                     | 0.76              |
| 1:D:900:MET:HE3   | 1:D:900:MET:HA    | 1.67                     | 0.75              |
| 1:C:1076:ALA:HB1  | 1:C:1077:PRO:HD2  | 1.69                     | 0.73              |
| 1:A:858:LEU:HD12  | 1:A:859:TYR:N     | 2.04                     | 0.72              |
| 1:D:1076:ALA:HB1  | 1:D:1077:PRO:HD2  | 1.72                     | 0.72              |
| 1:A:1076:ALA:HB1  | 1:A:1077:PRO:HD2  | 1.70                     | 0.72              |
| 1:B:506:VAL:O     | 1:B:510:LEU:HD12  | 1.89                     | 0.71              |
| 1:A:900:MET:HE3   | 1:A:900:MET:HA    | 1.72                     | 0.71              |
| 1:B:1076:ALA:HB1  | 1:B:1077:PRO:HD2  | 1.72                     | 0.71              |
| 1:C:352:GLU:O     | 1:C:355:MET:HE3   | 1.91                     | 0.70              |
| 1:D:394:LEU:HD12  | 1:D:399:LEU:HD21  | 1.73                     | 0.70              |
| 1:B:394:LEU:HD12  | 1:B:399:LEU:HD21  | 1.76                     | 0.68              |
| 1:D:858:LEU:HD12  | 1:D:859:TYR:N     | 2.07                     | 0.68              |
| 1:A:823:THR:HG21  | 1:A:1077:PRO:O    | 1.95                     | 0.67              |
| 1:D:823:THR:HG21  | 1:D:1077:PRO:O    | 1.94                     | 0.67              |
| 1:A:253:LEU:HD12  | 1:A:254:GLU:N     | 2.10                     | 0.66              |
| 1:A:1157:LEU:HD22 | 1:D:1159:LEU:HD21 | 1.77                     | 0.66              |
| 1:B:253:LEU:HD12  | 1:B:254:GLU:N     | 2.10                     | 0.66              |
| 1:D:138:LEU:HD12  | 1:D:139:ARG:N     | 2.10                     | 0.66              |
| 1:B:823:THR:HG21  | 1:B:1077:PRO:O    | 1.97                     | 0.65              |
| 1:B:292:THR:HG21  | 1:B:361:LEU:HD11  | 1.79                     | 0.65              |
| 1:A:292:THR:HG21  | 1:A:361:LEU:HD11  | 1.79                     | 0.64              |
| 1:C:823:THR:HG21  | 1:C:1077:PRO:O    | 1.97                     | 0.64              |
| 1:C:858:LEU:HD12  | 1:C:859:TYR:N     | 2.12                     | 0.64              |
| 1:A:394:LEU:HD12  | 1:A:399:LEU:HD21  | 1.79                     | 0.64              |
| 1:B:109:THR:HG23  | 1:B:110:TRP:CD1   | 2.33                     | 0.64              |
| 1:B:708:ILE:C     | 1:B:708:ILE:HD12  | 2.23                     | 0.64              |
| 1:C:292:THR:HG21  | 1:C:361:LEU:HD11  | 1.81                     | 0.63              |
| 1:B:858:LEU:HD12  | 1:B:859:TYR:N     | 2.14                     | 0.63              |
| 1:A:900:MET:HE1   | 1:D:943:ALA:HB1   | 1.81                     | 0.62              |
| 1:D:253:LEU:HD12  | 1:D:254:GLU:N     | 2.14                     | 0.62              |
| 1:A:1159:LEU:HD21 | 1:B:1157:LEU:HD22 | 1.82                     | 0.62              |
| 1:C:253:LEU:HD12  | 1:C:254:GLU:N     | 2.14                     | 0.62              |
| 1:B:277:LEU:HD22  | 1:B:288:ILE:CD1   | 2.29                     | 0.62              |
| 1:B:936:PHE:CD1   | 1:B:1035:LEU:HD11 | 2.35                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:277:LEU:HD22  | 1:D:288:ILE:CD1   | 2.30                     | 0.62              |
| 1:A:277:LEU:HD22  | 1:A:288:ILE:CD1   | 2.30                     | 0.62              |
| 1:C:1159:LEU:HD21 | 1:D:1157:LEU:HD22 | 1.82                     | 0.62              |
| 2:B:1307:CLR:H121 | 2:B:1307:CLR:H212 | 1.82                     | 0.61              |
| 1:A:472:LEU:O     | 1:A:476:LEU:HD22  | 2.00                     | 0.61              |
| 1:D:109:THR:HG23  | 1:D:110:TRP:CD1   | 2.35                     | 0.61              |
| 1:A:109:THR:HG23  | 1:A:110:TRP:CD1   | 2.34                     | 0.61              |
| 2:A:1302:CLR:H121 | 2:A:1302:CLR:H212 | 1.81                     | 0.61              |
| 1:C:277:LEU:HD22  | 1:C:288:ILE:CD1   | 2.29                     | 0.61              |
| 1:B:106:VAL:HG23  | 1:B:110:TRP:HE3   | 1.66                     | 0.61              |
| 1:A:106:VAL:HG23  | 1:A:110:TRP:HE3   | 1.66                     | 0.60              |
| 1:A:943:ALA:HB1   | 1:B:900:MET:HE1   | 1.82                     | 0.60              |
| 2:A:1304:CLR:H121 | 2:A:1304:CLR:H212 | 1.83                     | 0.60              |
| 1:C:106:VAL:HG23  | 1:C:110:TRP:HE3   | 1.66                     | 0.60              |
| 1:A:943:ALA:HB2   | 1:B:903:THR:HG21  | 1.84                     | 0.60              |
| 1:C:472:LEU:O     | 1:C:476:LEU:HD22  | 2.01                     | 0.60              |
| 2:D:1304:CLR:H121 | 2:D:1304:CLR:H212 | 1.83                     | 0.60              |
| 1:C:943:ALA:HB2   | 1:D:903:THR:HG21  | 1.84                     | 0.60              |
| 1:B:900:MET:HE3   | 1:B:900:MET:CA    | 2.32                     | 0.60              |
| 1:C:162:ILE:O     | 1:C:166:VAL:HG13  | 2.02                     | 0.60              |
| 1:C:109:THR:HG23  | 1:C:110:TRP:CD1   | 2.36                     | 0.60              |
| 1:D:472:LEU:O     | 1:D:476:LEU:HD22  | 2.01                     | 0.60              |
| 2:C:1305:CLR:H121 | 2:C:1305:CLR:H212 | 1.82                     | 0.60              |
| 2:B:1301:CLR:H121 | 2:B:1301:CLR:H212 | 1.84                     | 0.59              |
| 1:D:292:THR:HG21  | 1:D:361:LEU:HD11  | 1.83                     | 0.59              |
| 1:D:106:VAL:HG23  | 1:D:110:TRP:HE3   | 1.67                     | 0.59              |
| 1:D:162:ILE:O     | 1:D:166:VAL:HG13  | 2.01                     | 0.59              |
| 2:B:1305:CLR:H212 | 2:B:1305:CLR:H121 | 1.82                     | 0.59              |
| 1:C:119:VAL:HG21  | 1:C:142:LEU:HD11  | 1.84                     | 0.59              |
| 1:B:943:ALA:HB2   | 1:C:903:THR:HG21  | 1.85                     | 0.59              |
| 2:A:1303:CLR:H121 | 2:A:1303:CLR:H212 | 1.84                     | 0.59              |
| 1:A:162:ILE:O     | 1:A:166:VAL:HG13  | 2.02                     | 0.59              |
| 1:A:568:LEU:HD12  | 1:A:599:MET:HE1   | 1.83                     | 0.59              |
| 1:C:943:ALA:HB1   | 1:D:900:MET:HE1   | 1.85                     | 0.59              |
| 2:D:1301:CLR:H212 | 2:D:1301:CLR:H121 | 1.83                     | 0.59              |
| 1:C:936:PHE:CD2   | 1:C:1035:LEU:HD11 | 2.38                     | 0.58              |
| 2:B:1306:CLR:H121 | 2:B:1306:CLR:H212 | 1.85                     | 0.58              |
| 2:D:1302:CLR:H121 | 2:D:1302:CLR:H212 | 1.85                     | 0.58              |
| 1:A:249:PHE:CE2   | 1:A:253:LEU:HD23  | 2.38                     | 0.58              |
| 1:A:936:PHE:CD1   | 1:A:1035:LEU:HD11 | 2.38                     | 0.58              |
| 2:C:1303:CLR:H121 | 2:C:1303:CLR:H212 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:943:ALA:HB1   | 1:B:900:MET:CE    | 2.33                     | 0.58              |
| 1:A:900:MET:CE    | 1:D:943:ALA:HB1   | 2.34                     | 0.57              |
| 1:B:1159:LEU:HD21 | 1:C:1157:LEU:HD22 | 1.86                     | 0.57              |
| 1:D:900:MET:HE3   | 1:D:900:MET:CA    | 2.32                     | 0.57              |
| 1:A:460:LEU:HD23  | 1:A:460:LEU:O     | 2.05                     | 0.57              |
| 1:A:903:THR:HG21  | 1:D:943:ALA:HB2   | 1.86                     | 0.57              |
| 2:B:1304:CLR:H121 | 2:B:1304:CLR:H212 | 1.86                     | 0.57              |
| 1:D:936:PHE:HD1   | 1:D:1035:LEU:HD11 | 1.69                     | 0.57              |
| 2:A:1301:CLR:H121 | 2:A:1301:CLR:H212 | 1.87                     | 0.57              |
| 1:B:627:PHE:CZ    | 1:B:643:LEU:HD11  | 2.40                     | 0.57              |
| 1:A:627:PHE:CZ    | 1:A:643:LEU:HD11  | 2.40                     | 0.56              |
| 1:B:708:ILE:HD11  | 1:B:710:PHE:CE1   | 2.38                     | 0.56              |
| 1:C:460:LEU:O     | 1:C:460:LEU:HD23  | 2.05                     | 0.56              |
| 1:C:943:ALA:HB1   | 1:D:900:MET:CE    | 2.35                     | 0.56              |
| 1:D:936:PHE:CD1   | 1:D:1035:LEU:HD11 | 2.40                     | 0.56              |
| 1:B:460:LEU:HD23  | 1:B:460:LEU:O     | 2.05                     | 0.56              |
| 1:A:472:LEU:H     | 1:A:472:LEU:HD12  | 1.70                     | 0.56              |
| 2:C:1304:CLR:H212 | 2:C:1304:CLR:H121 | 1.86                     | 0.56              |
| 1:C:234:LEU:HD12  | 1:C:234:LEU:H     | 1.70                     | 0.56              |
| 2:D:1303:CLR:H121 | 2:D:1303:CLR:H212 | 1.86                     | 0.56              |
| 1:A:900:MET:HE3   | 1:A:900:MET:CA    | 2.34                     | 0.56              |
| 2:B:1303:CLR:H121 | 2:B:1303:CLR:H212 | 1.88                     | 0.56              |
| 1:C:627:PHE:CZ    | 1:C:643:LEU:HD11  | 2.40                     | 0.56              |
| 1:B:912:VAL:CG2   | 1:B:1065:LEU:HD22 | 2.36                     | 0.56              |
| 1:D:695:LEU:HD12  | 1:D:696:ALA:N     | 2.21                     | 0.56              |
| 2:A:1306:CLR:H212 | 2:A:1306:CLR:H121 | 1.88                     | 0.55              |
| 1:C:463:LEU:HD11  | 1:C:565:TRP:CZ2   | 2.41                     | 0.55              |
| 1:D:105:LEU:O     | 1:D:109:THR:HG22  | 2.06                     | 0.55              |
| 1:D:124:GLY:N     | 1:D:284:MET:HE1   | 2.21                     | 0.55              |
| 1:D:627:PHE:CZ    | 1:D:643:LEU:HD11  | 2.41                     | 0.55              |
| 1:D:912:VAL:CG2   | 1:D:1065:LEU:HD22 | 2.36                     | 0.55              |
| 1:B:234:LEU:HD12  | 1:B:234:LEU:H     | 1.71                     | 0.55              |
| 1:C:105:LEU:O     | 1:C:109:THR:HG22  | 2.06                     | 0.55              |
| 2:C:1302:CLR:H121 | 2:C:1302:CLR:H212 | 1.89                     | 0.55              |
| 1:B:985:VAL:HG12  | 1:B:985:VAL:O     | 2.06                     | 0.55              |
| 1:C:943:ALA:CB    | 1:D:903:THR:HG21  | 2.36                     | 0.54              |
| 1:D:463:LEU:HD11  | 1:D:565:TRP:CZ2   | 2.43                     | 0.54              |
| 1:A:105:LEU:O     | 1:A:109:THR:HG22  | 2.07                     | 0.54              |
| 1:A:277:LEU:HD11  | 1:A:279:ASP:O     | 2.07                     | 0.54              |
| 1:D:460:LEU:HD23  | 1:D:460:LEU:O     | 2.07                     | 0.54              |
| 1:A:943:ALA:CB    | 1:B:900:MET:HE1   | 2.37                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:472:LEU:O     | 1:B:476:LEU:HD22  | 2.07                     | 0.54              |
| 1:C:1077:PRO:HA   | 1:C:1080:ILE:HD12 | 1.90                     | 0.54              |
| 1:D:401:VAL:HG12  | 1:D:440:PHE:CD2   | 2.43                     | 0.54              |
| 1:B:943:ALA:CB    | 1:C:903:THR:HG21  | 2.38                     | 0.54              |
| 1:A:425:LEU:HB3   | 1:A:449:LEU:HD11  | 1.90                     | 0.54              |
| 1:C:912:VAL:CG2   | 1:C:1065:LEU:HD22 | 2.38                     | 0.54              |
| 2:D:1306:CLR:H121 | 2:D:1306:CLR:H212 | 1.90                     | 0.54              |
| 1:C:695:LEU:HD12  | 1:C:696:ALA:N     | 2.23                     | 0.54              |
| 1:A:985:VAL:HG12  | 1:A:985:VAL:O     | 2.08                     | 0.54              |
| 1:C:1157:LEU:HD23 | 1:C:1157:LEU:C    | 2.33                     | 0.54              |
| 1:A:900:MET:HE1   | 1:D:943:ALA:CB    | 2.38                     | 0.53              |
| 1:B:429:LEU:C     | 1:B:429:LEU:HD12  | 2.33                     | 0.53              |
| 1:B:249:PHE:CE1   | 1:B:253:LEU:HD23  | 2.43                     | 0.53              |
| 1:B:105:LEU:O     | 1:B:109:THR:HG22  | 2.08                     | 0.53              |
| 1:B:959:PHE:HB2   | 2:B:1306:CLR:H193 | 1.90                     | 0.53              |
| 1:D:670:ASP:OD1   | 1:D:670:ASP:C     | 2.52                     | 0.53              |
| 1:A:943:ALA:CB    | 1:B:903:THR:HG21  | 2.39                     | 0.53              |
| 1:C:985:VAL:HG12  | 1:C:985:VAL:O     | 2.09                     | 0.53              |
| 1:C:1032:ASN:O    | 1:C:1033:ILE:HD13 | 2.08                     | 0.53              |
| 1:A:670:ASP:OD1   | 1:A:670:ASP:C     | 2.52                     | 0.53              |
| 1:A:959:PHE:HB2   | 2:B:1301:CLR:H193 | 1.91                     | 0.53              |
| 1:B:941:LEU:HD12  | 1:B:941:LEU:C     | 2.34                     | 0.53              |
| 1:A:912:VAL:CG2   | 1:A:1065:LEU:HD22 | 2.37                     | 0.53              |
| 1:A:1157:LEU:HD23 | 1:A:1157:LEU:C    | 2.33                     | 0.53              |
| 1:A:936:PHE:HD1   | 1:A:1035:LEU:HD11 | 1.73                     | 0.52              |
| 1:B:936:PHE:HD1   | 1:B:1035:LEU:HD11 | 1.72                     | 0.52              |
| 1:D:941:LEU:HD12  | 1:D:941:LEU:C     | 2.34                     | 0.52              |
| 1:A:912:VAL:HG21  | 1:A:1065:LEU:HD22 | 1.92                     | 0.52              |
| 1:D:1157:LEU:C    | 1:D:1157:LEU:HD23 | 2.34                     | 0.52              |
| 1:D:234:LEU:HD12  | 1:D:234:LEU:H     | 1.75                     | 0.52              |
| 1:A:131:GLN:HG2   | 1:A:134:LEU:HD12  | 1.92                     | 0.52              |
| 1:B:1077:PRO:HG2  | 1:B:1078:PRO:HD3  | 1.91                     | 0.52              |
| 1:B:277:LEU:HD11  | 1:B:279:ASP:O     | 2.10                     | 0.52              |
| 1:B:695:LEU:HD12  | 1:B:696:ALA:N     | 2.25                     | 0.52              |
| 1:C:959:PHE:HB2   | 2:D:1302:CLR:H193 | 1.92                     | 0.52              |
| 1:A:903:THR:HG21  | 1:D:943:ALA:CB    | 2.41                     | 0.51              |
| 1:B:131:GLN:HG2   | 1:B:134:LEU:HD12  | 1.93                     | 0.51              |
| 1:B:285:LEU:C     | 1:B:285:LEU:HD23  | 2.35                     | 0.51              |
| 1:D:1077:PRO:HG2  | 1:D:1078:PRO:HD3  | 1.91                     | 0.51              |
| 1:B:1157:LEU:C    | 1:B:1157:LEU:HD23 | 2.36                     | 0.51              |
| 1:C:900:MET:HA    | 1:C:900:MET:HE3   | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:1303:CLR:H193 | 1:D:959:PHE:HB2   | 1.92                     | 0.51              |
| 1:B:1077:PRO:HA   | 1:B:1080:ILE:HD12 | 1.92                     | 0.51              |
| 1:C:1077:PRO:HG2  | 1:C:1078:PRO:HD3  | 1.93                     | 0.51              |
| 1:C:943:ALA:CB    | 1:D:900:MET:HE1   | 2.40                     | 0.51              |
| 1:C:936:PHE:HD2   | 1:C:1035:LEU:HD11 | 1.75                     | 0.51              |
| 1:D:131:GLN:HG2   | 1:D:134:LEU:HD12  | 1.92                     | 0.51              |
| 1:A:1077:PRO:HA   | 1:A:1080:ILE:HD12 | 1.93                     | 0.51              |
| 1:D:1077:PRO:HA   | 1:D:1080:ILE:HD12 | 1.93                     | 0.51              |
| 1:A:937:LEU:HD11  | 1:A:974:ILE:HD11  | 1.93                     | 0.51              |
| 1:A:1077:PRO:HG2  | 1:A:1078:PRO:HD3  | 1.92                     | 0.51              |
| 1:C:912:VAL:HG21  | 1:C:1065:LEU:HD22 | 1.92                     | 0.51              |
| 1:C:1076:ALA:HB1  | 1:C:1077:PRO:CD   | 2.41                     | 0.51              |
| 1:B:1076:ALA:HB1  | 1:B:1077:PRO:CD   | 2.41                     | 0.51              |
| 1:B:429:LEU:HD12  | 1:B:430:MET:N     | 2.26                     | 0.50              |
| 1:C:509:MET:HE2   | 1:C:509:MET:N     | 2.26                     | 0.50              |
| 1:D:510:LEU:HD12  | 1:D:510:LEU:H     | 1.76                     | 0.50              |
| 1:D:924:SER:OG    | 2:D:1304:CLR:H191 | 2.12                     | 0.50              |
| 1:B:912:VAL:HG21  | 1:B:1065:LEU:HD22 | 1.92                     | 0.50              |
| 1:A:134:LEU:HD11  | 1:A:304:SER:HA    | 1.93                     | 0.50              |
| 1:A:68:THR:HG22   | 1:A:69:GLU:H      | 1.76                     | 0.50              |
| 1:A:463:LEU:HD11  | 1:A:565:TRP:CZ2   | 2.47                     | 0.50              |
| 1:A:784:MET:HE1   | 2:A:1305:CLR:H181 | 1.94                     | 0.50              |
| 1:C:285:LEU:HD23  | 1:C:285:LEU:C     | 2.36                     | 0.50              |
| 1:D:106:VAL:HG23  | 1:D:110:TRP:CE3   | 2.46                     | 0.50              |
| 1:C:784:MET:HE1   | 2:C:1301:CLR:H181 | 1.95                     | 0.49              |
| 1:B:106:VAL:HG23  | 1:B:110:TRP:CE3   | 2.45                     | 0.49              |
| 1:B:130:LEU:HD21  | 1:B:278:ILE:HD11  | 1.95                     | 0.49              |
| 1:C:858:LEU:HD12  | 1:C:858:LEU:C     | 2.38                     | 0.49              |
| 1:A:886:GLY:O     | 1:A:887:LEU:HD23  | 2.11                     | 0.49              |
| 1:B:670:ASP:OD1   | 1:B:670:ASP:C     | 2.54                     | 0.49              |
| 1:D:912:VAL:HG21  | 1:D:1065:LEU:HD22 | 1.94                     | 0.49              |
| 1:C:149:THR:HG23  | 1:C:403:TRP:CG    | 2.48                     | 0.49              |
| 1:C:240:HIS:CG    | 1:C:240:HIS:O     | 2.65                     | 0.49              |
| 1:D:985:VAL:HG12  | 1:D:985:VAL:O     | 2.12                     | 0.49              |
| 1:C:277:LEU:HD11  | 1:C:279:ASP:O     | 2.13                     | 0.49              |
| 1:A:130:LEU:HD21  | 1:A:278:ILE:HD11  | 1.95                     | 0.48              |
| 1:B:510:LEU:HD12  | 1:B:510:LEU:H     | 1.77                     | 0.48              |
| 1:D:149:THR:HG23  | 1:D:403:TRP:CG    | 2.48                     | 0.48              |
| 1:D:277:LEU:HD11  | 1:D:279:ASP:O     | 2.13                     | 0.48              |
| 1:A:106:VAL:HG23  | 1:A:110:TRP:CE3   | 2.47                     | 0.48              |
| 1:C:941:LEU:C     | 1:C:941:LEU:HD12  | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:708:ILE:HD11  | 1:C:710:PHE:CE1   | 2.49                     | 0.48              |
| 1:B:1124:TRP:HE1  | 1:B:1128:HIS:CE1  | 2.31                     | 0.48              |
| 1:D:431:ASP:OD1   | 1:D:431:ASP:C     | 2.56                     | 0.48              |
| 1:B:943:ALA:HB1   | 1:C:900:MET:CE    | 2.43                     | 0.48              |
| 1:C:886:GLY:O     | 1:C:887:LEU:HD23  | 2.12                     | 0.48              |
| 1:B:431:ASP:OD2   | 1:B:431:ASP:C     | 2.57                     | 0.48              |
| 1:D:134:LEU:HD11  | 1:D:304:SER:HA    | 1.94                     | 0.48              |
| 1:A:429:LEU:HD12  | 1:A:430:MET:N     | 2.29                     | 0.48              |
| 1:A:311:LEU:HD22  | 1:A:311:LEU:H     | 1.78                     | 0.48              |
| 1:A:1024:LEU:HD12 | 1:A:1024:LEU:O    | 2.14                     | 0.48              |
| 1:B:568:LEU:HD12  | 1:B:599:MET:CE    | 2.41                     | 0.48              |
| 1:B:943:ALA:HB1   | 1:C:900:MET:HE1   | 1.96                     | 0.48              |
