



## Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:05 AM UTC

PDB ID : 7LQE / pdb\_00007lqe  
EMDB ID : EMD-23483  
Title : Cryo-EM of 1-protofilament of the KFE8 thinner nanotube  
Authors : Wang, F.; Gnewou, O.M.; Egelman, E.H.; Conticello, V.P.  
Deposited on : 2021-02-13  
Resolution : 3.40 Å(reported)

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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
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) : 2.49

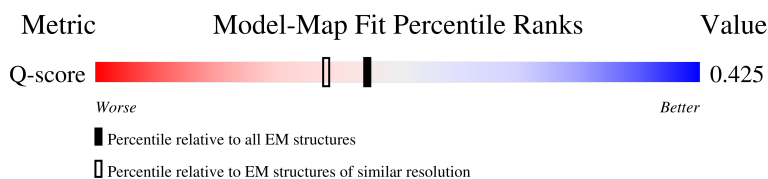
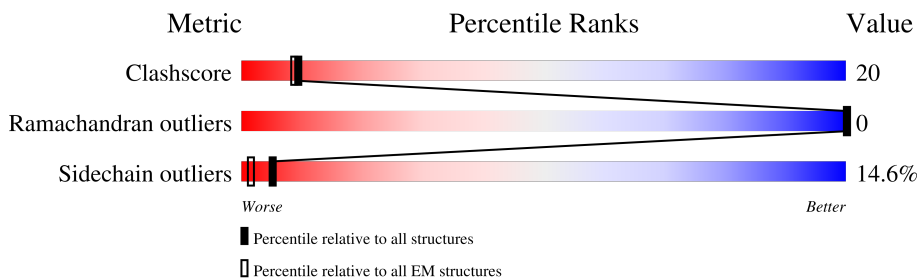
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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                       | 14717 ( 2.90 - 3.90 )                                    |

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   | 0     | 8      | <div> <div>50%</div> <div>25%</div> <div>75%</div> </div>                |
| 1   | 1     | 8      | <div> <div>50%</div> <div>88%</div> <div>12%</div> </div>                |
| 1   | 2     | 8      | <div> <div>50%</div> <div>25%</div> <div>50%</div> <div>25%</div> </div> |
| 1   | 3     | 8      | <div> <div>50%</div> <div>25%</div> <div>75%</div> </div>                |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 4     | 8      |                  |
| 1   | 5     | 8      |                  |
| 1   | 6     | 8      |                  |
| 1   | 7     | 8      |                  |
| 1   | 8     | 8      |                  |
| 1   | 9     | 8      |                  |
| 1   | A     | 8      |                  |
| 1   | AA    | 8      |                  |
| 1   | B     | 8      |                  |
| 1   | BA    | 8      |                  |
| 1   | C     | 8      |                  |
| 1   | CA    | 8      |                  |
| 1   | D     | 8      |                  |
| 1   | DA    | 8      |                  |
| 1   | E     | 8      |                  |
| 1   | EA    | 8      |                  |
| 1   | F     | 8      |                  |
| 1   | FA    | 8      |                  |
| 1   | G     | 8      |                  |
| 1   | GA    | 8      |                  |
| 1   | H     | 8      |                  |
| 1   | HA    | 8      |                  |
| 1   | I     | 8      |                  |
| 1   | IA    | 8      |                  |
| 1   | J     | 8      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | JA    | 8      |                  |
| 1   | K     | 8      |                  |
| 1   | L     | 8      |                  |
| 1   | M     | 8      |                  |
| 1   | N     | 8      |                  |
| 1   | O     | 8      |                  |
| 1   | P     | 8      |                  |
| 1   | Q     | 8      |                  |
| 1   | R     | 8      |                  |
| 1   | S     | 8      |                  |
| 1   | T     | 8      |                  |
| 1   | U     | 8      |                  |
| 1   | V     | 8      |                  |
| 1   | W     | 8      |                  |
| 1   | X     | 8      |                  |
| 1   | Y     | 8      |                  |
| 1   | Z     | 8      |                  |
| 1   | a     | 8      |                  |
| 1   | b     | 8      |                  |
| 1   | c     | 8      |                  |
| 1   | d     | 8      |                  |
| 1   | e     | 8      |                  |
| 1   | f     | 8      |                  |
| 1   | g     | 8      |                  |
| 1   | h     | 8      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | i     | 8      |                  |
| 1   | j     | 8      |                  |
| 1   | k     | 8      |                  |
| 1   | l     | 8      |                  |
| 1   | m     | 8      |                  |
| 1   | n     | 8      |                  |
| 1   | o     | 8      |                  |
| 1   | p     | 8      |                  |
| 1   | q     | 8      |                  |
| 1   | r     | 8      |                  |
| 1   | s     | 8      |                  |
| 1   | t     | 8      |                  |
| 1   | u     | 8      |                  |
| 1   | v     | 8      |                  |
| 1   | w     | 8      |                  |
| 1   | x     | 8      |                  |
| 1   | y     | 8      |                  |
| 1   | z     | 8      |                  |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6048 atoms, of which 0 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 KFE8 peptide.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | A     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | J     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | K     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | L     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | B     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | M     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | N     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | O     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | C     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | P     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | Q     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | R     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | D     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | S     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | T     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | U     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | E     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | V     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | W     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | X     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | F     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | Y     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | Z     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | j     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | G     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | k     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | l     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | m     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | H     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | n     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | o     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | p     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | I     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | q     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | r     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | s     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | a     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | t     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | u     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | v     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | b     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | w     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | x     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | y     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | c     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | z     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 0     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 1     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | d     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 2     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 3     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 4     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | e     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 5     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 6     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 7     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | f     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 8     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 9     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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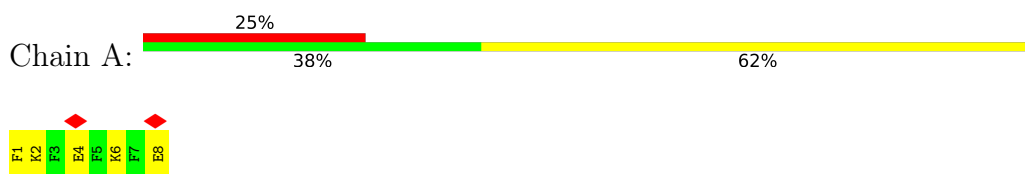
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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | AA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | g     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | BA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | CA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | DA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | h     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | EA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | FA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | GA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | i     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | HA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | IA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | JA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

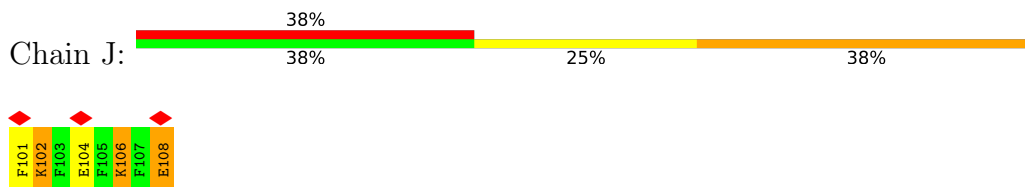
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

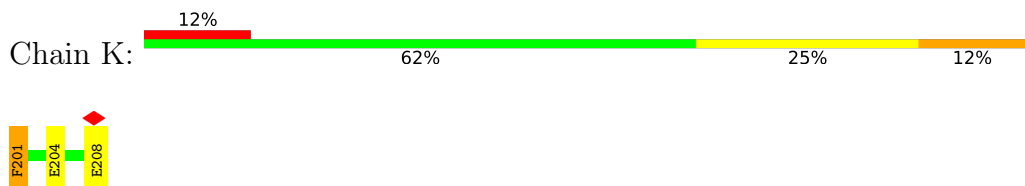
- Molecule 1: KFE8 peptide



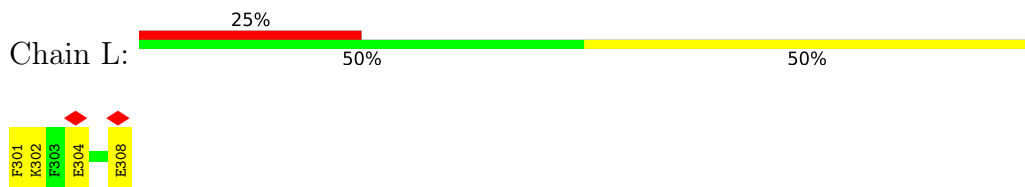
- Molecule 1: KFE8 peptide



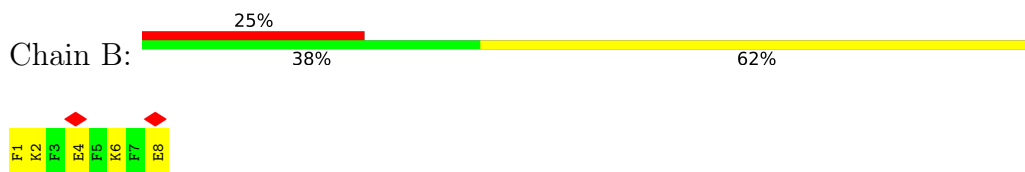
- Molecule 1: KFE8 peptide



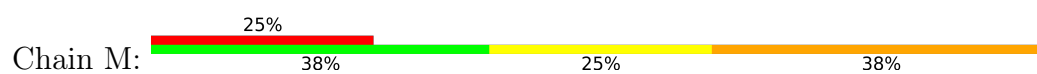
- Molecule 1: KFE8 peptide



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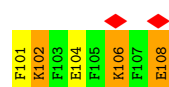
- Molecule 1: KFE8 peptide



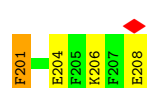
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



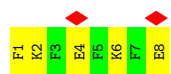
- Molecule 1: KFE8 peptide



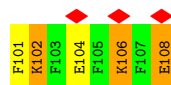
- Molecule 1: KFE8 peptide



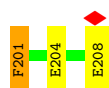
## ● Molecule 1: KFE8 peptide



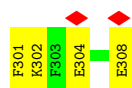
## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide



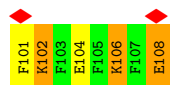
## ● Molecule 1: KFE8 peptide



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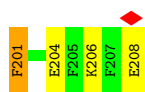


## ● Molecule 1: KFE8 peptide

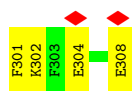


## ● Molecule 1: KFE8 peptide

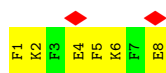




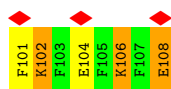
- Molecule 1: KFE8 peptide



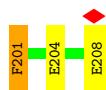
- Molecule 1: KFE8 peptide



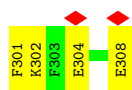
- Molecule 1: KFE8 peptide



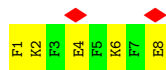
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



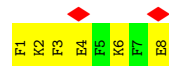
- Molecule 1: KFE8 peptide



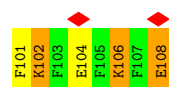
- Molecule 1: KFE8 peptide



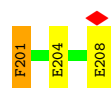
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



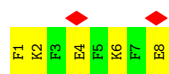
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



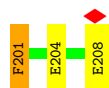
## ● Molecule 1: KFE8 peptide



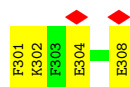
## ● Molecule 1: KFE8 peptide



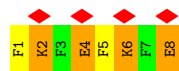
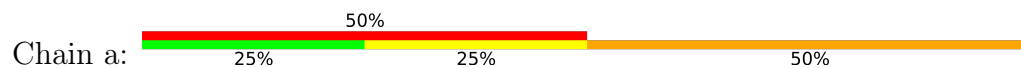
## ● Molecule 1: KFE8 peptide



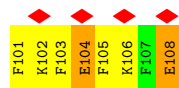
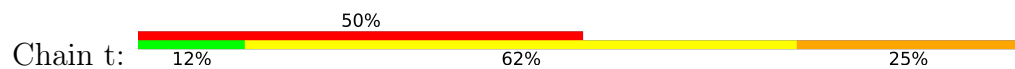
## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide

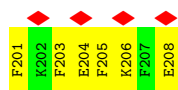


## ● Molecule 1: KFE8 peptide

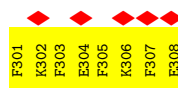


## ● Molecule 1: KFE8 peptide

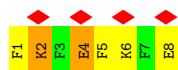




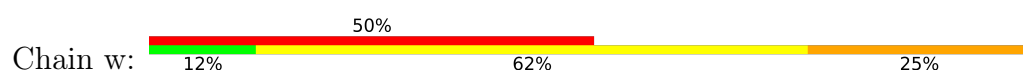
- Molecule 1: KFE8 peptide



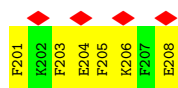
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



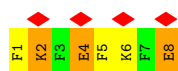
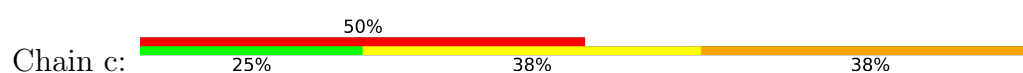
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

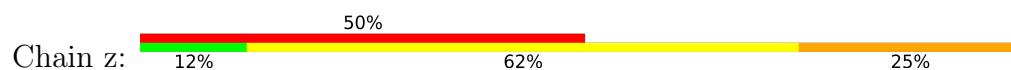


- Molecule 1: KFE8 peptide

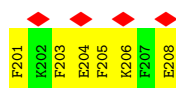


- Molecule 1: KFE8 peptide

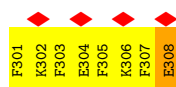
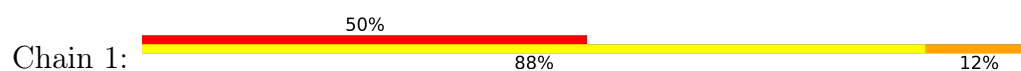




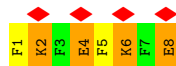
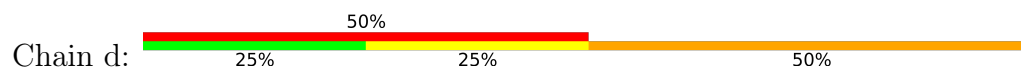
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



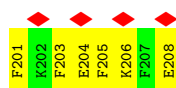
- Molecule 1: KFE8 peptide



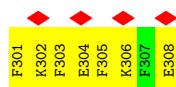
- Molecule 1: KFE8 peptide



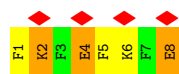
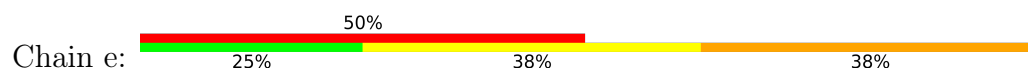
- Molecule 1: KFE8 peptide



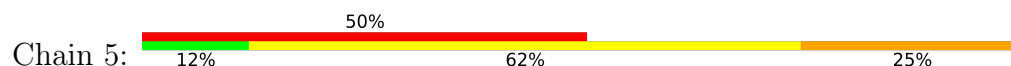
- Molecule 1: KFE8 peptide



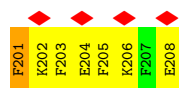
## ● Molecule 1: KFE8 peptide



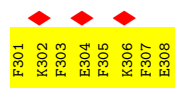
## ● Molecule 1: KFE8 peptide



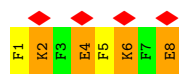
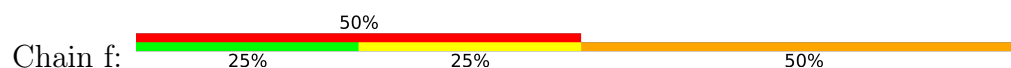
## ● Molecule 1: KFE8 peptide



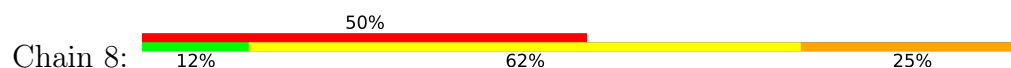
## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide

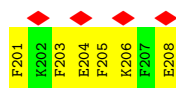


## ● Molecule 1: KFE8 peptide

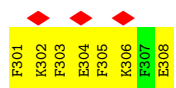


## ● Molecule 1: KFE8 peptide

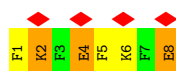
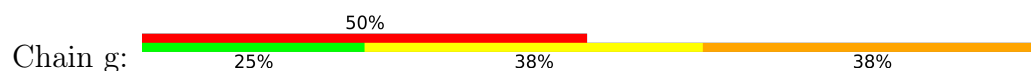




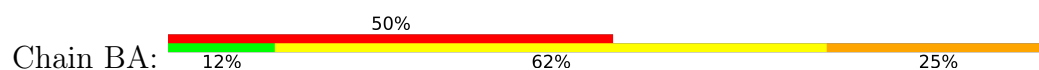
- Molecule 1: KFE8 peptide



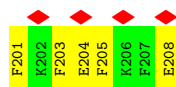
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



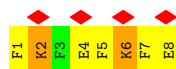
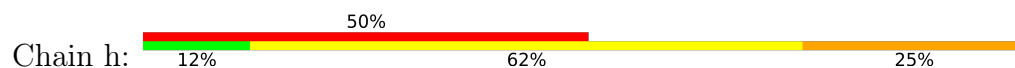
- Molecule 1: KFE8 peptide



