



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:52 PM UTC

PDB ID : 7LQH / pdb\_00007lqh  
EMDB ID : EMD-23486  
Title : Cryo-EM of KFE8 thinner nanotube (class 2, 2-sub-1)  
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:

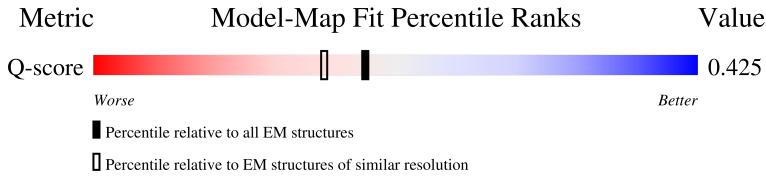
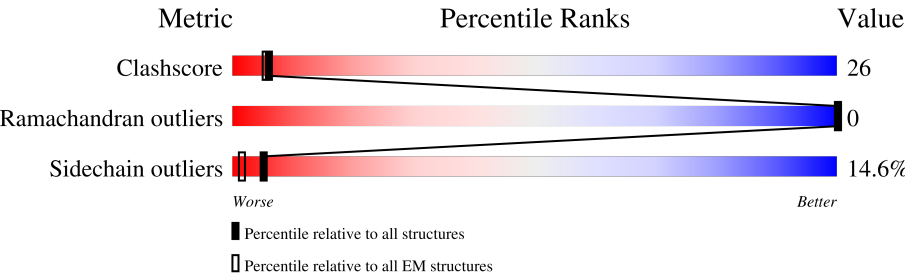
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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>38%</div> <div>50%</div> <div>38%</div> <div>12%</div> </div> |
| 1   | 0A    | 8      | <div> <div>62%</div> <div>12%</div> <div>75%</div> <div>12%</div> </div> |
| 1   | 1     | 8      | <div> <div>62%</div> <div>38%</div> <div>12%</div> <div>50%</div> </div> |
| 1   | 1A    | 8      | <div> <div>100%</div> <div>100%</div> </div>                             |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 2     | 8      |                  |
| 1   | 2A    | 8      |                  |
| 1   | 3     | 8      |                  |
| 1   | 3A    | 8      |                  |
| 1   | 4     | 8      |                  |
| 1   | 4A    | 8      |                  |
| 1   | 5     | 8      |                  |
| 1   | 5A    | 8      |                  |
| 1   | 6     | 8      |                  |
| 1   | 6A    | 8      |                  |
| 1   | 7     | 8      |                  |
| 1   | 7A    | 8      |                  |
| 1   | 8     | 8      |                  |
| 1   | 8A    | 8      |                  |
| 1   | 9     | 8      |                  |
| 1   | 9A    | 8      |                  |
| 1   | A     | 8      |                  |
| 1   | AA    | 8      |                  |
| 1   | AB    | 8      |                  |
| 1   | B     | 8      |                  |
| 1   | BA    | 8      |                  |
| 1   | BB    | 8      |                  |
| 1   | C     | 8      |                  |
| 1   | CA    | 8      |                  |
| 1   | CB    | 8      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | D     | 8      |                  |
| 1   | DA    | 8      |                  |
| 1   | DB    | 8      |                  |
| 1   | E     | 8      |                  |
| 1   | EA    | 8      |                  |
| 1   | EB    | 8      |                  |
| 1   | F     | 8      |                  |
| 1   | FA    | 8      |                  |
| 1   | FB    | 8      |                  |
| 1   | G     | 8      |                  |
| 1   | GA    | 8      |                  |
| 1   | GB    | 8      |                  |
| 1   | H     | 8      |                  |
| 1   | HA    | 8      |                  |
| 1   | HB    | 8      |                  |
| 1   | I     | 8      |                  |
| 1   | IA    | 8      |                  |
| 1   | IB    | 8      |                  |
| 1   | J     | 8      |                  |
| 1   | JA    | 8      |                  |
| 1   | JB    | 8      |                  |
| 1   | K     | 8      |                  |
| 1   | KA    | 8      |                  |
| 1   | KB    | 8      |                  |
| 1   | L     | 8      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | LA    | 8      |                  |
| 1   | LB    | 8      |                  |
| 1   | M     | 8      |                  |
| 1   | MA    | 8      |                  |
| 1   | MB    | 8      |                  |
| 1   | N     | 8      |                  |
| 1   | NA    | 8      |                  |
| 1   | NB    | 8      |                  |
| 1   | O     | 8      |                  |
| 1   | OA    | 8      |                  |
| 1   | OB    | 8      |                  |
| 1   | P     | 8      |                  |
| 1   | PA    | 8      |                  |
| 1   | PB    | 8      |                  |
| 1   | Q     | 8      |                  |
| 1   | QA    | 8      |                  |
| 1   | QB    | 8      |                  |
| 1   | R     | 8      |                  |
| 1   | RA    | 8      |                  |
| 1   | RB    | 8      |                  |
| 1   | S     | 8      |                  |
| 1   | SA    | 8      |                  |
| 1   | SB    | 8      |                  |
| 1   | T     | 8      |                  |
| 1   | TA    | 8      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | TB    | 8      |                  |
| 1   | U     | 8      |                  |
| 1   | UA    | 8      |                  |
| 1   | V     | 8      |                  |
| 1   | VA    | 8      |                  |
| 1   | W     | 8      |                  |
| 1   | WA    | 8      |                  |
| 1   | X     | 8      |                  |
| 1   | XA    | 8      |                  |
| 1   | Y     | 8      |                  |
| 1   | YA    | 8      |                  |
| 1   | Z     | 8      |                  |
| 1   | ZA    | 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      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | g     | 8      |                  |
| 1   | gA    | 8      |                  |
| 1   | h     | 8      |                  |
| 1   | hA    | 8      |                  |
| 1   | i     | 8      |                  |
| 1   | iA    | 8      |                  |
| 1   | j     | 8      |                  |
| 1   | jA    | 8      |                  |
| 1   | k     | 8      |                  |
| 1   | kA    | 8      |                  |
| 1   | l     | 8      |                  |
| 1   | lA    | 8      |                  |
| 1   | m     | 8      |                  |
| 1   | mA    | 8      |                  |
| 1   | n     | 8      |                  |
| 1   | nA    | 8      |                  |
| 1   | o     | 8      |                  |
| 1   | oA    | 8      |                  |
| 1   | p     | 8      |                  |
| 1   | pA    | 8      |                  |
| 1   | q     | 8      |                  |
| 1   | qA    | 8      |                  |
| 1   | r     | 8      |                  |
| 1   | rA    | 8      |                  |
| 1   | s     | 8      |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | sA    | 8      |                  |
| 1   | t     | 8      |                  |
| 1   | tA    | 8      |                  |
| 1   | u     | 8      |                  |
| 1   | uA    | 8      |                  |
| 1   | v     | 8      |                  |
| 1   | vA    | 8      |                  |
| 1   | w     | 8      |                  |
| 1   | wA    | 8      |                  |
| 1   | x     | 8      |                  |
| 1   | xA    | 8      |                  |
| 1   | y     | 8      |                  |
| 1   | yA    | 8      |                  |
| 1   | z     | 8      |                  |
| 1   | zA    | 8      |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | GMA  | 0     | 1308 | -         | -        | X       | -                |
| 1   | 5CR  | 1     | 101  | -         | -        | X       | -                |
| 1   | 5CR  | 5     | 1101 | -         | -        | X       | -                |
| 1   | GMA  | AA    | 308  | -         | -        | X       | -                |
| 1   | GMA  | EA    | 1308 | -         | -        | X       | -                |
| 1   | 5CR  | FA    | 101  | -         | -        | X       | -                |
| 1   | 5CR  | J     | 101  | -         | -        | X       | -                |
| 1   | GMA  | L     | 308  | -         | -        | X       | -                |
| 1   | 5CR  | N     | 1101 | -         | -        | X       | -                |
| 1   | GMA  | OA    | 308  | -         | -        | X       | -                |
| 1   | GMA  | P     | 1308 | -         | -        | X       | -                |
| 1   | 5CR  | Q     | 101  | -         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | GMA  | S     | 308  | -         | -        | X       | -                |
| 1   | GMA  | SA    | 1308 | -         | -        | X       | -                |
| 1   | GMA  | Z     | 308  | -         | -        | X       | -                |
| 1   | 5CR  | k     | 1101 | -         | -        | X       | -                |
| 1   | GMA  | m     | 1308 | -         | -        | X       | -                |
| 1   | 5CR  | r     | 1101 | -         | -        | X       | -                |
| 1   | GMA  | w     | 308  | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 12096 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   | 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   | P     | 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   | 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   | 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   | 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   | C     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 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   | 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   | 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   | D     | 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   | 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   | t     | 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   | 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   | 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 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 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   | F     | 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   | 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   | 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   | G     | 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 |         |       |
| 1   | AA    | 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   | EA    | 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   | 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 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 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 |         |       |
| 1   | KA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | LA    | 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   | MA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | NA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | OA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | PA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | QA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | RA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | SA    | 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   | TA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | UA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | VA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | WA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | XA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | YA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | ZA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | b     | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | aA    | 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   | 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   | c     | 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 |         |       |
| 1   | kA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | lA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | mA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | nA    | 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   | oA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | pA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | qA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | rA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | sA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | tA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | uA    | 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   | vA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | wA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | xA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | yA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | zA    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 0A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 1A    | 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   | 2A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 3A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 4A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 5A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 6A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 7A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | 8A    | 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   | 9A    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | AB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | BB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | CB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | DB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | EB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | FB    | 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   | GB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | HB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | IB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | JB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | KB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | LB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | MB    | 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   | NB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | OB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | PB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | QB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | RB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |
| 1   | SB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

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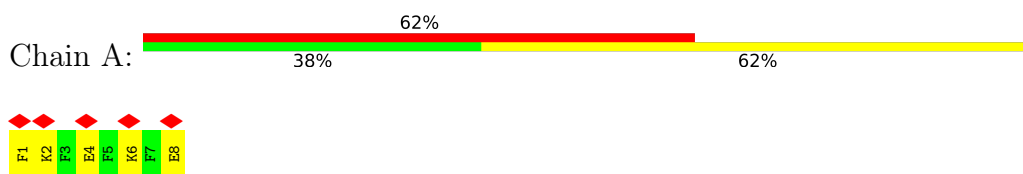
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| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1   | TB    | 8        | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 84    | 60 | 11 | 13 |         |       |

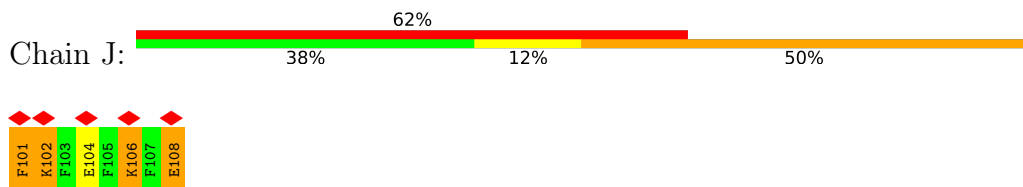
### 3 Residue-property plots [i](#)

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.

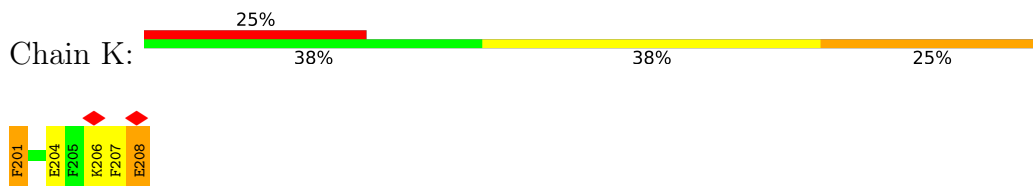
- Molecule 1: KFE8 peptide



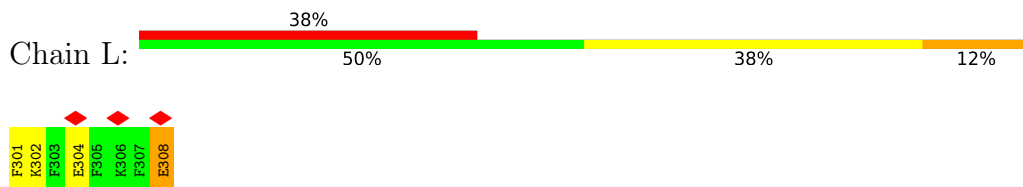
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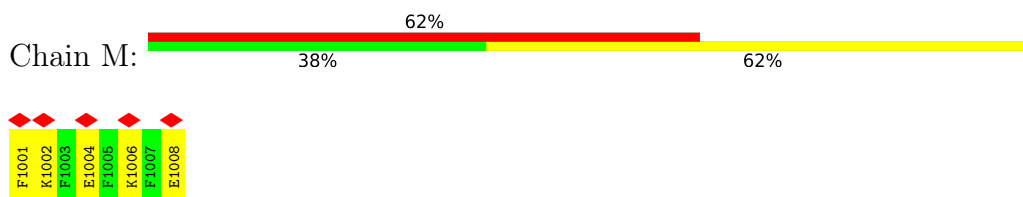
- Molecule 1: KFE8 peptide



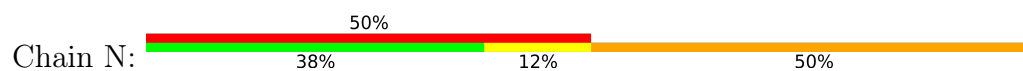
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



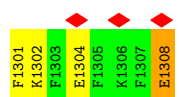
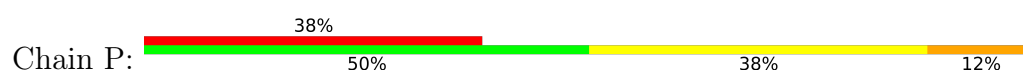
## ● Molecule 1: KFE8 peptide



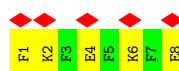
## ● Molecule 1: KFE8 peptide



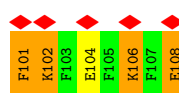
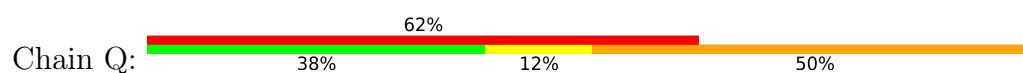
## ● Molecule 1: KFE8 peptide



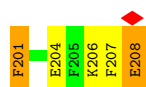
## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide





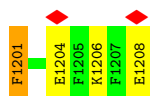
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



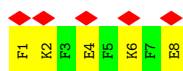
- Molecule 1: KFE8 peptide



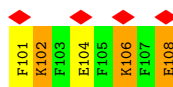
- Molecule 1: KFE8 peptide



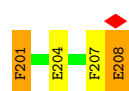
- Molecule 1: KFE8 peptide



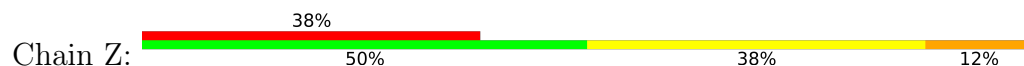
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