| 1:A:941:LEU:C     | 1:A:941:LEU:HD12  | 2.39                     | 0.47              |
| 1:B:463:LEU:HD11  | 1:B:565:TRP:CZ2   | 2.49                     | 0.47              |
| 1:C:137:LEU:O     | 1:C:137:LEU:HD12  | 2.14                     | 0.47              |
| 1:B:430:MET:HE1   | 1:B:434:LEU:HD11  | 1.96                     | 0.47              |
| 1:C:274:LEU:HD12  | 1:C:275:LEU:N     | 2.30                     | 0.47              |
| 1:A:277:LEU:HD12  | 1:A:278:ILE:N     | 2.28                     | 0.47              |
| 1:B:134:LEU:HD11  | 1:B:304:SER:HA    | 1.95                     | 0.47              |
| 1:D:253:LEU:HD12  | 1:D:253:LEU:C     | 2.40                     | 0.47              |
| 1:C:131:GLN:HG2   | 1:C:134:LEU:HD12  | 1.96                     | 0.47              |
| 1:C:201:ILE:HG23  | 1:C:201:ILE:O     | 2.15                     | 0.47              |
| 1:D:886:GLY:O     | 1:D:887:LEU:HD23  | 2.14                     | 0.47              |
| 1:C:134:LEU:HD11  | 1:C:304:SER:HA    | 1.97                     | 0.47              |
| 1:C:1024:LEU:O    | 1:C:1024:LEU:HD12 | 2.15                     | 0.47              |
| 1:C:106:VAL:HG23  | 1:C:110:TRP:CE3   | 2.46                     | 0.47              |
| 1:D:443:LEU:C     | 1:D:443:LEU:HD23  | 2.40                     | 0.47              |
| 1:D:506:VAL:O     | 1:D:510:LEU:HD12  | 2.15                     | 0.47              |
| 1:B:201:ILE:O     | 1:B:201:ILE:HG23  | 2.15                     | 0.47              |
| 1:D:138:LEU:HD12  | 1:D:138:LEU:C     | 2.40                     | 0.47              |
| 1:D:1076:ALA:HB1  | 1:D:1077:PRO:CD   | 2.42                     | 0.47              |
| 1:A:201:ILE:HG23  | 1:A:201:ILE:O     | 2.15                     | 0.46              |
| 1:B:225:LEU:HD13  | 1:B:232:PHE:CE2   | 2.50                     | 0.46              |
| 1:C:253:LEU:HD12  | 1:C:253:LEU:C     | 2.41                     | 0.46              |
| 1:D:140:ARG:O     | 1:D:140:ARG:HG2   | 2.15                     | 0.46              |
| 1:A:149:THR:HG23  | 1:A:403:TRP:CG    | 2.50                     | 0.46              |
| 1:A:700:PRO:N     | 1:A:701:PRO:CD    | 2.79                     | 0.46              |
| 1:C:149:THR:HG22  | 1:C:149:THR:O     | 2.14                     | 0.46              |
| 1:C:429:LEU:HD12  | 1:C:429:LEU:C     | 2.41                     | 0.46              |
| 1:C:877:LEU:O     | 1:C:877:LEU:HD23  | 2.15                     | 0.46              |
| 1:B:149:THR:HG22  | 1:B:149:THR:O     | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:443:LEU:HD23  | 1:B:443:LEU:C     | 2.41                     | 0.46              |
| 1:C:394:LEU:HD11  | 1:C:399:LEU:CD2   | 2.36                     | 0.46              |
| 1:C:900:MET:HE3   | 1:C:900:MET:CA    | 2.45                     | 0.46              |
| 1:C:937:LEU:HD11  | 1:C:974:ILE:HD11  | 1.97                     | 0.46              |
| 1:B:1024:LEU:HD12 | 1:B:1024:LEU:O    | 2.15                     | 0.46              |
| 1:C:394:LEU:HD12  | 1:C:395:ASP:H     | 1.81                     | 0.46              |
| 1:D:937:LEU:HD11  | 1:D:974:ILE:HD11  | 1.97                     | 0.46              |
| 1:C:249:PHE:CE2   | 1:C:253:LEU:HD23  | 2.51                     | 0.46              |
| 1:A:234:LEU:HD12  | 1:A:234:LEU:H     | 1.81                     | 0.45              |
| 1:A:708:ILE:HD11  | 1:A:710:PHE:CE1   | 2.50                     | 0.45              |
| 1:B:149:THR:HG23  | 1:B:403:TRP:CG    | 2.51                     | 0.45              |
| 1:B:886:GLY:O     | 1:B:887:LEU:HD23  | 2.16                     | 0.45              |
| 1:A:277:LEU:HD21  | 1:A:307:ALA:O     | 2.17                     | 0.45              |
| 1:C:924:SER:OG    | 2:C:1303:CLR:H191 | 2.15                     | 0.45              |
| 1:D:72:THR:HG23   | 1:D:92:ARG:HB3    | 1.99                     | 0.45              |
| 1:A:225:LEU:HD13  | 1:A:232:PHE:CE2   | 2.51                     | 0.45              |
| 1:B:459:ARG:HA    | 1:B:462:GLN:OE1   | 2.16                     | 0.45              |
| 1:A:1088:LEU:O    | 1:A:1089:LEU:HG   | 2.17                     | 0.45              |
| 1:D:1065:LEU:C    | 1:D:1065:LEU:HD23 | 2.42                     | 0.45              |
| 1:D:137:LEU:HD12  | 1:D:137:LEU:O     | 2.16                     | 0.45              |
| 1:D:149:THR:HG22  | 1:D:149:THR:O     | 2.16                     | 0.45              |
| 1:A:137:LEU:O     | 1:A:137:LEU:HD12  | 2.17                     | 0.45              |
| 1:A:509:MET:N     | 1:A:509:MET:HE2   | 2.31                     | 0.45              |
| 1:B:784:MET:HE1   | 2:B:1302:CLR:H181 | 1.99                     | 0.45              |
| 1:B:1088:LEU:O    | 1:B:1089:LEU:HG   | 2.17                     | 0.45              |
| 1:C:1080:ILE:HG22 | 1:C:1080:ILE:O    | 2.17                     | 0.45              |
| 1:C:1088:LEU:O    | 1:C:1089:LEU:HG   | 2.17                     | 0.45              |
| 1:D:1024:LEU:HD12 | 1:D:1024:LEU:O    | 2.16                     | 0.45              |
| 1:A:149:THR:HG22  | 1:A:149:THR:O     | 2.17                     | 0.45              |
| 1:B:1065:LEU:C    | 1:B:1065:LEU:HD23 | 2.42                     | 0.45              |
| 1:C:784:MET:HE2   | 1:C:784:MET:HA    | 1.99                     | 0.45              |
| 1:D:201:ILE:HG23  | 1:D:201:ILE:O     | 2.15                     | 0.45              |
| 1:A:1080:ILE:O    | 1:A:1080:ILE:HG22 | 2.16                     | 0.45              |
| 1:D:249:PHE:CE2   | 1:D:253:LEU:HD23  | 2.52                     | 0.45              |
| 1:D:68:THR:HG22   | 1:D:69:GLU:H      | 1.81                     | 0.45              |
| 1:D:130:LEU:HD21  | 1:D:278:ILE:HD11  | 1.99                     | 0.45              |
| 1:D:425:LEU:HB3   | 1:D:449:LEU:HD11  | 1.99                     | 0.45              |
| 1:D:225:LEU:HD13  | 1:D:232:PHE:CE2   | 2.53                     | 0.44              |
| 1:D:1080:ILE:O    | 1:D:1080:ILE:HG22 | 2.16                     | 0.44              |
| 1:D:1088:LEU:O    | 1:D:1089:LEU:HG   | 2.17                     | 0.44              |
| 1:A:253:LEU:HD12  | 1:A:253:LEU:C     | 2.42                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:924:SER:OG    | 2:B:1305:CLR:H191 | 2.16                     | 0.44              |
| 1:B:1080:ILE:O    | 1:B:1080:ILE:HG22 | 2.16                     | 0.44              |
| 1:D:942:VAL:HG22  | 1:D:967:PHE:CE1   | 2.53                     | 0.44              |
| 1:A:924:SER:OG    | 2:A:1302:CLR:H191 | 2.17                     | 0.44              |
| 1:C:225:LEU:HD13  | 1:C:232:PHE:CE2   | 2.53                     | 0.44              |
| 1:B:455:LEU:HD23  | 1:B:456:THR:N     | 2.32                     | 0.44              |
| 1:C:327:ARG:NE    | 1:C:327:ARG:HA    | 2.32                     | 0.44              |
| 1:C:379:LYS:HA    | 1:C:382:VAL:HG12  | 2.00                     | 0.44              |
| 1:D:277:LEU:HD12  | 1:D:278:ILE:N     | 2.32                     | 0.44              |
| 1:D:708:ILE:HD11  | 1:D:710:PHE:CE1   | 2.52                     | 0.44              |
| 1:A:1065:LEU:C    | 1:A:1065:LEU:HD23 | 2.43                     | 0.44              |
| 1:B:937:LEU:HD11  | 1:B:974:ILE:HD11  | 1.98                     | 0.44              |
| 1:C:153:ILE:HG23  | 1:C:153:ILE:O     | 2.18                     | 0.44              |
| 1:B:138:LEU:C     | 1:B:138:LEU:HD12  | 2.43                     | 0.44              |
| 1:C:311:LEU:HD22  | 1:C:311:LEU:H     | 1.83                     | 0.44              |
| 1:A:1076:ALA:HB1  | 1:A:1077:PRO:CD   | 2.44                     | 0.44              |
| 1:C:130:LEU:HD21  | 1:C:278:ILE:HD11  | 1.99                     | 0.44              |
| 1:D:451:LEU:H     | 1:D:451:LEU:HD23  | 1.83                     | 0.44              |
| 1:A:871:ALA:HB1   | 1:A:902:PHE:CE1   | 2.52                     | 0.44              |
| 1:B:311:LEU:H     | 1:B:311:LEU:HD22  | 1.83                     | 0.44              |
| 1:D:871:ALA:HB1   | 1:D:902:PHE:CE1   | 2.53                     | 0.43              |
| 1:D:644:ARG:O     | 1:D:644:ARG:HG2   | 2.18                     | 0.43              |
| 1:D:858:LEU:HD12  | 1:D:858:LEU:C     | 2.44                     | 0.43              |
| 1:B:68:THR:HG22   | 1:B:69:GLU:H      | 1.82                     | 0.43              |
| 2:B:1302:CLR:H121 | 2:B:1302:CLR:H212 | 2.00                     | 0.43              |
| 1:A:451:LEU:H     | 1:A:451:LEU:HD23  | 1.84                     | 0.43              |
| 1:A:794:LEU:HD23  | 1:A:794:LEU:HA    | 1.92                     | 0.43              |
| 1:B:277:LEU:HD21  | 1:B:307:ALA:O     | 2.19                     | 0.43              |
| 1:C:277:LEU:HD21  | 1:C:307:ALA:O     | 2.18                     | 0.43              |
| 1:C:871:ALA:HB1   | 1:C:902:PHE:CE1   | 2.53                     | 0.43              |
| 1:C:1065:LEU:HD23 | 1:C:1065:LEU:C    | 2.43                     | 0.43              |
| 1:D:154:VAL:HG12  | 1:D:186:MET:HB3   | 2.01                     | 0.43              |
| 1:D:568:LEU:HD23  | 1:D:599:MET:HE1   | 1.99                     | 0.43              |
| 1:D:985:VAL:HA    | 1:D:988:MET:SD    | 2.59                     | 0.43              |
| 1:A:258:SER:HB2   | 1:A:273:VAL:HG21  | 2.00                     | 0.43              |
| 1:A:784:MET:HE2   | 1:A:784:MET:HA    | 2.00                     | 0.43              |
| 1:C:234:LEU:HD12  | 1:C:234:LEU:N     | 2.33                     | 0.43              |
| 1:C:425:LEU:HB3   | 1:C:449:LEU:HD11  | 2.00                     | 0.43              |
| 1:A:924:SER:HB2   | 2:A:1302:CLR:H8   | 2.01                     | 0.43              |
| 1:B:871:ALA:HB1   | 1:B:902:PHE:CE1   | 2.53                     | 0.43              |
| 1:C:68:THR:HG22   | 1:C:69:GLU:H      | 1.81                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:277:LEU:HD21  | 1:D:307:ALA:O     | 2.18                     | 0.43              |
| 1:A:942:VAL:HG22  | 1:A:967:PHE:CE1   | 2.54                     | 0.43              |
| 1:B:277:LEU:HD12  | 1:B:278:ILE:N     | 2.33                     | 0.43              |
| 1:D:311:LEU:H     | 1:D:311:LEU:HD22  | 1.84                     | 0.43              |
| 1:D:700:PRO:N     | 1:D:701:PRO:CD    | 2.82                     | 0.43              |
| 1:A:119:VAL:HG21  | 1:A:142:LEU:HD11  | 2.01                     | 0.43              |
| 1:C:355:MET:SD    | 1:C:355:MET:C     | 3.01                     | 0.43              |
| 1:C:1032:ASN:O    | 1:C:1032:ASN:ND2  | 2.47                     | 0.43              |
| 2:A:1305:CLR:H121 | 2:A:1305:CLR:H212 | 2.00                     | 0.43              |
| 1:B:576:MET:SD    | 1:B:622:MET:HE1   | 2.58                     | 0.43              |
| 1:D:285:LEU:C     | 1:D:285:LEU:HD23  | 2.44                     | 0.43              |
| 1:A:394:LEU:HD12  | 1:A:399:LEU:CD2   | 2.46                     | 0.42              |
| 1:B:249:PHE:CD1   | 1:B:249:PHE:C     | 2.96                     | 0.42              |
| 1:C:216:ASP:N     | 1:C:217:PRO:HD2   | 2.34                     | 0.42              |
| 1:A:937:LEU:HD11  | 1:A:974:ILE:CD1   | 2.49                     | 0.42              |
| 1:B:425:LEU:HB3   | 1:B:449:LEU:HD11  | 2.01                     | 0.42              |
| 1:C:154:VAL:HG12  | 1:C:186:MET:HB3   | 2.00                     | 0.42              |
| 1:D:193:VAL:HG13  | 1:D:241:GLY:HA3   | 2.01                     | 0.42              |
| 1:D:509:MET:N     | 1:D:509:MET:HE2   | 2.34                     | 0.42              |
| 1:A:379:LYS:HA    | 1:A:382:VAL:HG12  | 2.01                     | 0.42              |
| 1:B:943:ALA:CB    | 1:C:900:MET:HE1   | 2.50                     | 0.42              |
| 1:D:119:VAL:HG21  | 1:D:142:LEU:HD11  | 2.02                     | 0.42              |
| 1:A:72:THR:HG23   | 1:A:92:ARG:HB3    | 2.02                     | 0.42              |
| 1:A:978:ILE:HD13  | 1:B:977:GLN:HG3   | 2.01                     | 0.42              |
| 1:C:700:PRO:N     | 1:C:701:PRO:CD    | 2.83                     | 0.42              |
| 1:D:959:PHE:CE1   | 1:D:963:LEU:HD22  | 2.55                     | 0.42              |
| 1:D:86:LYS:O      | 1:D:86:LYS:HG2    | 2.19                     | 0.42              |
| 1:A:138:LEU:HD12  | 1:A:138:LEU:C     | 2.45                     | 0.42              |
| 1:A:285:LEU:HD23  | 1:A:285:LEU:C     | 2.45                     | 0.42              |
| 1:B:216:ASP:N     | 1:B:217:PRO:HD2   | 2.35                     | 0.42              |
| 1:D:299:LEU:HD23  | 1:D:299:LEU:C     | 2.44                     | 0.42              |
| 1:D:953:ARG:O     | 1:D:953:ARG:HG2   | 2.20                     | 0.42              |
| 1:B:274:LEU:HD11  | 1:B:299:LEU:HB2   | 2.02                     | 0.42              |
| 1:B:700:PRO:N     | 1:B:701:PRO:CD    | 2.83                     | 0.42              |
| 1:B:942:VAL:HG22  | 1:B:967:PHE:CE1   | 2.54                     | 0.42              |
| 1:A:977:GLN:HG3   | 1:D:978:ILE:HD13  | 2.01                     | 0.41              |
| 1:C:72:THR:HG23   | 1:C:92:ARG:HB3    | 2.02                     | 0.41              |
| 1:C:871:ALA:HB1   | 1:C:902:PHE:CD1   | 2.55                     | 0.41              |
| 1:D:149:THR:HG23  | 1:D:403:TRP:HB3   | 2.02                     | 0.41              |
| 1:D:216:ASP:N     | 1:D:217:PRO:HD2   | 2.35                     | 0.41              |
| 1:A:240:HIS:O     | 1:A:240:HIS:CG    | 2.71                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:473:ILE:HD12  | 1:A:473:ILE:H     | 1.85                     | 0.41              |
| 1:B:90:PHE:CB     | 1:B:234:LEU:HD11  | 2.50                     | 0.41              |
| 1:C:800:VAL:HG11  | 1:C:817:LEU:HD22  | 2.02                     | 0.41              |
| 1:D:139:ARG:O     | 1:D:143:VAL:HB    | 2.20                     | 0.41              |
| 1:D:707:LEU:HD12  | 1:D:707:LEU:H     | 1.85                     | 0.41              |
| 1:A:871:ALA:HB1   | 1:A:902:PHE:CD1   | 2.55                     | 0.41              |
| 1:B:451:LEU:HD23  | 1:B:451:LEU:H     | 1.86                     | 0.41              |
| 1:A:81:THR:HG22   | 1:B:451:LEU:HD23  | 2.02                     | 0.41              |
| 1:C:670:ASP:OD1   | 1:C:670:ASP:C     | 2.63                     | 0.41              |
| 1:D:274:LEU:HD12  | 1:D:275:LEU:N     | 2.35                     | 0.41              |
| 1:A:300:LEU:HD22  | 1:A:300:LEU:N     | 2.36                     | 0.41              |
| 1:B:700:PRO:N     | 1:B:701:PRO:HD2   | 2.36                     | 0.41              |
| 1:C:576:MET:SD    | 1:C:622:MET:HE1   | 2.61                     | 0.41              |
| 1:D:158:LEU:HD12  | 1:D:160:THR:N     | 2.34                     | 0.41              |
| 1:A:216:ASP:N     | 1:A:217:PRO:HD2   | 2.35                     | 0.41              |
| 1:A:953:ARG:O     | 1:A:953:ARG:HG2   | 2.19                     | 0.41              |
| 1:B:959:PHE:CE1   | 1:B:963:LEU:HD22  | 2.56                     | 0.41              |
| 1:C:307:ALA:O     | 1:C:311:LEU:HD23  | 2.21                     | 0.41              |
| 1:D:90:PHE:CB     | 1:D:234:LEU:HD11  | 2.50                     | 0.41              |
| 1:A:154:VAL:HG12  | 1:A:186:MET:HB3   | 2.02                     | 0.41              |
| 1:A:959:PHE:CE1   | 1:A:963:LEU:HD22  | 2.55                     | 0.41              |
| 1:B:924:SER:HB2   | 2:B:1305:CLR:H8   | 2.03                     | 0.41              |
| 1:B:1032:ASN:O    | 1:B:1033:ILE:HD13 | 2.21                     | 0.41              |
| 1:C:953:ARG:O     | 1:C:953:ARG:HG2   | 2.19                     | 0.41              |
| 1:D:800:VAL:HG11  | 1:D:817:LEU:HD22  | 2.02                     | 0.41              |
| 1:D:871:ALA:HB1   | 1:D:902:PHE:CD1   | 2.56                     | 0.41              |
| 1:A:281:ASP:H     | 1:A:284:MET:HE3   | 1.86                     | 0.41              |
| 1:A:985:VAL:HA    | 1:A:988:MET:SD    | 2.61                     | 0.41              |
| 1:B:253:LEU:HD12  | 1:B:253:LEU:C     | 2.46                     | 0.41              |
| 1:B:379:LYS:HA    | 1:B:382:VAL:HG12  | 2.03                     | 0.41              |
| 1:B:772:TRP:O     | 1:B:776:TRP:HB2   | 2.21                     | 0.41              |
| 1:C:300:LEU:HD22  | 1:C:300:LEU:N     | 2.36                     | 0.41              |
| 1:C:1037:ASN:OD1  | 1:D:1040:ILE:HD11 | 2.21                     | 0.41              |
| 1:A:576:MET:SD    | 1:A:622:MET:HE1   | 2.61                     | 0.41              |
| 1:C:959:PHE:CE1   | 1:C:963:LEU:HD22  | 2.56                     | 0.41              |
| 2:D:1305:CLR:H121 | 2:D:1305:CLR:H212 | 2.03                     | 0.41              |
| 1:A:299:LEU:HD23  | 1:A:299:LEU:C     | 2.46                     | 0.40              |
| 1:B:307:ALA:O     | 1:B:311:LEU:HD23  | 2.21                     | 0.40              |
| 1:B:871:ALA:HB1   | 1:B:902:PHE:CD1   | 2.56                     | 0.40              |
| 1:C:700:PRO:N     | 1:C:701:PRO:HD2   | 2.36                     | 0.40              |
| 1:C:784:MET:CE    | 2:C:1301:CLR:H181 | 2.51                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:942:VAL:HG22  | 1:C:967:PHE:CE1  | 2.56                     | 0.40              |
| 1:A:149:THR:HG23  | 1:A:403:TRP:HB3  | 2.04                     | 0.40              |
| 1:A:207:PHE:HB2   | 1:A:208:PRO:HD3  | 2.04                     | 0.40              |
| 1:B:953:ARG:O     | 1:B:953:ARG:HG2  | 2.21                     | 0.40              |
| 1:C:1035:LEU:HD23 | 1:C:1035:LEU:HA  | 1.96                     | 0.40              |
| 1:D:379:LYS:HA    | 1:D:382:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:451:LEU:HD23  | 1:D:451:LEU:N    | 2.36                     | 0.40              |
| 1:A:249:PHE:CD2   | 1:A:249:PHE:C    | 2.98                     | 0.40              |
| 1:A:277:LEU:HD22  | 1:A:288:ILE:HD12 | 2.02                     | 0.40              |
| 1:B:473:ILE:H     | 1:B:473:ILE:HD12 | 1.87                     | 0.40              |
| 1:B:985:VAL:HA    | 1:B:988:MET:SD   | 2.61                     | 0.40              |
| 1:C:258:SER:HB2   | 1:C:273:VAL:HG21 | 2.03                     | 0.40              |
| 1:C:877:LEU:HD23  | 1:C:877:LEU:C    | 2.47                     | 0.40              |
| 1:A:274:LEU:HD12  | 1:A:297:PRO:HB2  | 2.03                     | 0.40              |
| 1:B:207:PHE:HB2   | 1:B:208:PRO:HD3  | 2.04                     | 0.40              |
| 1:B:509:MET:HE2   | 1:B:509:MET:HA   | 2.03                     | 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 PDB entries followed by that with respect to all EM entries.