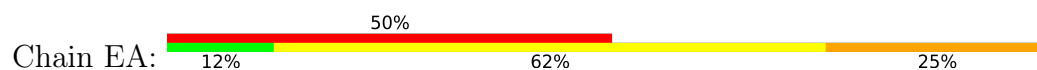
- Molecule 1: KFE8 peptide



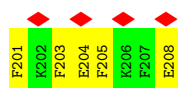
- Molecule 1: KFE8 peptide



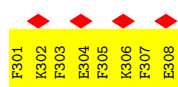
- Molecule 1: KFE8 peptide



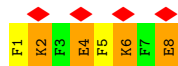
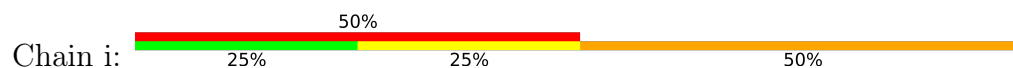
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



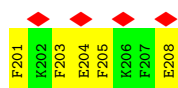
- Molecule 1: KFE8 peptide



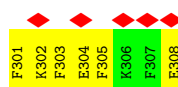
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



## 4 Experimental information

| Property                           | Value                                            | Source    |
|------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                          | Depositor |
| Imposed symmetry                   | HELICAL, twist=-15.8°, rise=7.93 Å, axial sym=C1 | Depositor |
| Number of segments used            | 64959                                            | Depositor |
| Resolution determination method    | OTHER                                            | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION          | Depositor |
| Microscope                         | FEI TITAN KRIOS                                  | Depositor |
| Voltage (kV)                       | 300                                              | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 50                                               | Depositor |
| Minimum defocus (nm)               | Not provided                                     |           |
| Maximum defocus (nm)               | Not provided                                     |           |
| Magnification                      | Not provided                                     |           |
| Image detector                     | GATAN K3 (6k x 4k)                               | Depositor |
| Maximum map value                  | 1.010                                            | Depositor |
| Minimum map value                  | -0.000                                           | Depositor |
| Average map value                  | 0.002                                            | Depositor |
| Map value standard deviation       | 0.026                                            | Depositor |
| Recommended contour level          | 0.264                                            | Depositor |
| Map size (Å)                       | 345.6, 345.6, 345.6                              | wwPDB     |
| Map dimensions                     | 320, 320, 320                                    | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                  | 1.08, 1.08, 1.08                                 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GMA, 5CR

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   | 0     | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | 1     | 0.32         | 0/62        | 0.39        | 0/79        |
| 1   | 2     | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | 3     | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | 4     | 0.32         | 0/62        | 0.39        | 0/79        |
| 1   | 5     | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | 6     | 0.32         | 0/62        | 0.46        | 0/79        |
| 1   | 7     | 0.32         | 0/62        | 0.39        | 0/79        |
| 1   | 8     | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | 9     | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | A     | 0.40         | 0/62        | 0.42        | 0/79        |
| 1   | AA    | 0.33         | 0/62        | 0.39        | 0/79        |
| 1   | B     | 0.40         | 0/62        | 0.42        | 0/79        |
| 1   | BA    | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | C     | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | CA    | 0.31         | 0/62        | 0.45        | 0/79        |
| 1   | D     | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | DA    | 0.33         | 0/62        | 0.39        | 0/79        |
| 1   | E     | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | EA    | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | F     | 0.40         | 0/62        | 0.42        | 0/79        |
| 1   | FA    | 0.32         | 0/62        | 0.46        | 0/79        |
| 1   | G     | 0.40         | 0/62        | 0.42        | 0/79        |
| 1   | GA    | 0.32         | 0/62        | 0.39        | 0/79        |
| 1   | H     | 0.40         | 0/62        | 0.42        | 0/79        |
| 1   | HA    | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | I     | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | IA    | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | J     | 0.38         | 0/62        | 0.38        | 0/79        |
| 1   | JA    | 0.32         | 0/62        | 0.39        | 0/79        |
| 1   | K     | 0.43         | 0/62        | 0.45        | 0/79        |
| 1   | L     | 0.39         | 0/62        | 0.33        | 0/79        |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | M     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | N     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | O     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | P     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | Q     | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | R     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | S     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | T     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | U     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | V     | 0.38         | 0/62    | 0.37        | 0/79    |
| 1   | W     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | X     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | Y     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | Z     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | a     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | b     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | c     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | d     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | e     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | f     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | g     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | h     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | i     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | j     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | k     | 0.39         | 0/62    | 0.38        | 0/79    |
| 1   | l     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | m     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | n     | 0.38         | 0/62    | 0.37        | 0/79    |
| 1   | o     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | p     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | q     | 0.39         | 0/62    | 0.38        | 0/79    |
| 1   | r     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | s     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | t     | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | u     | 0.32         | 0/62    | 0.46        | 0/79    |
| 1   | v     | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | w     | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | x     | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | y     | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | z     | 0.30         | 0/62    | 0.43        | 0/79    |
| All | All   | 0.36         | 0/4464  | 0.44        | 0/5688  |