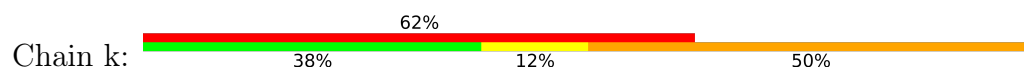
- Molecule 1: KFE8 peptide



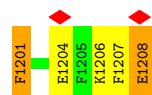
- Molecule 1: KFE8 peptide



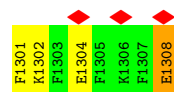
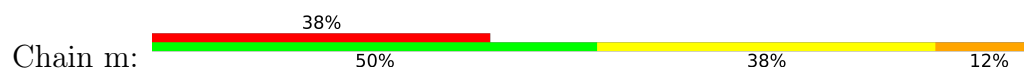
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

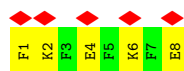


- Molecule 1: KFE8 peptide

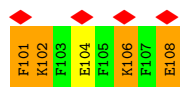
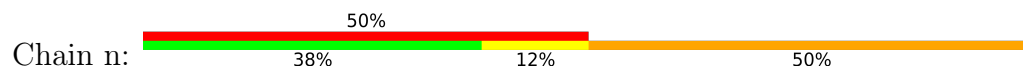


- Molecule 1: KFE8 peptide





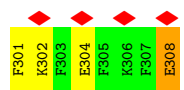
- Molecule 1: KFE8 peptide



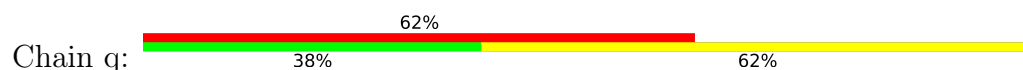
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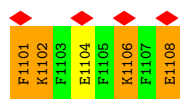
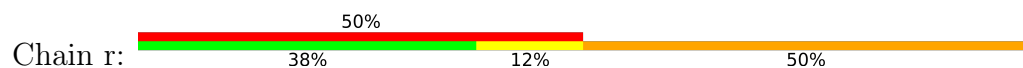
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



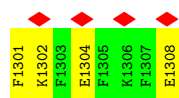
- Molecule 1: KFE8 peptide



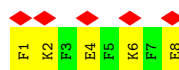
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



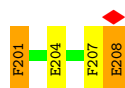
- Molecule 1: KFE8 peptide



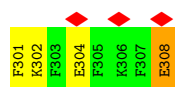
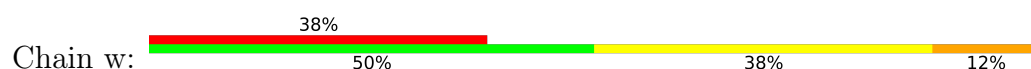
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

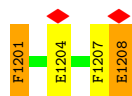


- Molecule 1: KFE8 peptide

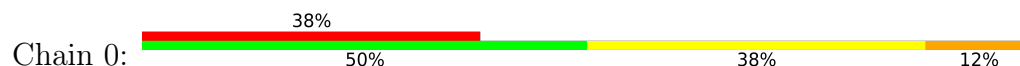




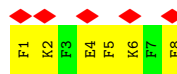
- Molecule 1: KFE8 peptide



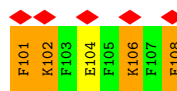
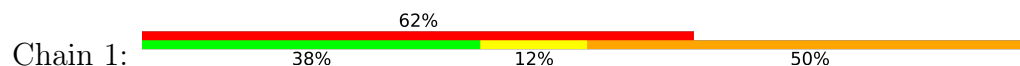
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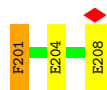
- Molecule 1: KFE8 peptide



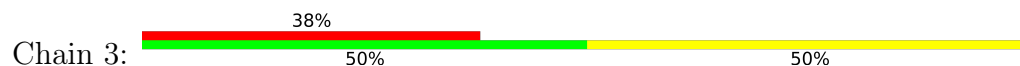
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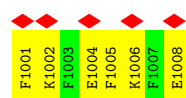
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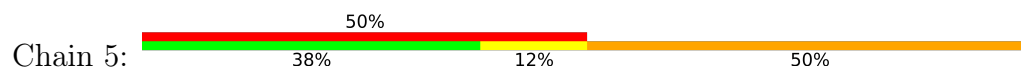
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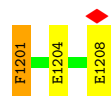
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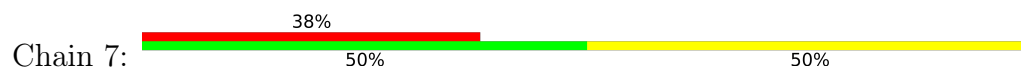
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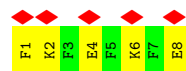
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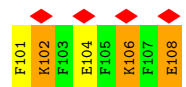
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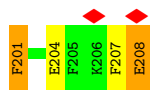


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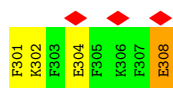
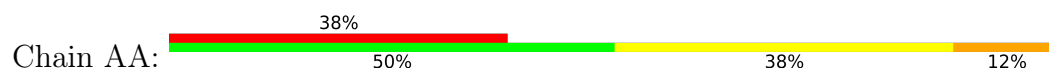


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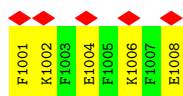




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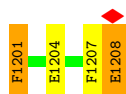
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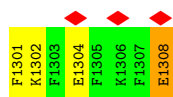
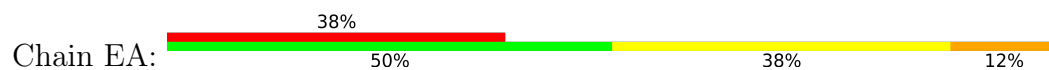
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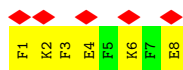
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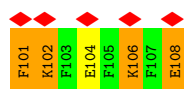
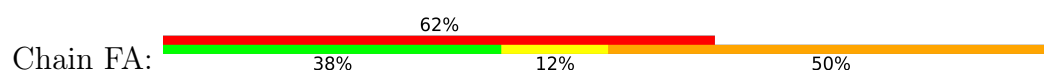
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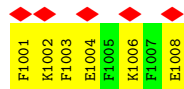
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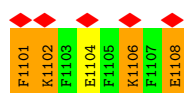
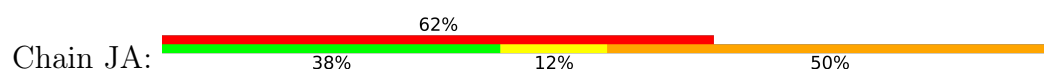
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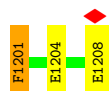
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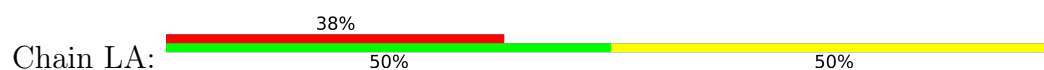
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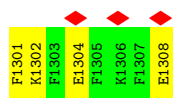


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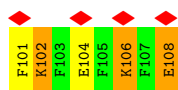




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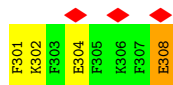
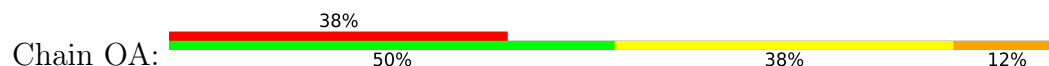
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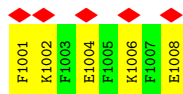
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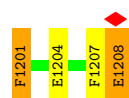
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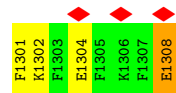
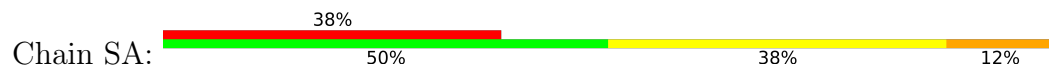
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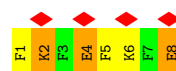
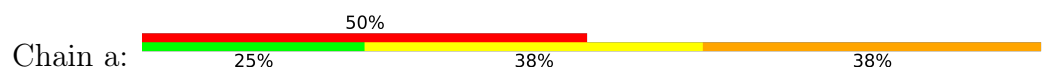
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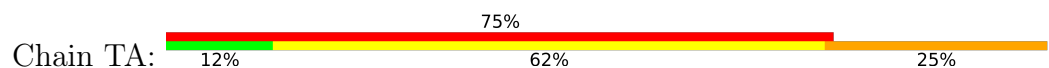
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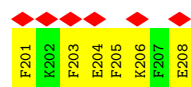
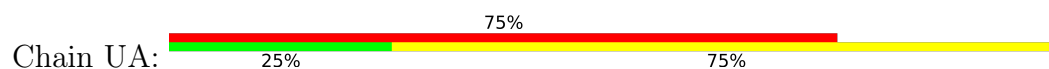
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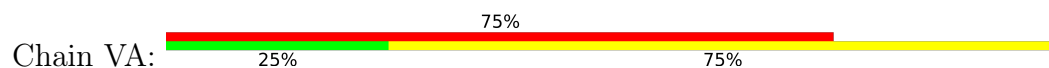
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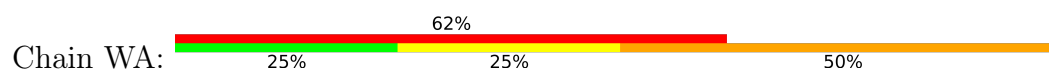
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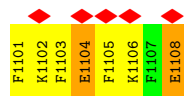
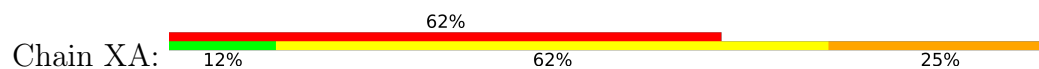


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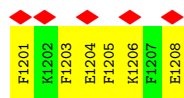




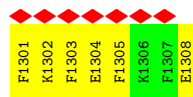
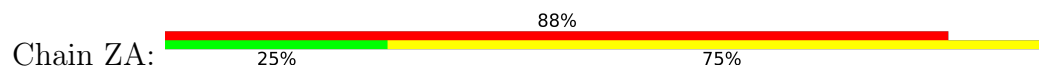
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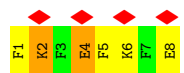
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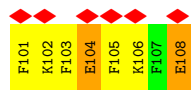
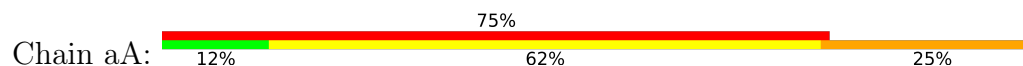
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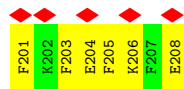
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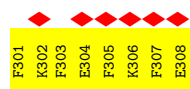
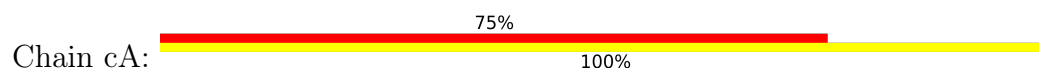
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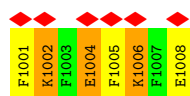
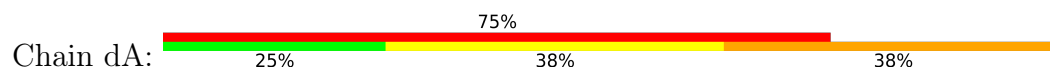
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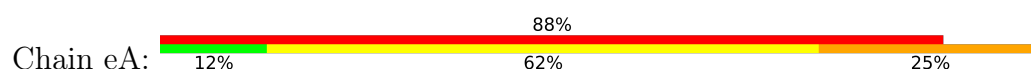
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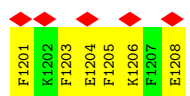
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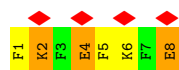
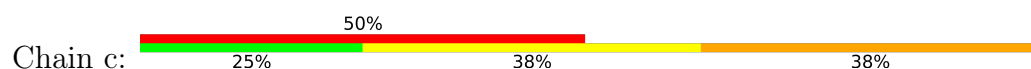
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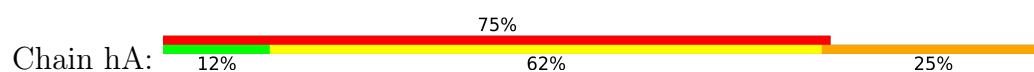
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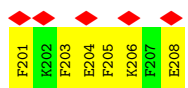


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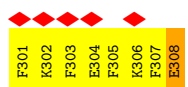
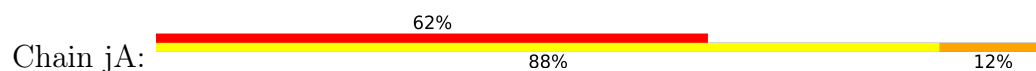




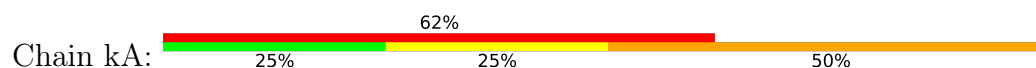
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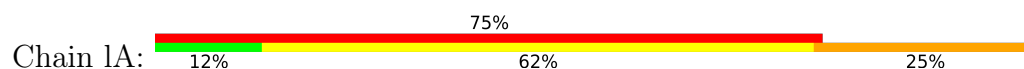
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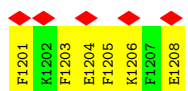
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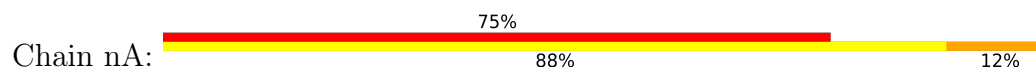
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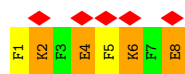
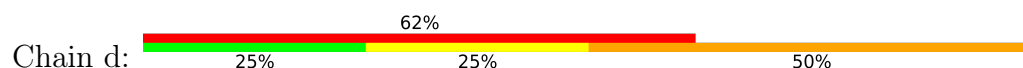
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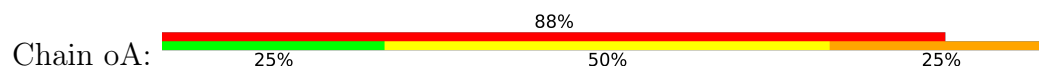
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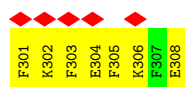
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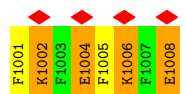
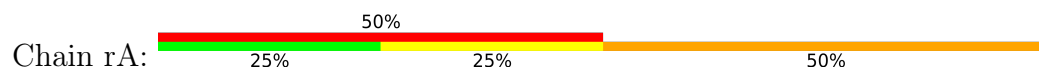
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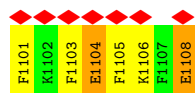
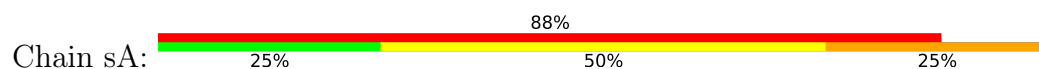
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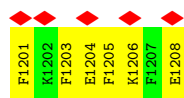