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     | 970/1214 (80%)  | 915 (94%)  | 54 (6%)  | 1 (0%)   | 48          | 78 |
| 1   | B     | 970/1214 (80%)  | 917 (94%)  | 52 (5%)  | 1 (0%)   | 48          | 78 |
| 1   | C     | 970/1214 (80%)  | 919 (95%)  | 50 (5%)  | 1 (0%)   | 48          | 78 |
| 1   | D     | 970/1214 (80%)  | 915 (94%)  | 54 (6%)  | 1 (0%)   | 48          | 78 |
| All | All   | 3880/4856 (80%) | 3666 (94%) | 210 (5%) | 4 (0%)   | 49          | 78 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 318 | THR  |
| 1   | B     | 318 | THR  |
| 1   | C     | 318 | THR  |
| 1   | D     | 318 | THR  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 729/1000 (73%)  | 711 (98%)  | 18 (2%)  | 42          | 61 |
| 1   | B     | 729/1000 (73%)  | 717 (98%)  | 12 (2%)  | 55          | 68 |
| 1   | C     | 729/1000 (73%)  | 715 (98%)  | 14 (2%)  | 50          | 65 |
| 1   | D     | 729/1000 (73%)  | 709 (97%)  | 20 (3%)  | 39          | 59 |
| All | All   | 2916/4000 (73%) | 2852 (98%) | 64 (2%)  | 45          | 63 |

All (64) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 8    | GLN  |
| 1   | A     | 138  | LEU  |
| 1   | A     | 423  | PHE  |
| 1   | A     | 449  | LEU  |
| 1   | A     | 454  | PHE  |
| 1   | A     | 456  | THR  |
| 1   | A     | 462  | GLN  |
| 1   | A     | 622  | MET  |
| 1   | A     | 653  | THR  |
| 1   | A     | 702  | LEU  |
| 1   | A     | 776  | TRP  |
| 1   | A     | 902  | PHE  |
| 1   | A     | 920  | ILE  |
| 1   | A     | 939  | VAL  |
| 1   | A     | 941  | LEU  |
| 1   | A     | 942  | VAL  |
| 1   | A     | 1069 | PHE  |
| 1   | A     | 1164 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 423  | PHE  |
| 1   | B     | 449  | LEU  |
| 1   | B     | 456  | THR  |
| 1   | B     | 653  | THR  |
| 1   | B     | 824  | LEU  |
| 1   | B     | 902  | PHE  |
| 1   | B     | 920  | ILE  |
| 1   | B     | 939  | VAL  |
| 1   | B     | 941  | LEU  |
| 1   | B     | 942  | VAL  |
| 1   | B     | 1069 | PHE  |
| 1   | B     | 1164 | HIS  |
| 1   | C     | 155  | THR  |
| 1   | C     | 423  | PHE  |
| 1   | C     | 449  | LEU  |
| 1   | C     | 456  | THR  |
| 1   | C     | 462  | GLN  |
| 1   | C     | 622  | MET  |
| 1   | C     | 653  | THR  |
| 1   | C     | 874  | CYS  |
| 1   | C     | 902  | PHE  |
| 1   | C     | 939  | VAL  |
| 1   | C     | 941  | LEU  |
| 1   | C     | 942  | VAL  |
| 1   | C     | 1032 | ASN  |
| 1   | C     | 1069 | PHE  |
| 1   | D     | 8    | GLN  |
| 1   | D     | 262  | THR  |
| 1   | D     | 285  | LEU  |
| 1   | D     | 423  | PHE  |
| 1   | D     | 449  | LEU  |
| 1   | D     | 454  | PHE  |
| 1   | D     | 456  | THR  |
| 1   | D     | 462  | GLN  |
| 1   | D     | 594  | LEU  |
| 1   | D     | 619  | PHE  |
| 1   | D     | 653  | THR  |
| 1   | D     | 776  | TRP  |
| 1   | D     | 784  | MET  |
| 1   | D     | 874  | CYS  |
| 1   | D     | 902  | PHE  |
| 1   | D     | 920  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 939  | VAL  |
| 1   | D     | 941  | LEU  |
| 1   | D     | 942  | VAL  |
| 1   | D     | 1069 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 435  | ASN  |
| 1   | A     | 447  | HIS  |
| 1   | A     | 673  | GLN  |
| 1   | A     | 1002 | HIS  |
| 1   | B     | 889  | HIS  |
| 1   | B     | 1084 | HIS  |
| 1   | C     | 1084 | HIS  |
| 1   | D     | 447  | HIS  |
| 1   | D     | 1032 | ASN  |
| 1   | D     | 1084 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | CLR  | B     | 1302 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.96 | 19 (39%) |
| 2   | CLR  | B     | 1301 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.83 | 12 (25%) |
| 2   | CLR  | B     | 1303 | -    | 31,31,31     | 4.01 | 14 (45%) | 48,48,48    | 1.84 | 13 (27%) |
| 2   | CLR  | D     | 1304 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.80 | 11 (22%) |
| 2   | CLR  | C     | 1305 | -    | 31,31,31     | 3.98 | 15 (48%) | 48,48,48    | 1.86 | 13 (27%) |
| 2   | CLR  | C     | 1303 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.82 | 12 (25%) |
| 2   | CLR  | A     | 1302 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.80 | 9 (18%)  |
| 2   | CLR  | D     | 1301 | -    | 31,31,31     | 3.98 | 15 (48%) | 48,48,48    | 1.86 | 12 (25%) |
| 2   | CLR  | C     | 1301 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.98 | 19 (39%) |
| 2   | CLR  | D     | 1302 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.83 | 12 (25%) |
| 2   | CLR  | C     | 1302 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.83 | 13 (27%) |
| 2   | CLR  | A     | 1305 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.96 | 19 (39%) |
| 2   | CLR  | A     | 1303 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.82 | 12 (25%) |
| 2   | CLR  | D     | 1306 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.85 | 13 (27%) |
| 2   | CLR  | D     | 1303 | -    | 31,31,31     | 3.98 | 15 (48%) | 48,48,48    | 1.75 | 12 (25%) |
| 2   | CLR  | A     | 1306 | -    | 31,31,31     | 4.01 | 15 (48%) | 48,48,48    | 1.86 | 13 (27%) |
| 2   | CLR  | C     | 1304 | -    | 31,31,31     | 3.99 | 15 (48%) | 48,48,48    | 1.76 | 12 (25%) |
| 2   | CLR  | D     | 1305 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.99 | 19 (39%) |
| 2   | CLR  | B     | 1307 | -    | 31,31,31     | 3.98 | 15 (48%) | 48,48,48    | 1.87 | 13 (27%) |
| 2   | CLR  | B     | 1306 | -    | 31,31,31     | 4.02 | 15 (48%) | 48,48,48    | 1.84 | 12 (25%) |
| 2   | CLR  | A     | 1304 | -    | 31,31,31     | 3.98 | 15 (48%) | 48,48,48    | 1.86 | 13 (27%) |
| 2   | CLR  | B     | 1304 | -    | 31,31,31     | 3.99 | 15 (48%) | 48,48,48    | 1.76 | 12 (25%) |
| 2   | CLR  | A     | 1301 | -    | 31,31,31     | 3.99 | 15 (48%) | 48,48,48    | 1.75 | 12 (25%) |
| 2   | CLR  | B     | 1305 | -    | 31,31,31     | 4.03 | 15 (48%) | 48,48,48    | 1.80 | 10 (20%) |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | CLR  | B     | 1302 | -    | -       | 2/10/68/68 | 0/4/4/4 |
| 2   | CLR  | B     | 1301 | -    | -       | 2/10/68/68 | 0/4/4/4 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | CLR  | B     | 1303 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | D     | 1304 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | C     | 1305 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | C     | 1303 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | A     | 1302 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 2   | CLR  | D     | 1301 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | C     | 1301 | -    | -       | 2/10/68/68 | 0/4/4/4 |
| 2   | CLR  | D     | 1302 | -    | -       | 2/10/68/68 | 0/4/4/4 |
| 2   | CLR  | C     | 1302 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | A     | 1305 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 2   | CLR  | A     | 1303 | -    | -       | 2/10/68/68 | 0/4/4/4 |
| 2   | CLR  | D     | 1306 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | D     | 1303 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | A     | 1306 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | C     | 1304 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | D     | 1305 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 2   | CLR  | B     | 1307 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | B     | 1306 | -    | -       | 2/10/68/68 | 0/4/4/4 |
| 2   | CLR  | A     | 1304 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | B     | 1304 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 2   | CLR  | A     | 1301 | -    | -       | 0/10/68/68 | 0/4/4/4 |
| 2   | CLR  | B     | 1305 | -    | -       | 1/10/68/68 | 0/4/4/4 |