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

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   | 0     | 84    | 0        | 63       | 4       | 0            |
| 1   | 1     | 84    | 0        | 63       | 10      | 0            |
| 1   | 2     | 84    | 0        | 62       | 4       | 0            |
| 1   | 3     | 84    | 0        | 63       | 6       | 0            |
| 1   | 4     | 84    | 0        | 63       | 8       | 0            |
| 1   | 5     | 84    | 0        | 62       | 6       | 0            |
| 1   | 6     | 84    | 0        | 63       | 9       | 0            |
| 1   | 7     | 84    | 0        | 63       | 5       | 0            |
| 1   | 8     | 84    | 0        | 62       | 5       | 0            |
| 1   | 9     | 84    | 0        | 63       | 4       | 0            |
| 1   | A     | 84    | 0        | 63       | 7       | 0            |
| 1   | AA    | 84    | 0        | 63       | 7       | 0            |
| 1   | B     | 84    | 0        | 63       | 7       | 0            |
| 1   | BA    | 84    | 0        | 62       | 6       | 0            |
| 1   | C     | 84    | 0        | 63       | 7       | 0            |
| 1   | CA    | 84    | 0        | 63       | 3       | 0            |
| 1   | D     | 84    | 0        | 63       | 7       | 0            |
| 1   | DA    | 84    | 0        | 63       | 6       | 0            |
| 1   | E     | 84    | 0        | 63       | 7       | 0            |
| 1   | EA    | 84    | 0        | 62       | 7       | 0            |
| 1   | F     | 84    | 0        | 63       | 8       | 0            |
| 1   | FA    | 84    | 0        | 63       | 3       | 0            |
| 1   | G     | 84    | 0        | 63       | 7       | 0            |
| 1   | GA    | 84    | 0        | 63       | 6       | 0            |
| 1   | H     | 84    | 0        | 63       | 6       | 0            |
| 1   | HA    | 84    | 0        | 62       | 2       | 0            |
| 1   | I     | 84    | 0        | 63       | 7       | 0            |
| 1   | IA    | 84    | 0        | 63       | 5       | 0            |
| 1   | J     | 84    | 0        | 63       | 7       | 0            |
| 1   | JA    | 84    | 0        | 63       | 4       | 0            |
| 1   | K     | 84    | 0        | 63       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | L     | 84    | 0        | 63       | 1       | 0            |
| 1   | M     | 84    | 0        | 63       | 7       | 0            |
| 1   | N     | 84    | 0        | 63       | 3       | 0            |
| 1   | O     | 84    | 0        | 63       | 1       | 0            |
| 1   | P     | 84    | 0        | 63       | 8       | 0            |
| 1   | Q     | 84    | 0        | 63       | 3       | 0            |
| 1   | R     | 84    | 0        | 63       | 1       | 0            |
| 1   | S     | 84    | 0        | 63       | 8       | 0            |
| 1   | T     | 84    | 0        | 63       | 2       | 0            |
| 1   | U     | 84    | 0        | 63       | 1       | 0            |
| 1   | V     | 84    | 0        | 63       | 8       | 0            |
| 1   | W     | 84    | 0        | 63       | 3       | 0            |
| 1   | X     | 84    | 0        | 63       | 1       | 0            |
| 1   | Y     | 84    | 0        | 63       | 7       | 0            |
| 1   | Z     | 84    | 0        | 63       | 2       | 0            |
| 1   | a     | 84    | 0        | 63       | 6       | 0            |
| 1   | b     | 84    | 0        | 63       | 4       | 0            |
| 1   | c     | 84    | 0        | 63       | 5       | 0            |
| 1   | d     | 84    | 0        | 63       | 6       | 0            |
| 1   | e     | 84    | 0        | 63       | 5       | 0            |
| 1   | f     | 84    | 0        | 63       | 7       | 0            |
| 1   | g     | 84    | 0        | 63       | 6       | 0            |
| 1   | h     | 84    | 0        | 63       | 4       | 0            |
| 1   | i     | 84    | 0        | 63       | 6       | 0            |
| 1   | j     | 84    | 0        | 63       | 1       | 0            |
| 1   | k     | 84    | 0        | 63       | 8       | 0            |
| 1   | l     | 84    | 0        | 63       | 3       | 0            |
| 1   | m     | 84    | 0        | 63       | 1       | 0            |
| 1   | n     | 84    | 0        | 63       | 8       | 0            |
| 1   | o     | 84    | 0        | 63       | 2       | 0            |
| 1   | p     | 84    | 0        | 63       | 1       | 0            |
| 1   | q     | 84    | 0        | 63       | 6       | 0            |
| 1   | r     | 84    | 0        | 63       | 2       | 0            |
| 1   | s     | 84    | 0        | 63       | 1       | 0            |
| 1   | t     | 84    | 0        | 62       | 5       | 0            |
| 1   | u     | 84    | 0        | 63       | 4       | 0            |
| 1   | v     | 84    | 0        | 63       | 6       | 0            |
| 1   | w     | 84    | 0        | 62       | 5       | 0            |
| 1   | x     | 84    | 0        | 63       | 7       | 0            |
| 1   | y     | 84    | 0        | 63       | 5       | 0            |
| 1   | z     | 84    | 0        | 62       | 5       | 0            |
| All | All   | 6048  | 0        | 4527     | 214     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (214) 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:f:4:GLU:HB3    | 1:EA:106:LYS:HB3 | 1.58                     | 0.83              |
| 1:BA:106:LYS:HB3 | 1:i:4:GLU:HB3    | 1.66                     | 0.76              |
| 1:DA:302:LYS:HZ3 | 1:DA:304:GLU:HB2 | 1.51                     | 0.76              |
| 1:y:302:LYS:HZ1  | 1:y:304:GLU:HB2  | 1.51                     | 0.76              |
| 1:4:302:LYS:HZ1  | 1:4:304:GLU:HB2  | 1.51                     | 0.76              |
| 1:IA:205:PHE:HB3 | 1:JA:303:PHE:HB3 | 1.68                     | 0.76              |
| 1:CA:205:PHE:HB3 | 1:DA:303:PHE:HB3 | 1.68                     | 0.75              |
| 1:0:205:PHE:HB3  | 1:1:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:9:205:PHE:HB3  | 1:AA:303:PHE:HB3 | 1.68                     | 0.75              |
| 1:u:205:PHE:HB3  | 1:v:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:3:205:PHE:HB3  | 1:4:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:GA:302:LYS:HZ1 | 1:GA:304:GLU:HB2 | 1.51                     | 0.74              |
| 1:JA:302:LYS:HZ1 | 1:JA:304:GLU:HB2 | 1.52                     | 0.74              |
| 1:5:106:LYS:HB3  | 1:g:4:GLU:HB3    | 1.68                     | 0.74              |
| 1:7:302:LYS:HZ1  | 1:7:304:GLU:HB2  | 1.52                     | 0.74              |
| 1:6:205:PHE:HB3  | 1:7:303:PHE:HB3  | 1.68                     | 0.74              |
| 1:x:205:PHE:HB3  | 1:y:303:PHE:HB3  | 1.68                     | 0.74              |
| 1:FA:205:PHE:HB3 | 1:GA:303:PHE:HB3 | 1.68                     | 0.74              |
| 1:t:106:LYS:HB3  | 1:c:4:GLU:HB3    | 1.68                     | 0.73              |
| 1:v:302:LYS:HZ1  | 1:v:304:GLU:HB2  | 1.52                     | 0.73              |
| 1:CA:203:PHE:HB3 | 1:DA:305:PHE:HB3 | 1.71                     | 0.73              |
| 1:x:203:PHE:HB3  | 1:y:305:PHE:HB3  | 1.71                     | 0.73              |
| 1:0:203:PHE:HB3  | 1:1:305:PHE:HB3  | 1.71                     | 0.73              |
| 1:9:203:PHE:HB3  | 1:AA:305:PHE:HB3 | 1.71                     | 0.73              |
| 1:a:4:GLU:HB3    | 1:w:106:LYS:HB3  | 1.70                     | 0.72              |
| 1:AA:302:LYS:HZ1 | 1:AA:304:GLU:HB2 | 1.54                     | 0.72              |
| 1:6:203:PHE:HB3  | 1:7:305:PHE:HB3  | 1.71                     | 0.71              |
| 1:e:5:PHE:HB3    | 1:5:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:a:5:PHE:HB3    | 1:t:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:f:5:PHE:HB3    | 1:8:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:IA:203:PHE:HB3 | 1:JA:305:PHE:HB3 | 1.71                     | 0.71              |
| 1:i:5:PHE:HB3    | 1:HA:103:PHE:HB3 | 1.73                     | 0.71              |
| 1:u:203:PHE:HB3  | 1:v:305:PHE:HB3  | 1.71                     | 0.71              |
| 1:FA:203:PHE:HB3 | 1:GA:305:PHE:HB3 | 1.71                     | 0.71              |
| 1:b:5:PHE:HB3    | 1:w:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:d:5:PHE:HB3    | 1:2:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:3:203:PHE:HB3  | 1:4:305:PHE:HB3  | 1.71                     | 0.70              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:f:2:LYS:H     | 1:EA:108:GMA:HB2 | 1.55                     | 0.70              |
| 1:h:5:PHE:HB3   | 1:EA:103:PHE:HB3 | 1.73                     | 0.70              |
| 1:g:5:PHE:HB3   | 1:BA:103:PHE:HB3 | 1.73                     | 0.70              |
| 1:c:5:PHE:HB3   | 1:z:103:PHE:HB3  | 1.73                     | 0.70              |
| 1:d:4:GLU:HB3   | 1:8:106:LYS:HB3  | 1.72                     | 0.69              |
| 1:1:302:LYS:HZ1 | 1:1:304:GLU:HB2  | 1.56                     | 0.69              |
| 1:A:6:LYS:HG2   | 1:J:106:LYS:HB2  | 1.76                     | 0.68              |
| 1:B:6:LYS:HG2   | 1:M:106:LYS:HB2  | 1.76                     | 0.68              |
| 1:C:6:LYS:HG2   | 1:P:106:LYS:HB2  | 1.76                     | 0.68              |
| 1:D:6:LYS:HG2   | 1:S:106:LYS:HB2  | 1.76                     | 0.68              |
| 1:E:6:LYS:HG2   | 1:V:106:LYS:HB2  | 1.76                     | 0.67              |
| 1:G:6:LYS:HG2   | 1:k:106:LYS:HB2  | 1.76                     | 0.67              |
| 1:F:6:LYS:HG2   | 1:Y:106:LYS:HB2  | 1.76                     | 0.67              |
| 1:I:6:LYS:HG2   | 1:q:106:LYS:HB2  | 1.76                     | 0.67              |
| 1:H:6:LYS:HG2   | 1:n:106:LYS:HB2  | 1.76                     | 0.67              |
| 1:P:106:LYS:HD3 | 1:E:6:LYS:HE3    | 1.79                     | 0.63              |
| 1:F:6:LYS:HE3   | 1:n:106:LYS:HD3  | 1.80                     | 0.63              |
| 1:B:6:LYS:HE3   | 1:S:106:LYS:HD3  | 1.80                     | 0.62              |
| 1:D:6:LYS:HE3   | 1:Y:106:LYS:HD3  | 1.80                     | 0.62              |
| 1:t:108:GMA:HB2 | 1:c:2:LYS:H      | 1.63                     | 0.62              |
| 1:5:108:GMA:HB2 | 1:g:2:LYS:H      | 1.64                     | 0.62              |
| 1:A:6:LYS:HE3   | 1:M:106:LYS:HD3  | 1.80                     | 0.62              |
| 1:b:4:GLU:HB3   | 1:2:106:LYS:HB3  | 1.81                     | 0.62              |
| 1:V:106:LYS:HD3 | 1:G:6:LYS:HE3    | 1.80                     | 0.62              |
| 1:k:106:LYS:HD3 | 1:I:6:LYS:HE3    | 1.81                     | 0.62              |
| 1:J:106:LYS:HD3 | 1:C:6:LYS:HE3    | 1.80                     | 0.61              |
| 1:H:2:LYS:HE3   | 1:n:102:LYS:HE3  | 1.82                     | 0.61              |
| 1:z:106:LYS:HB3 | 1:e:4:GLU:HB3    | 1.83                     | 0.61              |
| 1:D:2:LYS:HE3   | 1:S:102:LYS:HE3  | 1.82                     | 0.60              |
| 1:F:2:LYS:HE3   | 1:Y:102:LYS:HE3  | 1.82                     | 0.60              |
| 1:E:2:LYS:HE3   | 1:V:102:LYS:HE3  | 1.82                     | 0.60              |
| 1:I:2:LYS:HE3   | 1:q:102:LYS:HE3  | 1.82                     | 0.60              |
| 1:A:2:LYS:HE3   | 1:J:102:LYS:HE3  | 1.82                     | 0.60              |
| 1:B:2:LYS:HE3   | 1:M:102:LYS:HE3  | 1.82                     | 0.59              |
| 1:C:2:LYS:HE3   | 1:P:102:LYS:HE3  | 1.82                     | 0.59              |
| 1:G:2:LYS:HE3   | 1:k:102:LYS:HE3  | 1.82                     | 0.59              |
| 1:d:2:LYS:H     | 1:8:108:GMA:HB2  | 1.66                     | 0.59              |
| 1:5:102:LYS:HB3 | 1:g:8:GMA:HB3    | 1.83                     | 0.59              |
| 1:o:204:GLU:HA  | 1:p:304:GLU:HB2  | 1.85                     | 0.59              |
| 1:Z:204:GLU:HA  | 1:j:304:GLU:HB2  | 1.85                     | 0.58              |
| 1:T:204:GLU:HA  | 1:U:304:GLU:HB2  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:4:GLU:HA     | 1:n:104:GLU:HB2  | 1.86                     | 0.58              |
| 1:k:102:LYS:HG3  | 1:I:2:LYS:HB3    | 1.85                     | 0.58              |
| 1:N:204:GLU:HA   | 1:O:304:GLU:HB2  | 1.85                     | 0.58              |
| 1:l:204:GLU:HA   | 1:m:304:GLU:HB2  | 1.85                     | 0.58              |
| 1:a:2:LYS:H      | 1:w:108:GMA:HB2  | 1.67                     | 0.58              |
| 1:F:4:GLU:HA     | 1:Y:104:GLU:HB2  | 1.86                     | 0.58              |
| 1:r:204:GLU:HA   | 1:s:304:GLU:HB2  | 1.85                     | 0.58              |
| 1:B:4:GLU:HA     | 1:M:104:GLU:HB2  | 1.86                     | 0.58              |
| 1:Q:204:GLU:HA   | 1:R:304:GLU:HB2  | 1.85                     | 0.58              |
| 1:K:204:GLU:HA   | 1:L:304:GLU:HB2  | 1.85                     | 0.57              |
| 1:D:4:GLU:HA     | 1:S:104:GLU:HB2  | 1.86                     | 0.57              |
| 1:V:102:LYS:HG3  | 1:G:2:LYS:HB3    | 1.85                     | 0.57              |
| 1:W:204:GLU:HA   | 1:X:304:GLU:HB2  | 1.85                     | 0.57              |
| 1:A:4:GLU:HA     | 1:J:104:GLU:HB2  | 1.86                     | 0.57              |
| 1:1:305:PHE:HE1  | 1:6:203:PHE:CZ   | 2.22                     | 0.57              |
| 1:C:4:GLU:HA     | 1:P:104:GLU:HB2  | 1.86                     | 0.57              |
| 1:A:2:LYS:HB3    | 1:M:102:LYS:HG3  | 1.86                     | 0.56              |
| 1:E:4:GLU:HA     | 1:V:104:GLU:HB2  | 1.86                     | 0.56              |
| 1:G:4:GLU:HA     | 1:k:104:GLU:HB2  | 1.86                     | 0.56              |
| 1:BA:108:GMA:HB2 | 1:i:2:LYS:H      | 1.71                     | 0.56              |
| 1:I:4:GLU:HA     | 1:q:104:GLU:HB2  | 1.86                     | 0.56              |
| 1:f:8:GMA:HB3    | 1:EA:102:LYS:HB3 | 1.88                     | 0.56              |
| 1:F:2:LYS:HB3    | 1:n:102:LYS:HG3  | 1.87                     | 0.55              |
| 1:D:2:LYS:HB3    | 1:Y:102:LYS:HG3  | 1.87                     | 0.55              |
| 1:b:2:LYS:H      | 1:2:108:GMA:HB2  | 1.71                     | 0.54              |
| 1:1:305:PHE:HE1  | 1:6:203:PHE:CE1  | 2.26                     | 0.54              |
| 1:J:102:LYS:HG3  | 1:C:2:LYS:HB3    | 1.87                     | 0.54              |
| 1:a:8:GMA:HB3    | 1:w:102:LYS:HB3  | 1.90                     | 0.54              |
| 1:z:108:GMA:HB2  | 1:e:2:LYS:H      | 1.73                     | 0.54              |
| 1:B:2:LYS:HB3    | 1:S:102:LYS:HG3  | 1.88                     | 0.54              |
| 1:D:4:GLU:OE1    | 1:D:4:GLU:N      | 2.42                     | 0.53              |
| 1:C:4:GLU:N      | 1:C:4:GLU:OE1    | 2.42                     | 0.53              |
| 1:G:4:GLU:OE1    | 1:G:4:GLU:N      | 2.42                     | 0.53              |
| 1:B:4:GLU:OE1    | 1:B:4:GLU:N      | 2.42                     | 0.53              |
| 1:A:4:GLU:N      | 1:A:4:GLU:OE1    | 2.42                     | 0.52              |
| 1:H:4:GLU:N      | 1:H:4:GLU:OE1    | 2.42                     | 0.52              |
| 1:F:4:GLU:N      | 1:F:4:GLU:OE1    | 2.42                     | 0.52              |
| 1:1:306:LYS:HB3  | 1:6:204:GLU:HB3  | 1.92                     | 0.52              |
| 1:E:4:GLU:N      | 1:E:4:GLU:OE1    | 2.42                     | 0.52              |
| 1:O:204:GLU:OE2  | 1:O:205:PHE:N    | 2.43                     | 0.52              |
| 1:CA:204:GLU:OE2 | 1:CA:205:PHE:N   | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:FA:204:GLU:OE2 | 1:FA:205:PHE:N   | 2.43                     | 0.52              |
| 1:I:4:GLU:OE1    | 1:I:4:GLU:N      | 2.42                     | 0.52              |
| 1:3:204:GLU:OE2  | 1:3:205:PHE:N    | 2.43                     | 0.51              |
| 1:9:204:GLU:OE2  | 1:9:205:PHE:N    | 2.43                     | 0.51              |
| 1:x:204:GLU:OE2  | 1:x:205:PHE:N    | 2.43                     | 0.51              |
| 1:IA:204:GLU:OE2 | 1:IA:205:PHE:N   | 2.43                     | 0.51              |
| 1:6:204:GLU:OE2  | 1:6:205:PHE:N    | 2.43                     | 0.51              |
| 1:D:6:LYS:HG2    | 1:S:106:LYS:CB   | 2.41                     | 0.51              |
| 1:B:6:LYS:HG2    | 1:M:106:LYS:CB   | 2.41                     | 0.51              |
| 1:u:204:GLU:OE2  | 1:u:205:PHE:N    | 2.43                     | 0.51              |
| 1:A:6:LYS:HG2    | 1:J:106:LYS:CB   | 2.41                     | 0.51              |
| 1:F:6:LYS:HG2    | 1:Y:106:LYS:CB   | 2.41                     | 0.51              |
| 1:H:6:LYS:HG2    | 1:n:106:LYS:CB   | 2.41                     | 0.51              |
| 1:x:203:PHE:CZ   | 1:4:305:PHE:HE1  | 2.30                     | 0.50              |
| 1:d:8:GMA:HB3    | 1:8:102:LYS:HB3  | 1.93                     | 0.50              |
| 1:BA:102:LYS:HB3 | 1:i:8:GMA:HB3    | 1.92                     | 0.50              |
| 1:I:6:LYS:HG2    | 1:q:106:LYS:CB   | 2.41                     | 0.50              |
| 1:G:6:LYS:HG2    | 1:k:106:LYS:CB   | 2.41                     | 0.50              |
| 1:1:304:GLU:HB3  | 1:6:206:LYS:HB3  | 1.93                     | 0.49              |
| 1:P:102:LYS:HG3  | 1:E:2:LYS:HB3    | 1.93                     | 0.49              |
| 1:E:6:LYS:HG2    | 1:V:106:LYS:CB   | 2.41                     | 0.49              |
| 1:GA:306:LYS:HZ3 | 1:GA:307:PHE:C   | 2.21                     | 0.48              |
| 1:C:6:LYS:HG2    | 1:P:106:LYS:CB   | 2.41                     | 0.48              |
| 1:x:203:PHE:CE1  | 1:4:305:PHE:HE1  | 2.30                     | 0.48              |
| 1:v:306:LYS:HZ3  | 1:v:307:PHE:C    | 2.22                     | 0.48              |
| 1:x:204:GLU:HB3  | 1:4:306:LYS:HB3  | 1.96                     | 0.48              |
| 1:t:102:LYS:HB3  | 1:c:8:GMA:HB3    | 1.96                     | 0.48              |
| 1:d:2:LYS:HE2    | 1:d:2:LYS:HB2    | 1.70                     | 0.48              |
| 1:h:6:LYS:HB2    | 1:h:6:LYS:HE2    | 1.71                     | 0.47              |
| 1:9:206:LYS:HB3  | 1:GA:304:GLU:HB3 | 1.95                     | 0.47              |
| 1:t:104:GLU:OE1  | 1:t:105:PHE:N    | 2.49                     | 0.46              |
| 1:5:104:GLU:OE1  | 1:5:105:PHE:N    | 2.49                     | 0.46              |
| 1:EA:104:GLU:OE1 | 1:EA:105:PHE:N   | 2.49                     | 0.46              |
| 1:2:104:GLU:OE1  | 1:2:105:PHE:N    | 2.49                     | 0.46              |
| 1:8:104:GLU:OE1  | 1:8:105:PHE:N    | 2.49                     | 0.46              |
| 1:z:104:GLU:OE1  | 1:z:105:PHE:N    | 2.49                     | 0.46              |
| 1:BA:104:GLU:OE1 | 1:BA:105:PHE:N   | 2.49                     | 0.46              |
| 1:HA:104:GLU:OE1 | 1:HA:105:PHE:N   | 2.49                     | 0.46              |
| 1:w:104:GLU:OE1  | 1:w:105:PHE:N    | 2.49                     | 0.46              |
| 1:x:206:LYS:HB3  | 1:4:304:GLU:HB3  | 1.96                     | 0.46              |
| 1:V:108:GMA:O1   | 1:W:201:5CR:N    | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:108:GMA:O1   | 1:Z:201:5CR:N    | 2.50                     | 0.45              |
| 1:q:108:GMA:O1   | 1:r:201:5CR:N    | 2.50                     | 0.45              |
| 1:3:206:LYS:HB3  | 1:AA:304:GLU:HB3 | 1.97                     | 0.45              |
| 1:J:108:GMA:O1   | 1:K:201:5CR:N    | 2.50                     | 0.45              |
| 1:h:2:LYS:HE2    | 1:h:2:LYS:HB2    | 1.70                     | 0.45              |
| 1:5:105:PHE:HA   | 1:g:4:GLU:O      | 2.16                     | 0.45              |
| 1:M:108:GMA:O1   | 1:N:201:5CR:N    | 2.50                     | 0.45              |
| 1:S:108:GMA:O1   | 1:T:201:5CR:N    | 2.50                     | 0.45              |
| 1:P:108:GMA:O1   | 1:Q:201:5CR:N    | 2.50                     | 0.45              |
| 1:k:108:GMA:O1   | 1:l:201:5CR:N    | 2.50                     | 0.44              |
| 1:1:308:GMA:HB2  | 1:6:202:LYS:HB3  | 2.00                     | 0.44              |
| 1:n:108:GMA:O1   | 1:o:201:5CR:N    | 2.50                     | 0.44              |
| 1:a:6:LYS:HB2    | 1:a:6:LYS:HE2    | 1.71                     | 0.44              |
| 1:v:302:LYS:HD2  | 1:v:303:PHE:H    | 1.82                     | 0.44              |
| 1:W:206:LYS:HB2  | 1:W:206:LYS:HE2  | 1.77                     | 0.44              |
| 1:y:302:LYS:HD2  | 1:y:303:PHE:H    | 1.82                     | 0.44              |
| 1:4:302:LYS:HD2  | 1:4:303:PHE:H    | 1.82                     | 0.44              |
| 1:DA:305:PHE:HE1 | 1:IA:203:PHE:CZ  | 2.36                     | 0.43              |
| 1:JA:302:LYS:HD2 | 1:JA:303:PHE:H   | 1.82                     | 0.43              |
| 1:S:106:LYS:HD2  | 1:S:106:LYS:HA   | 1.43                     | 0.43              |
| 1:l:206:LYS:HB2  | 1:l:206:LYS:HE2  | 1.77                     | 0.43              |
| 1:1:302:LYS:HD2  | 1:1:303:PHE:H    | 1.82                     | 0.43              |
| 1:AA:302:LYS:HD2 | 1:AA:303:PHE:H   | 1.82                     | 0.43              |
| 1:e:2:LYS:HB2    | 1:e:2:LYS:HE2    | 1.70                     | 0.43              |
| 1:7:302:LYS:HD2  | 1:7:303:PHE:H    | 1.82                     | 0.43              |
| 1:7:306:LYS:HZ3  | 1:7:307:PHE:C    | 2.27                     | 0.43              |
| 1:f:6:LYS:HE2    | 1:f:6:LYS:HB2    | 1.71                     | 0.43              |
| 1:g:2:LYS:HB2    | 1:g:2:LYS:HE2    | 1.70                     | 0.43              |
| 1:z:102:LYS:HB3  | 1:e:8:GMA:HB3    | 2.00                     | 0.43              |
| 1:k:106:LYS:HD2  | 1:k:106:LYS:HA   | 1.43                     | 0.43              |
| 1:DA:302:LYS:HD2 | 1:DA:303:PHE:H   | 1.82                     | 0.43              |
| 1:V:106:LYS:HD2  | 1:V:106:LYS:HA   | 1.43                     | 0.43              |
| 1:GA:302:LYS:HD2 | 1:GA:303:PHE:H   | 1.82                     | 0.43              |
| 1:i:6:LYS:HB2    | 1:i:6:LYS:HE2    | 1.71                     | 0.43              |
| 1:N:206:LYS:HB2  | 1:N:206:LYS:HE2  | 1.77                     | 0.42              |
| 1:P:106:LYS:HD2  | 1:P:106:LYS:HA   | 1.43                     | 0.42              |
| 1:3:203:PHE:CZ   | 1:AA:305:PHE:HE1 | 2.38                     | 0.41              |
| 1:BA:102:LYS:HB3 | 1:i:8:GMA:CB     | 2.49                     | 0.41              |
| 1:q:106:LYS:HD2  | 1:q:106:LYS:HA   | 1.43                     | 0.41              |
| 1:f:2:LYS:HB2    | 1:f:2:LYS:HE2    | 1.70                     | 0.41              |
| 1:Q:206:LYS:HB2  | 1:Q:206:LYS:HE2  | 1.77                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:2:LYS:HB2    | 1:c:2:LYS:HE2    | 1.70                     | 0.41              |
| 1:F:5:PHE:CE2    | 1:EA:103:PHE:CE1 | 3.08                     | 0.41              |
| 1:H:3:PHE:CZ     | 1:h:7:PHE:HZ     | 2.38                     | 0.41              |
| 1:b:2:LYS:HE2    | 1:b:2:LYS:HB2    | 1.70                     | 0.41              |
| 1:1:307:PHE:HE1  | 1:6:201:5CR:CZ   | 2.34                     | 0.41              |
| 1:3:204:GLU:HB3  | 1:AA:306:LYS:HB3 | 2.02                     | 0.41              |
| 1:DA:305:PHE:HE1 | 1:IA:203:PHE:CE1 | 2.39                     | 0.41              |
| 1:a:2:LYS:HE2    | 1:a:2:LYS:HB2    | 1.70                     | 0.41              |
| 1:u:206:LYS:HB3  | 1:y:304:GLU:HB3  | 2.02                     | 0.41              |
| 1:v:304:GLU:HB3  | 1:0:206:LYS:HB3  | 2.02                     | 0.41              |
| 1:d:6:LYS:HE2    | 1:d:6:LYS:HB2    | 1.71                     | 0.40              |
| 1:n:106:LYS:HA   | 1:n:106:LYS:HD2  | 1.43                     | 0.40              |
| 1:f:4:GLU:O      | 1:EA:105:PHE:HA  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | 0     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 1     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 2     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 3     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 4     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 5     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 6     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 7     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 8     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 9     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed  | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------|----------|---------|----------|-------------|-----|
| 1   | A     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | AA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | B     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | BA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | C     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | CA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | D     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | DA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | E     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | EA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | F     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | FA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | G     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | GA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | H     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | HA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | I     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | IA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | J     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | JA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | K     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | L     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | M     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | N     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | O     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | P     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | Q     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | R     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | S     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | T     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | U     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed  | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------|----------|---------|----------|-------------|-----|
| 1   | V     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | W     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | X     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | Y     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | Z     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | a     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | b     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | c     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | d     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | e     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | f     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | g     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | h     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | i     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | j     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | k     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | l     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | m     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | n     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | o     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | p     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | q     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | r     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | s     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | t     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | u     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | v     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | w     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | x     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | y     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | z     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| All | All   | 432/576 (75%) | 396 (92%) | 36 (8%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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   | 0     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 1     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 2     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 3     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 4     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 5     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 6     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 7     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 8     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 9     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | A     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | AA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | B     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | BA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | C     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | CA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | D     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | DA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | E     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | EA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | F     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed   | Rotameric | Outliers | Percentiles |     |
|-----|-------|------------|-----------|----------|-------------|-----|
| 1   | FA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | G     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | GA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | H     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | HA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | I     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | IA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | J     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | JA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | K     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | L     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | M     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | N     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | O     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | P     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | Q     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | R     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | S     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | T     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | U     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | V     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | W     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | X     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | Y     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | Z     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | a     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | b     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | c     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | d     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | e     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | f     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | g     | 6/6 (100%)     | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | h     | 6/6 (100%)     | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | i     | 6/6 (100%)     | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | j     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | k     | 6/6 (100%)     | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | l     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | m     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | n     | 6/6 (100%)     | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | o     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | p     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | q     | 6/6 (100%)     | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | r     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | s     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | t     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | u     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | v     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | w     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | x     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | y     | 6/6 (100%)     | 6 (100%)  | 0        | 100         | 100 |
| 1   | z     | 6/6 (100%)     | 5 (83%)   | 1 (17%)  | 2           | 9   |
| All | All   | 432/432 (100%) | 369 (85%) | 63 (15%) | 5           | 12  |