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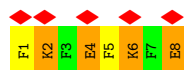
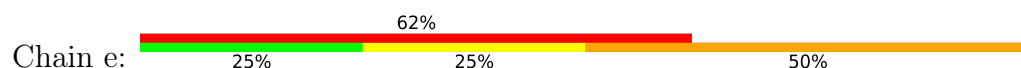




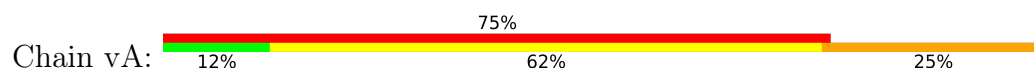
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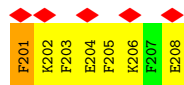
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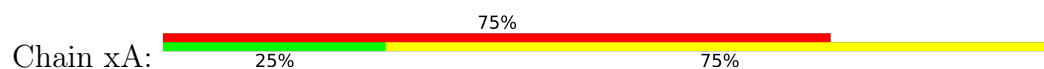
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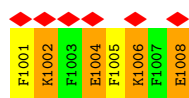
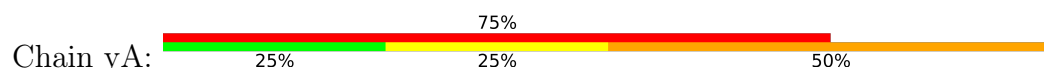
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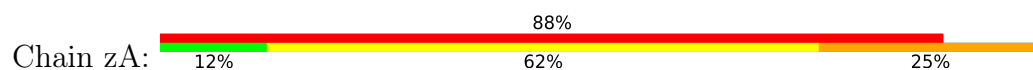
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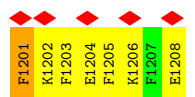
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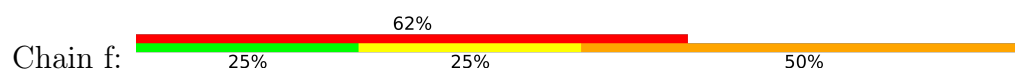
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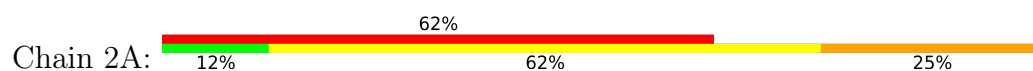
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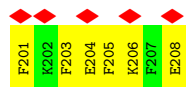
- Molecule 1: KFE8 peptide



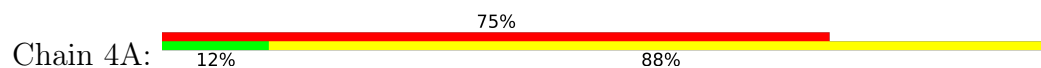
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

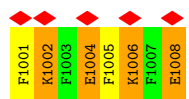
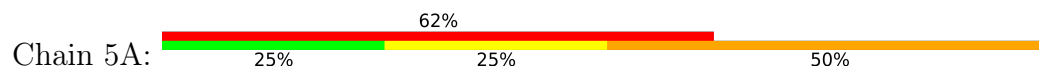


- Molecule 1: KFE8 peptide

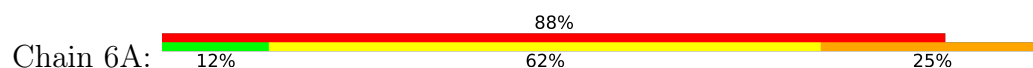




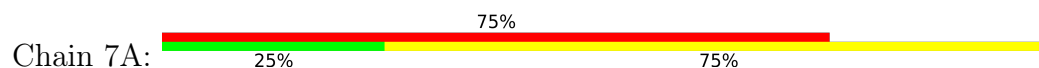
- Molecule 1: KFE8 peptide



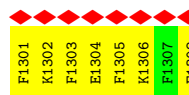
- Molecule 1: KFE8 peptide



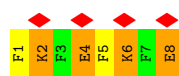
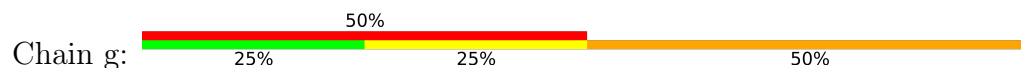
- Molecule 1: KFE8 peptide



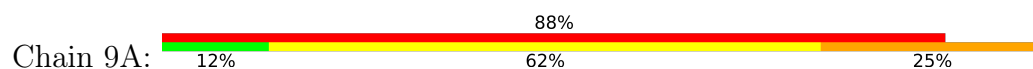
- Molecule 1: KFE8 peptide



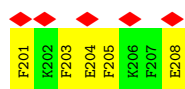
- Molecule 1: KFE8 peptide



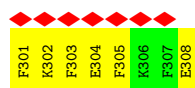
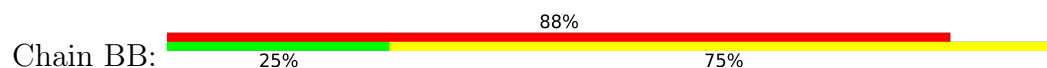
- Molecule 1: KFE8 peptide



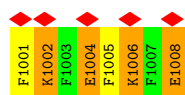
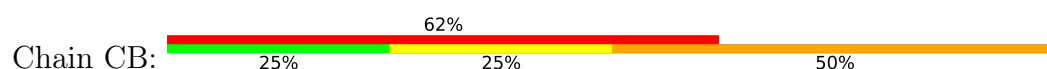
- Molecule 1: KFE8 peptide



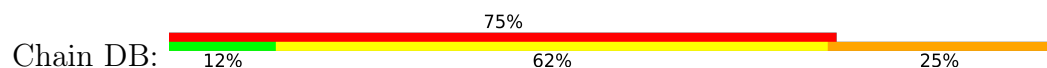
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

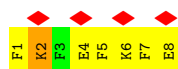


- Molecule 1: KFE8 peptide

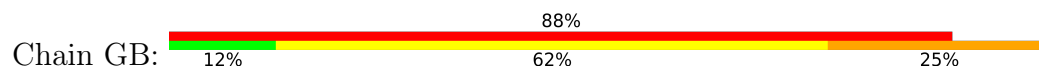


- Molecule 1: KFE8 peptide





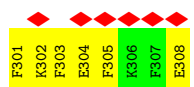
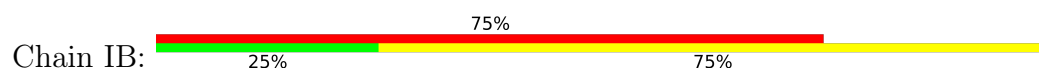
- Molecule 1: KFE8 peptide



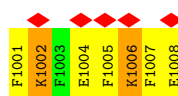
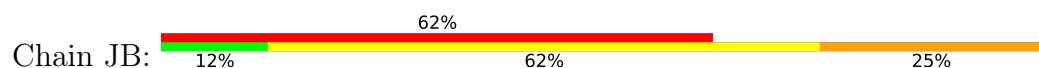
- Molecule 1: KFE8 peptide



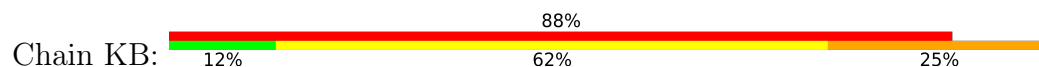
- Molecule 1: KFE8 peptide



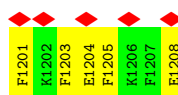
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



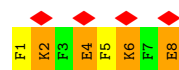
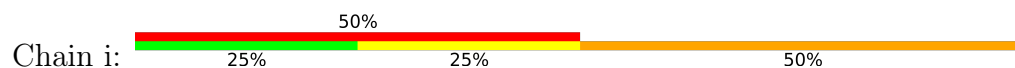
- Molecule 1: KFE8 peptide



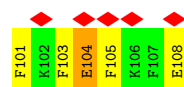
- Molecule 1: KFE8 peptide



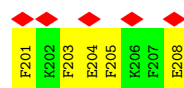
- Molecule 1: KFE8 peptide



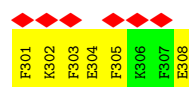
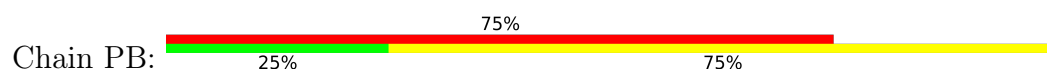
- Molecule 1: KFE8 peptide



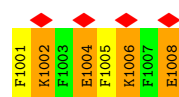
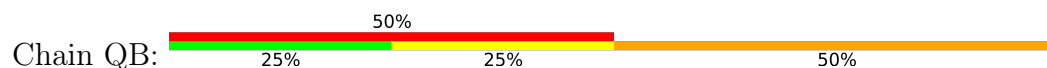
- Molecule 1: KFE8 peptide



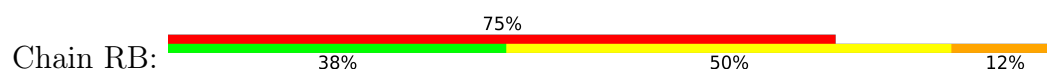
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

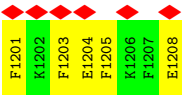
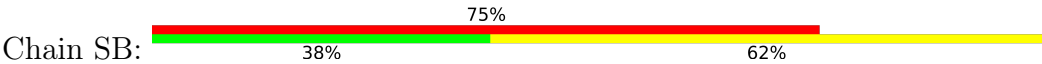


- Molecule 1: KFE8 peptide

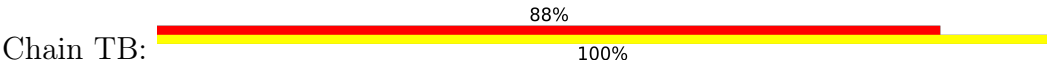




● Molecule 1: KFE8 peptide



● Molecule 1: KFE8 peptide



## 4 Experimental information

| Property                           | Value                                            | Source    |
|------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                          | Depositor |
| Imposed symmetry                   | HELICAL, twist=172.1°, rise=3.97 Å, axial sym=C2 | Depositor |
| Number of segments used            | 31760                                            | 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                  | 0.929                                            | Depositor |
| Minimum map value                  | -0.001                                           | Depositor |
| Average map value                  | 0.003                                            | Depositor |
| Map value standard deviation       | 0.029                                            | Depositor |
| Recommended contour level          | 0.273                                            | 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     | 0.39         | 0/62        | 0.33        | 0/79        |
| 1   | 0A    | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | 1     | 0.39         | 0/62        | 0.38        | 0/79        |
| 1   | 1A    | 0.32         | 0/62        | 0.39        | 0/79        |
| 1   | 2     | 0.43         | 0/62        | 0.44        | 0/79        |
| 1   | 2A    | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | 3     | 0.39         | 0/62        | 0.33        | 0/79        |
| 1   | 3A    | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | 4     | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | 4A    | 0.33         | 0/62        | 0.39        | 0/79        |
| 1   | 5     | 0.38         | 0/62        | 0.38        | 0/79        |
| 1   | 5A    | 0.33         | 0/62        | 0.61        | 0/79        |
| 1   | 6     | 0.43         | 0/62        | 0.44        | 0/79        |
| 1   | 6A    | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | 7     | 0.39         | 0/62        | 0.33        | 0/79        |
| 1   | 7A    | 0.32         | 0/62        | 0.45        | 0/79        |
| 1   | 8     | 0.39         | 0/62        | 0.38        | 0/79        |
| 1   | 8A    | 0.33         | 0/62        | 0.39        | 0/79        |
| 1   | 9     | 0.43         | 0/62        | 0.44        | 0/79        |
| 1   | 9A    | 0.30         | 0/62        | 0.43        | 0/79        |
| 1   | A     | 0.41         | 0/62        | 0.43        | 0/79        |
| 1   | AA    | 0.39         | 0/62        | 0.33        | 0/79        |
| 1   | AB    | 0.31         | 0/62        | 0.45        | 0/79        |
| 1   | B     | 0.41         | 0/62        | 0.43        | 0/79        |
| 1   | BA    | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | BB    | 0.33         | 0/62        | 0.39        | 0/79        |
| 1   | C     | 0.40         | 0/62        | 0.43        | 0/79        |
| 1   | CA    | 0.39         | 0/62        | 0.38        | 0/79        |
| 1   | CB    | 0.33         | 0/62        | 0.61        | 0/79        |
| 1   | D     | 0.40         | 0/62        | 0.42        | 0/79        |
| 1   | DA    | 0.43         | 0/62        | 0.44        | 0/79        |
| 1   | DB    | 0.30         | 0/62        | 0.43        | 0/79        |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | E     | 0.40         | 0/62    | 0.43        | 0/79    |
| 1   | EA    | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | EB    | 0.32         | 0/62    | 0.46        | 0/79    |
| 1   | F     | 0.40         | 0/62    | 0.43        | 0/79    |
| 1   | FA    | 0.38         | 0/62    | 0.37        | 0/79    |
| 1   | FB    | 0.33         | 0/62    | 0.39        | 0/79    |
| 1   | G     | 0.40         | 0/62    | 0.42        | 0/79    |
| 1   | GA    | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | GB    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | H     | 0.40         | 0/62    | 0.42        | 0/79    |
| 1   | HA    | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | HB    | 0.31         | 0/62    | 0.46        | 0/79    |
| 1   | I     | 0.40         | 0/62    | 0.43        | 0/79    |
| 1   | IA    | 0.40         | 0/62    | 0.42        | 0/79    |
| 1   | IB    | 0.33         | 0/62    | 0.39        | 0/79    |
| 1   | J     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | JA    | 0.38         | 0/62    | 0.37        | 0/79    |
| 1   | JB    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | K     | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | KA    | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | KB    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | L     | 0.38         | 0/62    | 0.33        | 0/79    |
| 1   | LA    | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | LB    | 0.31         | 0/62    | 0.46        | 0/79    |
| 1   | M     | 0.41         | 0/62    | 0.43        | 0/79    |
| 1   | MA    | 0.39         | 0/62    | 0.38        | 0/79    |
| 1   | MB    | 0.33         | 0/62    | 0.39        | 0/79    |
| 1   | N     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | NA    | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | NB    | 0.31         | 0/62    | 0.43        | 0/79    |
| 1   | O     | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | OA    | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | OB    | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | P     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | PA    | 0.40         | 0/62    | 0.43        | 0/79    |
| 1   | PB    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | Q     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | QA    | 0.39         | 0/62    | 0.38        | 0/79    |
| 1   | QB    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | R     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | RA    | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | RB    | 0.31         | 0/62    | 0.43        | 0/79    |
| 1   | S     | 0.39         | 0/62    | 0.33        | 0/79    |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | SA    | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | SB    | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | T     | 0.41         | 0/62    | 0.43        | 0/79    |
| 1   | TA    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | TB    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | U     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | UA    | 0.32         | 0/62    | 0.46        | 0/79    |
| 1   | V     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | VA    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | W     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | WA    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | X     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | XA    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | Y     | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | YA    | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | Z     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | ZA    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | a     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | aA    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | b     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | bA    | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | c     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | cA    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | d     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | dA    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | e     | 0.32         | 0/62    | 0.61        | 0/79    |
| 1   | eA    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | f     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | fA    | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | g     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | gA    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | h     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | hA    | 0.30         | 0/62    | 0.42        | 0/79    |
| 1   | i     | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | iA    | 0.32         | 0/62    | 0.46        | 0/79    |
| 1   | j     | 0.40         | 0/62    | 0.43        | 0/79    |
| 1   | jA    | 0.33         | 0/62    | 0.39        | 0/79    |
| 1   | k     | 0.38         | 0/62    | 0.38        | 0/79    |
| 1   | kA    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | l     | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | lA    | 0.30         | 0/62    | 0.42        | 0/79    |
| 1   | m     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | mA    | 0.32         | 0/62    | 0.45        | 0/79    |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | n     | 0.39         | 0/62    | 0.38        | 0/79    |
| 1   | nA    | 0.33         | 0/62    | 0.39        | 0/79    |
| 1   | o     | 0.44         | 0/62    | 0.43        | 0/79    |
| 1   | oA    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | p     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | pA    | 0.32         | 0/62    | 0.46        | 0/79    |
| 1   | q     | 0.40         | 0/62    | 0.42        | 0/79    |
| 1   | qA    | 0.32         | 0/62    | 0.40        | 0/79    |
| 1   | r     | 0.39         | 0/62    | 0.38        | 0/79    |
| 1   | rA    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | s     | 0.44         | 0/62    | 0.43        | 0/79    |
| 1   | sA    | 0.30         | 0/62    | 0.43        | 0/79    |
| 1   | t     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | tA    | 0.32         | 0/62    | 0.46        | 0/79    |
| 1   | u     | 0.38         | 0/62    | 0.37        | 0/79    |
| 1   | uA    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | v     | 0.43         | 0/62    | 0.45        | 0/79    |
| 1   | vA    | 0.31         | 0/62    | 0.43        | 0/79    |
| 1   | w     | 0.39         | 0/62    | 0.33        | 0/79    |
| 1   | wA    | 0.32         | 0/62    | 0.45        | 0/79    |
| 1   | x     | 0.40         | 0/62    | 0.43        | 0/79    |
| 1   | xA    | 0.32         | 0/62    | 0.39        | 0/79    |
| 1   | y     | 0.38         | 0/62    | 0.37        | 0/79    |
| 1   | yA    | 0.33         | 0/62    | 0.61        | 0/79    |
| 1   | z     | 0.43         | 0/62    | 0.44        | 0/79    |
| 1   | zA    | 0.30         | 0/62    | 0.43        | 0/79    |
| All | All   | 0.36         | 0/8928  | 0.44        | 0/11376 |