All (359) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | D     | 1304 | CLR  | C11-C9 | 9.96 | 1.70        | 1.53     |
| 2   | A     | 1302 | CLR  | C11-C9 | 9.95 | 1.70        | 1.53     |
| 2   | B     | 1305 | CLR  | C11-C9 | 9.94 | 1.70        | 1.53     |
| 2   | C     | 1303 | CLR  | C11-C9 | 9.93 | 1.70        | 1.53     |
| 2   | A     | 1303 | CLR  | C11-C9 | 9.85 | 1.70        | 1.53     |
| 2   | C     | 1301 | CLR  | C11-C9 | 9.85 | 1.70        | 1.53     |
| 2   | D     | 1305 | CLR  | C11-C9 | 9.85 | 1.70        | 1.53     |
| 2   | B     | 1301 | CLR  | C11-C9 | 9.85 | 1.70        | 1.53     |
| 2   | B     | 1302 | CLR  | C11-C9 | 9.84 | 1.70        | 1.53     |
| 2   | A     | 1305 | CLR  | C11-C9 | 9.83 | 1.70        | 1.53     |
| 2   | D     | 1302 | CLR  | C11-C9 | 9.83 | 1.70        | 1.53     |
| 2   | B     | 1306 | CLR  | C11-C9 | 9.83 | 1.70        | 1.53     |
| 2   | D     | 1306 | CLR  | C11-C9 | 9.73 | 1.70        | 1.53     |
| 2   | A     | 1306 | CLR  | C11-C9 | 9.67 | 1.70        | 1.53     |
| 2   | C     | 1302 | CLR  | C11-C9 | 9.63 | 1.69        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | D     | 1303 | CLR  | C11-C9 | 9.59 | 1.69        | 1.53     |
| 2   | A     | 1301 | CLR  | C11-C9 | 9.59 | 1.69        | 1.53     |
| 2   | B     | 1304 | CLR  | C11-C9 | 9.57 | 1.69        | 1.53     |
| 2   | C     | 1304 | CLR  | C11-C9 | 9.56 | 1.69        | 1.53     |
| 2   | B     | 1303 | CLR  | C11-C9 | 9.53 | 1.69        | 1.53     |
| 2   | D     | 1301 | CLR  | C11-C9 | 9.51 | 1.69        | 1.53     |
| 2   | A     | 1304 | CLR  | C11-C9 | 9.49 | 1.69        | 1.53     |
| 2   | C     | 1305 | CLR  | C11-C9 | 9.46 | 1.69        | 1.53     |
| 2   | B     | 1307 | CLR  | C11-C9 | 9.45 | 1.69        | 1.53     |
| 2   | D     | 1304 | CLR  | C2-C3  | 8.38 | 1.71        | 1.51     |
| 2   | A     | 1302 | CLR  | C2-C3  | 8.38 | 1.71        | 1.51     |
| 2   | B     | 1301 | CLR  | C2-C3  | 8.38 | 1.71        | 1.51     |
| 2   | B     | 1306 | CLR  | C2-C3  | 8.38 | 1.71        | 1.51     |
| 2   | D     | 1302 | CLR  | C2-C3  | 8.37 | 1.71        | 1.51     |
| 2   | B     | 1305 | CLR  | C2-C3  | 8.37 | 1.71        | 1.51     |
| 2   | A     | 1303 | CLR  | C2-C3  | 8.37 | 1.71        | 1.51     |
| 2   | C     | 1303 | CLR  | C2-C3  | 8.37 | 1.71        | 1.51     |
| 2   | C     | 1302 | CLR  | C2-C3  | 8.34 | 1.71        | 1.51     |
| 2   | A     | 1306 | CLR  | C2-C3  | 8.33 | 1.71        | 1.51     |
| 2   | D     | 1306 | CLR  | C2-C3  | 8.33 | 1.71        | 1.51     |
| 2   | B     | 1303 | CLR  | C2-C3  | 8.31 | 1.71        | 1.51     |
| 2   | C     | 1304 | CLR  | C2-C3  | 8.21 | 1.71        | 1.51     |
| 2   | A     | 1301 | CLR  | C2-C3  | 8.20 | 1.71        | 1.51     |
| 2   | D     | 1303 | CLR  | C2-C3  | 8.20 | 1.71        | 1.51     |
| 2   | B     | 1304 | CLR  | C2-C3  | 8.20 | 1.71        | 1.51     |
| 2   | A     | 1305 | CLR  | C2-C3  | 8.15 | 1.71        | 1.51     |
| 2   | B     | 1307 | CLR  | C6-C5  | 8.15 | 1.50        | 1.33     |
| 2   | C     | 1301 | CLR  | C6-C5  | 8.15 | 1.50        | 1.33     |
| 2   | C     | 1301 | CLR  | C2-C3  | 8.14 | 1.71        | 1.51     |
| 2   | B     | 1302 | CLR  | C2-C3  | 8.14 | 1.71        | 1.51     |
| 2   | C     | 1305 | CLR  | C6-C5  | 8.14 | 1.50        | 1.33     |
| 2   | A     | 1304 | CLR  | C6-C5  | 8.14 | 1.50        | 1.33     |
| 2   | D     | 1305 | CLR  | C2-C3  | 8.13 | 1.71        | 1.51     |
| 2   | D     | 1305 | CLR  | C6-C5  | 8.13 | 1.50        | 1.33     |
| 2   | D     | 1301 | CLR  | C6-C5  | 8.13 | 1.50        | 1.33     |
| 2   | B     | 1302 | CLR  | C6-C5  | 8.11 | 1.50        | 1.33     |
| 2   | A     | 1305 | CLR  | C6-C5  | 8.10 | 1.50        | 1.33     |
| 2   | B     | 1307 | CLR  | C2-C3  | 8.07 | 1.70        | 1.51     |
| 2   | A     | 1304 | CLR  | C2-C3  | 8.07 | 1.70        | 1.51     |
| 2   | C     | 1305 | CLR  | C2-C3  | 8.06 | 1.70        | 1.51     |
| 2   | D     | 1301 | CLR  | C2-C3  | 8.06 | 1.70        | 1.51     |
| 2   | A     | 1303 | CLR  | C6-C5  | 7.94 | 1.50        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | B     | 1304 | CLR  | C6-C5 | 7.94  | 1.50        | 1.33     |
| 2   | C     | 1304 | CLR  | C6-C5 | 7.93  | 1.50        | 1.33     |
| 2   | A     | 1301 | CLR  | C6-C5 | 7.93  | 1.50        | 1.33     |
| 2   | B     | 1301 | CLR  | C6-C5 | 7.93  | 1.50        | 1.33     |
| 2   | D     | 1303 | CLR  | C6-C5 | 7.93  | 1.50        | 1.33     |
| 2   | B     | 1303 | CLR  | C6-C5 | 7.92  | 1.50        | 1.33     |
| 2   | A     | 1306 | CLR  | C6-C5 | 7.92  | 1.50        | 1.33     |
| 2   | B     | 1306 | CLR  | C6-C5 | 7.92  | 1.50        | 1.33     |
| 2   | D     | 1304 | CLR  | C6-C5 | 7.92  | 1.50        | 1.33     |
| 2   | C     | 1303 | CLR  | C6-C5 | 7.91  | 1.50        | 1.33     |
| 2   | A     | 1302 | CLR  | C6-C5 | 7.91  | 1.50        | 1.33     |
| 2   | D     | 1302 | CLR  | C6-C5 | 7.91  | 1.50        | 1.33     |
| 2   | B     | 1305 | CLR  | C6-C5 | 7.90  | 1.50        | 1.33     |
| 2   | D     | 1306 | CLR  | C6-C5 | 7.90  | 1.50        | 1.33     |
| 2   | C     | 1302 | CLR  | C6-C5 | 7.86  | 1.50        | 1.33     |
| 2   | C     | 1302 | CLR  | C4-C5 | -7.53 | 1.35        | 1.51     |
| 2   | D     | 1305 | CLR  | C4-C5 | -7.48 | 1.35        | 1.51     |
| 2   | C     | 1301 | CLR  | C4-C5 | -7.47 | 1.35        | 1.51     |
| 2   | B     | 1302 | CLR  | C4-C5 | -7.45 | 1.35        | 1.51     |
| 2   | B     | 1303 | CLR  | C4-C5 | -7.45 | 1.35        | 1.51     |
| 2   | A     | 1305 | CLR  | C4-C5 | -7.45 | 1.35        | 1.51     |
| 2   | D     | 1306 | CLR  | C4-C5 | -7.38 | 1.35        | 1.51     |
| 2   | C     | 1303 | CLR  | C4-C5 | -7.37 | 1.35        | 1.51     |
| 2   | A     | 1302 | CLR  | C4-C5 | -7.36 | 1.35        | 1.51     |
| 2   | D     | 1304 | CLR  | C4-C5 | -7.36 | 1.35        | 1.51     |
| 2   | A     | 1306 | CLR  | C4-C5 | -7.36 | 1.35        | 1.51     |
| 2   | B     | 1305 | CLR  | C4-C5 | -7.36 | 1.35        | 1.51     |
| 2   | B     | 1304 | CLR  | C4-C5 | -7.34 | 1.35        | 1.51     |
| 2   | A     | 1301 | CLR  | C4-C5 | -7.33 | 1.35        | 1.51     |
| 2   | D     | 1302 | CLR  | C4-C5 | -7.33 | 1.35        | 1.51     |
| 2   | B     | 1306 | CLR  | C4-C5 | -7.33 | 1.35        | 1.51     |
| 2   | C     | 1304 | CLR  | C4-C5 | -7.32 | 1.35        | 1.51     |
| 2   | B     | 1307 | CLR  | C4-C5 | -7.32 | 1.35        | 1.51     |
| 2   | B     | 1301 | CLR  | C4-C5 | -7.32 | 1.35        | 1.51     |
| 2   | A     | 1303 | CLR  | C4-C5 | -7.32 | 1.35        | 1.51     |
| 2   | D     | 1303 | CLR  | C4-C5 | -7.32 | 1.35        | 1.51     |
| 2   | D     | 1301 | CLR  | C4-C5 | -7.30 | 1.35        | 1.51     |
| 2   | A     | 1304 | CLR  | C4-C5 | -7.30 | 1.35        | 1.51     |
| 2   | C     | 1305 | CLR  | C4-C5 | -7.30 | 1.35        | 1.51     |
| 2   | D     | 1304 | CLR  | C1-C2 | 6.44  | 1.67        | 1.53     |
| 2   | A     | 1302 | CLR  | C1-C2 | 6.43  | 1.67        | 1.53     |
| 2   | C     | 1302 | CLR  | C1-C2 | 6.43  | 1.67        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | B     | 1305 | CLR  | C1-C2   | 6.42 | 1.67        | 1.53     |
| 2   | C     | 1303 | CLR  | C1-C2   | 6.42 | 1.67        | 1.53     |
| 2   | D     | 1306 | CLR  | C1-C2   | 6.39 | 1.67        | 1.53     |
| 2   | B     | 1306 | CLR  | C1-C2   | 6.33 | 1.66        | 1.53     |
| 2   | D     | 1302 | CLR  | C1-C2   | 6.33 | 1.66        | 1.53     |
| 2   | C     | 1301 | CLR  | C1-C2   | 6.33 | 1.66        | 1.53     |
| 2   | A     | 1303 | CLR  | C1-C2   | 6.32 | 1.66        | 1.53     |
| 2   | A     | 1306 | CLR  | C1-C2   | 6.32 | 1.66        | 1.53     |
| 2   | B     | 1301 | CLR  | C1-C2   | 6.32 | 1.66        | 1.53     |
| 2   | A     | 1305 | CLR  | C1-C2   | 6.31 | 1.66        | 1.53     |
| 2   | B     | 1302 | CLR  | C1-C2   | 6.31 | 1.66        | 1.53     |
| 2   | D     | 1305 | CLR  | C1-C2   | 6.30 | 1.66        | 1.53     |
| 2   | B     | 1303 | CLR  | C1-C2   | 6.28 | 1.66        | 1.53     |
| 2   | B     | 1304 | CLR  | C1-C2   | 6.28 | 1.66        | 1.53     |
| 2   | C     | 1304 | CLR  | C1-C2   | 6.28 | 1.66        | 1.53     |
| 2   | D     | 1303 | CLR  | C1-C2   | 6.28 | 1.66        | 1.53     |
| 2   | A     | 1301 | CLR  | C1-C2   | 6.28 | 1.66        | 1.53     |
| 2   | B     | 1307 | CLR  | C1-C2   | 6.18 | 1.66        | 1.53     |
| 2   | D     | 1301 | CLR  | C1-C2   | 6.18 | 1.66        | 1.53     |
| 2   | A     | 1304 | CLR  | C1-C2   | 6.17 | 1.66        | 1.53     |
| 2   | C     | 1305 | CLR  | C1-C2   | 6.17 | 1.66        | 1.53     |
| 2   | B     | 1307 | CLR  | C16-C15 | 5.93 | 1.70        | 1.54     |
| 2   | C     | 1305 | CLR  | C16-C15 | 5.92 | 1.70        | 1.54     |
| 2   | A     | 1304 | CLR  | C16-C15 | 5.92 | 1.70        | 1.54     |
| 2   | D     | 1301 | CLR  | C16-C15 | 5.91 | 1.70        | 1.54     |
| 2   | A     | 1303 | CLR  | C16-C15 | 5.87 | 1.70        | 1.54     |
| 2   | B     | 1301 | CLR  | C16-C15 | 5.86 | 1.70        | 1.54     |
| 2   | B     | 1306 | CLR  | C16-C15 | 5.85 | 1.70        | 1.54     |
| 2   | D     | 1302 | CLR  | C16-C15 | 5.85 | 1.70        | 1.54     |
| 2   | C     | 1304 | CLR  | C16-C15 | 5.83 | 1.70        | 1.54     |
| 2   | B     | 1304 | CLR  | C16-C15 | 5.82 | 1.70        | 1.54     |
| 2   | A     | 1301 | CLR  | C16-C15 | 5.82 | 1.70        | 1.54     |
| 2   | D     | 1303 | CLR  | C16-C15 | 5.82 | 1.70        | 1.54     |
| 2   | A     | 1305 | CLR  | C16-C15 | 5.80 | 1.69        | 1.54     |
| 2   | C     | 1302 | CLR  | C16-C15 | 5.79 | 1.69        | 1.54     |
| 2   | B     | 1303 | CLR  | C16-C15 | 5.79 | 1.69        | 1.54     |
| 2   | C     | 1303 | CLR  | C16-C15 | 5.78 | 1.69        | 1.54     |
| 2   | B     | 1302 | CLR  | C16-C15 | 5.78 | 1.69        | 1.54     |
| 2   | A     | 1306 | CLR  | C16-C15 | 5.78 | 1.69        | 1.54     |
| 2   | C     | 1301 | CLR  | C16-C15 | 5.78 | 1.69        | 1.54     |
| 2   | D     | 1304 | CLR  | C16-C15 | 5.77 | 1.69        | 1.54     |
| 2   | A     | 1302 | CLR  | C16-C15 | 5.76 | 1.69        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 1306 | CLR  | C16-C15 | 5.76  | 1.69        | 1.54     |
| 2   | D     | 1305 | CLR  | C16-C15 | 5.76  | 1.69        | 1.54     |
| 2   | B     | 1305 | CLR  | C16-C15 | 5.76  | 1.69        | 1.54     |
| 2   | A     | 1305 | CLR  | C7-C8   | -5.39 | 1.44        | 1.53     |
| 2   | C     | 1302 | CLR  | C7-C8   | -5.39 | 1.44        | 1.53     |
| 2   | D     | 1305 | CLR  | C7-C8   | -5.38 | 1.44        | 1.53     |
| 2   | B     | 1302 | CLR  | C7-C8   | -5.38 | 1.44        | 1.53     |
| 2   | B     | 1303 | CLR  | C7-C8   | -5.38 | 1.44        | 1.53     |
| 2   | D     | 1306 | CLR  | C7-C8   | -5.37 | 1.44        | 1.53     |
| 2   | C     | 1303 | CLR  | C7-C8   | -5.37 | 1.44        | 1.53     |
| 2   | A     | 1306 | CLR  | C7-C8   | -5.37 | 1.44        | 1.53     |
| 2   | C     | 1301 | CLR  | C7-C8   | -5.36 | 1.44        | 1.53     |
| 2   | D     | 1304 | CLR  | C7-C8   | -5.36 | 1.44        | 1.53     |
| 2   | A     | 1302 | CLR  | C7-C8   | -5.35 | 1.44        | 1.53     |
| 2   | B     | 1305 | CLR  | C7-C8   | -5.35 | 1.44        | 1.53     |
| 2   | B     | 1306 | CLR  | C7-C8   | -5.32 | 1.44        | 1.53     |
| 2   | D     | 1302 | CLR  | C7-C8   | -5.32 | 1.44        | 1.53     |
| 2   | A     | 1303 | CLR  | C7-C8   | -5.31 | 1.44        | 1.53     |
| 2   | B     | 1301 | CLR  | C7-C8   | -5.31 | 1.44        | 1.53     |
| 2   | D     | 1301 | CLR  | C7-C8   | -5.28 | 1.44        | 1.53     |
| 2   | A     | 1304 | CLR  | C7-C8   | -5.28 | 1.44        | 1.53     |
| 2   | B     | 1307 | CLR  | C7-C8   | -5.28 | 1.44        | 1.53     |
| 2   | C     | 1305 | CLR  | C7-C8   | -5.26 | 1.44        | 1.53     |
| 2   | C     | 1304 | CLR  | C7-C8   | -5.23 | 1.44        | 1.53     |
| 2   | B     | 1304 | CLR  | C7-C8   | -5.23 | 1.44        | 1.53     |
| 2   | A     | 1301 | CLR  | C7-C8   | -5.23 | 1.44        | 1.53     |
| 2   | D     | 1303 | CLR  | C7-C8   | -5.20 | 1.44        | 1.53     |
| 2   | C     | 1301 | CLR  | O1-C3   | -5.08 | 1.28        | 1.43     |
| 2   | A     | 1305 | CLR  | O1-C3   | -5.08 | 1.28        | 1.43     |
| 2   | B     | 1302 | CLR  | O1-C3   | -5.08 | 1.28        | 1.43     |
| 2   | D     | 1305 | CLR  | O1-C3   | -5.08 | 1.28        | 1.43     |
| 2   | D     | 1301 | CLR  | O1-C3   | -5.07 | 1.28        | 1.43     |
| 2   | A     | 1304 | CLR  | O1-C3   | -5.07 | 1.28        | 1.43     |
| 2   | C     | 1305 | CLR  | O1-C3   | -5.06 | 1.28        | 1.43     |
| 2   | B     | 1307 | CLR  | O1-C3   | -5.06 | 1.28        | 1.43     |
| 2   | B     | 1304 | CLR  | O1-C3   | -5.05 | 1.28        | 1.43     |
| 2   | A     | 1301 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | D     | 1303 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | C     | 1303 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | B     | 1305 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | A     | 1302 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | D     | 1304 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | C     | 1304 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | C     | 1302 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | D     | 1302 | CLR  | O1-C3   | -5.04 | 1.28        | 1.43     |
| 2   | A     | 1303 | CLR  | O1-C3   | -5.03 | 1.28        | 1.43     |
| 2   | B     | 1303 | CLR  | O1-C3   | -5.03 | 1.28        | 1.43     |
| 2   | B     | 1306 | CLR  | O1-C3   | -5.03 | 1.28        | 1.43     |
| 2   | B     | 1301 | CLR  | O1-C3   | -5.03 | 1.28        | 1.43     |
| 2   | A     | 1306 | CLR  | O1-C3   | -5.01 | 1.28        | 1.43     |
| 2   | D     | 1306 | CLR  | O1-C3   | -5.01 | 1.28        | 1.43     |
| 2   | D     | 1305 | CLR  | C12-C13 | -4.75 | 1.45        | 1.54     |
| 2   | C     | 1301 | CLR  | C12-C13 | -4.73 | 1.45        | 1.54     |
| 2   | D     | 1301 | CLR  | C12-C13 | -4.73 | 1.45        | 1.54     |
| 2   | B     | 1307 | CLR  | C12-C13 | -4.71 | 1.45        | 1.54     |
| 2   | A     | 1305 | CLR  | C12-C13 | -4.71 | 1.45        | 1.54     |
| 2   | C     | 1305 | CLR  | C12-C13 | -4.71 | 1.45        | 1.54     |
| 2   | A     | 1304 | CLR  | C12-C13 | -4.71 | 1.45        | 1.54     |
| 2   | B     | 1302 | CLR  | C12-C13 | -4.69 | 1.45        | 1.54     |
| 2   | C     | 1304 | CLR  | C12-C13 | -4.66 | 1.45        | 1.54     |
| 2   | B     | 1306 | CLR  | C1-C10  | -4.65 | 1.45        | 1.54     |
| 2   | B     | 1304 | CLR  | C12-C13 | -4.65 | 1.45        | 1.54     |
| 2   | D     | 1302 | CLR  | C1-C10  | -4.65 | 1.45        | 1.54     |
| 2   | B     | 1303 | CLR  | C12-C13 | -4.64 | 1.45        | 1.54     |
| 2   | A     | 1301 | CLR  | C12-C13 | -4.64 | 1.45        | 1.54     |
| 2   | B     | 1301 | CLR  | C1-C10  | -4.64 | 1.45        | 1.54     |
| 2   | D     | 1303 | CLR  | C12-C13 | -4.64 | 1.45        | 1.54     |
| 2   | C     | 1302 | CLR  | C12-C13 | -4.63 | 1.45        | 1.54     |
| 2   | A     | 1303 | CLR  | C1-C10  | -4.62 | 1.45        | 1.54     |
| 2   | D     | 1304 | CLR  | C1-C10  | -4.61 | 1.45        | 1.54     |
| 2   | A     | 1306 | CLR  | C12-C13 | -4.60 | 1.45        | 1.54     |
| 2   | A     | 1302 | CLR  | C1-C10  | -4.60 | 1.45        | 1.54     |
| 2   | D     | 1306 | CLR  | C12-C13 | -4.60 | 1.45        | 1.54     |
| 2   | C     | 1303 | CLR  | C1-C10  | -4.60 | 1.45        | 1.54     |
| 2   | B     | 1305 | CLR  | C1-C10  | -4.59 | 1.45        | 1.54     |
| 2   | B     | 1303 | CLR  | C1-C10  | -4.56 | 1.45        | 1.54     |
| 2   | A     | 1306 | CLR  | C1-C10  | -4.56 | 1.45        | 1.54     |
| 2   | D     | 1306 | CLR  | C1-C10  | -4.52 | 1.45        | 1.54     |
| 2   | C     | 1302 | CLR  | C1-C10  | -4.51 | 1.45        | 1.54     |
| 2   | D     | 1303 | CLR  | C1-C10  | -4.49 | 1.45        | 1.54     |
| 2   | A     | 1301 | CLR  | C1-C10  | -4.49 | 1.45        | 1.54     |
| 2   | C     | 1304 | CLR  | C1-C10  | -4.48 | 1.45        | 1.54     |
| 2   | C     | 1305 | CLR  | C1-C10  | -4.47 | 1.45        | 1.54     |
| 2   | A     | 1304 | CLR  | C1-C10  | -4.47 | 1.45        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1304 | CLR  | C1-C10  | -4.47 | 1.45        | 1.54     |
| 2   | D     | 1301 | CLR  | C1-C10  | -4.46 | 1.45        | 1.54     |
| 2   | B     | 1307 | CLR  | C1-C10  | -4.45 | 1.45        | 1.54     |
| 2   | D     | 1302 | CLR  | C12-C13 | -4.43 | 1.46        | 1.54     |
| 2   | B     | 1306 | CLR  | C12-C13 | -4.43 | 1.46        | 1.54     |
| 2   | A     | 1302 | CLR  | C12-C13 | -4.42 | 1.46        | 1.54     |
| 2   | A     | 1303 | CLR  | C12-C13 | -4.42 | 1.46        | 1.54     |
| 2   | B     | 1305 | CLR  | C12-C13 | -4.41 | 1.46        | 1.54     |
| 2   | B     | 1301 | CLR  | C12-C13 | -4.41 | 1.46        | 1.54     |
| 2   | D     | 1304 | CLR  | C12-C13 | -4.41 | 1.46        | 1.54     |
| 2   | C     | 1303 | CLR  | C12-C13 | -4.41 | 1.46        | 1.54     |
| 2   | B     | 1302 | CLR  | C1-C10  | -4.40 | 1.45        | 1.54     |
| 2   | A     | 1305 | CLR  | C1-C10  | -4.40 | 1.45        | 1.54     |
| 2   | D     | 1305 | CLR  | C1-C10  | -4.40 | 1.45        | 1.54     |
| 2   | C     | 1301 | CLR  | C1-C10  | -4.38 | 1.45        | 1.54     |
| 2   | D     | 1305 | CLR  | C10-C9  | -3.64 | 1.49        | 1.56     |
| 2   | C     | 1301 | CLR  | C10-C9  | -3.62 | 1.50        | 1.56     |
| 2   | B     | 1303 | CLR  | C10-C9  | -3.60 | 1.50        | 1.56     |
| 2   | B     | 1302 | CLR  | C10-C9  | -3.60 | 1.50        | 1.56     |
| 2   | A     | 1305 | CLR  | C10-C9  | -3.58 | 1.50        | 1.56     |
| 2   | B     | 1307 | CLR  | C10-C9  | -3.56 | 1.50        | 1.56     |
| 2   | A     | 1304 | CLR  | C10-C9  | -3.54 | 1.50        | 1.56     |
| 2   | C     | 1305 | CLR  | C10-C9  | -3.54 | 1.50        | 1.56     |
| 2   | C     | 1304 | CLR  | C10-C9  | -3.54 | 1.50        | 1.56     |
| 2   | B     | 1304 | CLR  | C10-C9  | -3.54 | 1.50        | 1.56     |
| 2   | A     | 1301 | CLR  | C10-C9  | -3.53 | 1.50        | 1.56     |
| 2   | D     | 1303 | CLR  | C10-C9  | -3.53 | 1.50        | 1.56     |
| 2   | D     | 1301 | CLR  | C10-C9  | -3.52 | 1.50        | 1.56     |
| 2   | A     | 1306 | CLR  | C10-C9  | -3.52 | 1.50        | 1.56     |
| 2   | D     | 1306 | CLR  | C10-C9  | -3.46 | 1.50        | 1.56     |
| 2   | C     | 1302 | CLR  | C10-C9  | -3.37 | 1.50        | 1.56     |
| 2   | C     | 1303 | CLR  | C10-C5  | 3.32  | 1.59        | 1.52     |
| 2   | D     | 1304 | CLR  | C10-C5  | 3.32  | 1.59        | 1.52     |
| 2   | B     | 1305 | CLR  | C10-C5  | 3.30  | 1.59        | 1.52     |
| 2   | A     | 1302 | CLR  | C10-C5  | 3.30  | 1.59        | 1.52     |
| 2   | D     | 1306 | CLR  | C10-C5  | 3.25  | 1.59        | 1.52     |
| 2   | C     | 1303 | CLR  | C10-C9  | -3.18 | 1.50        | 1.56     |
| 2   | B     | 1304 | CLR  | C10-C5  | 3.17  | 1.59        | 1.52     |
| 2   | B     | 1305 | CLR  | C10-C9  | -3.17 | 1.50        | 1.56     |
| 2   | D     | 1302 | CLR  | C10-C9  | -3.17 | 1.50        | 1.56     |
| 2   | A     | 1303 | CLR  | C10-C5  | 3.17  | 1.59        | 1.52     |
| 2   | B     | 1306 | CLR  | C10-C5  | 3.17  | 1.59        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 1304 | CLR  | C10-C9  | -3.16 | 1.50        | 1.56     |
| 2   | B     | 1306 | CLR  | C10-C9  | -3.16 | 1.50        | 1.56     |
| 2   | A     | 1306 | CLR  | C10-C5  | 3.16  | 1.59        | 1.52     |
| 2   | D     | 1303 | CLR  | C10-C5  | 3.16  | 1.59        | 1.52     |
| 2   | D     | 1302 | CLR  | C10-C5  | 3.16  | 1.59        | 1.52     |
| 2   | A     | 1303 | CLR  | C10-C9  | -3.16 | 1.50        | 1.56     |
| 2   | B     | 1301 | CLR  | C10-C5  | 3.16  | 1.59        | 1.52     |
| 2   | A     | 1301 | CLR  | C10-C5  | 3.15  | 1.59        | 1.52     |
| 2   | C     | 1304 | CLR  | C10-C5  | 3.15  | 1.59        | 1.52     |
| 2   | A     | 1302 | CLR  | C10-C9  | -3.15 | 1.50        | 1.56     |
| 2   | B     | 1301 | CLR  | C10-C9  | -3.14 | 1.50        | 1.56     |
| 2   | C     | 1302 | CLR  | C10-C5  | 3.13  | 1.59        | 1.52     |
| 2   | B     | 1302 | CLR  | C10-C5  | 3.12  | 1.59        | 1.52     |
| 2   | C     | 1301 | CLR  | C10-C5  | 3.12  | 1.59        | 1.52     |
| 2   | A     | 1305 | CLR  | C10-C5  | 3.12  | 1.59        | 1.52     |
| 2   | B     | 1301 | CLR  | C4-C3   | 3.09  | 1.57        | 1.52     |
| 2   | B     | 1303 | CLR  | C10-C5  | 3.09  | 1.59        | 1.52     |
| 2   | D     | 1305 | CLR  | C10-C5  | 3.08  | 1.59        | 1.52     |
| 2   | A     | 1303 | CLR  | C4-C3   | 3.05  | 1.57        | 1.52     |
| 2   | B     | 1306 | CLR  | C4-C3   | 3.05  | 1.57        | 1.52     |
| 2   | B     | 1307 | CLR  | C10-C5  | 3.04  | 1.58        | 1.52     |
| 2   | D     | 1302 | CLR  | C4-C3   | 3.03  | 1.57        | 1.52     |
| 2   | C     | 1305 | CLR  | C10-C5  | 3.03  | 1.58        | 1.52     |
| 2   | A     | 1304 | CLR  | C10-C5  | 3.03  | 1.58        | 1.52     |
| 2   | D     | 1301 | CLR  | C10-C5  | 3.02  | 1.58        | 1.52     |
| 2   | A     | 1306 | CLR  | C4-C3   | 2.98  | 1.57        | 1.52     |
| 2   | A     | 1302 | CLR  | C4-C3   | 2.96  | 1.57        | 1.52     |
| 2   | D     | 1304 | CLR  | C4-C3   | 2.95  | 1.57        | 1.52     |
| 2   | C     | 1303 | CLR  | C4-C3   | 2.94  | 1.57        | 1.52     |
| 2   | B     | 1305 | CLR  | C4-C3   | 2.93  | 1.57        | 1.52     |
| 2   | C     | 1302 | CLR  | C13-C14 | -2.92 | 1.49        | 1.55     |
| 2   | B     | 1303 | CLR  | C4-C3   | 2.90  | 1.57        | 1.52     |
| 2   | D     | 1306 | CLR  | C13-C14 | -2.90 | 1.49        | 1.55     |
| 2   | A     | 1306 | CLR  | C13-C14 | -2.89 | 1.49        | 1.55     |
| 2   | D     | 1305 | CLR  | C13-C14 | -2.89 | 1.49        | 1.55     |
| 2   | D     | 1306 | CLR  | C4-C3   | 2.88  | 1.57        | 1.52     |
| 2   | B     | 1303 | CLR  | C13-C14 | -2.88 | 1.49        | 1.55     |
| 2   | D     | 1302 | CLR  | C13-C14 | -2.87 | 1.49        | 1.55     |
| 2   | C     | 1301 | CLR  | C13-C14 | -2.86 | 1.49        | 1.55     |
| 2   | B     | 1306 | CLR  | C13-C14 | -2.86 | 1.49        | 1.55     |
| 2   | B     | 1301 | CLR  | C13-C14 | -2.86 | 1.49        | 1.55     |
| 2   | B     | 1302 | CLR  | C13-C14 | -2.85 | 1.49        | 1.55     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1303 | CLR  | C13-C14 | -2.85 | 1.49        | 1.55     |
| 2   | C     | 1303 | CLR  | C13-C14 | -2.85 | 1.49        | 1.55     |
| 2   | C     | 1305 | CLR  | C4-C3   | 2.84  | 1.57        | 1.52     |
| 2   | A     | 1305 | CLR  | C13-C14 | -2.84 | 1.49        | 1.55     |
| 2   | A     | 1304 | CLR  | C4-C3   | 2.84  | 1.57        | 1.52     |
| 2   | C     | 1302 | CLR  | C4-C3   | 2.84  | 1.57        | 1.52     |
| 2   | A     | 1302 | CLR  | C13-C14 | -2.84 | 1.49        | 1.55     |
| 2   | D     | 1301 | CLR  | C4-C3   | 2.83  | 1.57        | 1.52     |
| 2   | B     | 1305 | CLR  | C13-C14 | -2.83 | 1.49        | 1.55     |
| 2   | B     | 1307 | CLR  | C4-C3   | 2.83  | 1.57        | 1.52     |
| 2   | D     | 1304 | CLR  | C13-C14 | -2.82 | 1.49        | 1.55     |
| 2   | B     | 1304 | CLR  | C13-C14 | -2.82 | 1.49        | 1.55     |
| 2   | B     | 1307 | CLR  | C13-C14 | -2.82 | 1.49        | 1.55     |
| 2   | A     | 1304 | CLR  | C13-C14 | -2.82 | 1.49        | 1.55     |
| 2   | C     | 1305 | CLR  | C13-C14 | -2.81 | 1.49        | 1.55     |
| 2   | D     | 1301 | CLR  | C13-C14 | -2.81 | 1.49        | 1.55     |
| 2   | A     | 1301 | CLR  | C13-C14 | -2.80 | 1.49        | 1.55     |
| 2   | C     | 1304 | CLR  | C13-C14 | -2.79 | 1.49        | 1.55     |
| 2   | D     | 1303 | CLR  | C13-C14 | -2.76 | 1.49        | 1.55     |
| 2   | C     | 1304 | CLR  | C4-C3   | 2.74  | 1.56        | 1.52     |
| 2   | D     | 1303 | CLR  | C4-C3   | 2.74  | 1.56        | 1.52     |
| 2   | A     | 1301 | CLR  | C4-C3   | 2.73  | 1.56        | 1.52     |
| 2   | B     | 1302 | CLR  | C4-C3   | 2.73  | 1.56        | 1.52     |
| 2   | A     | 1305 | CLR  | C4-C3   | 2.73  | 1.56        | 1.52     |
| 2   | B     | 1304 | CLR  | C4-C3   | 2.72  | 1.56        | 1.52     |
| 2   | C     | 1301 | CLR  | C4-C3   | 2.72  | 1.56        | 1.52     |
| 2   | D     | 1305 | CLR  | C4-C3   | 2.72  | 1.56        | 1.52     |
| 2   | C     | 1301 | CLR  | C12-C11 | 2.24  | 1.58        | 1.53     |
| 2   | D     | 1305 | CLR  | C12-C11 | 2.24  | 1.58        | 1.53     |
| 2   | B     | 1302 | CLR  | C12-C11 | 2.23  | 1.58        | 1.53     |
| 2   | A     | 1305 | CLR  | C12-C11 | 2.23  | 1.58        | 1.53     |
| 2   | B     | 1306 | CLR  | C12-C11 | 2.23  | 1.58        | 1.53     |
| 2   | B     | 1301 | CLR  | C12-C11 | 2.23  | 1.58        | 1.53     |
| 2   | D     | 1302 | CLR  | C12-C11 | 2.22  | 1.58        | 1.53     |
| 2   | A     | 1303 | CLR  | C12-C11 | 2.21  | 1.58        | 1.53     |
| 2   | A     | 1302 | CLR  | C12-C11 | 2.17  | 1.58        | 1.53     |
| 2   | B     | 1305 | CLR  | C12-C11 | 2.17  | 1.58        | 1.53     |
| 2   | D     | 1304 | CLR  | C12-C11 | 2.16  | 1.58        | 1.53     |
| 2   | C     | 1303 | CLR  | C12-C11 | 2.14  | 1.58        | 1.53     |
| 2   | D     | 1306 | CLR  | C12-C11 | 2.09  | 1.57        | 1.53     |
| 2   | A     | 1306 | CLR  | C12-C11 | 2.06  | 1.57        | 1.53     |
| 2   | D     | 1303 | CLR  | C12-C11 | 2.04  | 1.57        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | A     | 1301 | CLR  | C12-C11 | 2.04 | 1.57        | 1.53     |
| 2   | D     | 1301 | CLR  | C12-C11 | 2.04 | 1.57        | 1.53     |
| 2   | B     | 1304 | CLR  | C12-C11 | 2.03 | 1.57        | 1.53     |
| 2   | C     | 1304 | CLR  | C12-C11 | 2.02 | 1.57        | 1.53     |
| 2   | A     | 1304 | CLR  | C12-C11 | 2.02 | 1.57        | 1.53     |
| 2   | C     | 1305 | CLR  | C12-C11 | 2.01 | 1.57        | 1.53     |
| 2   | B     | 1307 | CLR  | C12-C11 | 2.00 | 1.57        | 1.53     |
| 2   | C     | 1302 | CLR  | C12-C11 | 2.00 | 1.57        | 1.53     |