All (63) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 102 | LYS  |
| 1   | J     | 106 | LYS  |
| 1   | L     | 302 | LYS  |
| 1   | M     | 102 | LYS  |
| 1   | M     | 106 | LYS  |
| 1   | O     | 302 | LYS  |
| 1   | P     | 102 | LYS  |
| 1   | P     | 106 | LYS  |
| 1   | R     | 302 | LYS  |
| 1   | S     | 102 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 106 | LYS  |
| 1   | U     | 302 | LYS  |
| 1   | V     | 102 | LYS  |
| 1   | V     | 106 | LYS  |
| 1   | X     | 302 | LYS  |
| 1   | Y     | 102 | LYS  |
| 1   | Y     | 106 | LYS  |
| 1   | j     | 302 | LYS  |
| 1   | k     | 102 | LYS  |
| 1   | k     | 106 | LYS  |
| 1   | m     | 302 | LYS  |
| 1   | n     | 102 | LYS  |
| 1   | n     | 106 | LYS  |
| 1   | p     | 302 | LYS  |
| 1   | q     | 102 | LYS  |
| 1   | q     | 106 | LYS  |
| 1   | s     | 302 | LYS  |
| 1   | a     | 2   | LYS  |
| 1   | a     | 4   | GLU  |
| 1   | a     | 6   | LYS  |
| 1   | t     | 104 | GLU  |
| 1   | b     | 2   | LYS  |
| 1   | b     | 4   | GLU  |
| 1   | b     | 6   | LYS  |
| 1   | w     | 104 | GLU  |
| 1   | c     | 2   | LYS  |
| 1   | c     | 4   | GLU  |
| 1   | c     | 6   | LYS  |
| 1   | z     | 104 | GLU  |
| 1   | d     | 2   | LYS  |
| 1   | d     | 4   | GLU  |
| 1   | d     | 6   | LYS  |
| 1   | 2     | 104 | GLU  |
| 1   | e     | 2   | LYS  |
| 1   | e     | 4   | GLU  |
| 1   | e     | 6   | LYS  |
| 1   | 5     | 104 | GLU  |
| 1   | f     | 2   | LYS  |
| 1   | f     | 4   | GLU  |
| 1   | f     | 6   | LYS  |
| 1   | 8     | 104 | GLU  |
| 1   | g     | 2   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | g     | 4   | GLU  |
| 1   | g     | 6   | LYS  |
| 1   | BA    | 104 | GLU  |
| 1   | h     | 2   | LYS  |
| 1   | h     | 4   | GLU  |
| 1   | h     | 6   | LYS  |
| 1   | EA    | 104 | GLU  |
| 1   | i     | 2   | LYS  |
| 1   | i     | 4   | GLU  |
| 1   | i     | 6   | LYS  |
| 1   | HA    | 104 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

144 non-standard protein/DNA/RNA residues 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 |
| 1   | GMA  | S     | 108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | GMA  | I     | 8   | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.28 | 0        |
| 1   | 5CR  | Z     | 201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | GMA  | M     | 108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | 5CR  | i     | 1   | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | L     | 308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | 0     | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.13 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | 5     | 101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | GMA  | E     | 8   | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | 1     | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | 5CR  | 8     | 101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | 5CR  | S     | 101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | EA    | 101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.06 | 1 (6%)   |
| 1   | GMA  | 3     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | GMA  | JA    | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | GMA  | n     | 108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 1 (10%)  |
| 1   | 5CR  | b     | 1   | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | r     | 201 | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | x     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.13 | 0        |
| 1   | GMA  | h     | 8   | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | D     | 8   | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | 5CR  | JA    | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | a     | 1   | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | g     | 1   | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | 5CR  | H     | 1   | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | GA    | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | 5CR  | d     | 1   | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | c     | 1   | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.69 | 3 (18%)  |
| 1   | 5CR  | U     | 301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | HA    | 101 | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | c     | 8   | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | GA    | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | GMA  | C     | 8   | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | G     | 8   | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | k     | 108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 1 (10%)  |
| 1   | 5CR  | N     | 201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | 5CR  | C     | 1   | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | GMA  | 4     | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | GMA  | CA    | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | v     | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | v     | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | GMA  | p     | 308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | 6     | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.13 | 1 (6%)   |
| 1   | 5CR  | BA    | 101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | 5CR  | e     | 1   | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | q     | 101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | GMA  | a     | 8   | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | n     | 101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | DA    | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | 5CR  | f     | 1   | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | K     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | GMA  | o     | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | GMA  | DA    | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | GMA  | 6     | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | GMA  | s     | 308 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | m     | 308 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | W     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | GMA  | d     | 8   | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | AA    | 308 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.32 | 0        |
| 1   | 5CR  | L     | 301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | h     | 1   | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | EA    | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | G     | 1   | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | IA    | 201 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | y     | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | 5CR  | j     | 301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | F     | 1   | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | GMA  | z     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | B     | 1   | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | 5CR  | l     | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | u     | 208 | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | M     | 101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | V     | 101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | GMA  | A     | 8   | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | g     | 8   | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | t     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | T     | 201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | m     | 301 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | GMA  | Y     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | GMA  | b     | 8   | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | q     | 108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | GMA  | l     | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | GMA  | 0     | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | GMA  | H     | 8   | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | 9     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | GMA  | N     | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | GMA  | V     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | GMA  | 2     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | Y     | 101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | FA    | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | X     | 301 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | GMA  | i     | 8   | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | 5CR  | 7     | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | GMA  | e     | 8   | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | BA    | 108 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | x     | 201 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | B     | 8   | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | GMA  | f     | 8   | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | 5CR  | u     | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | 4     | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | 5     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | 5CR  | J     | 101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | o     | 201 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | 8     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | K     | 201 | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | 5CR  | 3     | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | j     | 308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | R     | 308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | t     | 101 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | w     | 108 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.21 | 0        |
| 1   | 5CR  | k     | 101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | I     | 1   | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.58 | 2 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | A     | 1   | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | 5CR  | P     | 101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | s     | 301 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | 2     | 101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | 5CR  | O     | 301 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | GMA  | O     | 308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.24 | 0        |
| 1   | GMA  | FA    | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | w     | 101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | J     | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | 5CR  | y     | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | F     | 8   | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | Q     | 208 | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.29 | 2 (20%)  |
| 1   | 5CR  | l     | 201 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | GMA  | 7     | 308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | 5CR  | 9     | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | X     | 308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | Z     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | GMA  | HA    | 108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | 5CR  | D     | 1   | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | GMA  | U     | 308 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | p     | 301 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | z     | 101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | GMA  | r     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | GMA  | P     | 108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | GMA  | T     | 208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | 5CR  | W     | 201 | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | 5CR  | E     | 1   | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | GMA  | IA    | 208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | AA    | 301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | CA    | 201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | Q     | 201 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | 5CR  | R     | 301 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 1   | GMA  | S     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | I     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | Z     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | M     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | i     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | L     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | 0     | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 5     | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | E     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 1     | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | 8     | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | S     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | EA    | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 3     | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | JA    | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | n     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | b     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | r     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | x     | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | h     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | D     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | JA    | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | a     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | g     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | H     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | GA    | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | d     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | c     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | U     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | HA    | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | c     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | GA    | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | C     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | G     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | k     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | N     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 1   | 5CR  | C     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 4     | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | CA    | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | v     | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | v     | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | p     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | 6     | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | BA    | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | e     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | q     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | a     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | n     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | DA    | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | f     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | K     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | o     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | DA    | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | 6     | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | s     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | m     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | W     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | d     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | AA    | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | L     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | h     | 1   | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | EA    | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | G     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | IA    | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | y     | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | j     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | F     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | z     | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | B     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | l     | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | u     | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | M     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | V     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | A     | 8   | 1    | -       | 1/9/9/9   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 1   | GMA  | g     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | t     | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | T     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | m     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | Y     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | b     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | q     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | l     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 0     | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | H     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 9     | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | N     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | V     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | 2     | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | Y     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | FA    | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | X     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | i     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | 7     | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | e     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | BA    | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | x     | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | B     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | f     | 8   | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | u     | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 4     | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 5     | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | J     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | o     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 8     | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | K     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 3     | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | j     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | R     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | t     | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | w     | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | k     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 1   | 5CR  | I     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | A     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | P     | 101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | s     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 2     | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | O     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | O     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | FA    | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | w     | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | J     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | y     | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | F     | 8   | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | Q     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | l     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 7     | 308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | 9     | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | X     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | Z     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | HA    | 108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | D     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | U     | 308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | p     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | z     | 101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | r     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | P     | 108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | T     | 208 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | W     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | E     | 1   | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | IA    | 208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | AA    | 301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | CA    | 201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | Q     | 201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | R     | 301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |

All (176) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | e     | 1   | 5CR  | CAL-N | 3.72 | 1.46        | 1.34     |
| 1   | a     | 1   | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | i     | 1   | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | f     | 1   | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | h     | 1   | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | d     | 1   | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | b     | 1   | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | c     | 1   | 5CR  | CAL-N | 3.68 | 1.46        | 1.34     |
| 1   | g     | 1   | 5CR  | CAL-N | 3.68 | 1.46        | 1.34     |
| 1   | Y     | 101 | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | P     | 101 | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | S     | 101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | n     | 101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | M     | 101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | V     | 101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | q     | 101 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | J     | 101 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | FA    | 201 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | 6     | 201 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | k     | 101 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | 7     | 301 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | 4     | 301 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | GA    | 301 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | EA    | 101 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | JA    | 301 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | 3     | 201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | IA    | 201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | 2     | 101 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | CA    | 201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | 9     | 201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | AA    | 301 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | DA    | 301 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | v     | 301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | z     | 101 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | u     | 201 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | 0     | 201 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | BA    | 101 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | 1     | 301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | y     | 301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | HA    | 101 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | x     | 201 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | t     | 101 | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | 5     | 101 | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | 8     | 101 | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | w     | 101 | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | r     | 201 | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | Q     | 201 | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | N     | 201 | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | T     | 201 | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | K     | 201 | 5CR  | CAL-N | 3.33 | 1.45        | 1.34     |
| 1   | l     | 201 | 5CR  | CAL-N | 3.33 | 1.45        | 1.34     |
| 1   | W     | 201 | 5CR  | CAL-N | 3.32 | 1.45        | 1.34     |
| 1   | o     | 201 | 5CR  | CAL-N | 3.32 | 1.45        | 1.34     |
| 1   | Z     | 201 | 5CR  | CAL-N | 3.32 | 1.45        | 1.34     |
| 1   | F     | 1   | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | D     | 1   | 5CR  | CAL-N | 3.29 | 1.45        | 1.34     |
| 1   | C     | 1   | 5CR  | CAL-N | 3.29 | 1.45        | 1.34     |
| 1   | E     | 1   | 5CR  | CAL-N | 3.29 | 1.45        | 1.34     |
| 1   | B     | 1   | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | G     | 1   | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | A     | 1   | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | I     | 1   | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | H     | 1   | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | R     | 301 | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | X     | 301 | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | L     | 301 | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | m     | 301 | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | U     | 301 | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | s     | 301 | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | O     | 301 | 5CR  | CAL-N | 3.24 | 1.44        | 1.34     |
| 1   | j     | 301 | 5CR  | CAL-N | 3.24 | 1.44        | 1.34     |
| 1   | p     | 301 | 5CR  | CAL-N | 3.24 | 1.44        | 1.34     |
| 1   | o     | 208 | GMA  | CD-N2 | 2.34 | 1.38        | 1.32     |
| 1   | Q     | 208 | GMA  | CD-N2 | 2.33 | 1.38        | 1.32     |
| 1   | l     | 208 | GMA  | CD-N2 | 2.32 | 1.38        | 1.32     |
| 1   | N     | 208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | W     | 208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | Z     | 208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | r     | 208 | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | K     | 208 | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | e     | 8   | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | s     | 308 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | T     | 208 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | U     | 308 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | R     | 308 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | j     | 308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | h     | 8   | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | JA    | 308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | X     | 308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | 1     | 308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | u     | 208 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | O     | 308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | g     | 8   | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | i     | 8   | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | c     | 8   | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | DA    | 308 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | FA    | 208 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | d     | 8   | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | f     | 8   | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | p     | 308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | b     | 8   | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | L     | 308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | v     | 308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | 0     | 208 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | CA    | 208 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | GA    | 308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | 4     | 308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | IA    | 208 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | m     | 308 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | a     | 8   | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | 6     | 208 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | 9     | 208 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | 7     | 308 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | y     | 308 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | AA    | 308 | GMA  | CD-N2 | 2.23 | 1.38        | 1.32     |
| 1   | 3     | 208 | GMA  | CD-N2 | 2.23 | 1.38        | 1.32     |
| 1   | x     | 208 | GMA  | CD-N2 | 2.22 | 1.38        | 1.32     |
| 1   | I     | 8   | GMA  | CD-N2 | 2.21 | 1.38        | 1.32     |
| 1   | w     | 108 | GMA  | CD-N2 | 2.21 | 1.38        | 1.32     |
| 1   | B     | 8   | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | 5     | 108 | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | 8     | 108 | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | D     | 8   | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | q     | 108 | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | z     | 108 | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | J     | 108 | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | BA    | 108 | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | S     | 108 | GMA  | CD-N2 | 2.18 | 1.38        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 8   | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | 2     | 108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | t     | 108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | EA    | 108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | F     | 8   | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | HA    | 108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | Y     | 108 | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | V     | 108 | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | n     | 108 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | M     | 108 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | k     | 108 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | E     | 8   | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | A     | 8   | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | G     | 8   | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | P     | 108 | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | H     | 8   | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | X     | 301 | 5CR  | OAB-CAL | -2.11 | 1.18        | 1.23     |
| 1   | s     | 301 | 5CR  | OAB-CAL | -2.11 | 1.18        | 1.23     |
| 1   | m     | 301 | 5CR  | OAB-CAL | -2.10 | 1.18        | 1.23     |
| 1   | j     | 301 | 5CR  | OAB-CAL | -2.09 | 1.18        | 1.23     |
| 1   | R     | 301 | 5CR  | OAB-CAL | -2.08 | 1.18        | 1.23     |
| 1   | U     | 301 | 5CR  | OAB-CAL | -2.08 | 1.18        | 1.23     |
| 1   | L     | 301 | 5CR  | OAB-CAL | -2.07 | 1.18        | 1.23     |
| 1   | c     | 1   | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | O     | 301 | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | p     | 301 | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | a     | 1   | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | i     | 1   | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | b     | 1   | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | e     | 1   | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | f     | 1   | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | d     | 1   | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | E     | 1   | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | G     | 1   | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | B     | 1   | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | C     | 1   | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | Z     | 201 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | Q     | 201 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | I     | 1   | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | F     | 1   | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | H     | 1   | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | N     | 201 | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | g     | 1   | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | T     | 201 | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | h     | 1   | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | A     | 1   | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |
| 1   | t     | 101 | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |
| 1   | l     | 201 | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |