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       | 8       | 0            |
| 1   | 0A    | 84    | 0        | 63       | 9       | 0            |
| 1   | 1     | 84    | 0        | 62       | 13      | 0            |
| 1   | 1A    | 84    | 0        | 63       | 5       | 0            |
| 1   | 2     | 84    | 0        | 63       | 2       | 0            |
| 1   | 2A    | 84    | 0        | 62       | 5       | 0            |
| 1   | 3     | 84    | 0        | 63       | 1       | 0            |
| 1   | 3A    | 84    | 0        | 63       | 4       | 0            |
| 1   | 4     | 84    | 0        | 63       | 12      | 0            |
| 1   | 4A    | 84    | 0        | 63       | 7       | 0            |
| 1   | 5     | 84    | 0        | 62       | 15      | 0            |
| 1   | 5A    | 84    | 0        | 63       | 7       | 0            |
| 1   | 6     | 84    | 0        | 63       | 2       | 0            |
| 1   | 6A    | 84    | 0        | 62       | 5       | 0            |
| 1   | 7     | 84    | 0        | 63       | 1       | 0            |
| 1   | 7A    | 84    | 0        | 63       | 4       | 0            |
| 1   | 8     | 84    | 0        | 63       | 8       | 0            |
| 1   | 8A    | 84    | 0        | 63       | 7       | 0            |
| 1   | 9     | 84    | 0        | 63       | 6       | 0            |
| 1   | 9A    | 84    | 0        | 62       | 6       | 0            |
| 1   | A     | 84    | 0        | 63       | 11      | 0            |
| 1   | AA    | 84    | 0        | 63       | 8       | 0            |
| 1   | AB    | 84    | 0        | 63       | 3       | 0            |
| 1   | B     | 84    | 0        | 63       | 11      | 0            |
| 1   | BA    | 84    | 0        | 63       | 7       | 0            |
| 1   | BB    | 84    | 0        | 63       | 6       | 0            |
| 1   | C     | 84    | 0        | 63       | 11      | 0            |
| 1   | CA    | 84    | 0        | 63       | 8       | 0            |
| 1   | CB    | 84    | 0        | 63       | 7       | 0            |
| 1   | D     | 84    | 0        | 63       | 11      | 0            |
| 1   | DA    | 84    | 0        | 63       | 6       | 0            |
| 1   | DB    | 84    | 0        | 62       | 6       | 0            |
| 1   | E     | 84    | 0        | 63       | 7       | 0            |
| 1   | EA    | 84    | 0        | 63       | 8       | 0            |
| 1   | EB    | 84    | 0        | 63       | 3       | 0            |
| 1   | F     | 84    | 0        | 63       | 12      | 0            |
| 1   | FA    | 84    | 0        | 62       | 13      | 0            |
| 1   | FB    | 84    | 0        | 63       | 7       | 0            |
| 1   | G     | 84    | 0        | 63       | 7       | 0            |
| 1   | GA    | 84    | 0        | 63       | 3       | 0            |
| 1   | GB    | 84    | 0        | 62       | 7       | 0            |
| 1   | H     | 84    | 0        | 63       | 10      | 0            |
| 1   | HA    | 84    | 0        | 63       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | HB    | 84    | 0        | 63       | 3       | 0            |
| 1   | I     | 84    | 0        | 63       | 7       | 0            |
| 1   | IA    | 84    | 0        | 63       | 10      | 0            |
| 1   | IB    | 84    | 0        | 63       | 5       | 0            |
| 1   | J     | 84    | 0        | 62       | 14      | 0            |
| 1   | JA    | 84    | 0        | 62       | 14      | 0            |
| 1   | JB    | 84    | 0        | 63       | 4       | 0            |
| 1   | K     | 84    | 0        | 63       | 7       | 0            |
| 1   | KA    | 84    | 0        | 63       | 2       | 0            |
| 1   | KB    | 84    | 0        | 62       | 7       | 0            |
| 1   | L     | 84    | 0        | 63       | 8       | 0            |
| 1   | LA    | 84    | 0        | 63       | 1       | 0            |
| 1   | LB    | 84    | 0        | 63       | 3       | 0            |
| 1   | M     | 84    | 0        | 63       | 11      | 0            |
| 1   | MA    | 84    | 0        | 63       | 6       | 0            |
| 1   | MB    | 84    | 0        | 63       | 5       | 0            |
| 1   | N     | 84    | 0        | 62       | 15      | 0            |
| 1   | NA    | 84    | 0        | 63       | 7       | 0            |
| 1   | NB    | 84    | 0        | 62       | 2       | 0            |
| 1   | O     | 84    | 0        | 63       | 6       | 0            |
| 1   | OA    | 84    | 0        | 63       | 8       | 0            |
| 1   | OB    | 84    | 0        | 63       | 5       | 0            |
| 1   | P     | 84    | 0        | 63       | 7       | 0            |
| 1   | PA    | 84    | 0        | 63       | 7       | 0            |
| 1   | PB    | 84    | 0        | 63       | 4       | 0            |
| 1   | Q     | 84    | 0        | 62       | 15      | 0            |
| 1   | QA    | 84    | 0        | 63       | 6       | 0            |
| 1   | QB    | 84    | 0        | 63       | 6       | 0            |
| 1   | R     | 84    | 0        | 63       | 6       | 0            |
| 1   | RA    | 84    | 0        | 63       | 6       | 0            |
| 1   | RB    | 84    | 0        | 62       | 2       | 0            |
| 1   | S     | 84    | 0        | 63       | 8       | 0            |
| 1   | SA    | 84    | 0        | 63       | 7       | 0            |
| 1   | SB    | 84    | 0        | 63       | 5       | 0            |
| 1   | T     | 84    | 0        | 63       | 11      | 0            |
| 1   | TA    | 84    | 0        | 62       | 5       | 0            |
| 1   | TB    | 84    | 0        | 63       | 5       | 0            |
| 1   | U     | 84    | 0        | 62       | 14      | 0            |
| 1   | UA    | 84    | 0        | 63       | 4       | 0            |
| 1   | V     | 84    | 0        | 63       | 3       | 0            |
| 1   | VA    | 84    | 0        | 63       | 5       | 0            |
| 1   | W     | 84    | 0        | 63       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | WA    | 84    | 0        | 63       | 6       | 0            |
| 1   | X     | 84    | 0        | 63       | 8       | 0            |
| 1   | XA    | 84    | 0        | 62       | 5       | 0            |
| 1   | Y     | 84    | 0        | 63       | 6       | 0            |
| 1   | YA    | 84    | 0        | 63       | 4       | 0            |
| 1   | Z     | 84    | 0        | 63       | 8       | 0            |
| 1   | ZA    | 84    | 0        | 63       | 5       | 0            |
| 1   | a     | 84    | 0        | 63       | 5       | 0            |
| 1   | aA    | 84    | 0        | 62       | 5       | 0            |
| 1   | b     | 84    | 0        | 63       | 4       | 0            |
| 1   | bA    | 84    | 0        | 63       | 7       | 0            |
| 1   | c     | 84    | 0        | 63       | 5       | 0            |
| 1   | cA    | 84    | 0        | 63       | 6       | 0            |
| 1   | d     | 84    | 0        | 63       | 5       | 0            |
| 1   | dA    | 84    | 0        | 63       | 5       | 0            |
| 1   | e     | 84    | 0        | 63       | 6       | 0            |
| 1   | eA    | 84    | 0        | 62       | 5       | 0            |
| 1   | f     | 84    | 0        | 63       | 7       | 0            |
| 1   | fA    | 84    | 0        | 63       | 7       | 0            |
| 1   | g     | 84    | 0        | 63       | 7       | 0            |
| 1   | gA    | 84    | 0        | 63       | 5       | 0            |
| 1   | h     | 84    | 0        | 63       | 3       | 0            |
| 1   | hA    | 84    | 0        | 62       | 5       | 0            |
| 1   | i     | 84    | 0        | 63       | 7       | 0            |
| 1   | iA    | 84    | 0        | 63       | 4       | 0            |
| 1   | j     | 84    | 0        | 63       | 11      | 0            |
| 1   | jA    | 84    | 0        | 63       | 10      | 0            |
| 1   | k     | 84    | 0        | 62       | 16      | 0            |
| 1   | kA    | 84    | 0        | 63       | 6       | 0            |
| 1   | l     | 84    | 0        | 63       | 7       | 0            |
| 1   | lA    | 84    | 0        | 62       | 5       | 0            |
| 1   | m     | 84    | 0        | 63       | 7       | 0            |
| 1   | mA    | 84    | 0        | 63       | 4       | 0            |
| 1   | n     | 84    | 0        | 62       | 14      | 0            |
| 1   | nA    | 84    | 0        | 63       | 10      | 0            |
| 1   | o     | 84    | 0        | 63       | 3       | 0            |
| 1   | oA    | 84    | 0        | 62       | 4       | 0            |
| 1   | p     | 84    | 0        | 63       | 5       | 0            |
| 1   | pA    | 84    | 0        | 63       | 6       | 0            |
| 1   | q     | 84    | 0        | 63       | 11      | 0            |
| 1   | qA    | 84    | 0        | 63       | 8       | 0            |
| 1   | r     | 84    | 0        | 62       | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | rA    | 84    | 0        | 63       | 6       | 0            |
| 1   | s     | 84    | 0        | 63       | 2       | 0            |
| 1   | sA    | 84    | 0        | 62       | 4       | 0            |
| 1   | t     | 84    | 0        | 63       | 1       | 0            |
| 1   | tA    | 84    | 0        | 63       | 6       | 0            |
| 1   | u     | 84    | 0        | 63       | 8       | 0            |
| 1   | uA    | 84    | 0        | 63       | 8       | 0            |
| 1   | v     | 84    | 0        | 63       | 5       | 0            |
| 1   | vA    | 84    | 0        | 62       | 6       | 0            |
| 1   | w     | 84    | 0        | 63       | 8       | 0            |
| 1   | wA    | 84    | 0        | 63       | 9       | 0            |
| 1   | x     | 84    | 0        | 63       | 10      | 0            |
| 1   | xA    | 84    | 0        | 63       | 4       | 0            |
| 1   | y     | 84    | 0        | 63       | 8       | 0            |
| 1   | yA    | 84    | 0        | 63       | 6       | 0            |
| 1   | z     | 84    | 0        | 63       | 5       | 0            |
| 1   | zA    | 84    | 0        | 62       | 6       | 0            |
| All | All   | 12096 | 0        | 9043     | 556     | 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 26.