All (317) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | A     | 1306 | CLR  | C4-C5-C10  | 5.98  | 124.36      | 116.42   |
| 2   | D     | 1306 | CLR  | C4-C5-C10  | 5.83  | 124.16      | 116.42   |
| 2   | B     | 1303 | CLR  | C4-C5-C10  | 5.74  | 124.05      | 116.42   |
| 2   | D     | 1303 | CLR  | C4-C5-C10  | 5.57  | 123.81      | 116.42   |
| 2   | C     | 1304 | CLR  | C4-C5-C10  | 5.56  | 123.81      | 116.42   |
| 2   | B     | 1304 | CLR  | C4-C5-C10  | 5.55  | 123.80      | 116.42   |
| 2   | A     | 1301 | CLR  | C4-C5-C10  | 5.54  | 123.78      | 116.42   |
| 2   | B     | 1306 | CLR  | C4-C5-C10  | 5.53  | 123.77      | 116.42   |
| 2   | D     | 1302 | CLR  | C4-C5-C10  | 5.53  | 123.77      | 116.42   |
| 2   | B     | 1301 | CLR  | C4-C5-C10  | 5.50  | 123.73      | 116.42   |
| 2   | A     | 1303 | CLR  | C4-C5-C10  | 5.48  | 123.70      | 116.42   |
| 2   | B     | 1305 | CLR  | C4-C5-C10  | 5.39  | 123.58      | 116.42   |
| 2   | D     | 1304 | CLR  | C4-C5-C10  | 5.38  | 123.57      | 116.42   |
| 2   | D     | 1301 | CLR  | C4-C5-C10  | 5.38  | 123.56      | 116.42   |
| 2   | C     | 1305 | CLR  | C4-C5-C10  | 5.37  | 123.56      | 116.42   |
| 2   | A     | 1304 | CLR  | C4-C5-C10  | 5.37  | 123.55      | 116.42   |
| 2   | A     | 1302 | CLR  | C4-C5-C10  | 5.36  | 123.53      | 116.42   |
| 2   | C     | 1303 | CLR  | C4-C5-C10  | 5.35  | 123.52      | 116.42   |
| 2   | C     | 1302 | CLR  | C4-C5-C10  | 5.34  | 123.52      | 116.42   |
| 2   | B     | 1307 | CLR  | C4-C5-C10  | 5.31  | 123.47      | 116.42   |
| 2   | B     | 1302 | CLR  | C4-C5-C10  | 5.16  | 123.28      | 116.42   |
| 2   | A     | 1305 | CLR  | C4-C5-C10  | 5.14  | 123.25      | 116.42   |
| 2   | C     | 1301 | CLR  | C15-C14-C8 | -5.11 | 110.67      | 119.08   |
| 2   | D     | 1305 | CLR  | C4-C5-C10  | 5.10  | 123.19      | 116.42   |
| 2   | B     | 1302 | CLR  | C15-C14-C8 | -5.09 | 110.71      | 119.08   |
| 2   | C     | 1301 | CLR  | C4-C5-C10  | 5.08  | 123.17      | 116.42   |
| 2   | A     | 1305 | CLR  | C15-C14-C8 | -5.07 | 110.73      | 119.08   |
| 2   | D     | 1305 | CLR  | C15-C14-C8 | -5.02 | 110.81      | 119.08   |
| 2   | A     | 1306 | CLR  | C15-C14-C8 | -4.82 | 111.15      | 119.08   |
| 2   | B     | 1303 | CLR  | C15-C14-C8 | -4.80 | 111.18      | 119.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1306 | CLR  | C15-C14-C8  | -4.78 | 111.21      | 119.08   |
| 2   | A     | 1302 | CLR  | C15-C14-C8  | -4.74 | 111.27      | 119.08   |
| 2   | C     | 1304 | CLR  | C15-C14-C8  | -4.72 | 111.31      | 119.08   |
| 2   | B     | 1305 | CLR  | C15-C14-C8  | -4.72 | 111.31      | 119.08   |
| 2   | D     | 1303 | CLR  | C15-C14-C8  | -4.70 | 111.34      | 119.08   |
| 2   | B     | 1306 | CLR  | C15-C14-C8  | -4.69 | 111.35      | 119.08   |
| 2   | D     | 1302 | CLR  | C15-C14-C8  | -4.69 | 111.36      | 119.08   |
| 2   | A     | 1301 | CLR  | C15-C14-C8  | -4.68 | 111.38      | 119.08   |
| 2   | B     | 1304 | CLR  | C15-C14-C8  | -4.68 | 111.38      | 119.08   |
| 2   | D     | 1301 | CLR  | C15-C14-C8  | -4.67 | 111.39      | 119.08   |
| 2   | B     | 1301 | CLR  | C15-C14-C8  | -4.67 | 111.39      | 119.08   |
| 2   | D     | 1304 | CLR  | C15-C14-C8  | -4.66 | 111.41      | 119.08   |
| 2   | A     | 1303 | CLR  | C15-C14-C8  | -4.65 | 111.43      | 119.08   |
| 2   | B     | 1307 | CLR  | C15-C14-C8  | -4.65 | 111.43      | 119.08   |
| 2   | A     | 1304 | CLR  | C15-C14-C8  | -4.63 | 111.45      | 119.08   |
| 2   | C     | 1305 | CLR  | C15-C14-C8  | -4.63 | 111.46      | 119.08   |
| 2   | C     | 1302 | CLR  | C15-C14-C8  | -4.62 | 111.48      | 119.08   |
| 2   | C     | 1303 | CLR  | C15-C14-C8  | -4.61 | 111.50      | 119.08   |
| 2   | A     | 1302 | CLR  | C8-C7-C6    | -3.96 | 107.04      | 112.73   |
| 2   | B     | 1301 | CLR  | C17-C13-C14 | 3.92  | 104.71      | 100.07   |
| 2   | A     | 1303 | CLR  | C17-C13-C14 | 3.88  | 104.67      | 100.07   |
| 2   | C     | 1303 | CLR  | C8-C7-C6    | -3.86 | 107.18      | 112.73   |
| 2   | B     | 1306 | CLR  | C17-C13-C14 | 3.83  | 104.61      | 100.07   |
| 2   | D     | 1302 | CLR  | C17-C13-C14 | 3.82  | 104.60      | 100.07   |
| 2   | D     | 1305 | CLR  | C17-C13-C14 | 3.82  | 104.60      | 100.07   |
| 2   | A     | 1305 | CLR  | C17-C13-C14 | 3.82  | 104.60      | 100.07   |
| 2   | B     | 1307 | CLR  | C17-C13-C14 | 3.81  | 104.59      | 100.07   |
| 2   | D     | 1304 | CLR  | C8-C7-C6    | -3.81 | 107.26      | 112.73   |
| 2   | D     | 1301 | CLR  | C17-C13-C14 | 3.77  | 104.54      | 100.07   |
| 2   | C     | 1302 | CLR  | C17-C13-C14 | 3.76  | 104.53      | 100.07   |
| 2   | B     | 1305 | CLR  | C8-C7-C6    | -3.76 | 107.33      | 112.73   |
| 2   | B     | 1302 | CLR  | C17-C13-C14 | 3.73  | 104.50      | 100.07   |
| 2   | A     | 1304 | CLR  | C17-C13-C14 | 3.73  | 104.49      | 100.07   |
| 2   | C     | 1305 | CLR  | C17-C13-C14 | 3.67  | 104.42      | 100.07   |
| 2   | C     | 1301 | CLR  | C17-C13-C14 | 3.64  | 104.38      | 100.07   |
| 2   | C     | 1303 | CLR  | C17-C13-C14 | 3.56  | 104.29      | 100.07   |
| 2   | D     | 1304 | CLR  | C17-C13-C14 | 3.54  | 104.27      | 100.07   |
| 2   | B     | 1305 | CLR  | C17-C13-C14 | 3.47  | 104.19      | 100.07   |
| 2   | A     | 1302 | CLR  | C17-C13-C14 | 3.45  | 104.17      | 100.07   |
| 2   | D     | 1306 | CLR  | C17-C13-C14 | 3.37  | 104.07      | 100.07   |
| 2   | A     | 1306 | CLR  | C17-C13-C14 | 3.34  | 104.03      | 100.07   |
| 2   | B     | 1303 | CLR  | C17-C13-C14 | 3.24  | 103.91      | 100.07   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1305 | CLR  | C1-C2-C3    | -3.22 | 106.33      | 110.47   |
| 2   | C     | 1302 | CLR  | C8-C7-C6    | -3.22 | 108.11      | 112.73   |
| 2   | D     | 1301 | CLR  | C1-C2-C3    | -3.20 | 106.37      | 110.47   |
| 2   | A     | 1304 | CLR  | C1-C2-C3    | -3.13 | 106.45      | 110.47   |
| 2   | B     | 1306 | CLR  | C8-C7-C6    | -3.09 | 108.30      | 112.73   |
| 2   | A     | 1302 | CLR  | C7-C6-C5    | -3.09 | 119.37      | 125.06   |
| 2   | B     | 1307 | CLR  | C21-C20-C22 | -3.08 | 105.53      | 110.36   |
| 2   | A     | 1304 | CLR  | C21-C20-C22 | -3.08 | 105.54      | 110.36   |
| 2   | B     | 1307 | CLR  | C1-C2-C3    | -3.07 | 106.53      | 110.47   |
| 2   | C     | 1305 | CLR  | C21-C20-C22 | -3.07 | 105.55      | 110.36   |
| 2   | D     | 1303 | CLR  | C16-C15-C14 | -3.06 | 99.07       | 105.13   |
| 2   | D     | 1304 | CLR  | C7-C6-C5    | -3.05 | 119.43      | 125.06   |
| 2   | C     | 1303 | CLR  | C7-C6-C5    | -3.05 | 119.44      | 125.06   |
| 2   | B     | 1305 | CLR  | C7-C6-C5    | -3.03 | 119.48      | 125.06   |
| 2   | D     | 1301 | CLR  | C21-C20-C22 | -3.02 | 105.63      | 110.36   |
| 2   | B     | 1301 | CLR  | C8-C7-C6    | -3.02 | 108.40      | 112.73   |
| 2   | A     | 1301 | CLR  | C16-C15-C14 | -3.02 | 99.15       | 105.13   |
| 2   | C     | 1304 | CLR  | C16-C15-C14 | -3.02 | 99.15       | 105.13   |
| 2   | D     | 1306 | CLR  | C21-C20-C22 | -3.01 | 105.65      | 110.36   |
| 2   | B     | 1304 | CLR  | C16-C15-C14 | -3.01 | 99.17       | 105.13   |
| 2   | D     | 1302 | CLR  | C8-C7-C6    | -3.00 | 108.42      | 112.73   |
| 2   | A     | 1303 | CLR  | C8-C7-C6    | -2.95 | 108.49      | 112.73   |
| 2   | C     | 1304 | CLR  | C21-C20-C22 | -2.94 | 105.76      | 110.36   |
| 2   | C     | 1301 | CLR  | C7-C8-C9    | -2.93 | 106.16      | 109.71   |
| 2   | B     | 1304 | CLR  | C21-C20-C22 | -2.93 | 105.77      | 110.36   |
| 2   | B     | 1306 | CLR  | C21-C20-C22 | -2.92 | 105.78      | 110.36   |
| 2   | C     | 1302 | CLR  | C21-C20-C22 | -2.92 | 105.78      | 110.36   |
| 2   | A     | 1306 | CLR  | C21-C20-C22 | -2.92 | 105.79      | 110.36   |
| 2   | A     | 1301 | CLR  | C21-C20-C22 | -2.90 | 105.82      | 110.36   |
| 2   | B     | 1301 | CLR  | C21-C20-C22 | -2.90 | 105.82      | 110.36   |
| 2   | B     | 1303 | CLR  | C21-C20-C22 | -2.89 | 105.83      | 110.36   |
| 2   | A     | 1306 | CLR  | C4-C5-C6    | -2.89 | 116.44      | 120.61   |
| 2   | D     | 1302 | CLR  | C21-C20-C22 | -2.88 | 105.85      | 110.36   |
| 2   | D     | 1305 | CLR  | C21-C20-C22 | -2.88 | 105.85      | 110.36   |
| 2   | D     | 1305 | CLR  | C16-C15-C14 | -2.87 | 99.44       | 105.13   |
| 2   | B     | 1306 | CLR  | C7-C6-C5    | -2.87 | 119.76      | 125.06   |
| 2   | A     | 1303 | CLR  | C21-C20-C22 | -2.87 | 105.87      | 110.36   |
| 2   | B     | 1303 | CLR  | C16-C15-C14 | -2.86 | 99.46       | 105.13   |
| 2   | D     | 1303 | CLR  | C21-C20-C22 | -2.86 | 105.89      | 110.36   |
| 2   | D     | 1306 | CLR  | C4-C5-C6    | -2.85 | 116.51      | 120.61   |
| 2   | B     | 1304 | CLR  | C16-C17-C20 | -2.84 | 107.74      | 112.15   |
| 2   | C     | 1304 | CLR  | C16-C17-C20 | -2.84 | 107.75      | 112.15   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1301 | CLR  | C16-C17-C20 | -2.84 | 107.76      | 112.15   |
| 2   | D     | 1302 | CLR  | C7-C6-C5    | -2.83 | 119.84      | 125.06   |
| 2   | B     | 1301 | CLR  | C7-C6-C5    | -2.82 | 119.85      | 125.06   |
| 2   | C     | 1302 | CLR  | C7-C6-C5    | -2.82 | 119.86      | 125.06   |
| 2   | D     | 1306 | CLR  | C16-C15-C14 | -2.81 | 99.56       | 105.13   |
| 2   | D     | 1303 | CLR  | C16-C17-C20 | -2.81 | 107.80      | 112.15   |
| 2   | A     | 1305 | CLR  | C7-C8-C9    | -2.81 | 106.31      | 109.71   |
| 2   | A     | 1303 | CLR  | C7-C6-C5    | -2.80 | 119.89      | 125.06   |
| 2   | A     | 1306 | CLR  | C16-C15-C14 | -2.80 | 99.59       | 105.13   |
| 2   | A     | 1305 | CLR  | C21-C20-C22 | -2.79 | 105.98      | 110.36   |
| 2   | C     | 1301 | CLR  | C16-C15-C14 | -2.79 | 99.60       | 105.13   |
| 2   | B     | 1302 | CLR  | C21-C20-C22 | -2.78 | 106.01      | 110.36   |
| 2   | C     | 1301 | CLR  | C21-C20-C22 | -2.77 | 106.03      | 110.36   |
| 2   | D     | 1306 | CLR  | C8-C7-C6    | -2.77 | 108.76      | 112.73   |
| 2   | C     | 1302 | CLR  | C12-C13-C17 | -2.76 | 112.43      | 116.57   |
| 2   | D     | 1305 | CLR  | C7-C8-C9    | -2.76 | 106.37      | 109.71   |
| 2   | B     | 1303 | CLR  | C4-C5-C6    | -2.75 | 116.65      | 120.61   |
| 2   | C     | 1305 | CLR  | C10-C5-C6   | -2.75 | 118.70      | 122.90   |
| 2   | A     | 1304 | CLR  | C10-C5-C6   | -2.74 | 118.72      | 122.90   |
| 2   | D     | 1301 | CLR  | C10-C5-C6   | -2.74 | 118.72      | 122.90   |
| 2   | B     | 1302 | CLR  | C16-C15-C14 | -2.73 | 99.72       | 105.13   |
| 2   | B     | 1302 | CLR  | C7-C8-C9    | -2.71 | 106.42      | 109.71   |
| 2   | B     | 1302 | CLR  | C1-C2-C3    | -2.71 | 106.99      | 110.47   |
| 2   | D     | 1305 | CLR  | C1-C2-C3    | -2.70 | 107.01      | 110.47   |
| 2   | B     | 1307 | CLR  | C10-C5-C6   | -2.69 | 118.79      | 122.90   |
| 2   | C     | 1302 | CLR  | C16-C15-C14 | -2.69 | 99.81       | 105.13   |
| 2   | A     | 1305 | CLR  | C16-C15-C14 | -2.67 | 99.84       | 105.13   |
| 2   | C     | 1301 | CLR  | C16-C17-C20 | -2.67 | 108.02      | 112.15   |
| 2   | D     | 1306 | CLR  | C7-C6-C5    | -2.65 | 120.18      | 125.06   |
| 2   | D     | 1305 | CLR  | C12-C13-C17 | -2.64 | 112.62      | 116.57   |
| 2   | C     | 1302 | CLR  | C4-C5-C6    | -2.64 | 116.80      | 120.61   |
| 2   | D     | 1301 | CLR  | C16-C15-C14 | -2.62 | 99.94       | 105.13   |
| 2   | A     | 1305 | CLR  | C1-C2-C3    | -2.62 | 107.10      | 110.47   |
| 2   | B     | 1303 | CLR  | C12-C13-C17 | -2.62 | 112.65      | 116.57   |
| 2   | B     | 1301 | CLR  | C10-C5-C6   | -2.62 | 118.90      | 122.90   |
| 2   | A     | 1304 | CLR  | C16-C15-C14 | -2.61 | 99.95       | 105.13   |
| 2   | B     | 1306 | CLR  | C10-C5-C6   | -2.61 | 118.90      | 122.90   |
| 2   | D     | 1302 | CLR  | C10-C5-C6   | -2.61 | 118.91      | 122.90   |
| 2   | C     | 1305 | CLR  | C16-C15-C14 | -2.61 | 99.96       | 105.13   |
| 2   | A     | 1306 | CLR  | C8-C7-C6    | -2.61 | 108.99      | 112.73   |
| 2   | D     | 1305 | CLR  | C10-C5-C6   | -2.60 | 118.92      | 122.90   |
| 2   | C     | 1301 | CLR  | C8-C7-C6    | -2.60 | 109.00      | 112.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1301 | CLR  | C10-C5-C6   | -2.59 | 118.93      | 122.90   |
| 2   | B     | 1303 | CLR  | C8-C7-C6    | -2.59 | 109.01      | 112.73   |
| 2   | C     | 1304 | CLR  | C10-C5-C6   | -2.59 | 118.94      | 122.90   |
| 2   | A     | 1303 | CLR  | C10-C5-C6   | -2.59 | 118.94      | 122.90   |
| 2   | C     | 1301 | CLR  | C1-C2-C3    | -2.59 | 107.15      | 110.47   |
| 2   | A     | 1305 | CLR  | C10-C5-C6   | -2.58 | 118.95      | 122.90   |
| 2   | B     | 1302 | CLR  | C10-C5-C6   | -2.58 | 118.96      | 122.90   |
| 2   | A     | 1301 | CLR  | C10-C5-C6   | -2.56 | 118.98      | 122.90   |
| 2   | D     | 1303 | CLR  | C10-C5-C6   | -2.56 | 118.98      | 122.90   |
| 2   | A     | 1305 | CLR  | C8-C7-C6    | -2.56 | 109.06      | 112.73   |
| 2   | B     | 1304 | CLR  | C10-C5-C6   | -2.56 | 118.99      | 122.90   |
| 2   | B     | 1307 | CLR  | C16-C15-C14 | -2.55 | 100.08      | 105.13   |
| 2   | A     | 1304 | CLR  | C23-C22-C20 | -2.55 | 107.70      | 115.03   |
| 2   | D     | 1306 | CLR  | C12-C13-C17 | -2.55 | 112.76      | 116.57   |
| 2   | A     | 1306 | CLR  | C12-C13-C17 | -2.54 | 112.76      | 116.57   |
| 2   | B     | 1307 | CLR  | C23-C22-C20 | -2.54 | 107.75      | 115.03   |
| 2   | C     | 1303 | CLR  | C21-C20-C22 | -2.53 | 106.39      | 110.36   |
| 2   | C     | 1301 | CLR  | C14-C8-C9   | 2.53  | 112.48      | 109.09   |
| 2   | D     | 1301 | CLR  | C23-C22-C20 | -2.53 | 107.77      | 115.03   |
| 2   | C     | 1305 | CLR  | C23-C22-C20 | -2.51 | 107.80      | 115.03   |
| 2   | A     | 1306 | CLR  | C7-C6-C5    | -2.51 | 120.42      | 125.06   |
| 2   | B     | 1303 | CLR  | C7-C6-C5    | -2.50 | 120.44      | 125.06   |
| 2   | B     | 1302 | CLR  | C8-C7-C6    | -2.49 | 109.16      | 112.73   |
| 2   | D     | 1306 | CLR  | C16-C17-C20 | -2.46 | 108.34      | 112.15   |
| 2   | A     | 1305 | CLR  | C16-C17-C20 | -2.46 | 108.34      | 112.15   |
| 2   | B     | 1305 | CLR  | C4-C5-C6    | -2.45 | 117.08      | 120.61   |
| 2   | A     | 1306 | CLR  | C10-C5-C6   | -2.44 | 119.16      | 122.90   |
| 2   | D     | 1304 | CLR  | C4-C5-C6    | -2.44 | 117.08      | 120.61   |
| 2   | B     | 1302 | CLR  | C16-C17-C20 | -2.44 | 108.36      | 112.15   |
| 2   | C     | 1303 | CLR  | C4-C5-C6    | -2.43 | 117.11      | 120.61   |
| 2   | D     | 1305 | CLR  | C8-C7-C6    | -2.43 | 109.25      | 112.73   |
| 2   | D     | 1305 | CLR  | C3-C4-C5    | -2.42 | 107.92      | 112.03   |
| 2   | A     | 1301 | CLR  | C7-C6-C5    | -2.41 | 120.61      | 125.06   |
| 2   | A     | 1302 | CLR  | C4-C5-C6    | -2.41 | 117.13      | 120.61   |
| 2   | C     | 1304 | CLR  | C7-C6-C5    | -2.40 | 120.62      | 125.06   |
| 2   | B     | 1304 | CLR  | C7-C6-C5    | -2.40 | 120.63      | 125.06   |
| 2   | B     | 1306 | CLR  | C7-C8-C9    | -2.40 | 106.81      | 109.71   |
| 2   | D     | 1305 | CLR  | C1-C10-C5   | 2.40  | 113.15      | 108.75   |
| 2   | D     | 1301 | CLR  | C12-C13-C17 | -2.39 | 112.99      | 116.57   |
| 2   | D     | 1303 | CLR  | C7-C6-C5    | -2.39 | 120.65      | 125.06   |
| 2   | B     | 1303 | CLR  | C16-C17-C20 | -2.39 | 108.45      | 112.15   |
| 2   | A     | 1305 | CLR  | C3-C4-C5    | -2.39 | 107.98      | 112.03   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1301 | CLR  | C12-C13-C17 | -2.38 | 113.00      | 116.57   |
| 2   | D     | 1305 | CLR  | C16-C17-C20 | -2.38 | 108.47      | 112.15   |
| 2   | D     | 1303 | CLR  | C4-C5-C6    | -2.38 | 117.18      | 120.61   |
| 2   | A     | 1306 | CLR  | C16-C17-C20 | -2.38 | 108.47      | 112.15   |
| 2   | B     | 1303 | CLR  | C10-C5-C6   | -2.37 | 119.27      | 122.90   |
| 2   | A     | 1304 | CLR  | C12-C13-C17 | -2.37 | 113.02      | 116.57   |
| 2   | B     | 1304 | CLR  | C4-C5-C6    | -2.37 | 117.19      | 120.61   |
| 2   | A     | 1305 | CLR  | C23-C22-C20 | -2.37 | 108.23      | 115.03   |
| 2   | B     | 1306 | CLR  | C16-C15-C14 | -2.37 | 100.44      | 105.13   |
| 2   | C     | 1301 | CLR  | C3-C4-C5    | -2.37 | 108.01      | 112.03   |
| 2   | C     | 1301 | CLR  | C1-C10-C5   | 2.37  | 113.08      | 108.75   |
| 2   | B     | 1303 | CLR  | C1-C2-C3    | -2.36 | 107.44      | 110.47   |
| 2   | B     | 1302 | CLR  | C3-C4-C5    | -2.35 | 108.03      | 112.03   |
| 2   | A     | 1305 | CLR  | C14-C8-C9   | 2.35  | 112.24      | 109.09   |
| 2   | A     | 1301 | CLR  | C4-C5-C6    | -2.35 | 117.22      | 120.61   |
| 2   | D     | 1302 | CLR  | C16-C15-C14 | -2.35 | 100.47      | 105.13   |
| 2   | B     | 1302 | CLR  | C14-C8-C9   | 2.35  | 112.23      | 109.09   |
| 2   | D     | 1306 | CLR  | C10-C5-C6   | -2.34 | 119.31      | 122.90   |
| 2   | C     | 1305 | CLR  | C12-C13-C17 | -2.34 | 113.06      | 116.57   |
| 2   | C     | 1304 | CLR  | C4-C5-C6    | -2.34 | 117.23      | 120.61   |
| 2   | A     | 1302 | CLR  | C10-C5-C6   | -2.34 | 119.33      | 122.90   |
| 2   | B     | 1305 | CLR  | C10-C5-C6   | -2.33 | 119.34      | 122.90   |
| 2   | B     | 1302 | CLR  | C23-C22-C20 | -2.33 | 108.34      | 115.03   |
| 2   | D     | 1304 | CLR  | C10-C5-C6   | -2.33 | 119.34      | 122.90   |
| 2   | B     | 1307 | CLR  | C12-C13-C17 | -2.32 | 113.09      | 116.57   |
| 2   | C     | 1303 | CLR  | C16-C15-C14 | -2.32 | 100.53      | 105.13   |
| 2   | D     | 1305 | CLR  | C23-C22-C20 | -2.31 | 108.38      | 115.03   |
| 2   | C     | 1303 | CLR  | C10-C5-C6   | -2.31 | 119.37      | 122.90   |
| 2   | D     | 1305 | CLR  | C2-C3-C4    | -2.31 | 107.14      | 110.31   |
| 2   | B     | 1301 | CLR  | C16-C15-C14 | -2.30 | 100.57      | 105.13   |
| 2   | B     | 1301 | CLR  | C7-C8-C9    | -2.30 | 106.92      | 109.71   |
| 2   | A     | 1305 | CLR  | C12-C13-C17 | -2.30 | 113.13      | 116.57   |
| 2   | B     | 1302 | CLR  | C12-C13-C17 | -2.30 | 113.14      | 116.57   |
| 2   | A     | 1303 | CLR  | C12-C13-C17 | -2.29 | 113.14      | 116.57   |
| 2   | B     | 1306 | CLR  | C4-C5-C6    | -2.29 | 117.31      | 120.61   |
| 2   | D     | 1302 | CLR  | C4-C5-C6    | -2.29 | 117.31      | 120.61   |
| 2   | B     | 1306 | CLR  | C16-C17-C20 | -2.29 | 108.60      | 112.15   |
| 2   | D     | 1302 | CLR  | C7-C8-C9    | -2.29 | 106.94      | 109.71   |
| 2   | A     | 1305 | CLR  | C7-C6-C5    | -2.28 | 120.85      | 125.06   |
| 2   | B     | 1307 | CLR  | C13-C17-C20 | -2.28 | 115.92      | 119.49   |
| 2   | A     | 1303 | CLR  | C16-C15-C14 | -2.28 | 100.62      | 105.13   |
| 2   | C     | 1301 | CLR  | C23-C22-C20 | -2.28 | 108.48      | 115.03   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1302 | CLR  | C12-C13-C17 | -2.27 | 113.17      | 116.57   |
| 2   | B     | 1301 | CLR  | C12-C13-C17 | -2.27 | 113.17      | 116.57   |
| 2   | A     | 1303 | CLR  | C4-C5-C6    | -2.27 | 117.34      | 120.61   |
| 2   | D     | 1302 | CLR  | C16-C17-C20 | -2.27 | 108.64      | 112.15   |
| 2   | B     | 1301 | CLR  | C4-C5-C6    | -2.26 | 117.35      | 120.61   |
| 2   | A     | 1303 | CLR  | C7-C8-C9    | -2.26 | 106.97      | 109.71   |
| 2   | C     | 1301 | CLR  | C7-C6-C5    | -2.26 | 120.89      | 125.06   |
| 2   | B     | 1302 | CLR  | C7-C6-C5    | -2.26 | 120.89      | 125.06   |
| 2   | C     | 1301 | CLR  | C10-C9-C8   | -2.25 | 109.35      | 112.73   |
| 2   | C     | 1302 | CLR  | C16-C17-C20 | -2.25 | 108.66      | 112.15   |
| 2   | B     | 1306 | CLR  | C12-C13-C17 | -2.25 | 113.20      | 116.57   |
| 2   | D     | 1304 | CLR  | C16-C15-C14 | -2.25 | 100.68      | 105.13   |
| 2   | B     | 1304 | CLR  | C23-C22-C20 | -2.24 | 108.58      | 115.03   |
| 2   | D     | 1303 | CLR  | C1-C2-C3    | -2.24 | 107.59      | 110.47   |
| 2   | D     | 1304 | CLR  | C21-C20-C22 | -2.23 | 106.86      | 110.36   |
| 2   | A     | 1304 | CLR  | C13-C17-C20 | -2.23 | 115.99      | 119.49   |
| 2   | D     | 1305 | CLR  | C14-C8-C9   | 2.23  | 112.07      | 109.09   |
| 2   | C     | 1305 | CLR  | C13-C17-C20 | -2.22 | 116.00      | 119.49   |
| 2   | B     | 1305 | CLR  | C16-C15-C14 | -2.22 | 100.73      | 105.13   |
| 2   | B     | 1301 | CLR  | C16-C17-C20 | -2.22 | 108.71      | 112.15   |
| 2   | D     | 1301 | CLR  | C13-C17-C20 | -2.22 | 116.02      | 119.49   |
| 2   | C     | 1302 | CLR  | C1-C2-C3    | -2.22 | 107.62      | 110.47   |
| 2   | B     | 1304 | CLR  | C12-C13-C17 | -2.21 | 113.26      | 116.57   |
| 2   | A     | 1301 | CLR  | C12-C13-C17 | -2.20 | 113.27      | 116.57   |
| 2   | D     | 1305 | CLR  | C7-C6-C5    | -2.20 | 121.00      | 125.06   |
| 2   | A     | 1301 | CLR  | C23-C22-C20 | -2.19 | 108.74      | 115.03   |
| 2   | C     | 1304 | CLR  | C23-C22-C20 | -2.19 | 108.75      | 115.03   |
| 2   | A     | 1302 | CLR  | C16-C15-C14 | -2.19 | 100.80      | 105.13   |
| 2   | B     | 1302 | CLR  | C1-C10-C5   | 2.18  | 112.74      | 108.75   |
| 2   | C     | 1301 | CLR  | C2-C3-C4    | -2.17 | 107.33      | 110.31   |
| 2   | C     | 1302 | CLR  | C13-C17-C20 | -2.17 | 116.09      | 119.49   |
| 2   | D     | 1303 | CLR  | C12-C13-C17 | -2.17 | 113.33      | 116.57   |
| 2   | A     | 1306 | CLR  | C13-C17-C20 | -2.16 | 116.10      | 119.49   |
| 2   | B     | 1302 | CLR  | C2-C3-C4    | -2.16 | 107.35      | 110.31   |
| 2   | A     | 1306 | CLR  | C1-C2-C3    | -2.15 | 107.70      | 110.47   |
| 2   | A     | 1301 | CLR  | C17-C13-C14 | 2.15  | 102.62      | 100.07   |
| 2   | A     | 1305 | CLR  | C11-C12-C13 | -2.15 | 109.10      | 112.78   |
| 2   | B     | 1302 | CLR  | C11-C12-C13 | -2.14 | 109.10      | 112.78   |
| 2   | C     | 1304 | CLR  | C1-C2-C3    | -2.14 | 107.72      | 110.47   |
| 2   | A     | 1305 | CLR  | C1-C10-C5   | 2.14  | 112.67      | 108.75   |
| 2   | B     | 1304 | CLR  | C17-C13-C14 | 2.13  | 102.60      | 100.07   |
| 2   | C     | 1304 | CLR  | C12-C13-C17 | -2.13 | 113.38      | 116.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1303 | CLR  | C16-C17-C20 | -2.13 | 108.85      | 112.15   |
| 2   | D     | 1305 | CLR  | C10-C9-C8   | -2.12 | 109.55      | 112.73   |
| 2   | C     | 1301 | CLR  | C11-C12-C13 | -2.12 | 109.14      | 112.78   |
| 2   | D     | 1303 | CLR  | C23-C22-C20 | -2.12 | 108.95      | 115.03   |
| 2   | C     | 1302 | CLR  | C10-C5-C6   | -2.12 | 119.66      | 122.90   |
| 2   | A     | 1301 | CLR  | C1-C2-C3    | -2.11 | 107.76      | 110.47   |
| 2   | C     | 1303 | CLR  | C12-C13-C17 | -2.11 | 113.41      | 116.57   |
| 2   | D     | 1306 | CLR  | C13-C17-C20 | -2.10 | 116.19      | 119.49   |
| 2   | A     | 1305 | CLR  | C2-C3-C4    | -2.10 | 107.42      | 110.31   |
| 2   | D     | 1306 | CLR  | C1-C2-C3    | -2.10 | 107.77      | 110.47   |
| 2   | C     | 1303 | CLR  | C13-C17-C20 | -2.10 | 116.20      | 119.49   |
| 2   | A     | 1304 | CLR  | C7-C8-C9    | -2.09 | 107.17      | 109.71   |
| 2   | D     | 1304 | CLR  | C12-C13-C17 | -2.09 | 113.45      | 116.57   |
| 2   | C     | 1303 | CLR  | C16-C17-C20 | -2.09 | 108.92      | 112.15   |
| 2   | D     | 1305 | CLR  | C11-C12-C13 | -2.08 | 109.21      | 112.78   |
| 2   | B     | 1303 | CLR  | C13-C17-C20 | -2.07 | 116.24      | 119.49   |
| 2   | A     | 1302 | CLR  | C21-C20-C22 | -2.07 | 107.12      | 110.36   |
| 2   | A     | 1304 | CLR  | C7-C6-C5    | -2.06 | 121.26      | 125.06   |
| 2   | B     | 1305 | CLR  | C21-C20-C22 | -2.06 | 107.14      | 110.36   |
| 2   | D     | 1303 | CLR  | C17-C13-C14 | 2.06  | 102.51      | 100.07   |
| 2   | B     | 1307 | CLR  | C7-C8-C9    | -2.05 | 107.23      | 109.71   |
| 2   | D     | 1301 | CLR  | C7-C6-C5    | -2.05 | 121.28      | 125.06   |
| 2   | D     | 1304 | CLR  | C16-C17-C20 | -2.04 | 108.99      | 112.15   |
| 2   | B     | 1304 | CLR  | C1-C2-C3    | -2.03 | 107.86      | 110.47   |
| 2   | C     | 1304 | CLR  | C17-C13-C14 | 2.03  | 102.47      | 100.07   |
| 2   | C     | 1305 | CLR  | C7-C6-C5    | -2.03 | 121.32      | 125.06   |
| 2   | B     | 1305 | CLR  | C16-C17-C20 | -2.03 | 109.01      | 112.15   |
| 2   | B     | 1307 | CLR  | C7-C6-C5    | -2.03 | 121.32      | 125.06   |
| 2   | C     | 1305 | CLR  | C7-C8-C9    | -2.02 | 107.27      | 109.71   |
| 2   | B     | 1302 | CLR  | C10-C9-C8   | -2.02 | 109.71      | 112.73   |
| 2   | D     | 1301 | CLR  | C4-C5-C6    | -2.02 | 117.70      | 120.61   |
| 2   | A     | 1304 | CLR  | C4-C5-C6    | -2.01 | 117.71      | 120.61   |
| 2   | B     | 1307 | CLR  | C4-C5-C6    | -2.01 | 117.72      | 120.61   |
| 2   | A     | 1305 | CLR  | C10-C9-C8   | -2.01 | 109.73      | 112.73   |
| 2   | C     | 1305 | CLR  | C4-C5-C6    | -2.00 | 117.72      | 120.61   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1303 | CLR  | C20-C22-C23-C24 |
| 2   | B     | 1301 | CLR  | C20-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 1306 | CLR  | C20-C22-C23-C24 |
| 2   | D     | 1302 | CLR  | C20-C22-C23-C24 |
| 2   | C     | 1301 | CLR  | C21-C20-C22-C23 |
| 2   | B     | 1302 | CLR  | C21-C20-C22-C23 |
| 2   | D     | 1305 | CLR  | C21-C20-C22-C23 |
| 2   | A     | 1305 | CLR  | C21-C20-C22-C23 |
| 2   | C     | 1301 | CLR  | C17-C20-C22-C23 |
| 2   | B     | 1306 | CLR  | C23-C24-C25-C27 |
| 2   | B     | 1302 | CLR  | C17-C20-C22-C23 |
| 2   | B     | 1301 | CLR  | C23-C24-C25-C27 |
| 2   | A     | 1302 | CLR  | C20-C22-C23-C24 |
| 2   | B     | 1305 | CLR  | C20-C22-C23-C24 |
| 2   | D     | 1302 | CLR  | C23-C24-C25-C27 |
| 2   | A     | 1303 | CLR  | C23-C24-C25-C27 |
| 2   | B     | 1304 | CLR  | C20-C22-C23-C24 |