All (155) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | g     | 1   | 5CR  | CAA-CAL-N | 5.25  | 124.82      | 116.12   |
| 1   | h     | 1   | 5CR  | CAA-CAL-N | 5.22  | 124.78      | 116.12   |
| 1   | f     | 1   | 5CR  | CAA-CAL-N | 5.22  | 124.77      | 116.12   |
| 1   | b     | 1   | 5CR  | CAA-CAL-N | 5.22  | 124.77      | 116.12   |
| 1   | d     | 1   | 5CR  | CAA-CAL-N | 5.22  | 124.77      | 116.12   |
| 1   | a     | 1   | 5CR  | CAA-CAL-N | 5.21  | 124.76      | 116.12   |
| 1   | i     | 1   | 5CR  | CAA-CAL-N | 5.21  | 124.76      | 116.12   |
| 1   | e     | 1   | 5CR  | CAA-CAL-N | 5.20  | 124.75      | 116.12   |
| 1   | c     | 1   | 5CR  | CAA-CAL-N | 5.20  | 124.73      | 116.12   |
| 1   | B     | 1   | 5CR  | CG-CB-CA  | -4.71 | 106.81      | 113.51   |
| 1   | E     | 1   | 5CR  | CG-CB-CA  | -4.70 | 106.82      | 113.51   |
| 1   | I     | 1   | 5CR  | CG-CB-CA  | -4.70 | 106.82      | 113.51   |
| 1   | C     | 1   | 5CR  | CG-CB-CA  | -4.69 | 106.84      | 113.51   |
| 1   | A     | 1   | 5CR  | CG-CB-CA  | -4.69 | 106.84      | 113.51   |
| 1   | G     | 1   | 5CR  | CG-CB-CA  | -4.69 | 106.84      | 113.51   |
| 1   | F     | 1   | 5CR  | CG-CB-CA  | -4.68 | 106.84      | 113.51   |
| 1   | D     | 1   | 5CR  | CG-CB-CA  | -4.67 | 106.87      | 113.51   |
| 1   | H     | 1   | 5CR  | CG-CB-CA  | -4.65 | 106.90      | 113.51   |
| 1   | M     | 101 | 5CR  | CG-CB-CA  | -4.47 | 107.15      | 113.51   |
| 1   | Y     | 101 | 5CR  | CG-CB-CA  | -4.46 | 107.16      | 113.51   |
| 1   | k     | 101 | 5CR  | CG-CB-CA  | -4.45 | 107.17      | 113.51   |
| 1   | V     | 101 | 5CR  | CG-CB-CA  | -4.45 | 107.17      | 113.51   |
| 1   | q     | 101 | 5CR  | CG-CB-CA  | -4.44 | 107.19      | 113.51   |
| 1   | n     | 101 | 5CR  | CG-CB-CA  | -4.44 | 107.19      | 113.51   |
| 1   | P     | 101 | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | S     | 101 | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | J     | 101 | 5CR  | CG-CB-CA  | -4.40 | 107.25      | 113.51   |
| 1   | l     | 201 | 5CR  | CAA-CAL-N | 2.99  | 121.08      | 116.12   |
| 1   | Q     | 201 | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |
| 1   | W     | 201 | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |
| 1   | N     | 201 | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |
| 1   | r     | 201 | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | K     | 201 | 5CR  | CAA-CAL-N   | 2.97  | 121.04      | 116.12   |
| 1   | T     | 201 | 5CR  | CAA-CAL-N   | 2.96  | 121.03      | 116.12   |
| 1   | o     | 201 | 5CR  | CAA-CAL-N   | 2.96  | 121.03      | 116.12   |
| 1   | Z     | 201 | 5CR  | CAA-CAL-N   | 2.95  | 121.01      | 116.12   |
| 1   | u     | 201 | 5CR  | CG-CB-CA    | -2.88 | 109.41      | 113.51   |
| 1   | 0     | 201 | 5CR  | CG-CB-CA    | -2.86 | 109.44      | 113.51   |
| 1   | 6     | 201 | 5CR  | CG-CB-CA    | -2.86 | 109.44      | 113.51   |
| 1   | IA    | 201 | 5CR  | CG-CB-CA    | -2.86 | 109.44      | 113.51   |
| 1   | CA    | 201 | 5CR  | CG-CB-CA    | -2.86 | 109.44      | 113.51   |
| 1   | x     | 201 | 5CR  | CG-CB-CA    | -2.85 | 109.46      | 113.51   |
| 1   | 3     | 201 | 5CR  | CG-CB-CA    | -2.84 | 109.47      | 113.51   |
| 1   | 9     | 201 | 5CR  | CG-CB-CA    | -2.84 | 109.47      | 113.51   |
| 1   | FA    | 201 | 5CR  | CG-CB-CA    | -2.83 | 109.48      | 113.51   |
| 1   | F     | 1   | 5CR  | CAA-CAL-N   | 2.69  | 120.57      | 116.12   |
| 1   | I     | 1   | 5CR  | CAA-CAL-N   | 2.67  | 120.55      | 116.12   |
| 1   | B     | 1   | 5CR  | CAA-CAL-N   | 2.67  | 120.54      | 116.12   |
| 1   | A     | 1   | 5CR  | CAA-CAL-N   | 2.66  | 120.54      | 116.12   |
| 1   | D     | 1   | 5CR  | CAA-CAL-N   | 2.66  | 120.54      | 116.12   |
| 1   | H     | 1   | 5CR  | CAA-CAL-N   | 2.66  | 120.53      | 116.12   |
| 1   | E     | 1   | 5CR  | CAA-CAL-N   | 2.65  | 120.52      | 116.12   |
| 1   | C     | 1   | 5CR  | CAA-CAL-N   | 2.65  | 120.52      | 116.12   |
| 1   | G     | 1   | 5CR  | CAA-CAL-N   | 2.64  | 120.50      | 116.12   |
| 1   | z     | 101 | 5CR  | CAA-CAL-N   | 2.55  | 120.35      | 116.12   |
| 1   | 5     | 101 | 5CR  | CAA-CAL-N   | 2.55  | 120.35      | 116.12   |
| 1   | HA    | 101 | 5CR  | CAA-CAL-N   | 2.55  | 120.34      | 116.12   |
| 1   | w     | 101 | 5CR  | CAA-CAL-N   | 2.54  | 120.34      | 116.12   |
| 1   | BA    | 101 | 5CR  | CAA-CAL-N   | 2.54  | 120.33      | 116.12   |
| 1   | 2     | 101 | 5CR  | CAA-CAL-N   | 2.54  | 120.33      | 116.12   |
| 1   | 8     | 101 | 5CR  | CAA-CAL-N   | 2.53  | 120.32      | 116.12   |
| 1   | t     | 101 | 5CR  | CAA-CAL-N   | 2.53  | 120.32      | 116.12   |
| 1   | a     | 1   | 5CR  | OAB-CAL-N   | -2.52 | 117.53      | 121.98   |
| 1   | EA    | 101 | 5CR  | CAA-CAL-N   | 2.52  | 120.30      | 116.12   |
| 1   | d     | 1   | 5CR  | OAB-CAL-N   | -2.50 | 117.56      | 121.98   |
| 1   | f     | 1   | 5CR  | OAB-CAL-N   | -2.50 | 117.56      | 121.98   |
| 1   | g     | 1   | 5CR  | OAB-CAL-N   | -2.50 | 117.57      | 121.98   |
| 1   | e     | 1   | 5CR  | OAB-CAL-N   | -2.50 | 117.57      | 121.98   |
| 1   | g     | 1   | 5CR  | OAB-CAL-CAA | -2.50 | 117.61      | 122.05   |
| 1   | h     | 1   | 5CR  | OAB-CAL-N   | -2.49 | 117.57      | 121.98   |
| 1   | i     | 1   | 5CR  | OAB-CAL-N   | -2.49 | 117.58      | 121.98   |
| 1   | b     | 1   | 5CR  | OAB-CAL-CAA | -2.49 | 117.63      | 122.05   |
| 1   | c     | 1   | 5CR  | OAB-CAL-CAA | -2.48 | 117.64      | 122.05   |
| 1   | b     | 1   | 5CR  | OAB-CAL-N   | -2.48 | 117.60      | 121.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | h     | 1   | 5CR  | OAB-CAL-CAA | -2.48 | 117.64      | 122.05   |
| 1   | i     | 1   | 5CR  | OAB-CAL-CAA | -2.47 | 117.66      | 122.05   |
| 1   | c     | 1   | 5CR  | OAB-CAL-N   | -2.46 | 117.63      | 121.98   |
| 1   | f     | 1   | 5CR  | OAB-CAL-CAA | -2.46 | 117.67      | 122.05   |
| 1   | d     | 1   | 5CR  | OAB-CAL-CAA | -2.46 | 117.67      | 122.05   |
| 1   | e     | 1   | 5CR  | OAB-CAL-CAA | -2.45 | 117.68      | 122.05   |
| 1   | a     | 1   | 5CR  | OAB-CAL-CAA | -2.44 | 117.71      | 122.05   |
| 1   | W     | 201 | 5CR  | CG-CB-CA    | -2.31 | 110.23      | 113.51   |
| 1   | Q     | 201 | 5CR  | CG-CB-CA    | -2.31 | 110.23      | 113.51   |
| 1   | T     | 201 | 5CR  | CG-CB-CA    | -2.31 | 110.23      | 113.51   |
| 1   | K     | 201 | 5CR  | CG-CB-CA    | -2.30 | 110.24      | 113.51   |
| 1   | Z     | 201 | 5CR  | CG-CB-CA    | -2.29 | 110.25      | 113.51   |
| 1   | N     | 201 | 5CR  | CG-CB-CA    | -2.29 | 110.25      | 113.51   |
| 1   | r     | 201 | 5CR  | CG-CB-CA    | -2.29 | 110.26      | 113.51   |
| 1   | O     | 301 | 5CR  | CAA-CAL-N   | 2.28  | 119.90      | 116.12   |
| 1   | o     | 201 | 5CR  | CG-CB-CA    | -2.27 | 110.28      | 113.51   |
| 1   | p     | 301 | 5CR  | CAA-CAL-N   | 2.27  | 119.89      | 116.12   |
| 1   | j     | 301 | 5CR  | CAA-CAL-N   | 2.27  | 119.88      | 116.12   |
| 1   | L     | 301 | 5CR  | CAA-CAL-N   | 2.27  | 119.88      | 116.12   |
| 1   | R     | 301 | 5CR  | CAA-CAL-N   | 2.26  | 119.87      | 116.12   |
| 1   | JA    | 301 | 5CR  | CAA-CAL-N   | 2.26  | 119.86      | 116.12   |
| 1   | l     | 201 | 5CR  | CG-CB-CA    | -2.26 | 110.30      | 113.51   |
| 1   | m     | 301 | 5CR  | CAA-CAL-N   | 2.26  | 119.86      | 116.12   |
| 1   | DA    | 301 | 5CR  | CAA-CAL-N   | 2.26  | 119.86      | 116.12   |
| 1   | y     | 301 | 5CR  | CAA-CAL-N   | 2.25  | 119.86      | 116.12   |
| 1   | AA    | 301 | 5CR  | CAA-CAL-N   | 2.25  | 119.85      | 116.12   |
| 1   | U     | 301 | 5CR  | CAA-CAL-N   | 2.25  | 119.85      | 116.12   |
| 1   | s     | 301 | 5CR  | CAA-CAL-N   | 2.25  | 119.84      | 116.12   |
| 1   | 4     | 301 | 5CR  | CAA-CAL-N   | 2.25  | 119.84      | 116.12   |
| 1   | j     | 301 | 5CR  | O-C-CA      | -2.25 | 119.00      | 124.77   |
| 1   | 1     | 301 | 5CR  | CAA-CAL-N   | 2.24  | 119.84      | 116.12   |
| 1   | v     | 301 | 5CR  | CAA-CAL-N   | 2.24  | 119.84      | 116.12   |
| 1   | 7     | 301 | 5CR  | CAA-CAL-N   | 2.24  | 119.83      | 116.12   |
| 1   | U     | 301 | 5CR  | O-C-CA      | -2.24 | 119.01      | 124.77   |
| 1   | X     | 301 | 5CR  | CAA-CAL-N   | 2.24  | 119.83      | 116.12   |
| 1   | m     | 301 | 5CR  | O-C-CA      | -2.23 | 119.03      | 124.77   |
| 1   | GA    | 301 | 5CR  | CAA-CAL-N   | 2.23  | 119.82      | 116.12   |
| 1   | R     | 301 | 5CR  | O-C-CA      | -2.23 | 119.03      | 124.77   |
| 1   | X     | 301 | 5CR  | O-C-CA      | -2.23 | 119.04      | 124.77   |
| 1   | s     | 301 | 5CR  | O-C-CA      | -2.22 | 119.05      | 124.77   |
| 1   | L     | 301 | 5CR  | O-C-CA      | -2.21 | 119.07      | 124.77   |
| 1   | p     | 301 | 5CR  | O-C-CA      | -2.21 | 119.08      | 124.77   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 301 | 5CR  | O-C-CA    | -2.21 | 119.09      | 124.77   |
| 1   | P     | 101 | 5CR  | CAA-CAL-N | 2.16  | 119.70      | 116.12   |
| 1   | J     | 101 | 5CR  | CAA-CAL-N | 2.14  | 119.67      | 116.12   |
| 1   | M     | 101 | 5CR  | CAA-CAL-N | 2.13  | 119.66      | 116.12   |
| 1   | S     | 101 | 5CR  | CAA-CAL-N | 2.13  | 119.65      | 116.12   |
| 1   | V     | 101 | 5CR  | CAA-CAL-N | 2.13  | 119.65      | 116.12   |
| 1   | Y     | 101 | 5CR  | CAA-CAL-N | 2.12  | 119.63      | 116.12   |
| 1   | k     | 101 | 5CR  | CAA-CAL-N | 2.11  | 119.62      | 116.12   |
| 1   | n     | 101 | 5CR  | CAA-CAL-N | 2.10  | 119.61      | 116.12   |
| 1   | q     | 101 | 5CR  | CAA-CAL-N | 2.10  | 119.60      | 116.12   |
| 1   | o     | 208 | GMA  | O1-CD-CA  | 2.07  | 123.33      | 120.25   |
| 1   | Q     | 208 | GMA  | O1-CD-CA  | 2.06  | 123.31      | 120.25   |
| 1   | l     | 208 | GMA  | O1-CD-CA  | 2.06  | 123.31      | 120.25   |
| 1   | N     | 208 | GMA  | O1-CD-CA  | 2.04  | 123.29      | 120.25   |
| 1   | Z     | 208 | GMA  | O1-CD-CA  | 2.04  | 123.29      | 120.25   |
| 1   | Q     | 208 | GMA  | O1-CD-N2  | -2.04 | 119.45      | 123.04   |
| 1   | W     | 208 | GMA  | O1-CD-CA  | 2.03  | 123.28      | 120.25   |
| 1   | r     | 208 | GMA  | O1-CD-CA  | 2.03  | 123.28      | 120.25   |
| 1   | Y     | 108 | GMA  | O1-CD-CA  | 2.03  | 123.28      | 120.25   |
| 1   | o     | 201 | 5CR  | O-C-CA    | -2.03 | 119.55      | 124.77   |
| 1   | T     | 201 | 5CR  | O-C-CA    | -2.02 | 119.57      | 124.77   |
| 1   | o     | 208 | GMA  | O1-CD-N2  | -2.02 | 119.48      | 123.04   |
| 1   | r     | 201 | 5CR  | O-C-CA    | -2.01 | 119.59      | 124.77   |
| 1   | J     | 108 | GMA  | O1-CD-CA  | 2.01  | 123.25      | 120.25   |
| 1   | B     | 8   | GMA  | O1-CD-CA  | 2.01  | 123.25      | 120.25   |
| 1   | Q     | 201 | 5CR  | O-C-CA    | -2.01 | 119.60      | 124.77   |
| 1   | N     | 201 | 5CR  | O-C-CA    | -2.01 | 119.61      | 124.77   |
| 1   | l     | 201 | 5CR  | O-C-CA    | -2.01 | 119.61      | 124.77   |
| 1   | T     | 208 | GMA  | O1-CD-CA  | 2.01  | 123.24      | 120.25   |
| 1   | l     | 208 | GMA  | O1-CD-N2  | -2.01 | 119.50      | 123.04   |
| 1   | K     | 208 | GMA  | O1-CD-CA  | 2.01  | 123.24      | 120.25   |
| 1   | S     | 108 | GMA  | O1-CD-CA  | 2.01  | 123.24      | 120.25   |
| 1   | K     | 201 | 5CR  | O-C-CA    | -2.00 | 119.61      | 124.77   |
| 1   | W     | 201 | 5CR  | O-C-CA    | -2.00 | 119.62      | 124.77   |
| 1   | Z     | 201 | 5CR  | O-C-CA    | -2.00 | 119.62      | 124.77   |
| 1   | k     | 108 | GMA  | O1-CD-CA  | 2.00  | 123.23      | 120.25   |
| 1   | q     | 108 | GMA  | O1-CD-CA  | 2.00  | 123.23      | 120.25   |
| 1   | n     | 108 | GMA  | O1-CD-CA  | 2.00  | 123.23      | 120.25   |
| 1   | r     | 208 | GMA  | O1-CD-N2  | -2.00 | 119.51      | 123.04   |

There are no chirality outliers.