All (556) 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:k:1101:5CR:CAA | 1:NA:207:PHE:O    | 1.90                     | 1.19              |
| 1:N:1101:5CR:CAA | 1:9:207:PHE:O     | 1.89                     | 1.18              |
| 1:J:101:5CR:CAA  | 1:RA:1207:PHE:O   | 1.92                     | 1.18              |
| 1:K:207:PHE:O    | 1:5:1101:5CR:CAA  | 1.92                     | 1.18              |
| 1:U:1101:5CR:CAA | 1:v:207:PHE:O     | 1.92                     | 1.17              |
| 1:Q:101:5CR:CAA  | 1:DA:1207:PHE:O   | 1.93                     | 1.17              |
| 1:n:101:5CR:CAA  | 1:z:1207:PHE:O    | 1.93                     | 1.17              |
| 1:Y:207:PHE:O    | 1:r:1101:5CR:CAA  | 1.91                     | 1.16              |
| 1:l:1207:PHE:O   | 1:l:101:5CR:CAA   | 1.94                     | 1.16              |
| 1:R:207:PHE:O    | 1:JA:1101:5CR:CAA | 1.92                     | 1.15              |
| 1:O:1207:PHE:O   | 1:FA:101:5CR:CAA  | 1.94                     | 1.15              |
| 1:M:1002:LYS:NZ  | 1:w:308:GMA:OXT   | 1.94                     | 0.99              |
| 1:B:2:LYS:NZ     | 1:0:1308:GMA:OXT  | 1.97                     | 0.96              |
| 1:j:1002:LYS:NZ  | 1:AA:308:GMA:OXT  | 2.00                     | 0.92              |
| 1:S:308:GMA:OXT  | 1:4:1002:LYS:NZ   | 2.03                     | 0.92              |
| 1:A:2:LYS:NZ     | 1:EA:1308:GMA:OXT | 2.03                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:T:1002:LYS:NZ   | 1:Z:308:GMA:OXT   | 2.04                     | 0.90              |
| 1:L:308:GMA:OXT   | 1:q:1002:LYS:NZ   | 2.05                     | 0.88              |
| 1:p:308:GMA:OXT   | 1:IA:1002:LYS:NZ  | 2.06                     | 0.88              |
| 1:W:1308:GMA:OXT  | 1:H:2:LYS:NZ      | 2.06                     | 0.87              |
| 1:k:1101:5CR:CAA  | 1:OA:308:GMA:O1   | 2.22                     | 0.87              |
| 1:x:1002:LYS:NZ   | 1:OA:308:GMA:OXT  | 2.07                     | 0.87              |
| 1:P:1308:GMA:OXT  | 1:F:2:LYS:NZ      | 2.07                     | 0.86              |
| 1:J:101:5CR:CAA   | 1:SA:1308:GMA:O1  | 2.22                     | 0.86              |
| 1:m:1308:GMA:OXT  | 1:D:2:LYS:NZ      | 2.07                     | 0.86              |
| 1:5A:1004:GLU:HB3 | 1:KB:1106:LYS:HB3 | 1.58                     | 0.86              |
| 1:m:1308:GMA:O1   | 1:l:101:5CR:CAA   | 2.25                     | 0.85              |
| 1:P:1308:GMA:O1   | 1:FA:101:5CR:CAA  | 2.24                     | 0.85              |
| 1:Z:308:GMA:O1    | 1:r:1101:5CR:CAA  | 2.25                     | 0.85              |
| 1:C:2:LYS:NZ      | 1:SA:1308:GMA:OXT | 2.08                     | 0.84              |
| 1:L:308:GMA:O1    | 1:5:1101:5CR:CAA  | 2.25                     | 0.84              |
| 1:f:4:GLU:HB3     | 1:GB:106:LYS:HB3  | 1.58                     | 0.83              |
| 1:S:308:GMA:O1    | 1:JA:1101:5CR:CAA | 2.27                     | 0.82              |
| 1:Q:101:5CR:CAA   | 1:EA:1308:GMA:O1  | 2.29                     | 0.81              |
| 1:N:1101:5CR:CAA  | 1:AA:308:GMA:O1   | 2.30                     | 0.80              |
| 1:DB:1106:LYS:HB3 | 1:QB:1004:GLU:HB3 | 1.66                     | 0.77              |
| 1:fA:1205:PHE:HB3 | 1:gA:1303:PHE:HB3 | 1.68                     | 0.76              |
| 1:iA:205:PHE:HB3  | 1:jA:303:PHE:HB3  | 1.68                     | 0.76              |
| 1:OB:205:PHE:HB3  | 1:PB:303:PHE:HB3  | 1.68                     | 0.76              |
| 1:tA:1205:PHE:HB3 | 1:uA:1303:PHE:HB3 | 1.68                     | 0.76              |
| 1:9A:106:LYS:HB3  | 1:i:4:GLU:HB3     | 1.66                     | 0.76              |
| 1:EB:1205:PHE:HB3 | 1:FB:1303:PHE:HB3 | 1.68                     | 0.76              |
| 1:PB:302:LYS:HZ1  | 1:PB:304:GLU:HB2  | 1.51                     | 0.76              |
| 1:UA:205:PHE:HB3  | 1:VA:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:0A:1205:PHE:HB3 | 1:1A:1303:PHE:HB3 | 1.68                     | 0.75              |
| 1:YA:1205:PHE:HB3 | 1:ZA:1303:PHE:HB3 | 1.68                     | 0.75              |
| 1:cA:302:LYS:HZ3  | 1:cA:304:GLU:HB2  | 1.51                     | 0.75              |
| 1:uA:1302:LYS:HZ1 | 1:uA:1304:GLU:HB2 | 1.51                     | 0.75              |
| 1:wA:205:PHE:HB3  | 1:xA:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:pA:205:PHE:HB3  | 1:qA:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:3A:205:PHE:HB3  | 1:4A:303:PHE:HB3  | 1.68                     | 0.75              |
| 1:U:1101:5CR:CAA  | 1:w:308:GMA:O1    | 2.35                     | 0.75              |
| 1:MB:1302:LYS:HZ1 | 1:MB:1304:GLU:HB2 | 1.52                     | 0.75              |
| 1:SB:1205:PHE:HB3 | 1:TB:1303:PHE:HB3 | 1.68                     | 0.75              |
| 1:7A:1205:PHE:HB3 | 1:8A:1303:PHE:HB3 | 1.68                     | 0.74              |
| 1:XA:1106:LYS:HB3 | 1:kA:1004:GLU:HB3 | 1.69                     | 0.74              |
| 1:n:101:5CR:CAA   | 1:0:1308:GMA:O1   | 2.35                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FB:1302:LYS:HZ3 | 1:FB:1304:GLU:HB2 | 1.51                     | 0.74              |
| 1:gA:1302:LYS:HZ1 | 1:gA:1304:GLU:HB2 | 1.51                     | 0.74              |
| 1:LB:1205:PHE:HB3 | 1:MB:1303:PHE:HB3 | 1.68                     | 0.74              |
| 1:bA:205:PHE:HB3  | 1:cA:303:PHE:HB3  | 1.68                     | 0.74              |
| 1:mA:1205:PHE:HB3 | 1:nA:1303:PHE:HB3 | 1.68                     | 0.74              |
| 1:AB:205:PHE:HB3  | 1:BB:303:PHE:HB3  | 1.68                     | 0.74              |
| 1:TB:1302:LYS:HZ3 | 1:TB:1304:GLU:HB2 | 1.51                     | 0.74              |
| 1:BB:302:LYS:HZ3  | 1:BB:304:GLU:HB2  | 1.52                     | 0.74              |
| 1:ZA:1302:LYS:HZ1 | 1:ZA:1304:GLU:HB2 | 1.53                     | 0.74              |
| 1:VA:302:LYS:HZ1  | 1:VA:304:GLU:HB2  | 1.52                     | 0.74              |
| 1:1A:1302:LYS:HZ1 | 1:1A:1304:GLU:HB2 | 1.51                     | 0.74              |
| 1:HB:205:PHE:HB3  | 1:IB:303:PHE:HB3  | 1.68                     | 0.73              |
| 1:nA:1302:LYS:HZ1 | 1:nA:1304:GLU:HB2 | 1.51                     | 0.73              |
| 1:wA:203:PHE:HB3  | 1:xA:305:PHE:HB3  | 1.71                     | 0.73              |
| 1:0A:1203:PHE:HB3 | 1:1A:1305:PHE:HB3 | 1.71                     | 0.73              |
| 1:4A:302:LYS:HZ1  | 1:4A:304:GLU:HB2  | 1.53                     | 0.73              |
| 1:YA:1203:PHE:HB3 | 1:ZA:1305:PHE:HB3 | 1.71                     | 0.73              |
| 1:zA:1106:LYS:HB3 | 1:CB:1004:GLU:HB3 | 1.68                     | 0.73              |
| 1:OB:203:PHE:HB3  | 1:PB:305:PHE:HB3  | 1.71                     | 0.73              |
| 1:UA:203:PHE:HB3  | 1:VA:305:PHE:HB3  | 1.71                     | 0.73              |
| 1:WA:1004:GLU:HB3 | 1:eA:1106:LYS:HB3 | 1.70                     | 0.73              |
| 1:SB:1203:PHE:HB3 | 1:TB:1305:PHE:HB3 | 1.71                     | 0.73              |
| 1:TA:106:LYS:HB3  | 1:c:4:GLU:HB3     | 1.69                     | 0.73              |
| 1:vA:106:LYS:HB3  | 1:g:4:GLU:HB3     | 1.68                     | 0.73              |
| 1:pA:203:PHE:HB3  | 1:qA:305:PHE:HB3  | 1.71                     | 0.73              |
| 1:tA:1203:PHE:HB3 | 1:uA:1305:PHE:HB3 | 1.71                     | 0.73              |
| 1:8A:1302:LYS:HZ1 | 1:8A:1304:GLU:HB2 | 1.54                     | 0.72              |
| 1:7A:1203:PHE:HB3 | 1:8A:1305:PHE:HB3 | 1.71                     | 0.72              |
| 1:fA:1203:PHE:HB3 | 1:gA:1305:PHE:HB3 | 1.71                     | 0.72              |
| 1:HB:203:PHE:HB3  | 1:IB:305:PHE:HB3  | 1.71                     | 0.72              |
| 1:LB:1203:PHE:HB3 | 1:MB:1305:PHE:HB3 | 1.71                     | 0.72              |
| 1:bA:203:PHE:HB3  | 1:cA:305:PHE:HB3  | 1.71                     | 0.72              |
| 1:iA:203:PHE:HB3  | 1:jA:305:PHE:HB3  | 1.71                     | 0.72              |
| 1:AB:203:PHE:HB3  | 1:BB:305:PHE:HB3  | 1.71                     | 0.71              |
| 1:b:5:PHE:HB3     | 1:aA:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:rA:1004:GLU:HB3 | 1:6A:1106:LYS:HB3 | 1.72                     | 0.71              |
| 1:EB:1203:PHE:HB3 | 1:FB:1305:PHE:HB3 | 1.71                     | 0.71              |
| 1:mA:1203:PHE:HB3 | 1:nA:1305:PHE:HB3 | 1.71                     | 0.71              |
| 1:c:5:PHE:HB3     | 1:hA:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:f:5:PHE:HB3     | 1:2A:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:QB:1005:PHE:HB3 | 1:RB:1103:PHE:HB3 | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3A:203:PHE:HB3  | 1:4A:305:PHE:HB3  | 1.71                     | 0.71              |
| 1:5A:1002:LYS:H   | 1:KB:1108:GMA:HB2 | 1.55                     | 0.71              |
| 1:yA:1005:PHE:HB3 | 1:zA:1103:PHE:HB3 | 1.73                     | 0.71              |
| 1:g:5:PHE:HB3     | 1:9A:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:a:4:GLU:HB3     | 1:aA:106:LYS:HB3  | 1.70                     | 0.71              |
| 1:jA:302:LYS:HZ1  | 1:jA:304:GLU:HB2  | 1.55                     | 0.71              |
| 1:xA:302:LYS:HZ1  | 1:xA:304:GLU:HB2  | 1.55                     | 0.71              |
| 1:f:2:LYS:H       | 1:GB:108:GMA:HB2  | 1.55                     | 0.71              |
| 1:h:5:PHE:HB3     | 1:GB:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:i:5:PHE:HB3     | 1:NB:103:PHE:HB3  | 1.73                     | 0.71              |
| 1:d:4:GLU:HB3     | 1:2A:106:LYS:HB3  | 1.72                     | 0.70              |
| 1:JB:1005:PHE:HB3 | 1:KB:1103:PHE:HB3 | 1.73                     | 0.70              |
| 1:WA:1005:PHE:HB3 | 1:XA:1103:PHE:HB3 | 1.73                     | 0.70              |
| 1:e:5:PHE:HB3     | 1:vA:103:PHE:HB3  | 1.73                     | 0.70              |
| 1:rA:1005:PHE:HB3 | 1:sA:1103:PHE:HB3 | 1.73                     | 0.70              |
| 1:a:5:PHE:HB3     | 1:TA:103:PHE:HB3  | 1.73                     | 0.70              |
| 1:d:5:PHE:HB3     | 1:oA:103:PHE:HB3  | 1.73                     | 0.70              |
| 1:IB:302:LYS:HZ1  | 1:IB:304:GLU:HB2  | 1.56                     | 0.70              |
| 1:CB:1005:PHE:HB3 | 1:DB:1103:PHE:HB3 | 1.73                     | 0.69              |
| 1:dA:1005:PHE:HB3 | 1:eA:1103:PHE:HB3 | 1.73                     | 0.69              |
| 1:5A:1005:PHE:HB3 | 1:6A:1103:PHE:HB3 | 1.73                     | 0.69              |
| 1:kA:1005:PHE:HB3 | 1:lA:1103:PHE:HB3 | 1.73                     | 0.69              |
| 1:qA:302:LYS:HZ1  | 1:qA:304:GLU:HB2  | 1.57                     | 0.68              |
| 1:B:6:LYS:HG2     | 1:Q:106:LYS:HB2   | 1.76                     | 0.68              |
| 1:D:6:LYS:HG2     | 1:n:106:LYS:HB2   | 1.76                     | 0.68              |
| 1:F:6:LYS:HG2     | 1:1:106:LYS:HB2   | 1.76                     | 0.68              |
| 1:A:6:LYS:HG2     | 1:J:106:LYS:HB2   | 1.76                     | 0.68              |
| 1:H:6:LYS:HG2     | 1:FA:106:LYS:HB2  | 1.76                     | 0.68              |
| 1:C:6:LYS:HG2     | 1:X:106:LYS:HB2   | 1.76                     | 0.67              |
| 1:E:6:LYS:HG2     | 1:u:106:LYS:HB2   | 1.76                     | 0.67              |
| 1:4:1006:LYS:HG2  | 1:5:1106:LYS:HB2  | 1.76                     | 0.66              |
| 1:G:6:LYS:HG2     | 1:8:106:LYS:HB2   | 1.76                     | 0.66              |
| 1:PA:1006:LYS:HG2 | 1:QA:1106:LYS:HB2 | 1.76                     | 0.66              |
| 1:IA:1006:LYS:HG2 | 1:JA:1106:LYS:HB2 | 1.76                     | 0.66              |
| 1:M:1006:LYS:HG2  | 1:N:1106:LYS:HB2  | 1.76                     | 0.66              |
| 1:T:1006:LYS:HG2  | 1:U:1106:LYS:HB2  | 1.76                     | 0.66              |