There are no ring outliers.

24 monomers are involved in 37 short contacts:

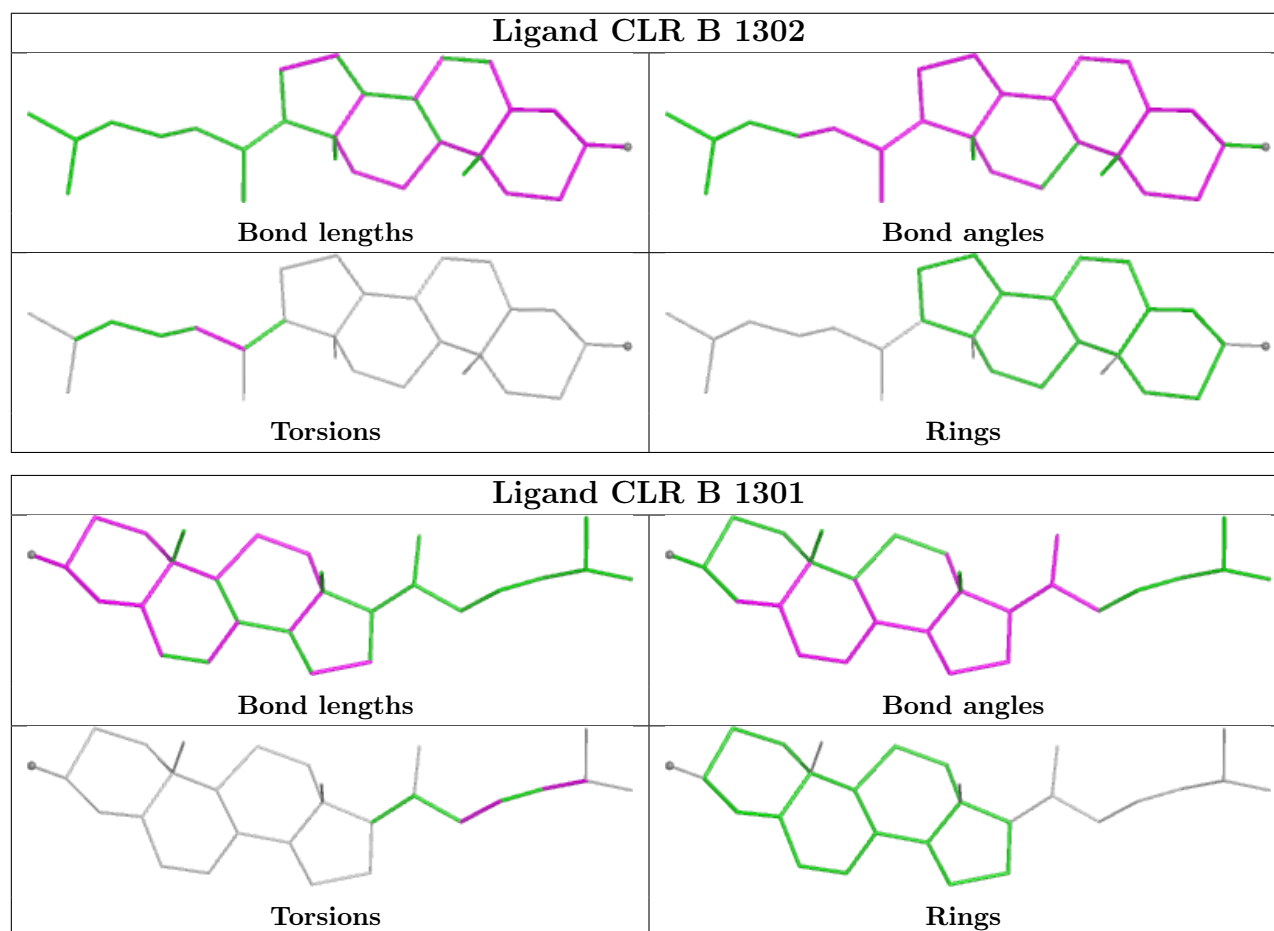
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | B     | 1302 | CLR  | 2       | 0            |
| 2   | B     | 1301 | CLR  | 2       | 0            |
| 2   | B     | 1303 | CLR  | 1       | 0            |
| 2   | D     | 1304 | CLR  | 2       | 0            |
| 2   | C     | 1305 | CLR  | 1       | 0            |
| 2   | C     | 1303 | CLR  | 2       | 0            |
| 2   | A     | 1302 | CLR  | 3       | 0            |
| 2   | D     | 1301 | CLR  | 1       | 0            |
| 2   | C     | 1301 | CLR  | 2       | 0            |
| 2   | D     | 1302 | CLR  | 2       | 0            |
| 2   | C     | 1302 | CLR  | 1       | 0            |
| 2   | A     | 1305 | CLR  | 2       | 0            |
| 2   | A     | 1303 | CLR  | 2       | 0            |
| 2   | D     | 1306 | CLR  | 1       | 0            |
| 2   | D     | 1303 | CLR  | 1       | 0            |
| 2   | A     | 1306 | CLR  | 1       | 0            |
| 2   | C     | 1304 | CLR  | 1       | 0            |
| 2   | D     | 1305 | CLR  | 1       | 0            |
| 2   | B     | 1307 | CLR  | 1       | 0            |
| 2   | B     | 1306 | CLR  | 2       | 0            |
| 2   | A     | 1304 | CLR  | 1       | 0            |
| 2   | B     | 1304 | CLR  | 1       | 0            |

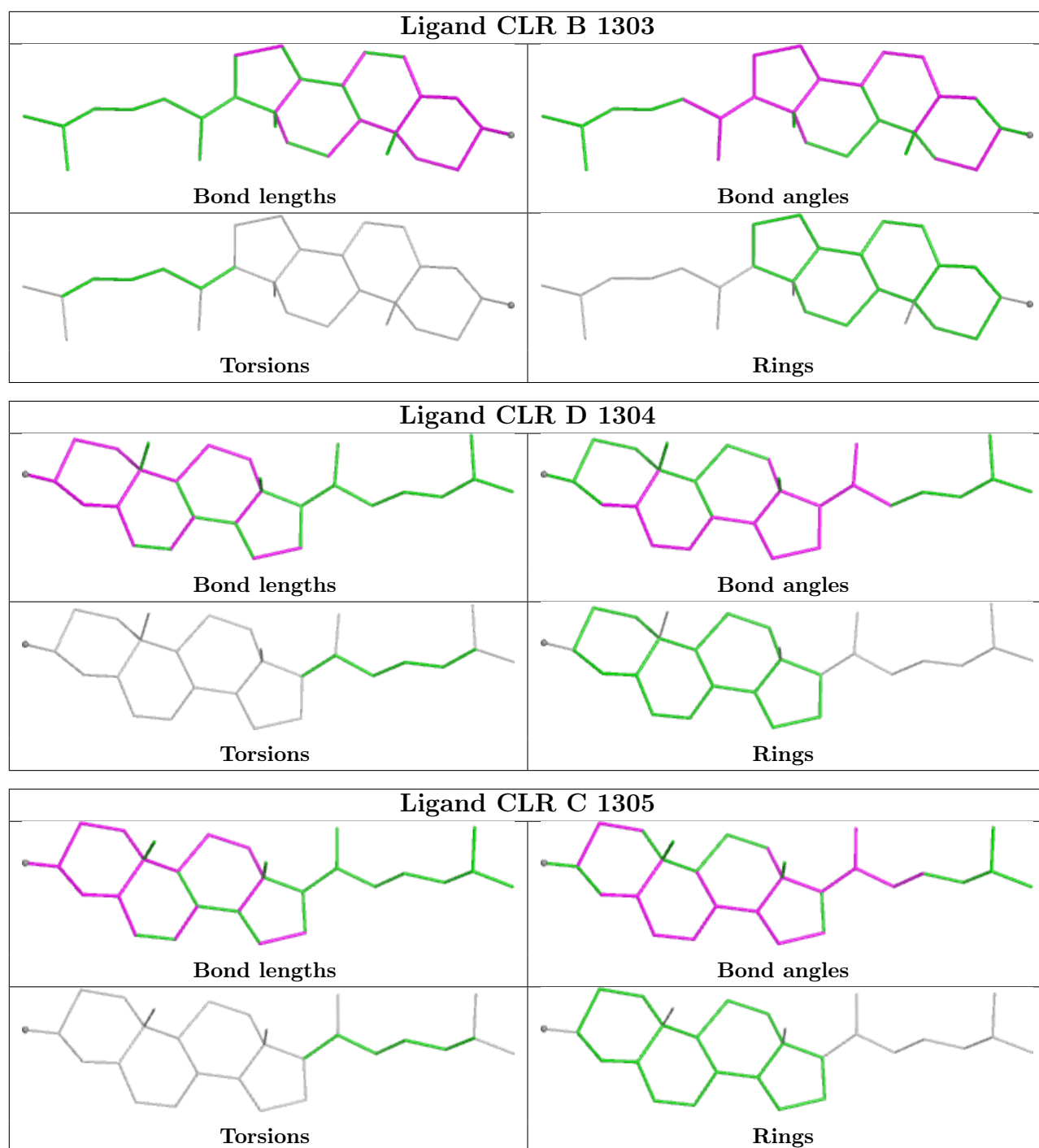
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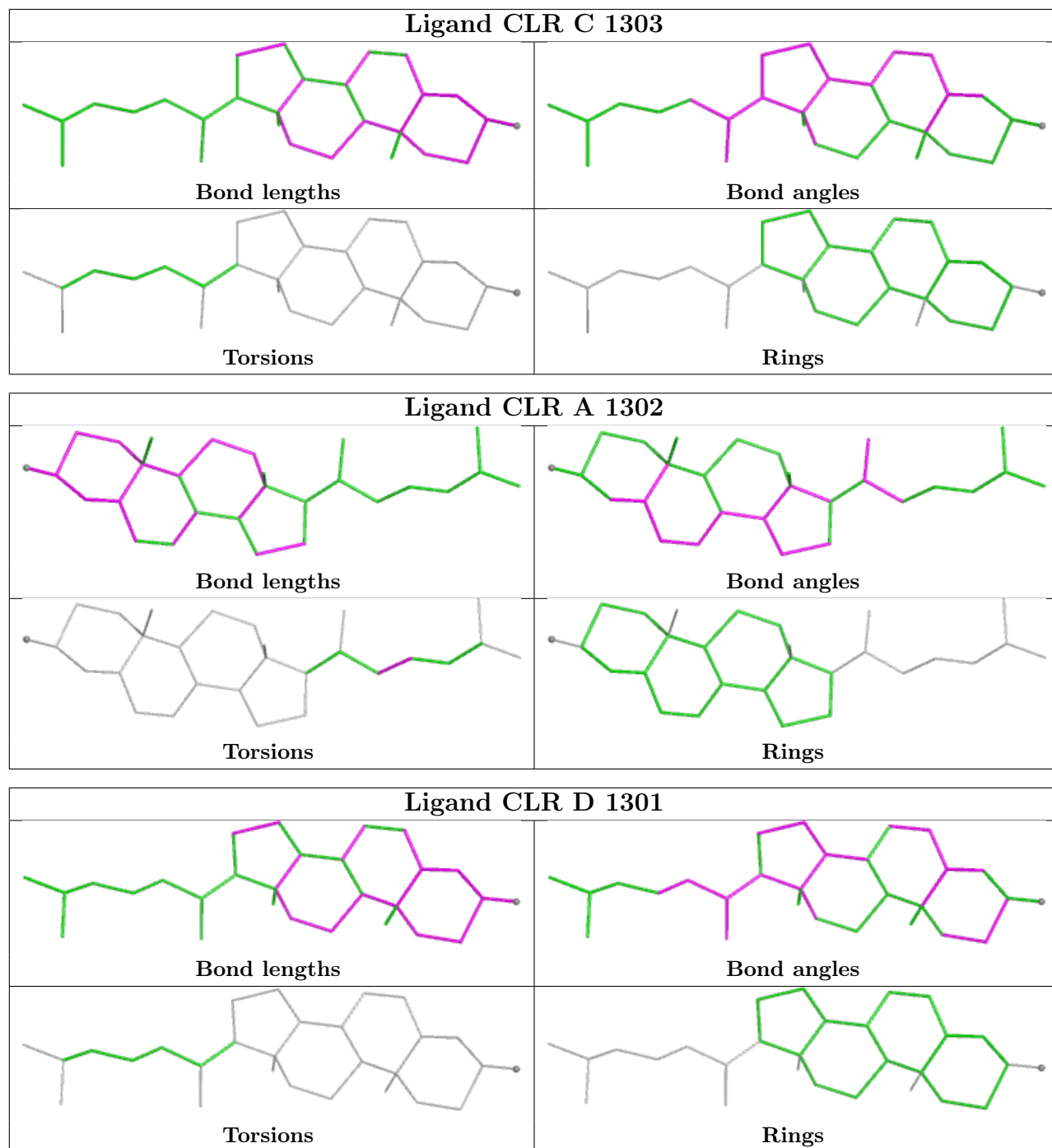
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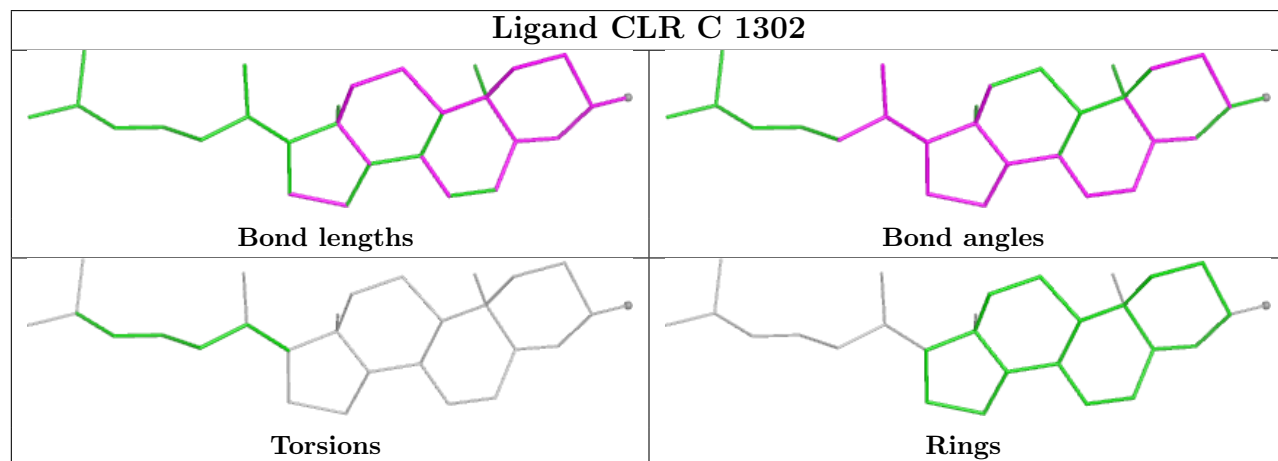
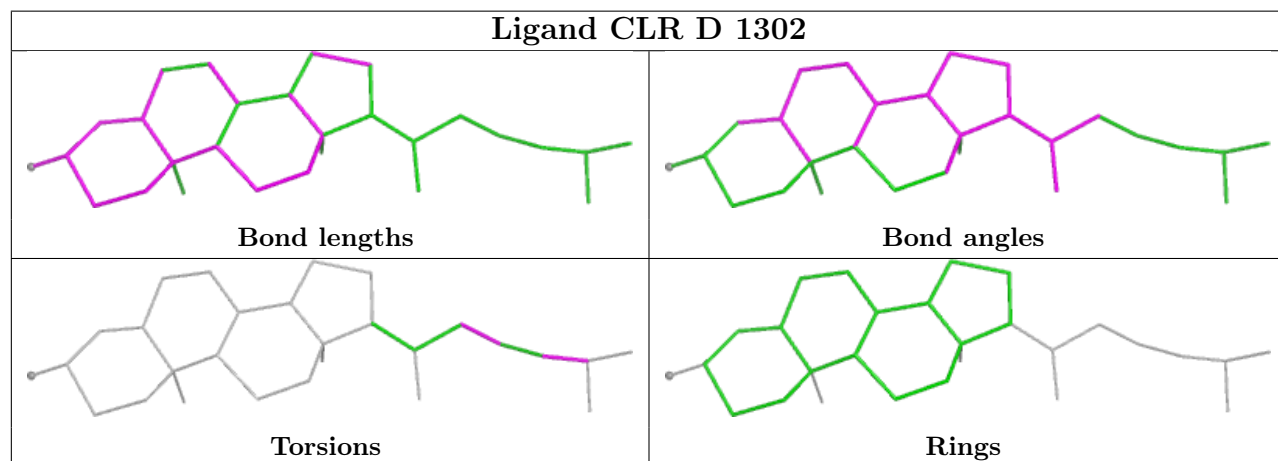
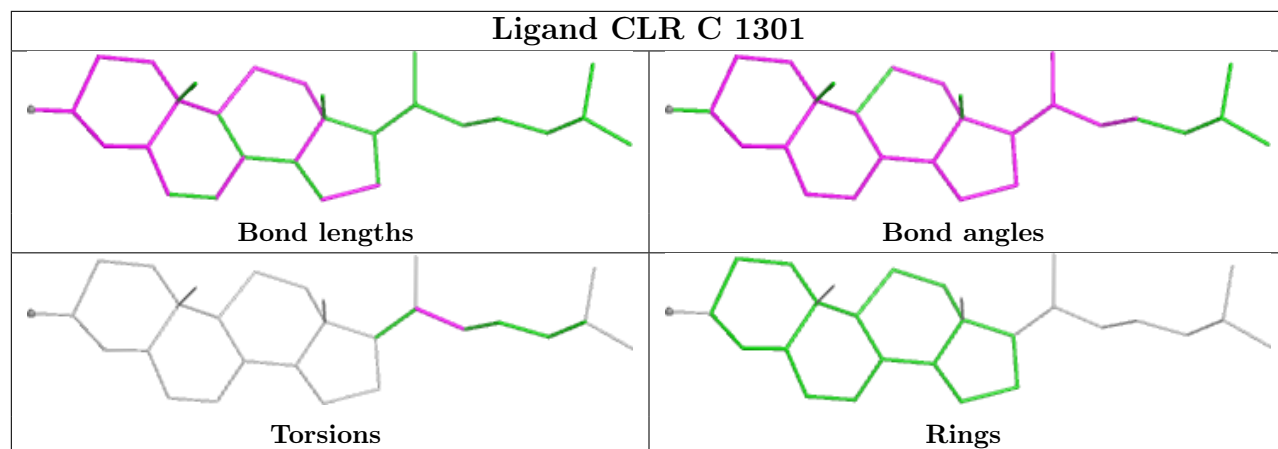
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1301 | CLR  | 1       | 0            |
| 2   | B     | 1305 | CLR  | 3       | 0            |

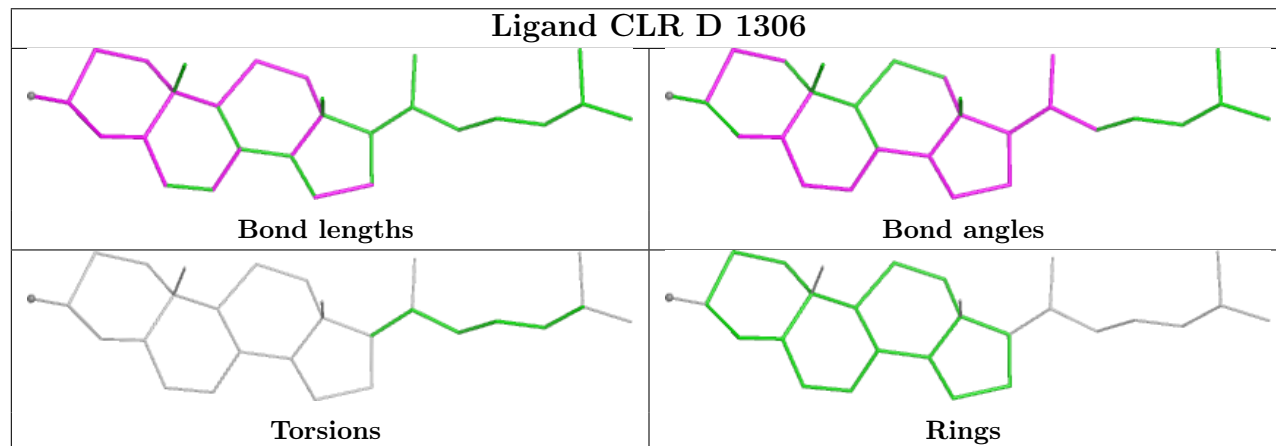
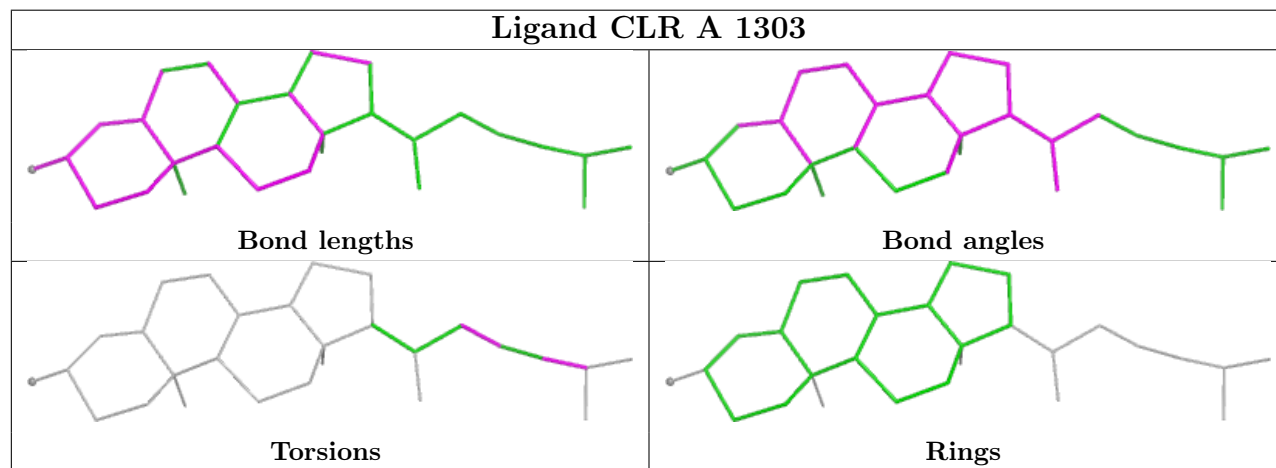
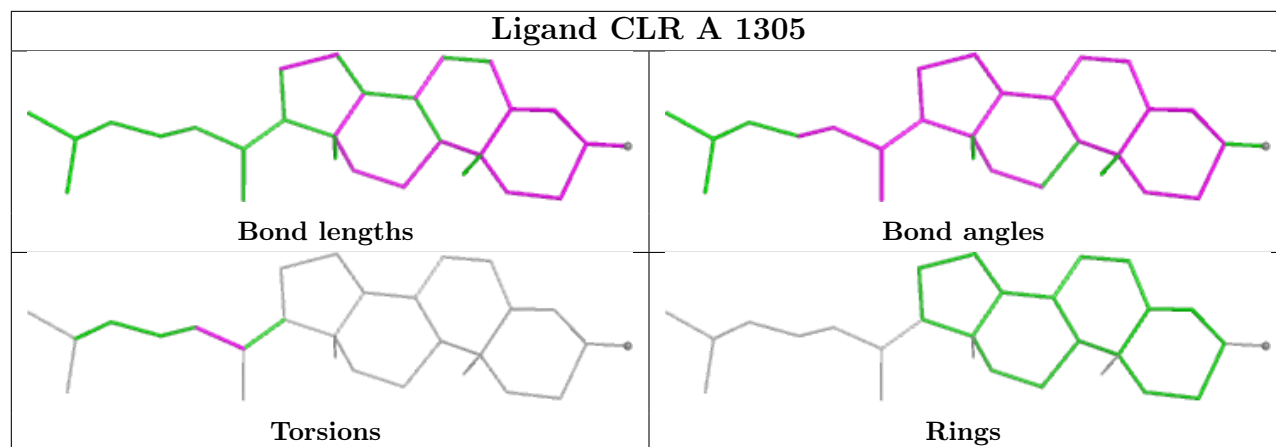
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