All (351) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 1   | J     | 101 | 5CR  | C-CA-N-CAL |
| 1   | J     | 101 | 5CR  | N-CA-CB-CG |
| 1   | K     | 201 | 5CR  | N-CA-CB-CG |
| 1   | L     | 301 | 5CR  | N-CA-CB-CG |
| 1   | L     | 301 | 5CR  | C-CA-CB-CG |
| 1   | M     | 101 | 5CR  | C-CA-N-CAL |
| 1   | M     | 101 | 5CR  | N-CA-CB-CG |
| 1   | N     | 201 | 5CR  | N-CA-CB-CG |
| 1   | O     | 301 | 5CR  | N-CA-CB-CG |
| 1   | O     | 301 | 5CR  | C-CA-CB-CG |
| 1   | P     | 101 | 5CR  | C-CA-N-CAL |
| 1   | P     | 101 | 5CR  | N-CA-CB-CG |
| 1   | Q     | 201 | 5CR  | N-CA-CB-CG |
| 1   | R     | 301 | 5CR  | N-CA-CB-CG |
| 1   | R     | 301 | 5CR  | C-CA-CB-CG |
| 1   | S     | 101 | 5CR  | C-CA-N-CAL |
| 1   | S     | 101 | 5CR  | N-CA-CB-CG |
| 1   | T     | 201 | 5CR  | N-CA-CB-CG |
| 1   | U     | 301 | 5CR  | N-CA-CB-CG |
| 1   | U     | 301 | 5CR  | C-CA-CB-CG |
| 1   | V     | 101 | 5CR  | C-CA-N-CAL |
| 1   | V     | 101 | 5CR  | N-CA-CB-CG |
| 1   | W     | 201 | 5CR  | N-CA-CB-CG |
| 1   | X     | 301 | 5CR  | N-CA-CB-CG |
| 1   | X     | 301 | 5CR  | C-CA-CB-CG |
| 1   | Y     | 101 | 5CR  | C-CA-N-CAL |
| 1   | Y     | 101 | 5CR  | N-CA-CB-CG |
| 1   | Z     | 201 | 5CR  | N-CA-CB-CG |
| 1   | j     | 301 | 5CR  | N-CA-CB-CG |
| 1   | j     | 301 | 5CR  | C-CA-CB-CG |
| 1   | k     | 101 | 5CR  | C-CA-N-CAL |
| 1   | k     | 101 | 5CR  | N-CA-CB-CG |
| 1   | l     | 201 | 5CR  | N-CA-CB-CG |
| 1   | m     | 301 | 5CR  | N-CA-CB-CG |
| 1   | m     | 301 | 5CR  | C-CA-CB-CG |
| 1   | n     | 101 | 5CR  | C-CA-N-CAL |
| 1   | n     | 101 | 5CR  | N-CA-CB-CG |
| 1   | o     | 201 | 5CR  | N-CA-CB-CG |
| 1   | p     | 301 | 5CR  | N-CA-CB-CG |
| 1   | p     | 301 | 5CR  | C-CA-CB-CG |
| 1   | q     | 101 | 5CR  | C-CA-N-CAL |
| 1   | q     | 101 | 5CR  | N-CA-CB-CG |
| 1   | r     | 201 | 5CR  | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | s     | 301 | 5CR  | N-CA-CB-CG  |
| 1   | s     | 301 | 5CR  | C-CA-CB-CG  |
| 1   | a     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | u     | 201 | 5CR  | C-CA-N-CAL  |
| 1   | b     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | x     | 201 | 5CR  | C-CA-N-CAL  |
| 1   | c     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | 0     | 201 | 5CR  | C-CA-N-CAL  |
| 1   | d     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | 3     | 201 | 5CR  | C-CA-N-CAL  |
| 1   | e     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | 6     | 201 | 5CR  | C-CA-N-CAL  |
| 1   | f     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | 9     | 201 | 5CR  | C-CA-N-CAL  |
| 1   | g     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | CA    | 201 | 5CR  | C-CA-N-CAL  |
| 1   | h     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | FA    | 201 | 5CR  | C-CA-N-CAL  |
| 1   | i     | 1   | 5CR  | C-CA-CB-CG  |
| 1   | IA    | 201 | 5CR  | C-CA-N-CAL  |
| 1   | A     | 8   | GMA  | N-CA-CD-N2  |
| 1   | B     | 8   | GMA  | N-CA-CD-N2  |
| 1   | C     | 8   | GMA  | N-CA-CD-N2  |
| 1   | D     | 8   | GMA  | N-CA-CD-N2  |
| 1   | E     | 8   | GMA  | N-CA-CD-N2  |
| 1   | F     | 8   | GMA  | N-CA-CD-N2  |
| 1   | G     | 8   | GMA  | N-CA-CD-N2  |
| 1   | H     | 8   | GMA  | N-CA-CD-N2  |
| 1   | I     | 8   | GMA  | N-CA-CD-N2  |
| 1   | a     | 8   | GMA  | N-CA-CB-CG  |
| 1   | a     | 8   | GMA  | CD-CA-CB-CG |
| 1   | u     | 208 | GMA  | N-CA-CB-CG  |
| 1   | u     | 208 | GMA  | CD-CA-CB-CG |
| 1   | b     | 8   | GMA  | N-CA-CB-CG  |
| 1   | b     | 8   | GMA  | CD-CA-CB-CG |
| 1   | x     | 208 | GMA  | N-CA-CB-CG  |
| 1   | x     | 208 | GMA  | CD-CA-CB-CG |
| 1   | c     | 8   | GMA  | N-CA-CB-CG  |
| 1   | c     | 8   | GMA  | CD-CA-CB-CG |
| 1   | 0     | 208 | GMA  | N-CA-CB-CG  |
| 1   | 0     | 208 | GMA  | CD-CA-CB-CG |
| 1   | d     | 8   | GMA  | N-CA-CB-CG  |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | d     | 8   | GMA  | CD-CA-CB-CG  |
| 1   | 3     | 208 | GMA  | N-CA-CB-CG   |
| 1   | 3     | 208 | GMA  | CD-CA-CB-CG  |
| 1   | e     | 8   | GMA  | N-CA-CB-CG   |
| 1   | e     | 8   | GMA  | CD-CA-CB-CG  |
| 1   | 6     | 208 | GMA  | N-CA-CB-CG   |
| 1   | 6     | 208 | GMA  | CD-CA-CB-CG  |
| 1   | f     | 8   | GMA  | N-CA-CB-CG   |
| 1   | f     | 8   | GMA  | CD-CA-CB-CG  |
| 1   | 9     | 208 | GMA  | N-CA-CB-CG   |
| 1   | 9     | 208 | GMA  | CD-CA-CB-CG  |
| 1   | g     | 8   | GMA  | N-CA-CB-CG   |
| 1   | g     | 8   | GMA  | CD-CA-CB-CG  |
| 1   | CA    | 208 | GMA  | N-CA-CB-CG   |
| 1   | CA    | 208 | GMA  | CD-CA-CB-CG  |
| 1   | h     | 8   | GMA  | N-CA-CB-CG   |
| 1   | h     | 8   | GMA  | CD-CA-CB-CG  |
| 1   | FA    | 208 | GMA  | N-CA-CB-CG   |
| 1   | FA    | 208 | GMA  | CD-CA-CB-CG  |
| 1   | i     | 8   | GMA  | N-CA-CB-CG   |
| 1   | i     | 8   | GMA  | CD-CA-CB-CG  |
| 1   | IA    | 208 | GMA  | N-CA-CB-CG   |
| 1   | IA    | 208 | GMA  | CD-CA-CB-CG  |
| 1   | K     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | K     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | N     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | N     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | Q     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | Q     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | T     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | T     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | W     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | W     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | Z     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | Z     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | l     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | l     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | o     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | o     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | r     | 201 | 5CR  | CAA-CAL-N-CA |
| 1   | r     | 201 | 5CR  | OAB-CAL-N-CA |
| 1   | a     | 1   | 5CR  | CAA-CAL-N-CA |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | a     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | b     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | b     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | c     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | c     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | d     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | d     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | e     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | e     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | f     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | f     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | g     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | g     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | h     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | h     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | i     | 1   | 5CR  | CAA-CAL-N-CA |
| 1   | i     | 1   | 5CR  | OAB-CAL-N-CA |
| 1   | L     | 308 | GMA  | CA-CB-CG-C   |
| 1   | O     | 308 | GMA  | CA-CB-CG-C   |
| 1   | R     | 308 | GMA  | CA-CB-CG-C   |
| 1   | U     | 308 | GMA  | CA-CB-CG-C   |
| 1   | X     | 308 | GMA  | CA-CB-CG-C   |
| 1   | j     | 308 | GMA  | CA-CB-CG-C   |
| 1   | m     | 308 | GMA  | CA-CB-CG-C   |
| 1   | p     | 308 | GMA  | CA-CB-CG-C   |
| 1   | s     | 308 | GMA  | CA-CB-CG-C   |
| 1   | K     | 208 | GMA  | CA-CB-CG-C   |
| 1   | N     | 208 | GMA  | CA-CB-CG-C   |
| 1   | Q     | 208 | GMA  | CA-CB-CG-C   |
| 1   | T     | 208 | GMA  | CA-CB-CG-C   |
| 1   | W     | 208 | GMA  | CA-CB-CG-C   |
| 1   | Z     | 208 | GMA  | CA-CB-CG-C   |
| 1   | l     | 208 | GMA  | CA-CB-CG-C   |
| 1   | o     | 208 | GMA  | CA-CB-CG-C   |
| 1   | r     | 208 | GMA  | CA-CB-CG-C   |
| 1   | L     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | O     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | R     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | U     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | X     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | j     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | m     | 301 | 5CR  | C-CA-N-CAL   |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | p     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | s     | 301 | 5CR  | C-CA-N-CAL   |
| 1   | 4     | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | 7     | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | AA    | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | DA    | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | v     | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | y     | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | 1     | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | GA    | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | JA    | 301 | 5CR  | CA-CB-CG-CD2 |
| 1   | v     | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | y     | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | 1     | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | 4     | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | 7     | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | AA    | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | DA    | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | GA    | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | JA    | 301 | 5CR  | CA-CB-CG-CD1 |
| 1   | a     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | v     | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | b     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | y     | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | c     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | 1     | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | d     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | 4     | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | e     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | 7     | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | f     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | AA    | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | g     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | DA    | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | h     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | GA    | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | i     | 1   | 5CR  | CB-CA-N-CAL  |
| 1   | JA    | 301 | 5CR  | CB-CA-N-CAL  |
| 1   | J     | 108 | GMA  | N-CA-CB-CG   |
| 1   | M     | 108 | GMA  | N-CA-CB-CG   |
| 1   | P     | 108 | GMA  | N-CA-CB-CG   |
| 1   | S     | 108 | GMA  | N-CA-CB-CG   |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | V     | 108 | GMA  | N-CA-CB-CG  |
| 1   | Y     | 108 | GMA  | N-CA-CB-CG  |
| 1   | k     | 108 | GMA  | N-CA-CB-CG  |
| 1   | n     | 108 | GMA  | N-CA-CB-CG  |
| 1   | q     | 108 | GMA  | N-CA-CB-CG  |
| 1   | a     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | a     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | b     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | b     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | c     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | c     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | d     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | d     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | e     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | e     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | f     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | f     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | g     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | g     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | h     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | h     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | i     | 8   | GMA  | CB-CA-CD-O1 |
| 1   | i     | 8   | GMA  | CB-CA-CD-N2 |
| 1   | J     | 108 | GMA  | CD-CA-CB-CG |
| 1   | M     | 108 | GMA  | CD-CA-CB-CG |
| 1   | P     | 108 | GMA  | CD-CA-CB-CG |
| 1   | S     | 108 | GMA  | CD-CA-CB-CG |
| 1   | V     | 108 | GMA  | CD-CA-CB-CG |
| 1   | Y     | 108 | GMA  | CD-CA-CB-CG |
| 1   | k     | 108 | GMA  | CD-CA-CB-CG |
| 1   | n     | 108 | GMA  | CD-CA-CB-CG |
| 1   | q     | 108 | GMA  | CD-CA-CB-CG |
| 1   | a     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | b     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | c     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | d     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | e     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | f     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | g     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | h     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | i     | 1   | 5CR  | N-CA-CB-CG  |
| 1   | a     | 1   | 5CR  | C-CA-N-CAL  |

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| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 1   | t     | 101 | 5CR  | C-CA-N-CAL |
| 1   | v     | 301 | 5CR  | C-CA-N-CAL |
| 1   | b     | 1   | 5CR  | C-CA-N-CAL |
| 1   | w     | 101 | 5CR  | C-CA-N-CAL |
| 1   | y     | 301 | 5CR  | C-CA-N-CAL |
| 1   | c     | 1   | 5CR  | C-CA-N-CAL |
| 1   | z     | 101 | 5CR  | C-CA-N-CAL |
| 1   | 1     | 301 | 5CR  | C-CA-N-CAL |
| 1   | d     | 1   | 5CR  | C-CA-N-CAL |
| 1   | 2     | 101 | 5CR  | C-CA-N-CAL |
| 1   | 4     | 301 | 5CR  | C-CA-N-CAL |
| 1   | e     | 1   | 5CR  | C-CA-N-CAL |
| 1   | 5     | 101 | 5CR  | C-CA-N-CAL |
| 1   | 7     | 301 | 5CR  | C-CA-N-CAL |
| 1   | f     | 1   | 5CR  | C-CA-N-CAL |
| 1   | 8     | 101 | 5CR  | C-CA-N-CAL |
| 1   | AA    | 301 | 5CR  | C-CA-N-CAL |
| 1   | g     | 1   | 5CR  | C-CA-N-CAL |
| 1   | BA    | 101 | 5CR  | C-CA-N-CAL |
| 1   | DA    | 301 | 5CR  | C-CA-N-CAL |
| 1   | h     | 1   | 5CR  | C-CA-N-CAL |
| 1   | EA    | 101 | 5CR  | C-CA-N-CAL |
| 1   | GA    | 301 | 5CR  | C-CA-N-CAL |
| 1   | i     | 1   | 5CR  | C-CA-N-CAL |
| 1   | HA    | 101 | 5CR  | C-CA-N-CAL |
| 1   | JA    | 301 | 5CR  | C-CA-N-CAL |
| 1   | a     | 8   | GMA  | CA-CB-CG-C |
| 1   | b     | 8   | GMA  | CA-CB-CG-C |
| 1   | c     | 8   | GMA  | CA-CB-CG-C |
| 1   | d     | 8   | GMA  | CA-CB-CG-C |
| 1   | e     | 8   | GMA  | CA-CB-CG-C |
| 1   | f     | 8   | GMA  | CA-CB-CG-C |
| 1   | g     | 8   | GMA  | CA-CB-CG-C |
| 1   | h     | 8   | GMA  | CA-CB-CG-C |
| 1   | i     | 8   | GMA  | CA-CB-CG-C |
| 1   | a     | 8   | GMA  | N-CA-CD-O1 |
| 1   | b     | 8   | GMA  | N-CA-CD-O1 |
| 1   | c     | 8   | GMA  | N-CA-CD-O1 |
| 1   | d     | 8   | GMA  | N-CA-CD-O1 |
| 1   | e     | 8   | GMA  | N-CA-CD-O1 |
| 1   | f     | 8   | GMA  | N-CA-CD-O1 |
| 1   | g     | 8   | GMA  | N-CA-CD-O1 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | h     | 8   | GMA  | N-CA-CD-O1  |
| 1   | i     | 8   | GMA  | N-CA-CD-O1  |
| 1   | K     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | N     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | Q     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | T     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | W     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | Z     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | l     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | o     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | r     | 201 | 5CR  | C-CA-CB-CG  |
| 1   | u     | 201 | 5CR  | CB-CA-N-CAL |
| 1   | x     | 201 | 5CR  | CB-CA-N-CAL |
| 1   | 0     | 201 | 5CR  | CB-CA-N-CAL |
| 1   | 3     | 201 | 5CR  | CB-CA-N-CAL |
| 1   | 6     | 201 | 5CR  | CB-CA-N-CAL |
| 1   | 9     | 201 | 5CR  | CB-CA-N-CAL |
| 1   | CA    | 201 | 5CR  | CB-CA-N-CAL |
| 1   | FA    | 201 | 5CR  | CB-CA-N-CAL |
| 1   | IA    | 201 | 5CR  | CB-CA-N-CAL |
| 1   | a     | 8   | GMA  | O-C-CG-CB   |
| 1   | b     | 8   | GMA  | O-C-CG-CB   |
| 1   | d     | 8   | GMA  | O-C-CG-CB   |
| 1   | f     | 8   | GMA  | O-C-CG-CB   |
| 1   | g     | 8   | GMA  | O-C-CG-CB   |
| 1   | i     | 8   | GMA  | O-C-CG-CB   |
| 1   | a     | 8   | GMA  | OXT-C-CG-CB |
| 1   | b     | 8   | GMA  | OXT-C-CG-CB |
| 1   | c     | 8   | GMA  | O-C-CG-CB   |
| 1   | c     | 8   | GMA  | OXT-C-CG-CB |
| 1   | d     | 8   | GMA  | OXT-C-CG-CB |
| 1   | e     | 8   | GMA  | O-C-CG-CB   |
| 1   | e     | 8   | GMA  | OXT-C-CG-CB |
| 1   | f     | 8   | GMA  | OXT-C-CG-CB |
| 1   | g     | 8   | GMA  | OXT-C-CG-CB |
| 1   | h     | 8   | GMA  | O-C-CG-CB   |
| 1   | h     | 8   | GMA  | OXT-C-CG-CB |
| 1   | i     | 8   | GMA  | OXT-C-CG-CB |
| 1   | 3     | 208 | GMA  | OXT-C-CG-CB |
| 1   | u     | 208 | GMA  | OXT-C-CG-CB |
| 1   | x     | 208 | GMA  | OXT-C-CG-CB |
| 1   | 0     | 208 | GMA  | OXT-C-CG-CB |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | 6     | 208 | GMA  | OXT-C-CG-CB |
| 1   | 9     | 208 | GMA  | OXT-C-CG-CB |
| 1   | FA    | 208 | GMA  | OXT-C-CG-CB |
| 1   | IA    | 208 | GMA  | OXT-C-CG-CB |
| 1   | CA    | 208 | GMA  | OXT-C-CG-CB |
| 1   | 0     | 208 | GMA  | O-C-CG-CB   |
| 1   | 3     | 208 | GMA  | O-C-CG-CB   |
| 1   | 9     | 208 | GMA  | O-C-CG-CB   |
| 1   | CA    | 208 | GMA  | O-C-CG-CB   |
| 1   | FA    | 208 | GMA  | O-C-CG-CB   |
| 1   | IA    | 208 | GMA  | O-C-CG-CB   |
| 1   | u     | 208 | GMA  | O-C-CG-CB   |
| 1   | x     | 208 | GMA  | O-C-CG-CB   |
| 1   | 6     | 208 | GMA  | O-C-CG-CB   |

There are no ring outliers.