| 1:q:1006:LYS:HG2  | 1:r:1106:LYS:HB2  | 1.76                     | 0.66              |
| 1:j:1006:LYS:HG2  | 1:k:1106:LYS:HB2  | 1.76                     | 0.66              |
| 1:I:6:LYS:HG2     | 1:MA:106:LYS:HB2  | 1.76                     | 0.66              |
| 1:BA:1006:LYS:HG2 | 1:CA:1106:LYS:HB2 | 1.76                     | 0.66              |
| 1:O:1208:GMA:N2   | 1:FA:101:5CR:CAA  | 2.59                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:x:1006:LYS:HG2  | 1:y:1106:LYS:HB2  | 1.76                     | 0.66              |
| 1:k:1106:LYS:HD3  | 1:x:1006:LYS:HE3  | 1.79                     | 0.65              |
| 1:l:1208:GMA:N2   | 1:1:101:5CR:CAA   | 2.60                     | 0.65              |
| 1:XA:1108:GMA:HB2 | 1:kA:1002:LYS:H   | 1.63                     | 0.64              |
| 1:M:1006:LYS:HE3  | 1:U:1106:LYS:HD3  | 1.80                     | 0.64              |
| 1:J:101:5CR:CAA   | 1:RA:1208:GMA:N2  | 2.61                     | 0.63              |
| 1:T:1006:LYS:HE3  | 1:r:1106:LYS:HD3  | 1.80                     | 0.63              |
| 1:X:106:LYS:HD3   | 1:E:6:LYS:HE3     | 1.79                     | 0.63              |
| 1:q:1006:LYS:HE3  | 1:5:1106:LYS:HD3  | 1.80                     | 0.63              |
| 1:dA:1004:GLU:HB3 | 1:sA:1106:LYS:HB3 | 1.81                     | 0.63              |
| 1:4:1006:LYS:HE3  | 1:JA:1106:LYS:HD3 | 1.80                     | 0.63              |
| 1:y:1106:LYS:HD3  | 1:BA:1006:LYS:HE3 | 1.80                     | 0.62              |
| 1:CA:1106:LYS:HD3 | 1:PA:1006:LYS:HE3 | 1.81                     | 0.62              |
| 1:zA:1108:GMA:HB2 | 1:CB:1002:LYS:H   | 1.64                     | 0.62              |
| 1:N:1106:LYS:HD3  | 1:j:1006:LYS:HE3  | 1.80                     | 0.62              |
| 1:J:106:LYS:HD3   | 1:C:6:LYS:HE3     | 1.80                     | 0.62              |
| 1:K:208:GMA:N2    | 1:5:1101:5CR:CAA  | 2.63                     | 0.62              |
| 1:u:106:LYS:HD3   | 1:G:6:LYS:HE3     | 1.80                     | 0.62              |
| 1:B:6:LYS:HE3     | 1:n:106:LYS:HD3   | 1.80                     | 0.62              |
| 1:F:6:LYS:HE3     | 1:FA:106:LYS:HD3  | 1.80                     | 0.62              |
| 1:A:6:LYS:HE3     | 1:Q:106:LYS:HD3   | 1.80                     | 0.62              |
| 1:M:1002:LYS:HE3  | 1:N:1102:LYS:HE3  | 1.82                     | 0.62              |
| 1:q:1002:LYS:HE3  | 1:r:1102:LYS:HE3  | 1.82                     | 0.61              |
| 1:TA:108:GMA:HB2  | 1:c:2:LYS:H       | 1.63                     | 0.61              |
| 1:T:1002:LYS:HE3  | 1:U:1102:LYS:HE3  | 1.82                     | 0.61              |
| 1:D:6:LYS:HE3     | 1:1:106:LYS:HD3   | 1.80                     | 0.61              |
| 1:x:1002:LYS:HE3  | 1:y:1102:LYS:HE3  | 1.82                     | 0.61              |
| 1:b:4:GLU:HB3     | 1:oA:106:LYS:HB3  | 1.81                     | 0.61              |
| 1:4:1002:LYS:HE3  | 1:5:1102:LYS:HE3  | 1.82                     | 0.61              |
| 1:8:106:LYS:HD3   | 1:I:6:LYS:HE3     | 1.81                     | 0.61              |
| 1:j:1002:LYS:HE3  | 1:k:1102:LYS:HE3  | 1.82                     | 0.61              |
| 1:BA:1002:LYS:HE3 | 1:CA:1102:LYS:HE3 | 1.82                     | 0.61              |
| 1:IA:1002:LYS:HE3 | 1:JA:1102:LYS:HE3 | 1.82                     | 0.61              |
| 1:vA:108:GMA:HB2  | 1:g:2:LYS:H       | 1.64                     | 0.61              |
| 1:Y:208:GMA:N2    | 1:r:1101:5CR:CAA  | 2.64                     | 0.61              |
| 1:PA:1002:LYS:HE3 | 1:QA:1102:LYS:HE3 | 1.82                     | 0.61              |
| 1:Q:101:5CR:CAA   | 1:DA:1208:GMA:N2  | 2.64                     | 0.61              |
| 1:R:208:GMA:N2    | 1:JA:1101:5CR:CAA | 2.65                     | 0.60              |
| 1:k:1101:5CR:CAA  | 1:NA:208:GMA:N2   | 2.64                     | 0.60              |
| 1:I:2:LYS:HE3     | 1:MA:102:LYS:HE3  | 1.82                     | 0.60              |
| 1:vA:102:LYS:HB3  | 1:g:8:GMA:HB3     | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2:LYS:HE3     | 1:Q:102:LYS:HE3   | 1.82                     | 0.60              |
| 1:zA:1102:LYS:HB3 | 1:CB:1008:GMA:HB3 | 1.83                     | 0.60              |
| 1:d:2:LYS:H       | 1:2A:108:GMA:HB2  | 1.66                     | 0.60              |
| 1:C:2:LYS:HE3     | 1:X:102:LYS:HE3   | 1.82                     | 0.60              |
| 1:E:2:LYS:HE3     | 1:u:102:LYS:HE3   | 1.82                     | 0.60              |
| 1:G:2:LYS:HE3     | 1:8:102:LYS:HE3   | 1.82                     | 0.60              |
| 1:lA:1106:LYS:HB3 | 1:yA:1004:GLU:HB3 | 1.83                     | 0.60              |
| 1:F:2:LYS:HE3     | 1:1:102:LYS:HE3   | 1.82                     | 0.60              |
| 1:H:2:LYS:HE3     | 1:FA:102:LYS:HE3  | 1.82                     | 0.59              |
| 1:j:1002:LYS:CD   | 1:AA:308:GMA:OXT  | 2.50                     | 0.59              |
| 1:A:2:LYS:HE3     | 1:J:102:LYS:HE3   | 1.82                     | 0.59              |
| 1:hA:106:LYS:HB3  | 1:e:4:GLU:HB3     | 1.83                     | 0.59              |
| 1:V:1204:GLU:HA   | 1:W:1304:GLU:HB2  | 1.85                     | 0.59              |
| 1:D:2:LYS:HE3     | 1:n:102:LYS:HE3   | 1.82                     | 0.59              |
| 1:s:1204:GLU:HA   | 1:t:1304:GLU:HB2  | 1.85                     | 0.59              |
| 1:l:1204:GLU:HA   | 1:m:1304:GLU:HB2  | 1.85                     | 0.59              |
| 1:DA:1204:GLU:HA  | 1:EA:1304:GLU:HB2 | 1.85                     | 0.59              |
| 1:KA:1204:GLU:HA  | 1:LA:1304:GLU:HB2 | 1.85                     | 0.59              |
| 1:O:1204:GLU:HA   | 1:P:1304:GLU:HB2  | 1.85                     | 0.59              |
| 1:a:2:LYS:H       | 1:aA:108:GMA:HB2  | 1.67                     | 0.59              |
| 1:6:1204:GLU:HA   | 1:7:1304:GLU:HB2  | 1.85                     | 0.59              |
| 1:M:1002:LYS:CD   | 1:w:308:GMA:OXT   | 2.51                     | 0.59              |
| 1:z:1204:GLU:HA   | 1:0:1304:GLU:HB2  | 1.85                     | 0.59              |
| 1:rA:1002:LYS:H   | 1:6A:1108:GMA:HB2 | 1.66                     | 0.59              |
| 1:L:308:GMA:OXT   | 1:q:1002:LYS:CD   | 2.51                     | 0.59              |
| 1:9:204:GLU:HA    | 1:AA:304:GLU:HB2  | 1.85                     | 0.59              |
| 1:NA:204:GLU:HA   | 1:OA:304:GLU:HB2  | 1.84                     | 0.59              |
| 1:RA:1204:GLU:HA  | 1:SA:1304:GLU:HB2 | 1.85                     | 0.59              |
| 1:WA:1002:LYS:H   | 1:eA:1108:GMA:HB2 | 1.67                     | 0.58              |
| 1:v:204:GLU:HA    | 1:w:304:GLU:HB2   | 1.85                     | 0.58              |
| 1:T:1002:LYS:CD   | 1:Z:308:GMA:OXT   | 2.51                     | 0.58              |
| 1:y:1102:LYS:HG3  | 1:BA:1002:LYS:HB3 | 1.85                     | 0.58              |
| 1:S:308:GMA:OXT   | 1:4:1002:LYS:CD   | 2.52                     | 0.58              |
| 1:8:102:LYS:HG3   | 1:I:2:LYS:HB3     | 1.85                     | 0.58              |
| 1:PA:1004:GLU:HA  | 1:QA:1104:GLU:HB2 | 1.86                     | 0.58              |
| 1:Y:204:GLU:HA    | 1:Z:304:GLU:HB2   | 1.85                     | 0.58              |
| 1:j:1004:GLU:HA   | 1:k:1104:GLU:HB2  | 1.86                     | 0.58              |
| 1:BA:1004:GLU:HA  | 1:CA:1104:GLU:HB2 | 1.86                     | 0.58              |
| 1:C:2:LYS:CD      | 1:SA:1308:GMA:OXT | 2.52                     | 0.58              |
| 1:H:4:GLU:HA      | 1:FA:104:GLU:HB2  | 1.86                     | 0.58              |
| 1:GA:204:GLU:HA   | 1:HA:304:GLU:HB2  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2:LYS:CD      | 1:EA:1308:GMA:OXT | 2.52                     | 0.58              |
| 1:o:204:GLU:HA    | 1:p:304:GLU:HB2   | 1.85                     | 0.58              |
| 1:p:308:GMA:OXT   | 1:IA:1002:LYS:CD  | 2.51                     | 0.58              |
| 1:K:204:GLU:HA    | 1:L:304:GLU:HB2   | 1.85                     | 0.57              |
| 1:x:1004:GLU:HA   | 1:y:1104:GLU:HB2  | 1.86                     | 0.57              |
| 1:T:1004:GLU:HA   | 1:U:1104:GLU:HB2  | 1.86                     | 0.57              |
| 1:jA:305:PHE:HE1  | 1:wA:203:PHE:CZ   | 2.22                     | 0.57              |
| 1:N:1101:5CR:CAA  | 1:9:208:GMA:N2    | 2.67                     | 0.57              |
| 1:2:204:GLU:HA    | 1:3:304:GLU:HB2   | 1.85                     | 0.57              |
| 1:M:1004:GLU:HA   | 1:N:1104:GLU:HB2  | 1.86                     | 0.57              |
| 1:R:204:GLU:HA    | 1:S:304:GLU:HB2   | 1.85                     | 0.57              |
| 1:u:102:LYS:HG3   | 1:G:2:LYS:HB3     | 1.85                     | 0.57              |
| 1:nA:1305:PHE:HE1 | 1:0A:1203:PHE:CZ  | 2.22                     | 0.57              |
| 1:M:1002:LYS:HB3  | 1:U:1102:LYS:HG3  | 1.86                     | 0.57              |
| 1:F:4:GLU:HA      | 1:1:104:GLU:HB2   | 1.86                     | 0.57              |
| 1:D:4:GLU:HA      | 1:n:104:GLU:HB2   | 1.86                     | 0.57              |
| 1:CA:1102:LYS:HG3 | 1:PA:1002:LYS:HB3 | 1.85                     | 0.57              |
| 1:I:4:GLU:HA      | 1:MA:104:GLU:HB2  | 1.86                     | 0.57              |
| 1:P:1308:GMA:OXT  | 1:F:2:LYS:CD      | 2.53                     | 0.57              |
| 1:4:1004:GLU:HA   | 1:5:1104:GLU:HB2  | 1.86                     | 0.57              |
| 1:q:1004:GLU:HA   | 1:r:1104:GLU:HB2  | 1.86                     | 0.56              |
| 1:G:4:GLU:HA      | 1:8:104:GLU:HB2   | 1.86                     | 0.56              |
| 1:C:2:LYS:HD2     | 1:SA:1308:GMA:OXT | 2.05                     | 0.56              |
| 1:E:4:GLU:HA      | 1:u:104:GLU:HB2   | 1.86                     | 0.56              |
| 1:B:4:GLU:HA      | 1:Q:104:GLU:HB2   | 1.86                     | 0.56              |
| 1:m:1308:GMA:OXT  | 1:D:2:LYS:CD      | 2.53                     | 0.56              |
| 1:p:308:GMA:OXT   | 1:IA:1002:LYS:HD2 | 2.05                     | 0.56              |
| 1:IA:1004:GLU:HA  | 1:JA:1104:GLU:HB2 | 1.86                     | 0.56              |
| 1:A:4:GLU:HA      | 1:J:104:GLU:HB2   | 1.86                     | 0.56              |
| 1:N:1102:LYS:HG3  | 1:j:1002:LYS:HB3  | 1.87                     | 0.56              |
| 1:C:4:GLU:HA      | 1:X:104:GLU:HB2   | 1.86                     | 0.56              |
| 1:j:1002:LYS:HD2  | 1:AA:308:GMA:OXT  | 2.06                     | 0.56              |
| 1:q:1002:LYS:HB3  | 1:5:1102:LYS:HG3  | 1.87                     | 0.56              |
| 1:L:308:GMA:OXT   | 1:q:1002:LYS:HD2  | 2.06                     | 0.56              |
| 1:A:2:LYS:HB3     | 1:Q:102:LYS:HG3   | 1.86                     | 0.56              |
| 1:J:102:LYS:HG3   | 1:C:2:LYS:HB3     | 1.87                     | 0.56              |
| 1:W:1308:GMA:OXT  | 1:H:2:LYS:CD      | 2.54                     | 0.56              |
| 1:f:8:GMA:HB3     | 1:GB:102:LYS:HB3  | 1.88                     | 0.56              |
| 1:n:101:5CR:CAA   | 1:z:1208:GMA:N2   | 2.69                     | 0.56              |
| 1:4:1002:LYS:HB3  | 1:JA:1102:LYS:HG3 | 1.87                     | 0.56              |
| 1:l:1208:GMA:N2   | 1:1:101:5CR:CAL   | 2.69                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:2:LYS:HB3     | 1:FA:102:LYS:HG3  | 1.87                     | 0.55              |
| 1:J:101:5CR:CAL   | 1:RA:1208:GMA:N2  | 2.69                     | 0.55              |
| 1:O:1208:GMA:N2   | 1:FA:101:5CR:CAL  | 2.69                     | 0.55              |
| 1:B:2:LYS:CD      | 1:O:1308:GMA:OXT  | 2.55                     | 0.55              |
| 1:P:1308:GMA:OXT  | 1:F:2:LYS:HD2     | 2.07                     | 0.55              |