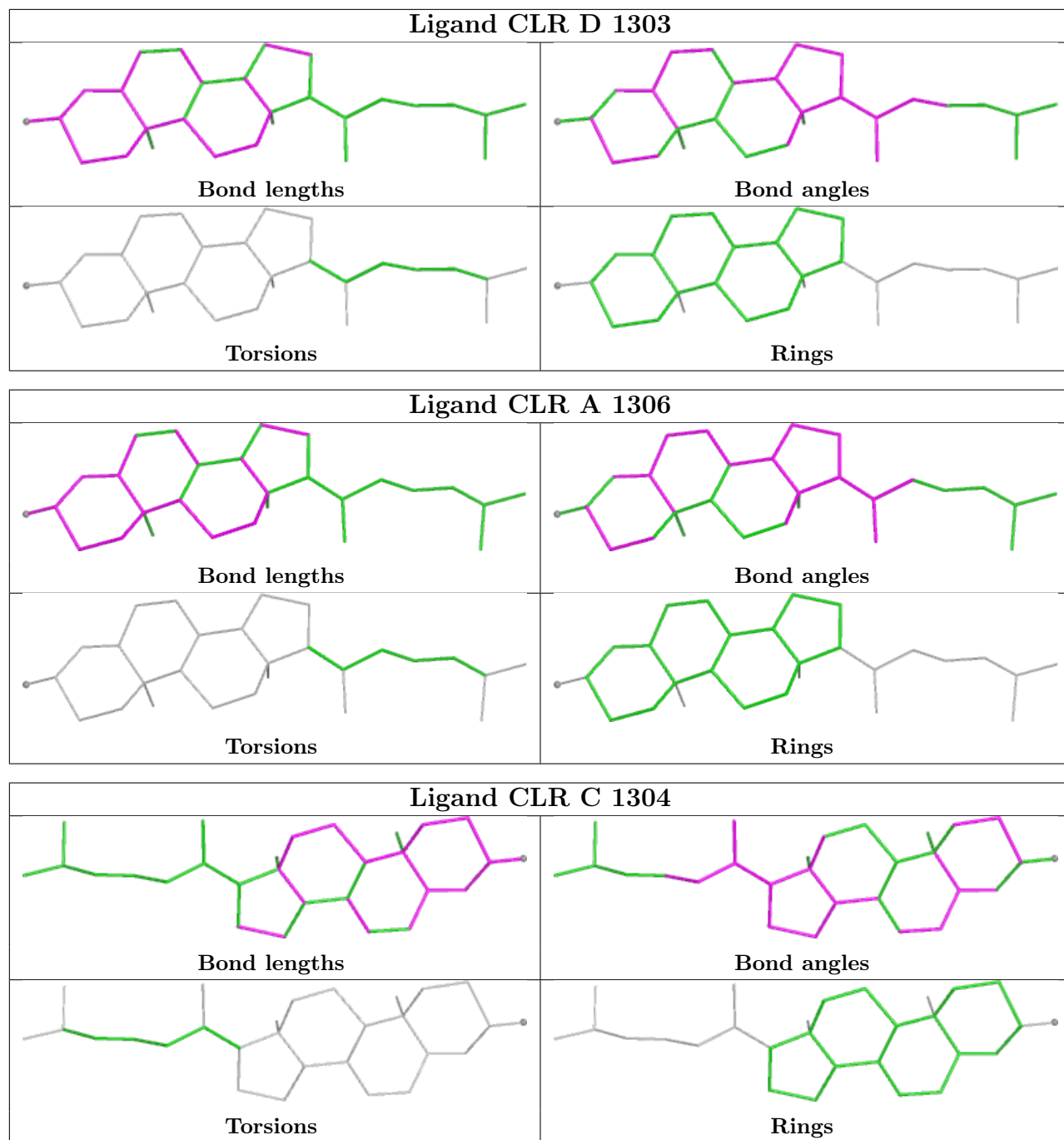


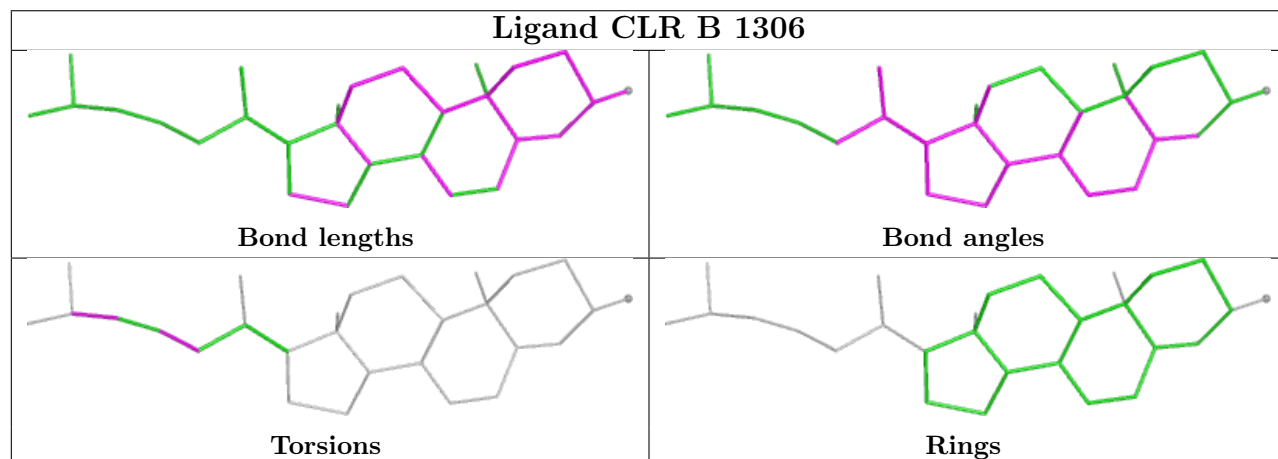
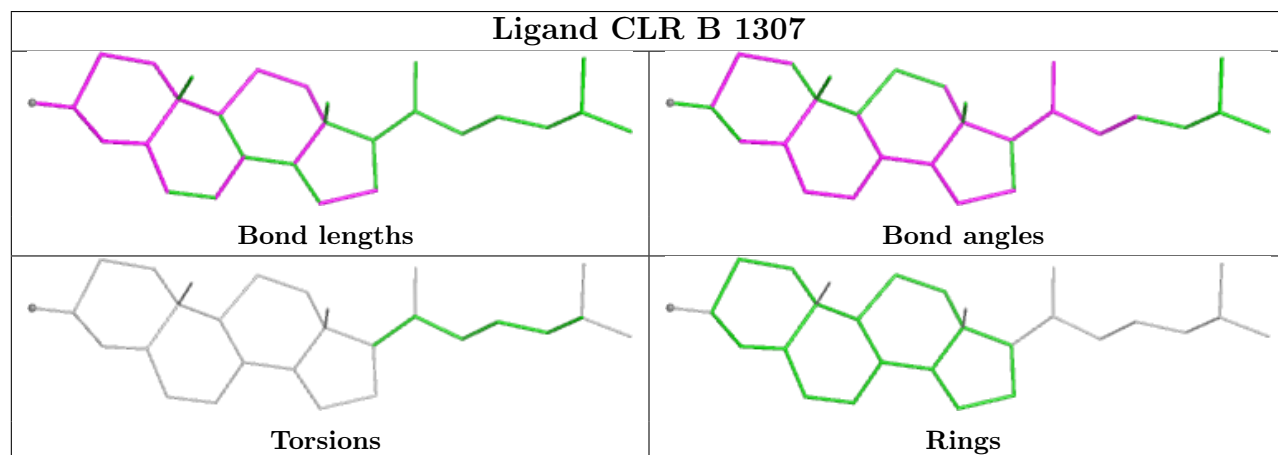
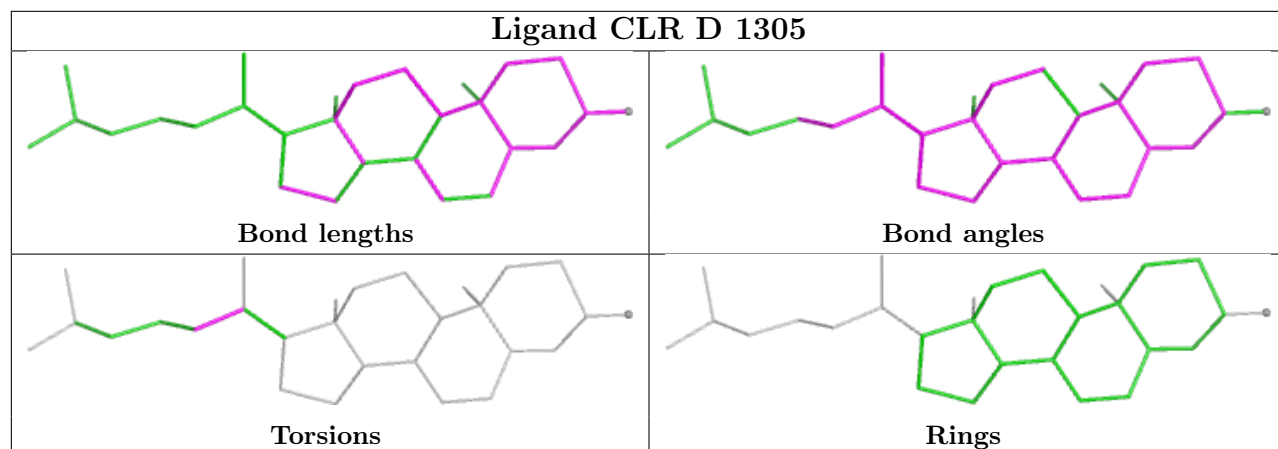


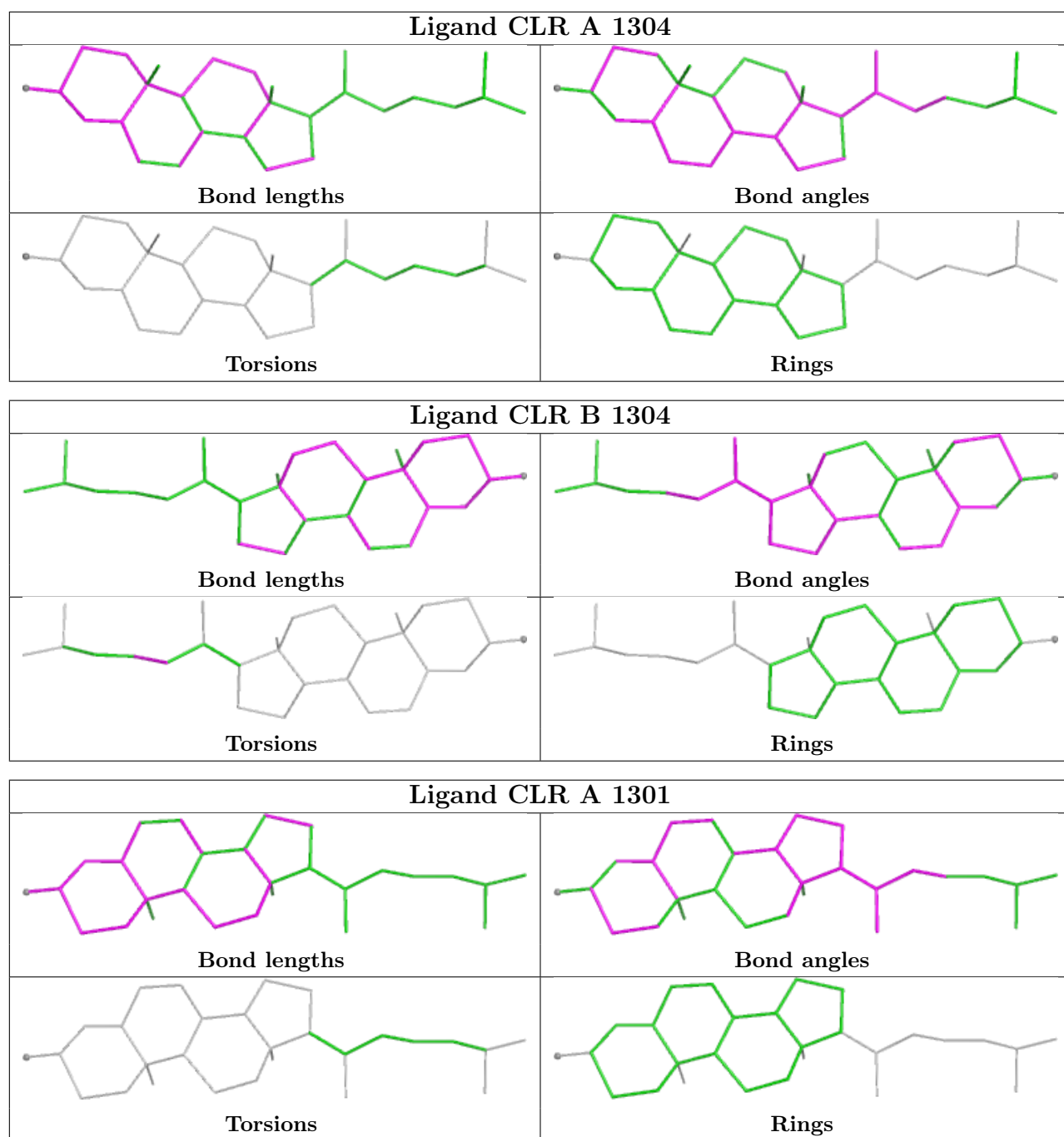


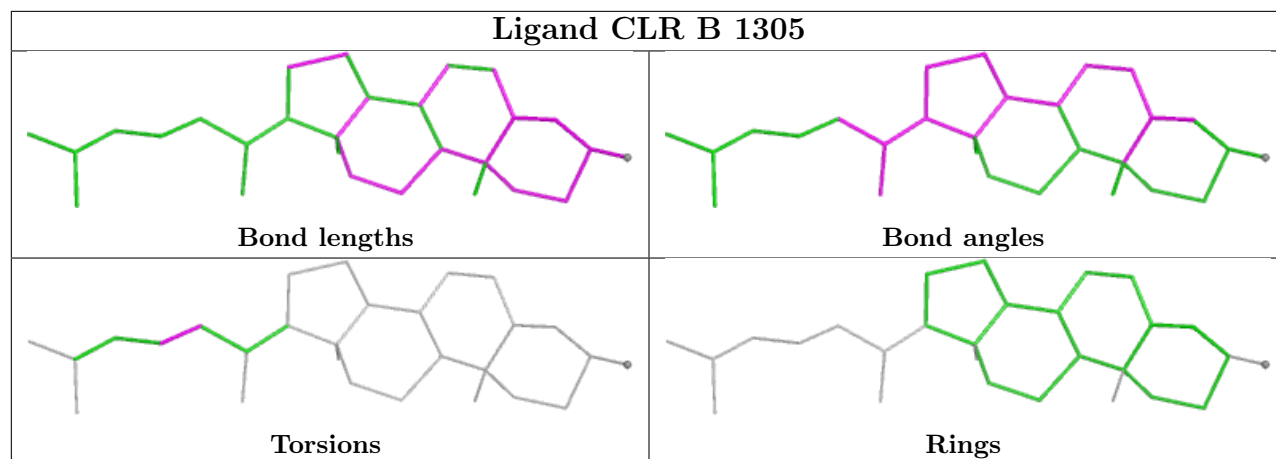












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

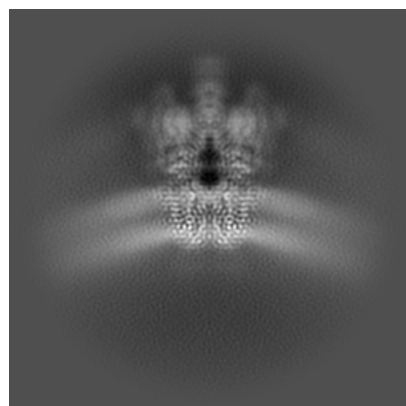
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57856. These allow visual inspection of the internal detail of the map and identification of artifacts.

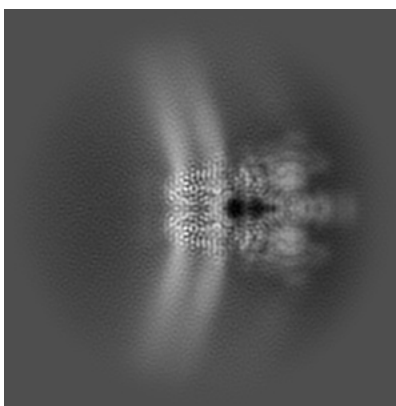
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

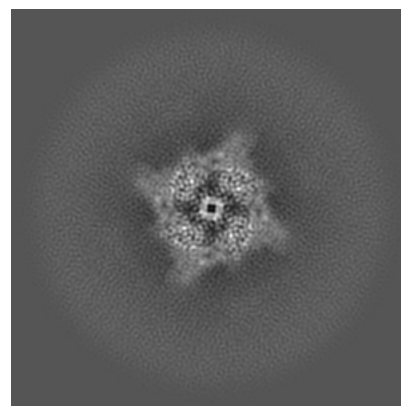
#### 6.1.1 Primary map



X

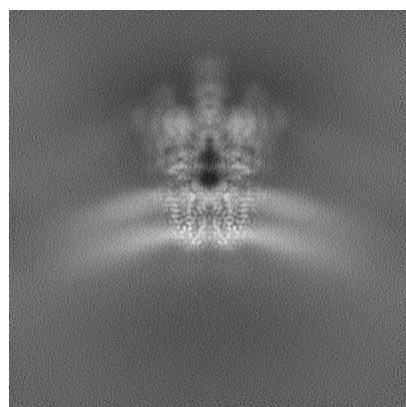


Y

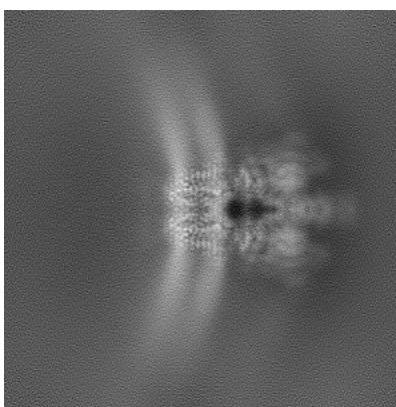


Z

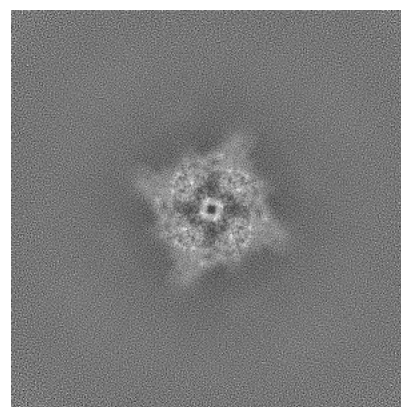
#### 6.1.2 Raw map



X



Y

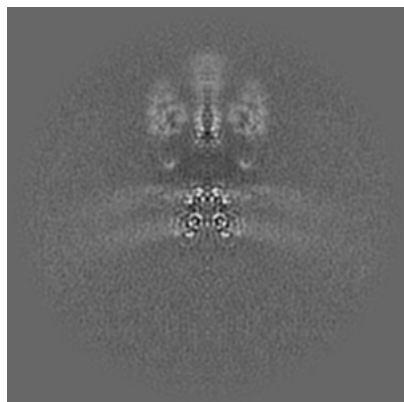


Z

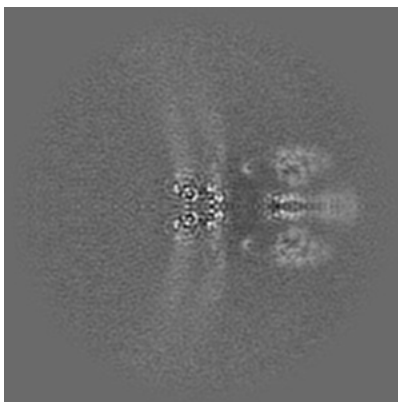
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

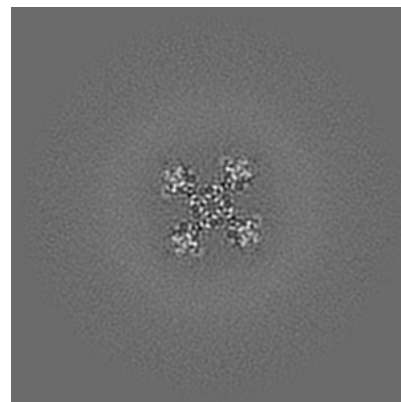
### 6.2.1 Primary map



X Index: 200



Y Index: 200

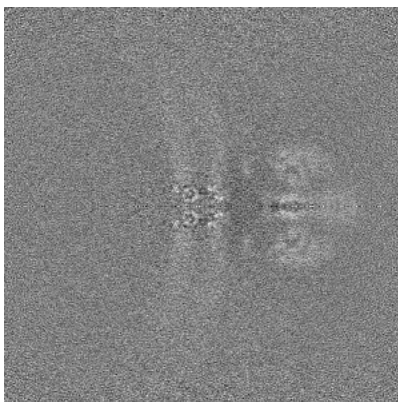


Z Index: 200

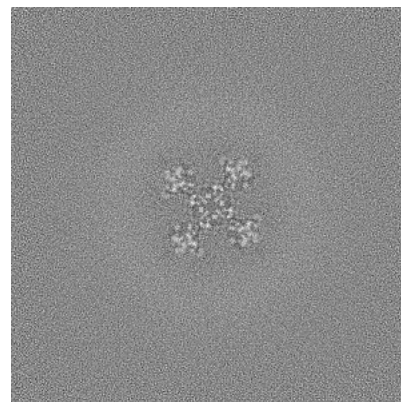
### 6.2.2 Raw map



X Index: 200



Y Index: 200

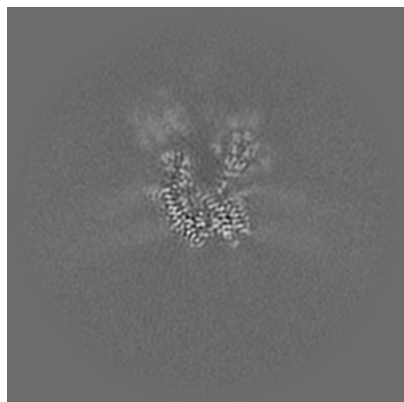


Z Index: 200

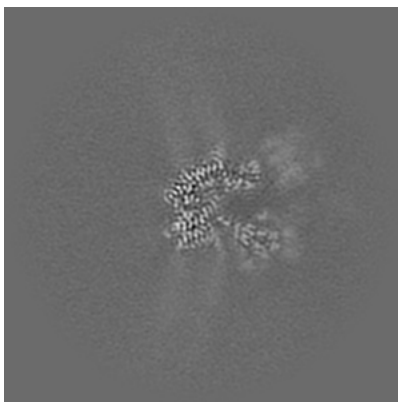
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

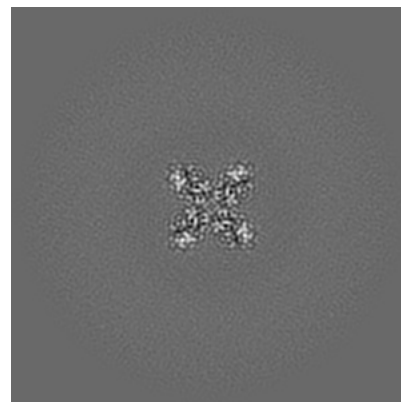
### 6.3.1 Primary map



X Index: 180

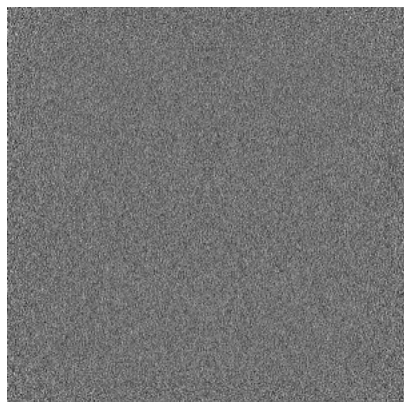


Y Index: 180

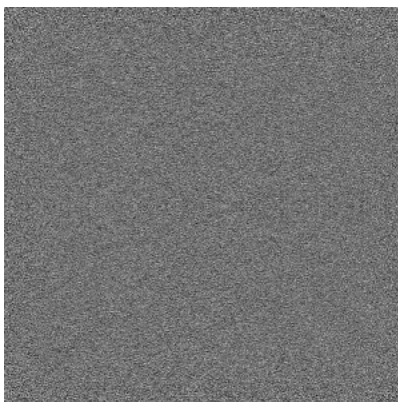


Z Index: 188

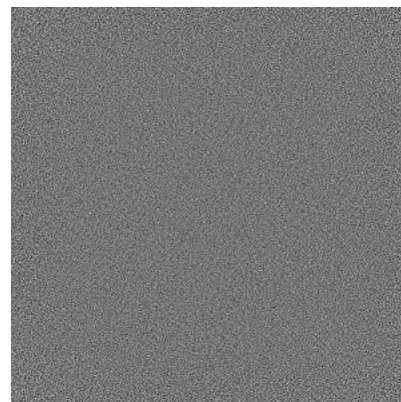
### 6.3.2 Raw map



X Index: 0



Y Index: 0

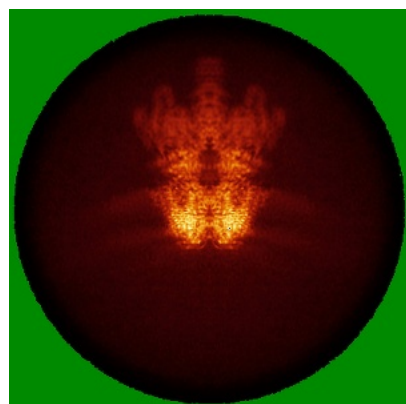


Z Index: 399

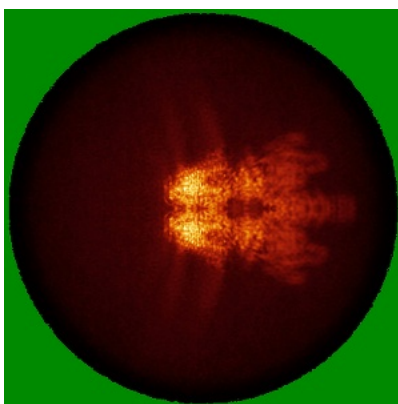
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

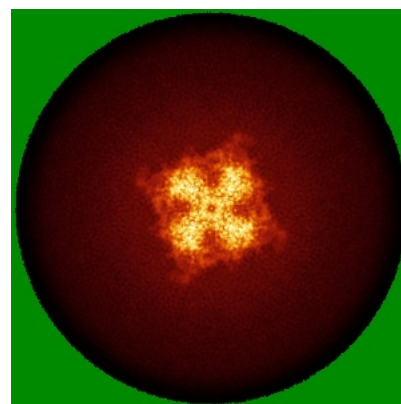
### 6.4.1 Primary map



X

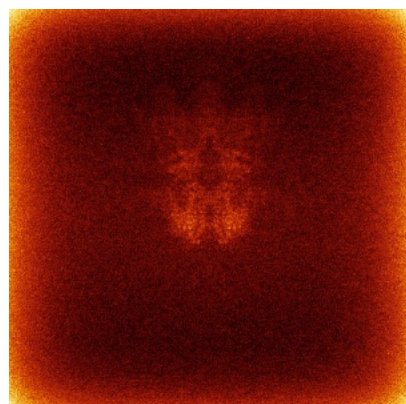


Y

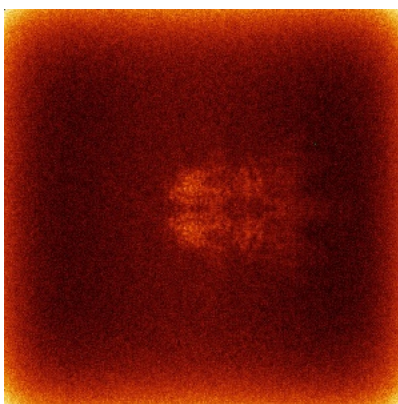


Z

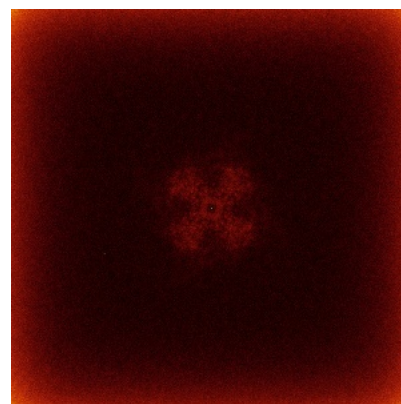
### 6.4.2 Raw map



X



Y

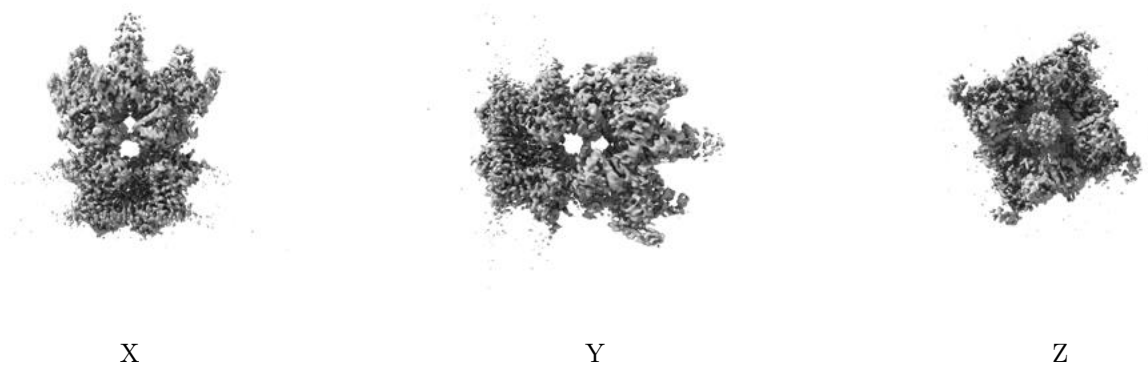


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

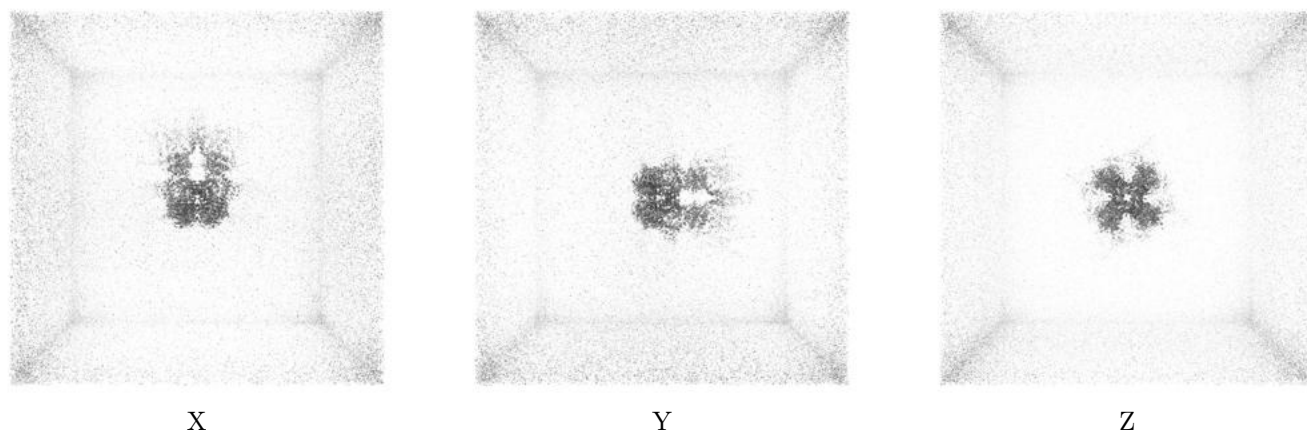
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