35 monomers are involved in 27 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | S     | 108 | GMA  | 1       | 0            |
| 1   | Z     | 201 | 5CR  | 1       | 0            |
| 1   | M     | 108 | GMA  | 1       | 0            |
| 1   | l     | 308 | GMA  | 1       | 0            |
| 1   | n     | 108 | GMA  | 1       | 0            |
| 1   | r     | 201 | 5CR  | 1       | 0            |
| 1   | c     | 8   | GMA  | 1       | 0            |
| 1   | k     | 108 | GMA  | 1       | 0            |
| 1   | N     | 201 | 5CR  | 1       | 0            |
| 1   | 6     | 201 | 5CR  | 1       | 0            |
| 1   | a     | 8   | GMA  | 1       | 0            |
| 1   | d     | 8   | GMA  | 1       | 0            |
| 1   | EA    | 108 | GMA  | 1       | 0            |
| 1   | z     | 108 | GMA  | 1       | 0            |
| 1   | g     | 8   | GMA  | 1       | 0            |
| 1   | t     | 108 | GMA  | 1       | 0            |
| 1   | T     | 201 | 5CR  | 1       | 0            |
| 1   | Y     | 108 | GMA  | 1       | 0            |
| 1   | q     | 108 | GMA  | 1       | 0            |
| 1   | V     | 108 | GMA  | 1       | 0            |
| 1   | 2     | 108 | GMA  | 1       | 0            |
| 1   | i     | 8   | GMA  | 2       | 0            |
| 1   | e     | 8   | GMA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | BA    | 108 | GMA  | 1       | 0            |
| 1   | f     | 8   | GMA  | 1       | 0            |
| 1   | 5     | 108 | GMA  | 1       | 0            |
| 1   | o     | 201 | 5CR  | 1       | 0            |
| 1   | 8     | 108 | GMA  | 1       | 0            |
| 1   | K     | 201 | 5CR  | 1       | 0            |
| 1   | w     | 108 | GMA  | 1       | 0            |
| 1   | J     | 108 | GMA  | 1       | 0            |
| 1   | l     | 201 | 5CR  | 1       | 0            |
| 1   | P     | 108 | GMA  | 1       | 0            |
| 1   | W     | 201 | 5CR  | 1       | 0            |
| 1   | Q     | 201 | 5CR  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.



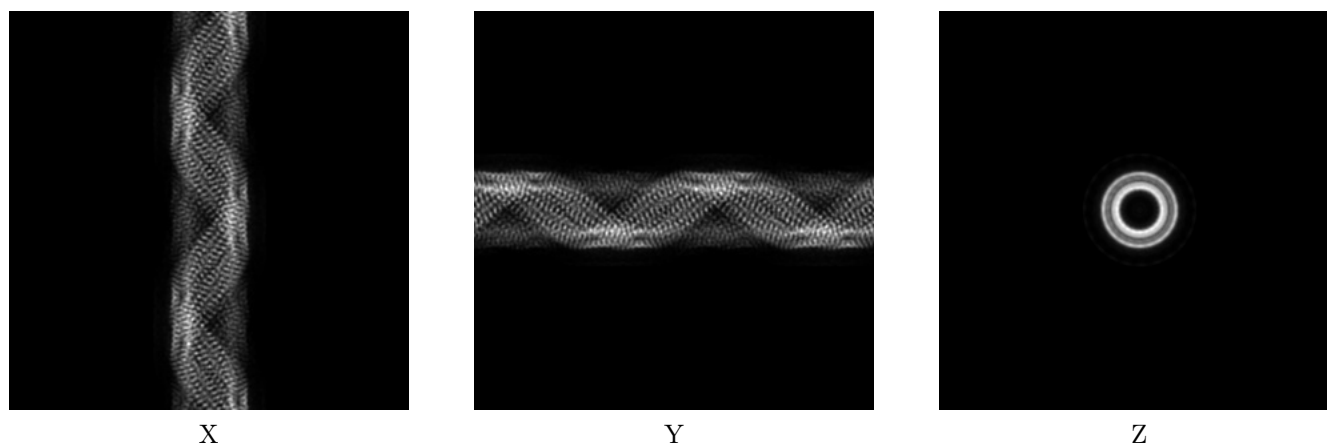
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23483. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

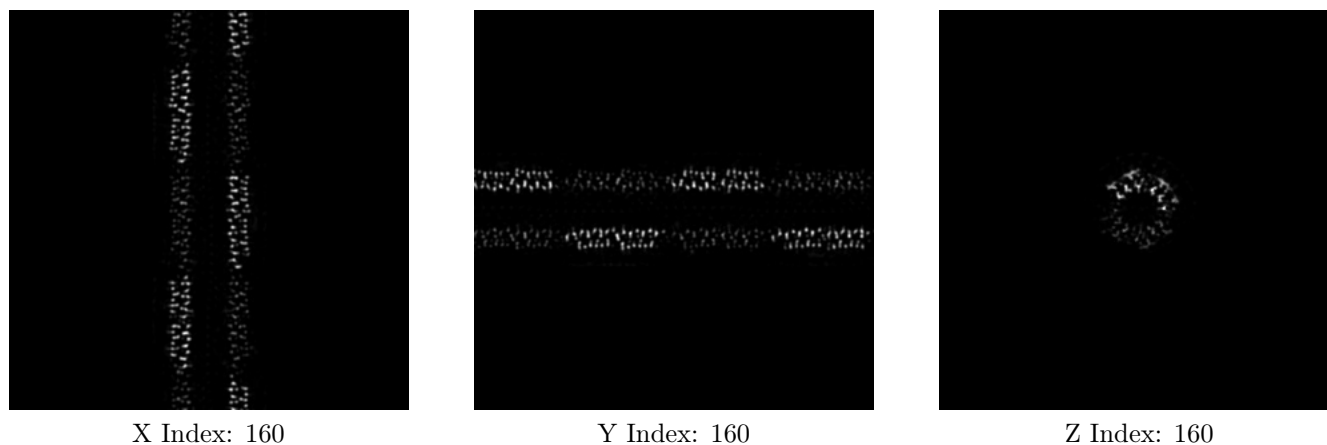
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



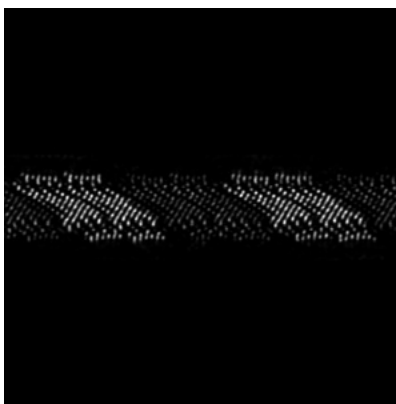
The images above show central slices of the map in three orthogonal directions.

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

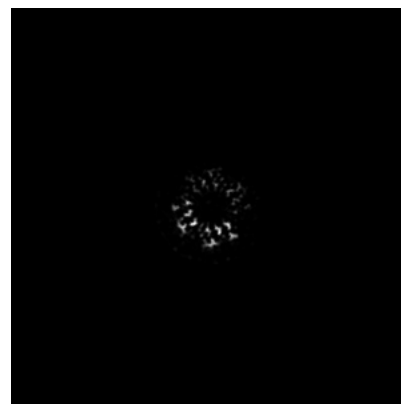
### 6.3.1 Primary map



X Index: 177



Y Index: 143

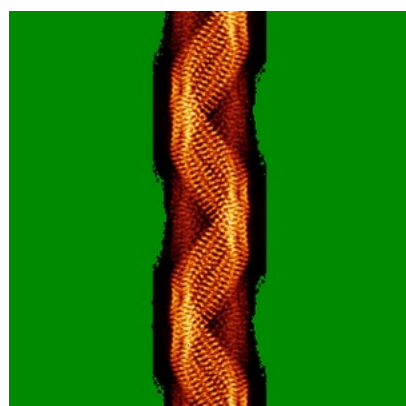


Z Index: 83

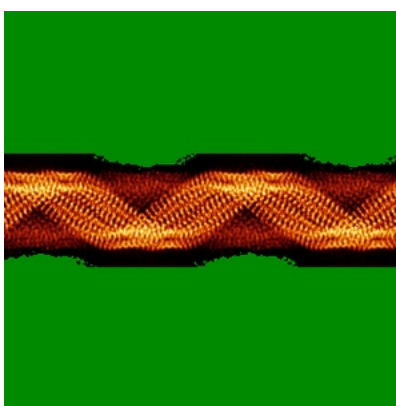
The images above show the largest variance slices of the map in three orthogonal directions.

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

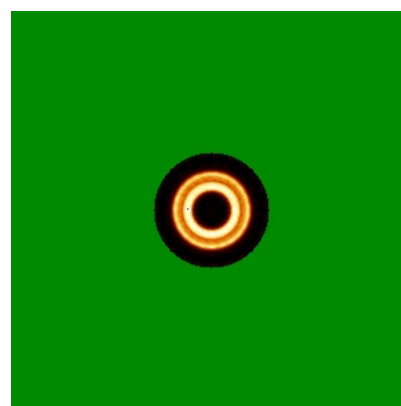
### 6.4.1 Primary map



X



Y

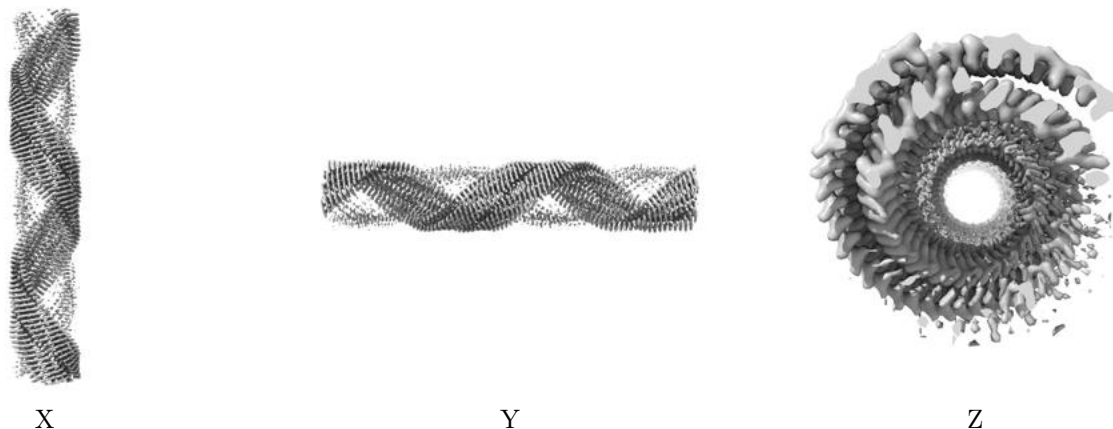


Z

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 0.264. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

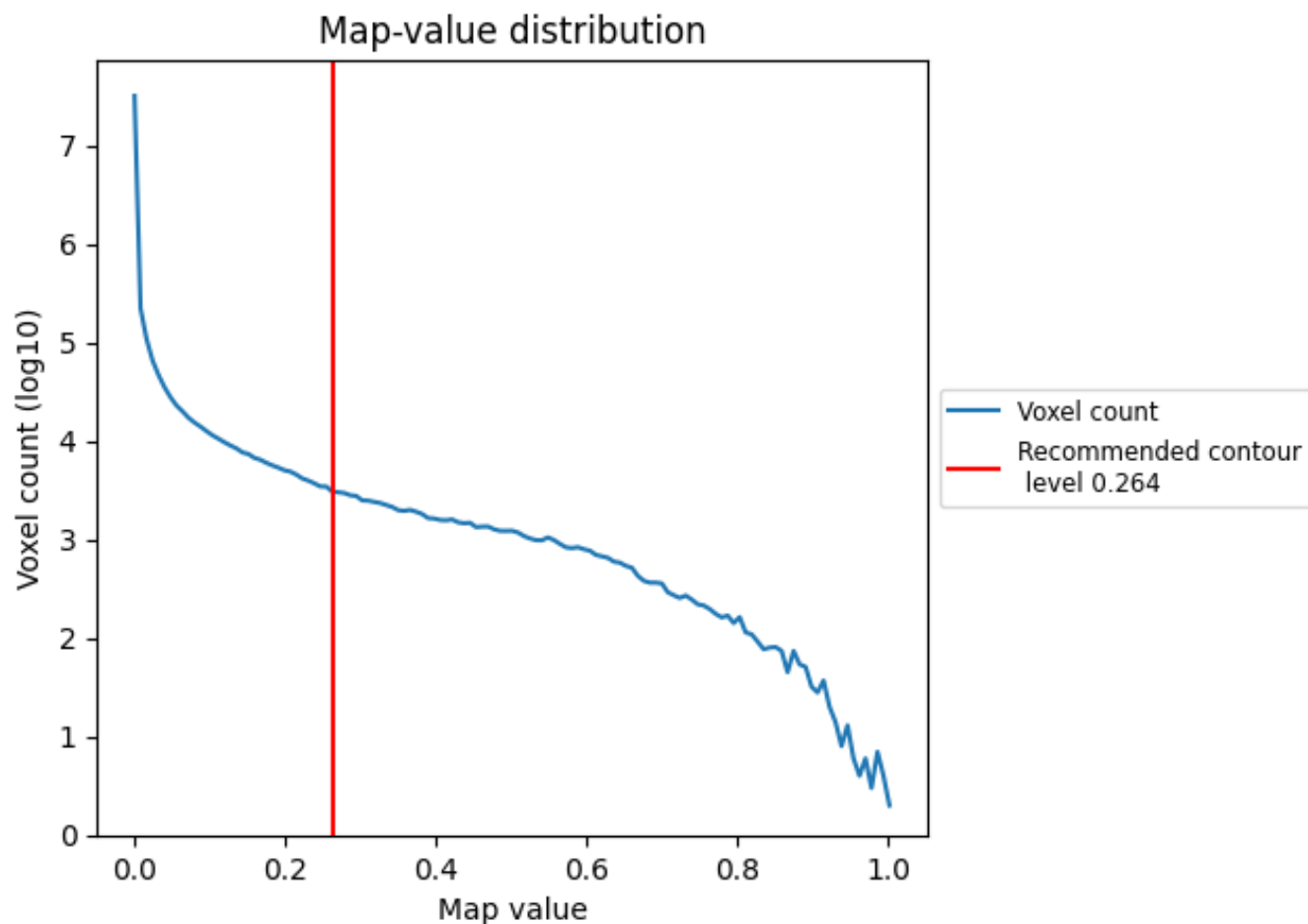
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

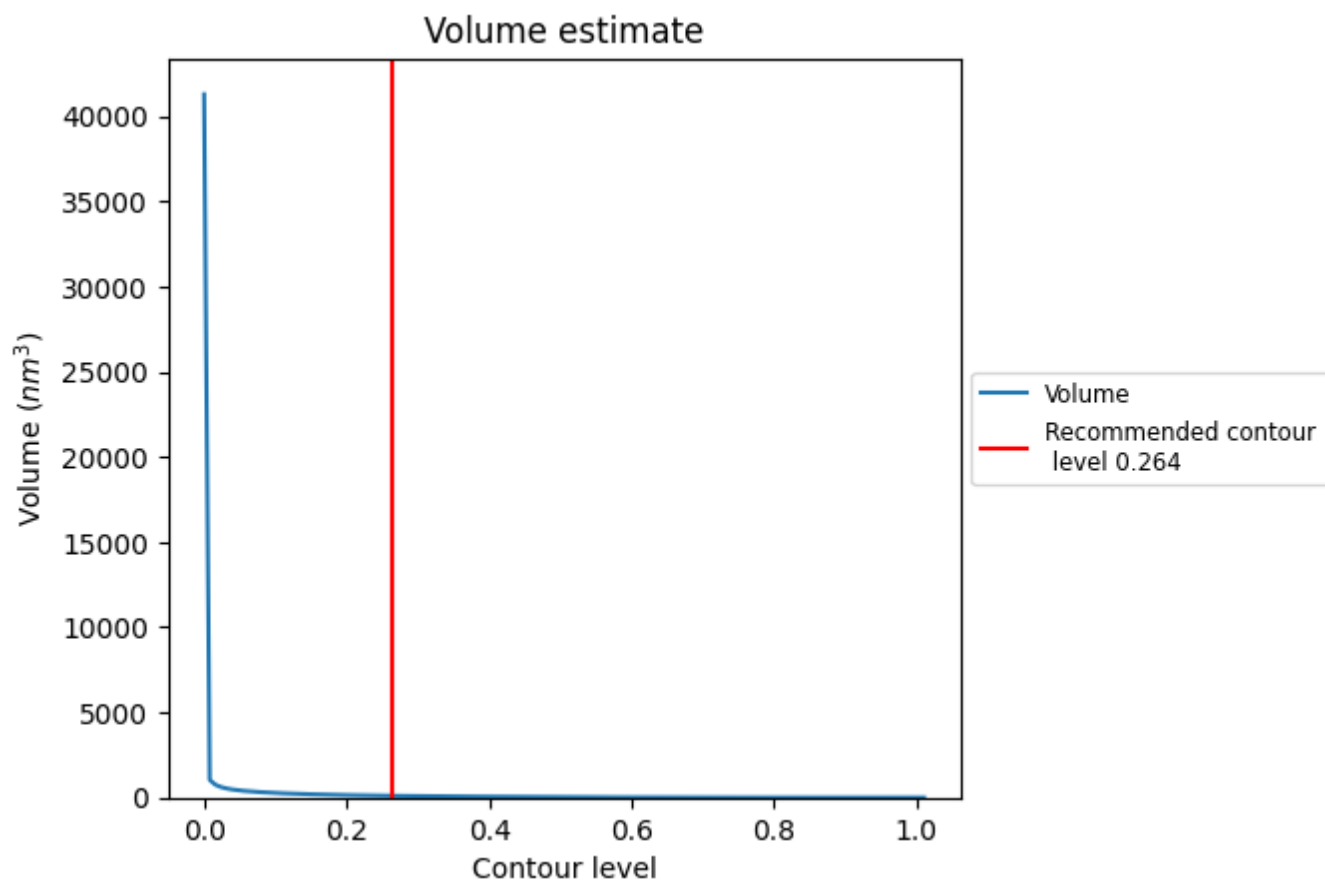
This section contains the results of statistical analysis of the map.