| 1:m:1308:GMA:OXT  | 1:D:2:LYS:HD2     | 2.07                     | 0.55              |
| 1:A:2:LYS:HD2     | 1:EA:1308:GMA:OXT | 2.07                     | 0.55              |
| 1:T:1002:LYS:HB3  | 1:r:1102:LYS:HG3  | 1.88                     | 0.55              |
| 1:9A:108:GMA:HB2  | 1:i:2:LYS:H       | 1.71                     | 0.55              |
| 1:B:2:LYS:HB3     | 1:n:102:LYS:HG3   | 1.89                     | 0.55              |
| 1:S:308:GMA:OXT   | 1:4:1002:LYS:HD2  | 2.08                     | 0.54              |
| 1:b:2:LYS:H       | 1:oA:108:GMA:HB2  | 1.71                     | 0.54              |
| 1:T:1002:LYS:HD2  | 1:Z:308:GMA:OXT   | 2.06                     | 0.54              |
| 1:DB:1108:GMA:HB2 | 1:QB:1002:LYS:H   | 1.71                     | 0.54              |
| 1:K:208:GMA:N2    | 1:5:1101:5CR:CAL  | 2.71                     | 0.54              |
| 1:5A:1008:GMA:HB3 | 1:KB:1102:LYS:HB3 | 1.88                     | 0.54              |
| 1:D:2:LYS:HB3     | 1:1:102:LYS:HG3   | 1.87                     | 0.54              |
| 1:jA:305:PHE:HE1  | 1:wA:203:PHE:CE1  | 2.26                     | 0.54              |
| 1:k:1101:5CR:CAL  | 1:NA:208:GMA:N2   | 2.71                     | 0.54              |
| 1:a:8:GMA:HB3     | 1:aA:102:LYS:HB3  | 1.90                     | 0.54              |
| 1:W:1308:GMA:OXT  | 1:H:2:LYS:HD2     | 2.09                     | 0.53              |
| 1:Y:208:GMA:N2    | 1:r:1101:5CR:CAL  | 2.71                     | 0.53              |
| 1:dA:1002:LYS:H   | 1:sA:1108:GMA:HB2 | 1.71                     | 0.53              |
| 1:nA:1305:PHE:HE1 | 1:0A:1203:PHE:CE1 | 2.26                     | 0.53              |
| 1:hA:108:GMA:HB2  | 1:e:2:LYS:H       | 1.73                     | 0.53              |
| 1:A:4:GLU:N       | 1:A:4:GLU:OE1     | 2.42                     | 0.53              |
| 1:D:4:GLU:OE1     | 1:D:4:GLU:N       | 2.42                     | 0.53              |
| 1:x:1002:LYS:CD   | 1:OA:308:GMA:OXT  | 2.57                     | 0.53              |
| 1:M:1002:LYS:CE   | 1:w:308:GMA:OXT   | 2.57                     | 0.53              |
| 1:F:4:GLU:N       | 1:F:4:GLU:OE1     | 2.42                     | 0.53              |
| 1:H:4:GLU:N       | 1:H:4:GLU:OE1     | 2.42                     | 0.53              |
| 1:E:4:GLU:N       | 1:E:4:GLU:OE1     | 2.42                     | 0.52              |
| 1:B:4:GLU:OE1     | 1:B:4:GLU:N       | 2.42                     | 0.52              |
| 1:I:4:GLU:OE1     | 1:I:4:GLU:N       | 2.42                     | 0.52              |
| 1:G:4:GLU:OE1     | 1:G:4:GLU:N       | 2.42                     | 0.52              |
| 1:BA:1004:GLU:OE1 | 1:BA:1004:GLU:N   | 2.42                     | 0.52              |
| 1:C:4:GLU:N       | 1:C:4:GLU:OE1     | 2.42                     | 0.52              |
| 1:IA:1108:GMA:HB2 | 1:yA:1002:LYS:H   | 1.73                     | 0.52              |
| 1:nA:1306:LYS:HB3 | 1:0A:1204:GLU:HB3 | 1.92                     | 0.52              |
| 1:EB:1204:GLU:OE2 | 1:EB:1205:PHE:N   | 2.43                     | 0.52              |
| 1:M:1004:GLU:N    | 1:M:1004:GLU:OE1  | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:9A:102:LYS:HB3  | 1:i:8:GMA:HB3     | 1.92                     | 0.52              |
| 1:N:1101:5CR:CAL  | 1:9:208:GMA:N2    | 2.73                     | 0.52              |
| 1:x:1004:GLU:OE1  | 1:x:1004:GLU:N    | 2.42                     | 0.52              |
| 1:PA:1004:GLU:N   | 1:PA:1004:GLU:OE1 | 2.42                     | 0.52              |
| 1:UA:204:GLU:OE2  | 1:UA:205:PHE:N    | 2.43                     | 0.52              |
| 1:WA:1008:GMA:HB3 | 1:eA:1102:LYS:HB3 | 1.90                     | 0.52              |
| 1:wA:204:GLU:OE2  | 1:wA:205:PHE:N    | 2.43                     | 0.52              |
| 1:0A:1204:GLU:OE2 | 1:0A:1205:PHE:N   | 2.43                     | 0.52              |
| 1:LB:1204:GLU:OE2 | 1:LB:1205:PHE:N   | 2.43                     | 0.52              |
| 1:T:1004:GLU:N    | 1:T:1004:GLU:OE1  | 2.42                     | 0.52              |
| 1:q:1004:GLU:OE1  | 1:q:1004:GLU:N    | 2.42                     | 0.52              |
| 1:IA:1004:GLU:OE1 | 1:IA:1004:GLU:N   | 2.42                     | 0.52              |
| 1:fA:1204:GLU:OE2 | 1:fA:1205:PHE:N   | 2.43                     | 0.52              |
| 1:7A:1204:GLU:OE2 | 1:7A:1205:PHE:N   | 2.43                     | 0.52              |
| 1:4:1004:GLU:OE1  | 1:4:1004:GLU:N    | 2.42                     | 0.51              |
| 1:YA:1204:GLU:OE2 | 1:YA:1205:PHE:N   | 2.43                     | 0.51              |
| 1:iA:204:GLU:OE2  | 1:iA:205:PHE:N    | 2.43                     | 0.51              |
| 1:pA:204:GLU:OE2  | 1:pA:205:PHE:N    | 2.43                     | 0.51              |
| 1:AB:204:GLU:OE2  | 1:AB:205:PHE:N    | 2.43                     | 0.51              |
| 1:SB:1204:GLU:OE2 | 1:SB:1205:PHE:N   | 2.43                     | 0.51              |
| 1:M:1002:LYS:HD2  | 1:w:308:GMA:OXT   | 2.10                     | 0.51              |
| 1:R:208:GMA:N2    | 1:JA:1101:5CR:CAL | 2.73                     | 0.51              |
| 1:j:1004:GLU:N    | 1:j:1004:GLU:OE1  | 2.42                     | 0.51              |
| 1:mA:1204:GLU:OE2 | 1:mA:1205:PHE:N   | 2.43                     | 0.51              |
| 1:bA:204:GLU:OE2  | 1:bA:205:PHE:N    | 2.43                     | 0.51              |
| 1:OB:204:GLU:OE2  | 1:OB:205:PHE:N    | 2.43                     | 0.51              |
| 1:Q:101:5CR:CAL   | 1:DA:1208:GMA:N2  | 2.73                     | 0.51              |
| 1:tA:1204:GLU:OE2 | 1:tA:1205:PHE:N   | 2.43                     | 0.51              |
| 1:3A:204:GLU:OE2  | 1:3A:205:PHE:N    | 2.43                     | 0.51              |
| 1:U:1101:5CR:CAA  | 1:v:208:GMA:N2    | 2.73                     | 0.51              |
| 1:k:1101:5CR:N    | 1:OA:308:GMA:O1   | 2.44                     | 0.51              |
| 1:H:6:LYS:HG2     | 1:FA:106:LYS:CB   | 2.41                     | 0.51              |
| 1:k:1102:LYS:HG3  | 1:x:1002:LYS:HB3  | 1.93                     | 0.51              |
| 1:HB:204:GLU:OE2  | 1:HB:205:PHE:N    | 2.43                     | 0.51              |
| 1:F:6:LYS:HG2     | 1:1:106:LYS:CB    | 2.41                     | 0.51              |
| 1:DB:1102:LYS:HB3 | 1:QB:1008:GMA:HB3 | 1.92                     | 0.51              |
| 1:jA:306:LYS:HB3  | 1:wA:204:GLU:HB3  | 1.92                     | 0.51              |
| 1:nA:1304:GLU:HB3 | 1:0A:1206:LYS:HB3 | 1.93                     | 0.51              |
| 1:I:6:LYS:HG2     | 1:MA:106:LYS:CB   | 2.41                     | 0.51              |
| 1:d:8:GMA:HB3     | 1:2A:102:LYS:HB3  | 1.93                     | 0.51              |
| 1:G:6:LYS:HG2     | 1:8:106:LYS:CB    | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:6:LYS:HG2     | 1:u:106:LYS:CB    | 2.41                     | 0.50              |
| 1:PA:1006:LYS:HG2 | 1:QA:1106:LYS:CB  | 2.41                     | 0.50              |
| 1:j:1002:LYS:CE   | 1:AA:308:GMA:OXT  | 2.59                     | 0.50              |
| 1:jA:304:GLU:HB3  | 1:wA:206:LYS:HB3  | 1.93                     | 0.50              |
| 1:C:6:LYS:HG2     | 1:X:106:LYS:CB    | 2.41                     | 0.50              |
| 1:BA:1006:LYS:HG2 | 1:CA:1106:LYS:CB  | 2.41                     | 0.50              |
| 1:fA:1203:PHE:CZ  | 1:uA:1305:PHE:HE1 | 2.30                     | 0.50              |
| 1:A:6:LYS:HG2     | 1:J:106:LYS:CB    | 2.41                     | 0.50              |
| 1:B:2:LYS:HD2     | 1:O:1308:GMA:OXT  | 2.12                     | 0.49              |
| 1:bA:203:PHE:CE1  | 1:qA:305:PHE:HE1  | 2.30                     | 0.49              |
| 1:bA:203:PHE:CZ   | 1:qA:305:PHE:HE1  | 2.30                     | 0.49              |
| 1:x:1006:LYS:HG2  | 1:y:1106:LYS:CB   | 2.41                     | 0.49              |
| 1:X:102:LYS:HG3   | 1:E:2:LYS:HB3     | 1.93                     | 0.49              |
| 1:x:1002:LYS:HD2  | 1:OA:308:GMA:OXT  | 2.13                     | 0.49              |
| 1:rA:1008:GMA:HB3 | 1:6A:1102:LYS:HB3 | 1.93                     | 0.49              |
| 1:B:6:LYS:HG2     | 1:Q:106:LYS:CB    | 2.41                     | 0.49              |
| 1:B:2:LYS:CE      | 1:O:1308:GMA:OXT  | 2.60                     | 0.49              |
| 1:Z:308:GMA:O1    | 1:r:1101:5CR:N    | 2.46                     | 0.49              |
| 1:7A:1206:LYS:HB3 | 1:MB:1304:GLU:HB3 | 1.95                     | 0.49              |
| 1:J:101:5CR:N     | 1:SA:1308:GMA:O1  | 2.46                     | 0.48              |
| 1:j:1006:LYS:HG2  | 1:k:1106:LYS:CB   | 2.41                     | 0.48              |
| 1:IA:1006:LYS:HG2 | 1:JA:1106:LYS:CB  | 2.41                     | 0.48              |
| 1:T:1006:LYS:HG2  | 1:U:1106:LYS:CB   | 2.41                     | 0.48              |
| 1:fA:1203:PHE:CE1 | 1:uA:1305:PHE:HE1 | 2.30                     | 0.48              |
| 1:M:1006:LYS:HG2  | 1:N:1106:LYS:CB   | 2.41                     | 0.48              |
| 1:D:6:LYS:HG2     | 1:n:106:LYS:CB    | 2.41                     | 0.48              |
| 1:A:2:LYS:CE      | 1:EA:1308:GMA:OXT | 2.62                     | 0.48              |
| 1:L:308:GMA:O1    | 1:5:1101:5CR:N    | 2.47                     | 0.48              |
| 1:q:1006:LYS:HG2  | 1:r:1106:LYS:CB   | 2.41                     | 0.48              |
| 1:4:1006:LYS:HG2  | 1:5:1106:LYS:CB   | 2.41                     | 0.48              |
| 1:XA:1102:LYS:HB3 | 1:kA:1008:GMA:HB3 | 1.96                     | 0.48              |
| 1:e:2:LYS:HE2     | 1:e:2:LYS:HB2     | 1.70                     | 0.48              |
| 1:1A:1306:LYS:HZ3 | 1:1A:1307:PHE:C   | 2.21                     | 0.48              |
| 1:N:1101:5CR:N    | 1:AA:308:GMA:O1   | 2.46                     | 0.48              |
| 1:L:308:GMA:OXT   | 1:q:1002:LYS:CE   | 2.62                     | 0.47              |
| 1:fA:1206:LYS:HB3 | 1:uA:1304:GLU:HB3 | 1.96                     | 0.47              |
| 1:cA:306:LYS:HZ3  | 1:cA:307:PHE:C    | 2.23                     | 0.47              |
| 1:3A:206:LYS:HB3  | 1:IB:304:GLU:HB3  | 1.95                     | 0.47              |
| 1:S:308:GMA:OXT   | 1:4:1002:LYS:CE   | 2.62                     | 0.47              |
| 1:n:101:5CR:CAL   | 1:z:1208:GMA:N2   | 2.78                     | 0.47              |
| 1:tA:1206:LYS:HB3 | 1:8A:1304:GLU:HB3 | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FB:1306:LYS:HZ3 | 1:FB:1307:PHE:C   | 2.22                     | 0.47              |
| 1:S:308:GMA:O1    | 1:JA:1101:5CR:N   | 2.48                     | 0.47              |
| 1:8:106:LYS:HD2   | 1:8:106:LYS:HA    | 1.43                     | 0.47              |
| 1:fA:1204:GLU:HB3 | 1:uA:1306:LYS:HB3 | 1.96                     | 0.47              |
| 1:TB:1306:LYS:HZ3 | 1:TB:1307:PHE:C   | 2.22                     | 0.47              |
| 1:bA:204:GLU:HB3  | 1:qA:306:LYS:HB3  | 1.96                     | 0.47              |
| 1:T:1002:LYS:CE   | 1:Z:308:GMA:OXT   | 2.63                     | 0.46              |
| 1:p:308:GMA:OXT   | 1:IA:1002:LYS:CE  | 2.64                     | 0.46              |
| 1:NB:104:GLU:OE1  | 1:NB:105:PHE:N    | 2.48                     | 0.46              |
| 1:RB:1104:GLU:OE1 | 1:RB:1105:PHE:N   | 2.49                     | 0.46              |
| 1:KB:1104:GLU:OE1 | 1:KB:1105:PHE:N   | 2.49                     | 0.46              |
| 1:TA:102:LYS:HB3  | 1:c:8:GMA:HB3     | 1.96                     | 0.46              |
| 1:TA:104:GLU:OE1  | 1:TA:105:PHE:N    | 2.48                     | 0.46              |
| 1:bA:206:LYS:HB3  | 1:qA:304:GLU:HB3  | 1.96                     | 0.46              |
| 1:2A:104:GLU:OE1  | 1:2A:105:PHE:N    | 2.49                     | 0.46              |