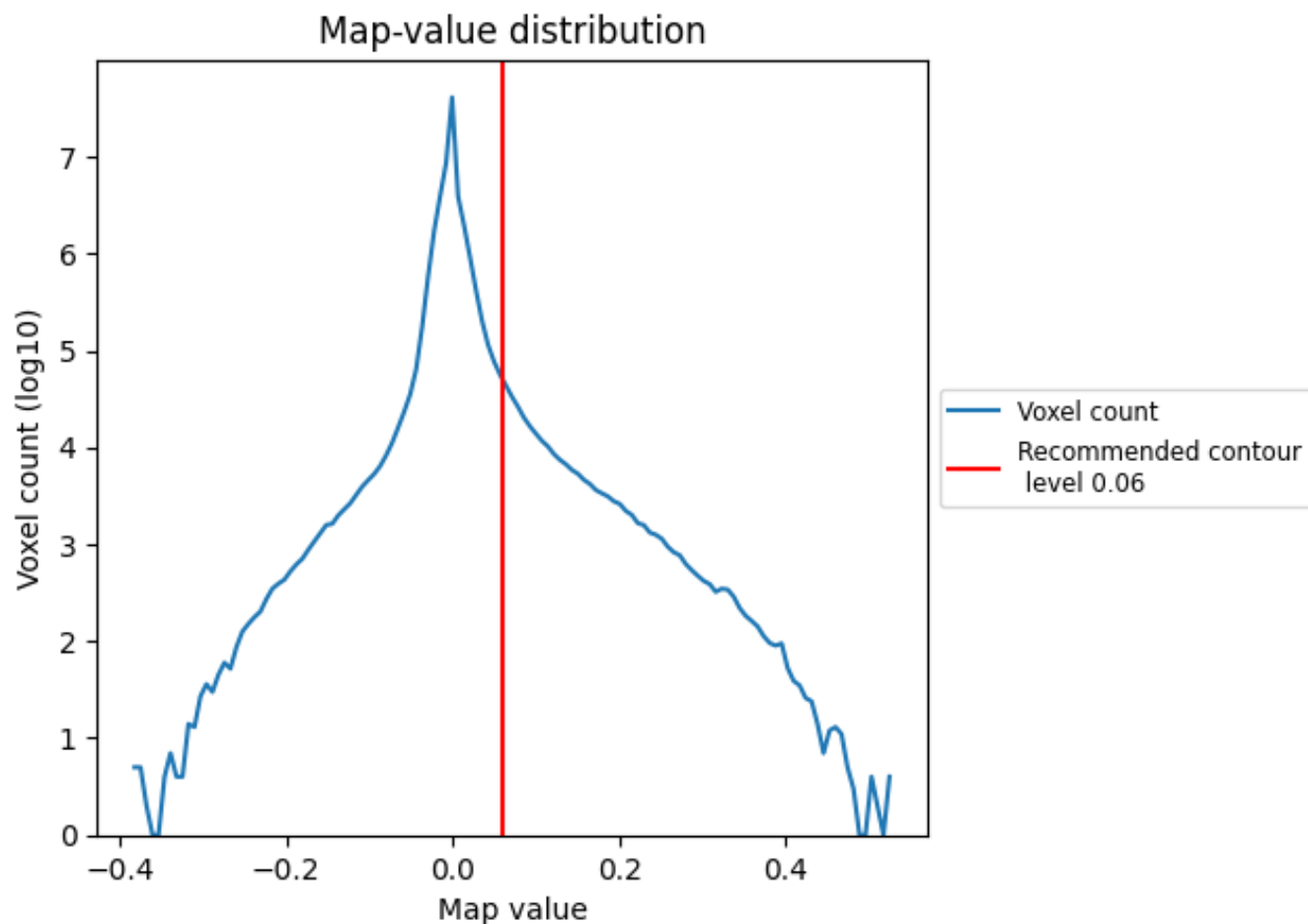
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

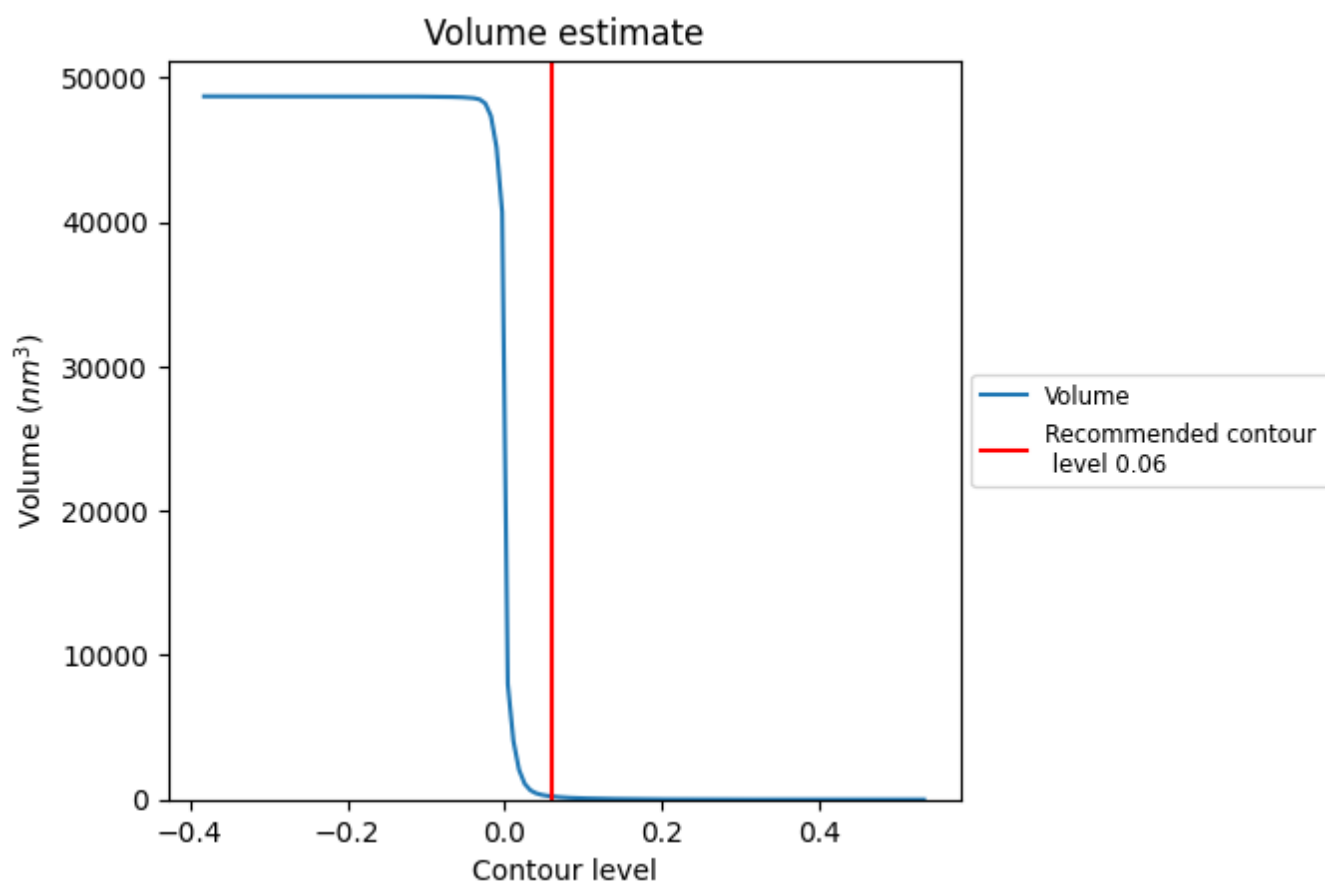
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

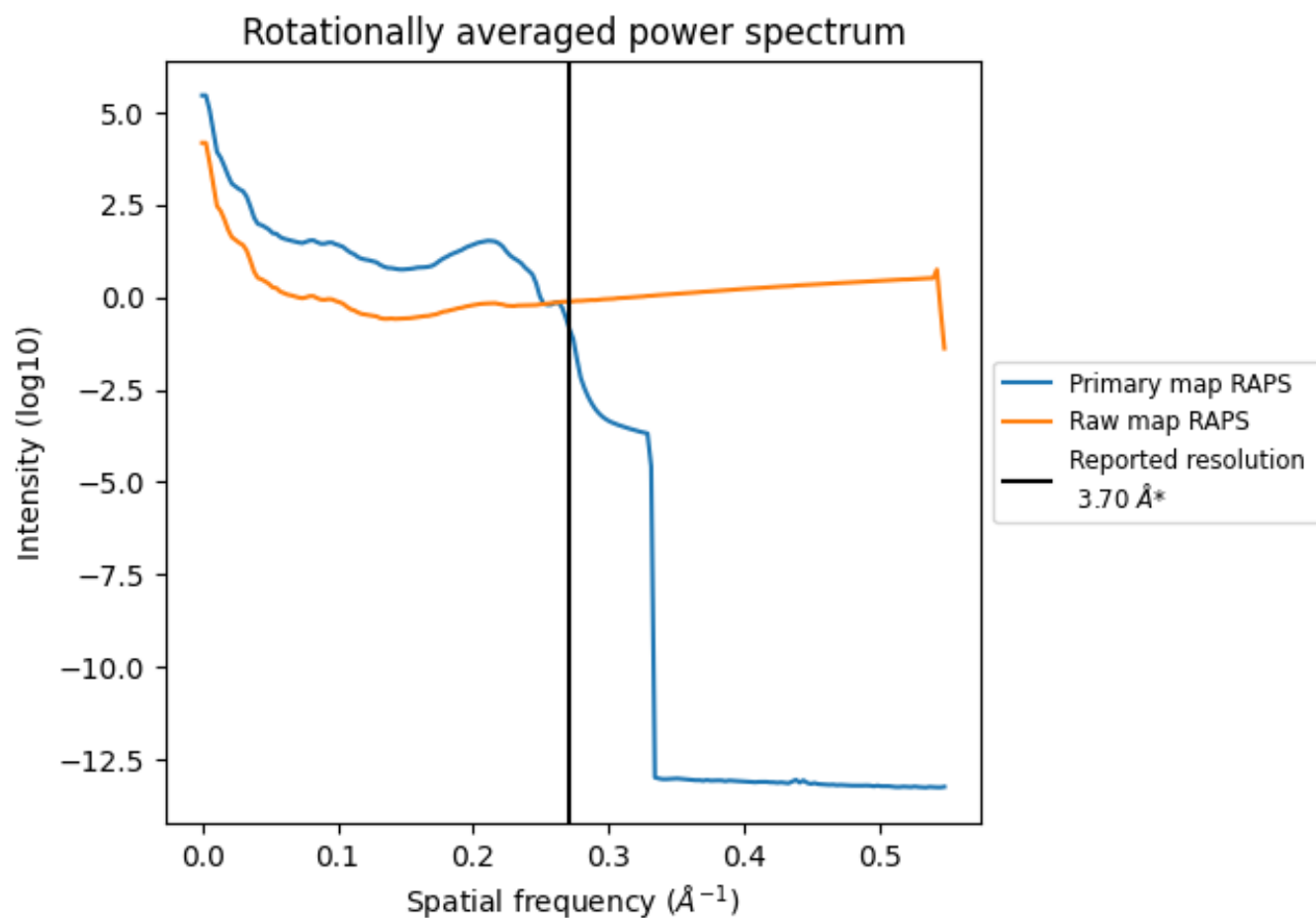
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm<sup>3</sup>; this corresponds to an approximate mass of 197 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

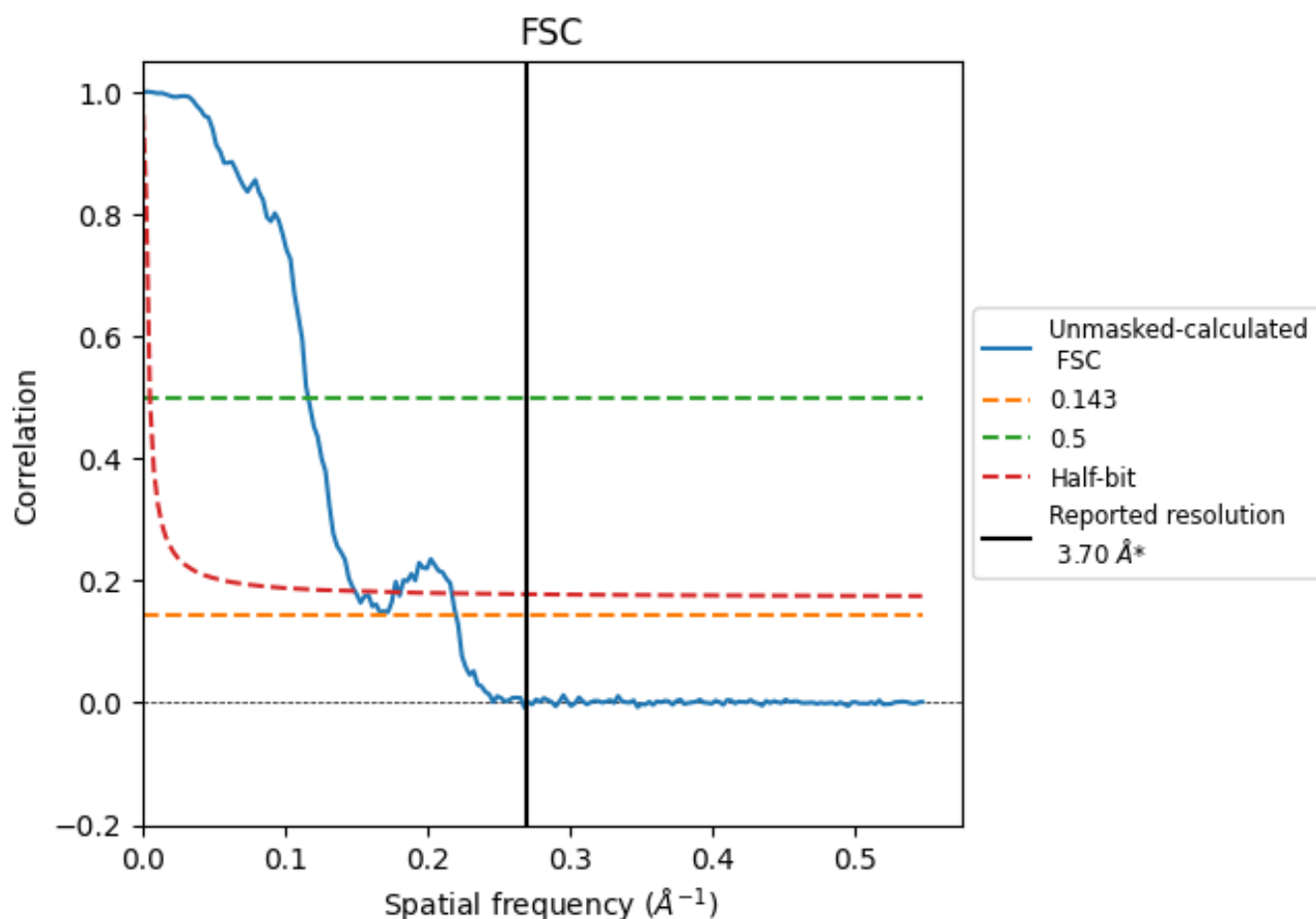


\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.270 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

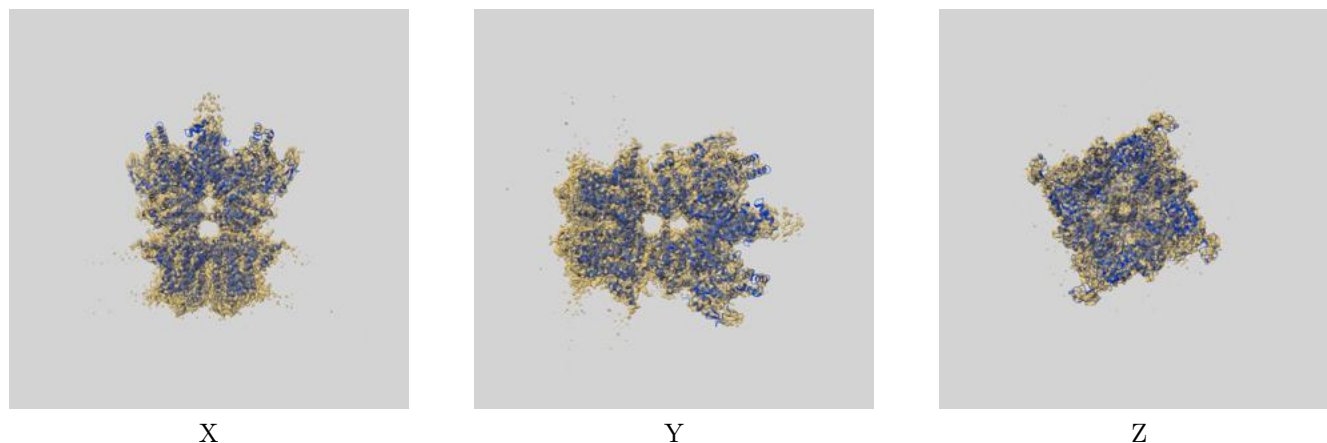
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.54                               | 8.58 | 6.69     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.54 differs from the reported value 3.7 by more than 10 %

## 9 Map-model fit [i](#)

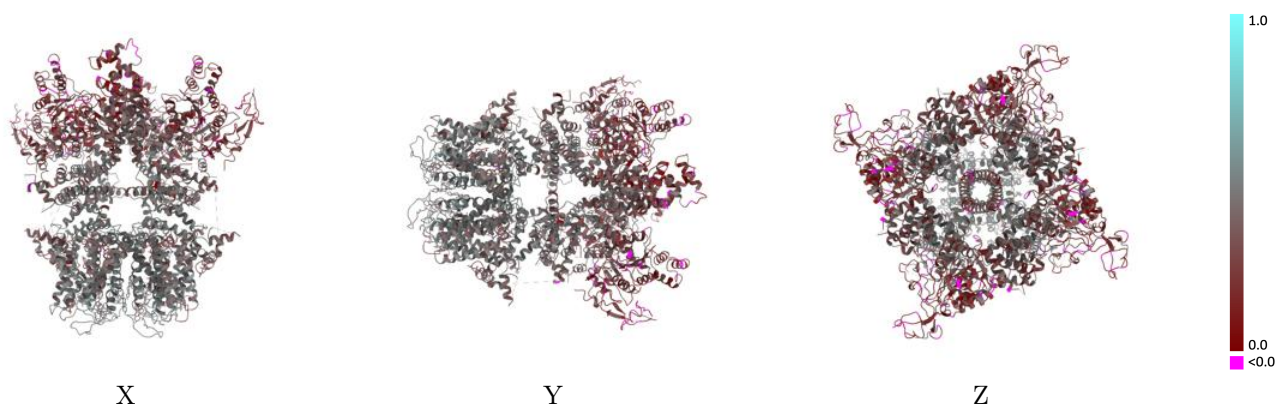
This section contains information regarding the fit between EMDB map EMD-57856 and PDB model 30KH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



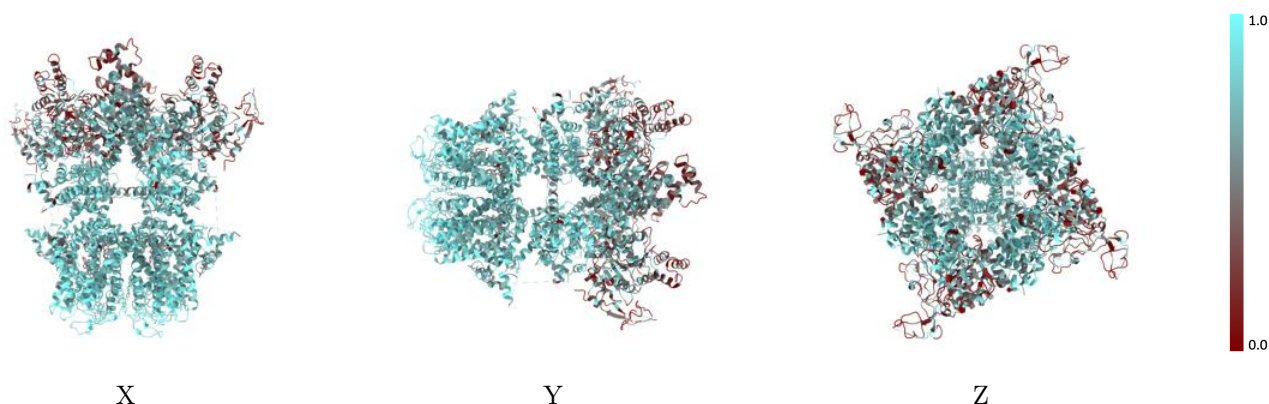
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



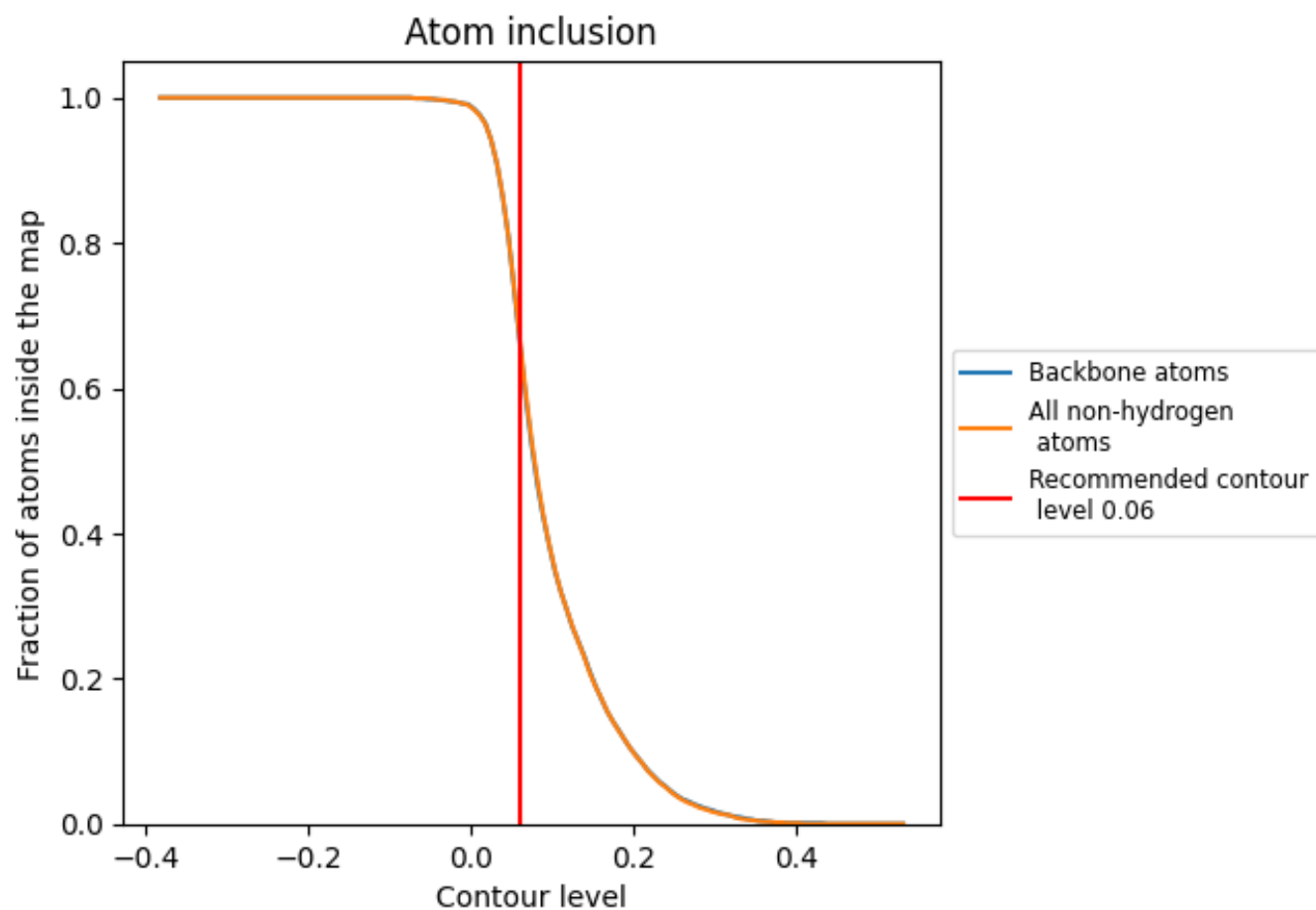
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6750 | <div></div> 0.3720 |
| A     | <div></div> 0.6850 | <div></div> 0.3740 |
| B     | <div></div> 0.6820 | <div></div> 0.3720 |
| C     | <div></div> 0.6850 | <div></div> 0.3700 |
| D     | <div></div> 0.6860 | <div></div> 0.3710 |