### 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.

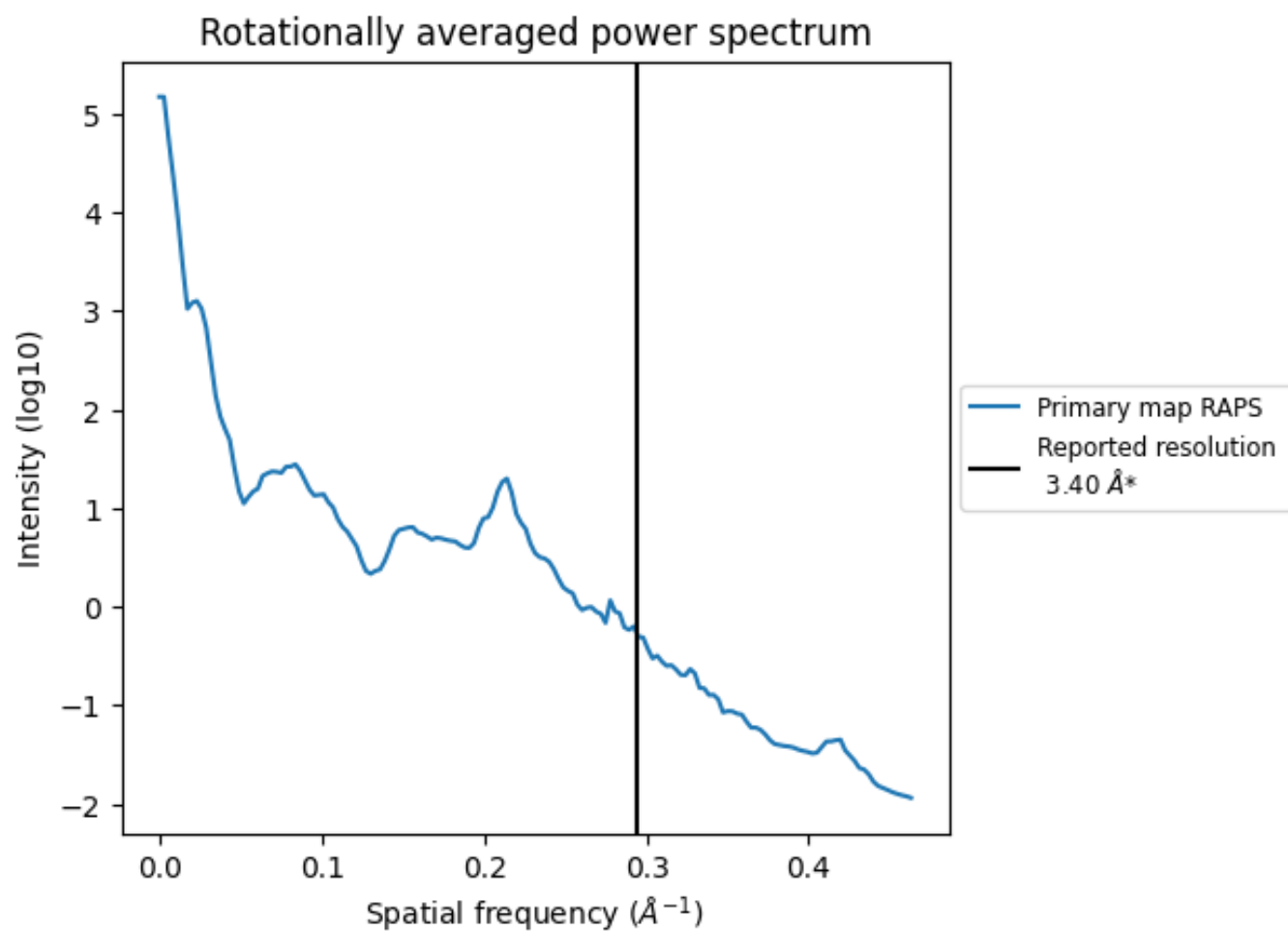
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103  $\text{nm}^3$ ; this corresponds to an approximate mass of 93 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 0.294 Å<sup>-1</sup>

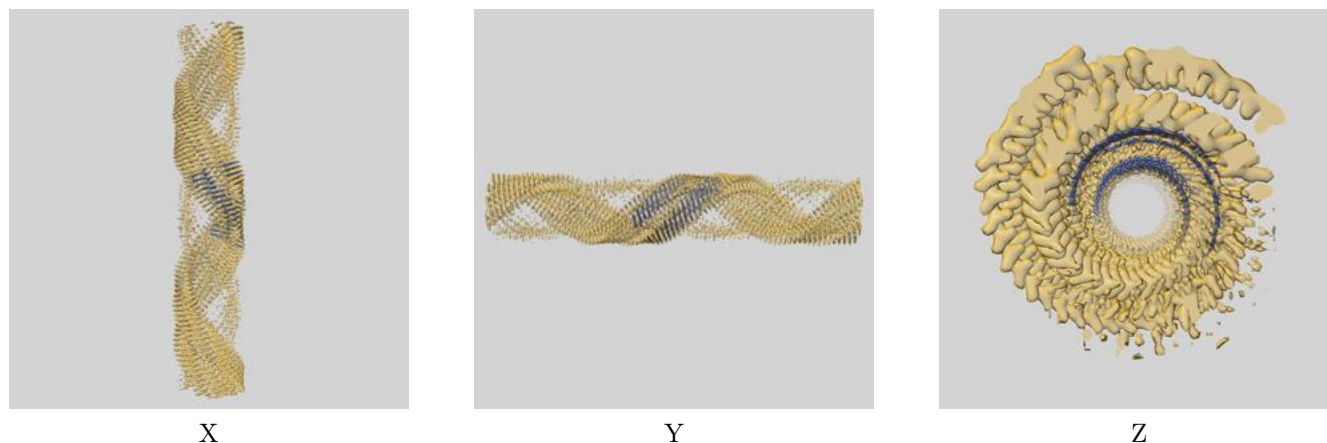
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-23483 and PDB model 7LQE. Per-residue inclusion information can be found in section 3 on page 10.

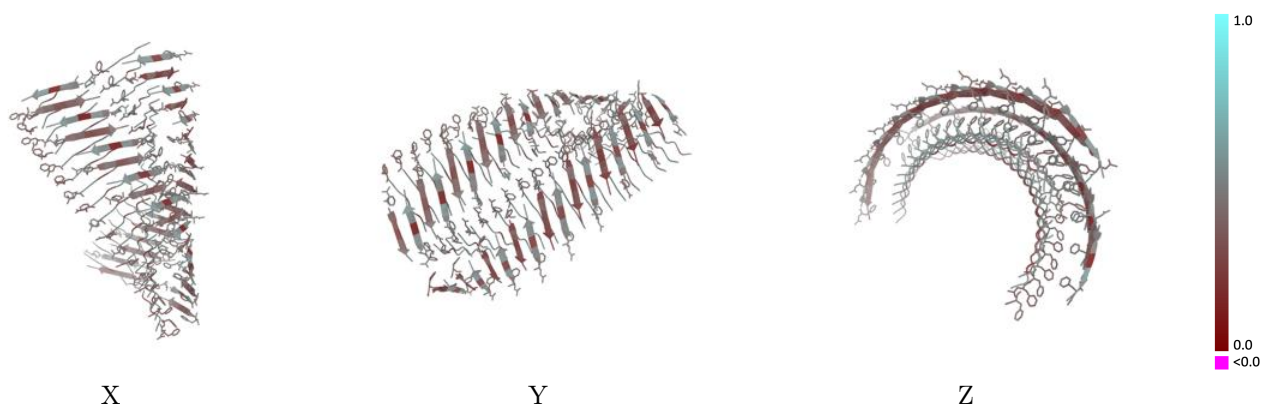
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.264 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.

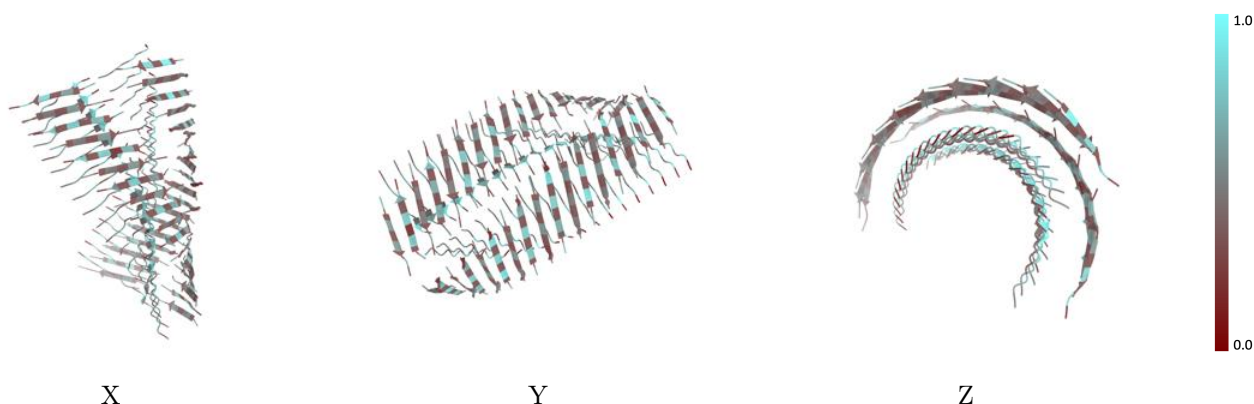


## 9.2 Q-score mapped to coordinate model [i](#)



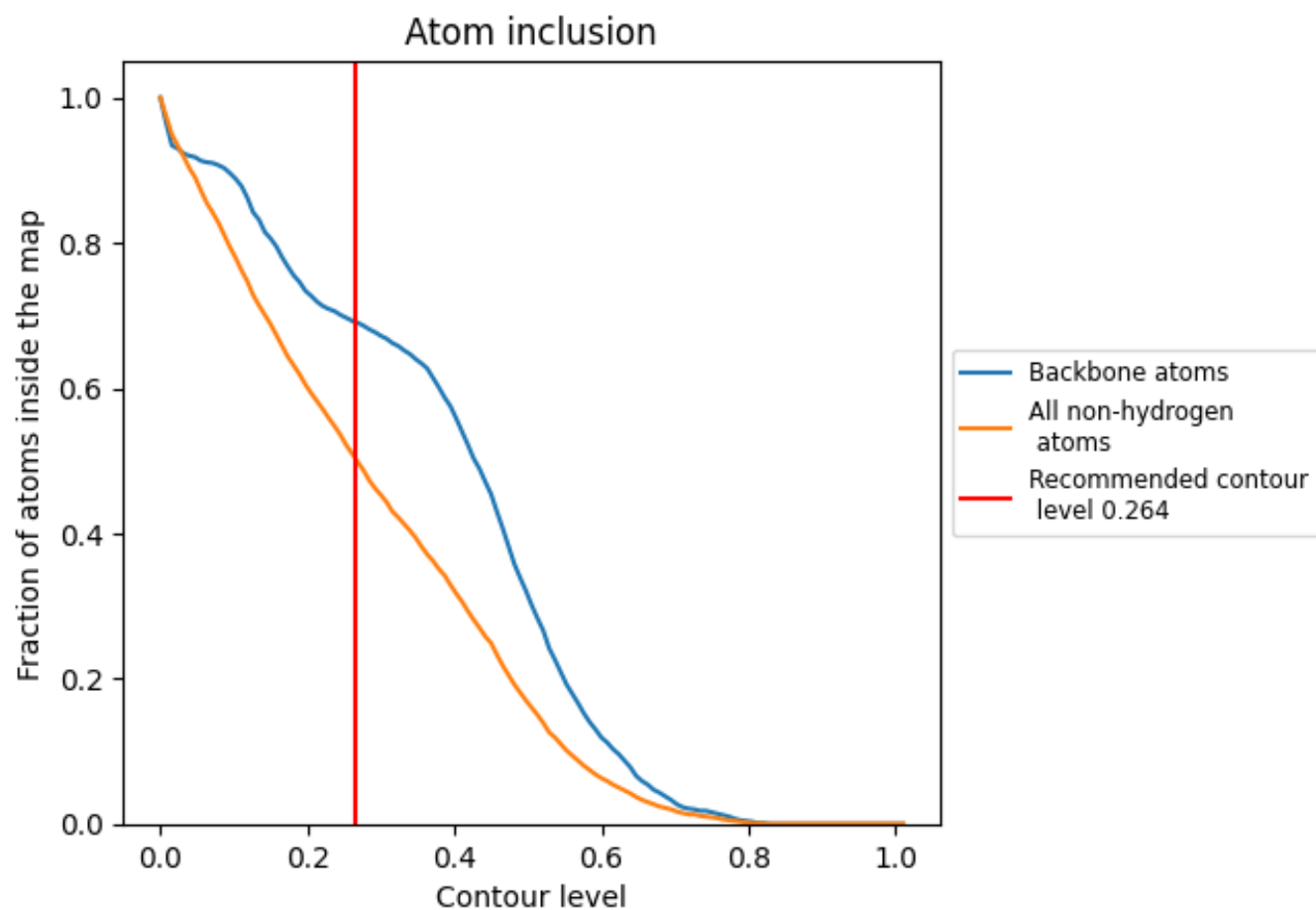
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.264).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 50% 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 (0.264) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5050   |  0.4250   |
| 0     |  0.5120   |  0.4370   |
| 1     |  0.4410   |  0.3390   |
| 2     |  0.4290   |  0.4070   |
| 3     |  0.5360   |  0.4470   |
| 4     |  0.4410   |  0.3420   |
| 5     |  0.4170   |  0.3870   |
| 6     |  0.5360   |  0.4570   |
| 7     |  0.4520   |  0.3410   |
| 8     |  0.4290   |  0.3860   |
| 9     |  0.5240   |  0.4510   |
| A     |  0.5120   |  0.4420   |
| AA    |  0.4520   |  0.3400   |
| B     |  0.5360   |  0.4280   |
| BA    |  0.4290  |  0.3960  |
| C     |  0.5120 |  0.4330 |
| CA    |  0.5120 |  0.4520 |
| D     |  0.5240 |  0.4270 |
| DA    |  0.4520 |  0.3520 |
| E     |  0.5000 |  0.4320 |
| EA    |  0.4170 |  0.3910 |
| F     |  0.5360 |  0.4310 |
| FA    |  0.5480 |  0.4570 |
| G     |  0.5480 |  0.4370 |
| GA    |  0.4170 |  0.3380 |
| H     |  0.5360 |  0.4250 |
| HA    |  0.4760 |  0.3980 |
| I     |  0.5000 |  0.4240 |
| IA    |  0.5120 |  0.4450 |
| J     |  0.5590 |  0.4260 |
| JA    |  0.4050 |  0.3180 |
| K     |  0.5480 |  0.4850 |
| L     |  0.5590 |  0.4410 |
| M     |  0.5590 |  0.4090 |
| N     |  0.5360 |  0.4850 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| O     |  0.5480   |  0.4460   |
| P     |  0.5590   |  0.4260   |
| Q     |  0.5120   |  0.4830   |
| R     |  0.5590   |  0.4480   |
| S     |  0.5240   |  0.4210   |
| T     |  0.5240   |  0.4660   |
| U     |  0.5710   |  0.4500   |
| V     |  0.5590   |  0.4330   |
| W     |  0.5480   |  0.4760   |
| X     |  0.5590   |  0.4380   |
| Y     |  0.5360   |  0.4160   |
| Z     |  0.5360   |  0.4790   |
| a     |  0.5000   |  0.4430   |
| b     |  0.4640   |  0.4340   |
| c     |  0.4640   |  0.4510   |
| d     |  0.4880   |  0.4420   |
| e     |  0.4880   |  0.4370   |
| f     |  0.5000   |  0.4430   |
| g     |  0.4760   |  0.4490   |
| h     |  0.5000  |  0.4250  |
| i     |  0.4880 |  0.4420 |
| j     |  0.5360 |  0.4500 |
| k     |  0.5590 |  0.4260 |
| l     |  0.5480 |  0.4790 |
| m     |  0.5360 |  0.4320 |
| n     |  0.5360 |  0.4230 |
| o     |  0.5120 |  0.4580 |
| p     |  0.5590 |  0.4430 |
| q     |  0.5590 |  0.4170 |
| r     |  0.5360 |  0.4770 |
| s     |  0.5360 |  0.4350 |
| t     |  0.4520 |  0.3960 |
| u     |  0.5240 |  0.4440 |
| v     |  0.4290 |  0.3380 |
| w     |  0.4290 |  0.4030 |
| x     |  0.5120 |  0.4580 |
| y     |  0.4170 |  0.3500 |
| z     |  0.4640 |  0.3980 |