| 1:aA:104:GLU:OE1  | 1:aA:105:PHE:N    | 2.49                     | 0.46              |
| 1:hA:104:GLU:OE1  | 1:hA:105:PHE:N    | 2.49                     | 0.46              |
| 1:vA:104:GLU:OE1  | 1:vA:105:PHE:N    | 2.49                     | 0.46              |
| 1:9A:104:GLU:OE1  | 1:9A:105:PHE:N    | 2.49                     | 0.46              |
| 1:m:1308:GMA:O1   | 1:1:101:5CR:N     | 2.49                     | 0.46              |
| 1:XA:1104:GLU:OE1 | 1:XA:1105:PHE:N   | 2.49                     | 0.46              |
| 1:zA:1104:GLU:OE1 | 1:zA:1105:PHE:N   | 2.49                     | 0.46              |
| 1:U:1102:LYS:HD3  | 1:w:308:GMA:HG2   | 1.97                     | 0.46              |
| 1:i:6:LYS:HB2     | 1:i:6:LYS:HE2     | 1.71                     | 0.46              |
| 1:DB:1104:GLU:OE1 | 1:DB:1105:PHE:N   | 2.49                     | 0.46              |
| 1:rA:1002:LYS:HE2 | 1:rA:1002:LYS:HB2 | 1.70                     | 0.46              |
| 1:k:1106:LYS:HD2  | 1:k:1106:LYS:HA   | 1.43                     | 0.46              |
| 1:sA:1104:GLU:OE1 | 1:sA:1105:PHE:N   | 2.49                     | 0.46              |
| 1:GB:104:GLU:OE1  | 1:GB:105:PHE:N    | 2.49                     | 0.46              |
| 1:5:1106:LYS:HD2  | 1:5:1106:LYS:HA   | 1.43                     | 0.46              |
| 1:oA:104:GLU:OE1  | 1:oA:105:PHE:N    | 2.49                     | 0.46              |
| 1:zA:1105:PHE:HA  | 1:CB:1004:GLU:O   | 2.16                     | 0.46              |
| 1:X:108:GMA:O1    | 1:Y:201:5CR:N     | 2.50                     | 0.45              |
| 1:lA:1104:GLU:OE1 | 1:lA:1105:PHE:N   | 2.49                     | 0.45              |
| 1:vA:105:PHE:HA   | 1:g:4:GLU:O       | 2.16                     | 0.45              |
| 1:Q:108:GMA:O1    | 1:R:201:5CR:N     | 2.50                     | 0.45              |
| 1:pA:206:LYS:HB3  | 1:4A:304:GLU:HB3  | 1.97                     | 0.45              |
| 1:CB:1006:LYS:HB2 | 1:CB:1006:LYS:HE2 | 1.71                     | 0.45              |
| 1:8:108:GMA:O1    | 1:9:201:5CR:N     | 2.50                     | 0.45              |
| 1:QA:1108:GMA:O1  | 1:RA:1201:5CR:N   | 2.50                     | 0.45              |
| 1:U:1101:5CR:N    | 1:w:308:GMA:O1    | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:1108:GMA:O1   | 1:l:1201:5CR:N    | 2.50                     | 0.45              |
| 1:1:108:GMA:O1    | 1:2:201:5CR:N     | 2.50                     | 0.45              |
| 1:5:1108:GMA:O1   | 1:6:1201:5CR:N    | 2.50                     | 0.45              |
| 1:FA:108:GMA:O1   | 1:GA:201:5CR:N    | 2.50                     | 0.45              |
| 1:MA:108:GMA:O1   | 1:NA:201:5CR:N    | 2.49                     | 0.45              |
| 1:eA:1104:GLU:OE1 | 1:eA:1105:PHE:N   | 2.49                     | 0.45              |
| 1:JB:1002:LYS:HE2 | 1:JB:1002:LYS:HB2 | 1.70                     | 0.45              |
| 1:U:1108:GMA:O1   | 1:V:1201:5CR:N    | 2.50                     | 0.45              |
| 1:CA:1108:GMA:O1  | 1:DA:1201:5CR:N   | 2.50                     | 0.45              |
| 1:uA:1302:LYS:HD2 | 1:uA:1303:PHE:H   | 1.82                     | 0.45              |
| 1:P:1308:GMA:O1   | 1:FA:101:5CR:N    | 2.50                     | 0.45              |
| 1:gA:1302:LYS:HD2 | 1:gA:1303:PHE:H   | 1.82                     | 0.45              |
| 1:6A:1104:GLU:OE1 | 1:6A:1105:PHE:N   | 2.49                     | 0.45              |
| 1:m:1308:GMA:OXT  | 1:D:2:LYS:CE      | 2.65                     | 0.45              |
| 1:u:108:GMA:O1    | 1:v:201:5CR:N     | 2.50                     | 0.45              |
| 1:y:1108:GMA:O1   | 1:z:1201:5CR:N    | 2.50                     | 0.45              |
| 1:QA:1106:LYS:HD2 | 1:QA:1106:LYS:HA  | 1.43                     | 0.45              |
| 1:b:2:LYS:HE2     | 1:b:2:LYS:HB2     | 1.70                     | 0.45              |
| 1:8A:1302:LYS:HD2 | 1:8A:1303:PHE:H   | 1.82                     | 0.45              |
| 1:Q:101:5CR:N     | 1:EA:1308:GMA:O1  | 2.50                     | 0.45              |
| 1:n:108:GMA:O1    | 1:o:201:5CR:N     | 2.50                     | 0.45              |
| 1:N:1108:GMA:O1   | 1:O:1201:5CR:N    | 2.50                     | 0.44              |
| 1:MB:1302:LYS:HD2 | 1:MB:1303:PHE:H   | 1.82                     | 0.44              |
| 1:W:1308:GMA:OXT  | 1:H:2:LYS:CE      | 2.65                     | 0.44              |
| 1:QB:1006:LYS:HB2 | 1:QB:1006:LYS:HE2 | 1.71                     | 0.44              |
| 1:ZA:1302:LYS:HD2 | 1:ZA:1303:PHE:H   | 1.82                     | 0.44              |
| 1:kA:1006:LYS:HB2 | 1:kA:1006:LYS:HE2 | 1.71                     | 0.44              |
| 1:r:1108:GMA:O1   | 1:s:1201:5CR:N    | 2.50                     | 0.44              |
| 1:xA:302:LYS:HD2  | 1:xA:303:PHE:H    | 1.82                     | 0.44              |
| 1:J:108:GMA:O1    | 1:K:201:5CR:N     | 2.50                     | 0.44              |
| 1:JA:1108:GMA:O1  | 1:KA:1201:5CR:N   | 2.50                     | 0.44              |
| 1:hA:102:LYS:HB3  | 1:e:8:GMA:HB3     | 2.00                     | 0.44              |
| 1:e:6:LYS:HB2     | 1:e:6:LYS:HE2     | 1.70                     | 0.44              |
| 1:1A:1302:LYS:HD2 | 1:1A:1303:PHE:H   | 1.82                     | 0.44              |
| 1:BB:302:LYS:HD2  | 1:BB:303:PHE:H    | 1.82                     | 0.44              |
| 1:PB:302:LYS:HD2  | 1:PB:303:PHE:H    | 1.82                     | 0.44              |
| 1:P:1308:GMA:OXT  | 1:F:2:LYS:CE      | 2.65                     | 0.44              |
| 1:IB:302:LYS:HD2  | 1:IB:303:PHE:H    | 1.82                     | 0.44              |
| 1:jA:308:GMA:HB2  | 1:wA:202:LYS:HB3  | 2.00                     | 0.44              |
| 1:lA:1102:LYS:HB3 | 1:yA:1008:GMA:HB3 | 2.00                     | 0.44              |
| 1:FB:1302:LYS:HD2 | 1:FB:1303:PHE:H   | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:WA:1006:LYS:HB2 | 1:WA:1006:LYS:HE2 | 1.71                     | 0.44              |
| 1:nA:1302:LYS:HD2 | 1:nA:1303:PHE:H   | 1.82                     | 0.44              |
| 1:qA:302:LYS:HD2  | 1:qA:303:PHE:H    | 1.82                     | 0.44              |
| 1:4A:302:LYS:HD2  | 1:4A:303:PHE:H    | 1.82                     | 0.44              |
| 1:rA:1006:LYS:HB2 | 1:rA:1006:LYS:HE2 | 1.70                     | 0.44              |
| 1:yA:1002:LYS:HE2 | 1:yA:1002:LYS:HB2 | 1.70                     | 0.44              |
| 1:FB:1305:PHE:HE1 | 1:SB:1203:PHE:CZ  | 2.36                     | 0.44              |
| 1:BB:305:PHE:HE1  | 1:OB:203:PHE:CZ   | 2.36                     | 0.43              |
| 1:N:1102:LYS:HD3  | 1:AA:308:GMA:HG2  | 2.00                     | 0.43              |
| 1:JB:1006:LYS:HB2 | 1:JB:1006:LYS:HE2 | 1.71                     | 0.43              |
| 1:WA:1002:LYS:HE2 | 1:WA:1002:LYS:HB2 | 1.70                     | 0.43              |
| 1:C:2:LYS:CE      | 1:SA:1308:GMA:OXT | 2.65                     | 0.43              |
| 1:cA:302:LYS:HD2  | 1:cA:303:PHE:H    | 1.82                     | 0.43              |
| 1:dA:1006:LYS:HB2 | 1:dA:1006:LYS:HE2 | 1.70                     | 0.43              |
| 1:TB:1302:LYS:HD2 | 1:TB:1303:PHE:H   | 1.82                     | 0.43              |
| 1:U:1101:5CR:CAL  | 1:v:208:GMA:N2    | 2.81                     | 0.43              |
| 1:jA:302:LYS:HD2  | 1:jA:303:PHE:H    | 1.82                     | 0.43              |
| 1:5A:1006:LYS:HB2 | 1:5A:1006:LYS:HE2 | 1.71                     | 0.43              |
| 1:kA:1002:LYS:HE2 | 1:kA:1002:LYS:HB2 | 1.70                     | 0.43              |
| 1:J:106:LYS:HD2   | 1:J:106:LYS:HA    | 1.43                     | 0.43              |
| 1:VA:302:LYS:HD2  | 1:VA:303:PHE:H    | 1.82                     | 0.43              |
| 1:yA:1006:LYS:HB2 | 1:yA:1006:LYS:HE2 | 1.71                     | 0.43              |
| 1:Q:106:LYS:HD2   | 1:Q:106:LYS:HA    | 1.43                     | 0.43              |
| 1:u:106:LYS:HD2   | 1:u:106:LYS:HA    | 1.43                     | 0.43              |
| 1:n:102:LYS:HD3   | 1:0:1308:GMA:HG2  | 2.01                     | 0.43              |
| 1:a:2:LYS:HB2     | 1:a:2:LYS:HE2     | 1.70                     | 0.43              |
| 1:g:2:LYS:HE2     | 1:g:2:LYS:HB2     | 1.70                     | 0.43              |
| 1:R:206:LYS:HB2   | 1:R:206:LYS:HE2   | 1.77                     | 0.42              |
| 1:V:1206:LYS:HB2  | 1:V:1206:LYS:HE2  | 1.77                     | 0.42              |
| 1:n:101:5CR:N     | 1:0:1308:GMA:O1   | 2.52                     | 0.42              |
| 1:c:2:LYS:HE2     | 1:c:2:LYS:HB2     | 1.70                     | 0.42              |
| 1:f:6:LYS:HB2     | 1:f:6:LYS:HE2     | 1.71                     | 0.42              |
| 1:DB:1102:LYS:HB3 | 1:QB:1008:GMA:CB  | 2.49                     | 0.42              |
| 1:i:2:LYS:HE2     | 1:i:2:LYS:HB2     | 1.70                     | 0.42              |
| 1:y:1106:LYS:HA   | 1:y:1106:LYS:HD2  | 1.43                     | 0.42              |
| 1:k:1102:LYS:HD3  | 1:OA:308:GMA:HG2  | 2.01                     | 0.42              |
| 1:tA:1203:PHE:CZ  | 1:8A:1305:PHE:HE1 | 2.38                     | 0.42              |
| 1:h:2:LYS:HE2     | 1:h:2:LYS:HB2     | 1.70                     | 0.42              |
| 1:f:2:LYS:HE2     | 1:f:2:LYS:HB2     | 1.70                     | 0.42              |
| 1:pA:203:PHE:CZ   | 1:4A:305:PHE:HE1  | 2.38                     | 0.42              |
| 1:K:206:LYS:HB2   | 1:K:206:LYS:HE2   | 1.77                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:5:PHE:CE2     | 1:GB:103:PHE:CE1  | 3.08                     | 0.42              |
| 1:5A:1002:LYS:HE2 | 1:5A:1002:LYS:HB2 | 1.70                     | 0.42              |
| 1:nA:1308:GMA:HB2 | 1:0A:1202:LYS:HB3 | 2.00                     | 0.42              |
| 1:N:1106:LYS:HD2  | 1:N:1106:LYS:HA   | 1.43                     | 0.41              |
| 1:l:1206:LYS:HB2  | 1:l:1206:LYS:HE2  | 1.77                     | 0.41              |
| 1:JA:1106:LYS:HD2 | 1:JA:1106:LYS:HA  | 1.43                     | 0.41              |
| 1:g:6:LYS:HB2     | 1:g:6:LYS:HE2     | 1.71                     | 0.41              |
| 1:N:1101:5CR:N    | 1:9:208:GMA:N2    | 2.68                     | 0.41              |
| 1:S:308:GMA:HG2   | 1:JA:1102:LYS:HD3 | 2.02                     | 0.41              |
| 1:Z:308:GMA:HG2   | 1:r:1102:LYS:HD3  | 2.02                     | 0.41              |
| 1:l:1208:GMA:N2   | 1:1:101:5CR:N     | 2.68                     | 0.41              |
| 1:n:106:LYS:HD2   | 1:n:106:LYS:HA    | 1.43                     | 0.41              |
| 1:YA:1206:LYS:HB3 | 1:gA:1304:GLU:HB3 | 2.02                     | 0.41              |
| 1:ZA:1304:GLU:HB3 | 1:mA:1206:LYS:HB3 | 2.03                     | 0.41              |
| 1:X:106:LYS:HD2   | 1:X:106:LYS:HA    | 1.43                     | 0.41              |
| 1:4:1005:PHE:CE2  | 1:KB:1103:PHE:CE1 | 3.08                     | 0.41              |
| 1:9A:102:LYS:HB3  | 1:i:8:GMA:CB      | 2.49                     | 0.41              |
| 1:J:101:5CR:N     | 1:RA:1208:GMA:N2  | 2.68                     | 0.41              |
| 1:GA:206:LYS:HB2  | 1:GA:206:LYS:HE2  | 1.77                     | 0.41              |
| 1:pA:204:GLU:HB3  | 1:4A:306:LYS:HB3  | 2.02                     | 0.41              |
| 1:K:208:GMA:N2    | 1:5:1101:5CR:N    | 2.68                     | 0.41              |
| 1:O:1208:GMA:N2   | 1:FA:101:5CR:N    | 2.68                     | 0.41              |
| 1:nA:1307:PHE:HE1 | 1:0A:1201:5CR:CZ  | 2.34                     | 0.41              |
| 1:k:1101:5CR:CAL  | 1:OA:308:GMA:O1   | 2.68                     | 0.41              |
| 1:5A:1004:GLU:O   | 1:KB:1105:PHE:HA  | 2.21                     | 0.41              |
| 1:MA:106:LYS:HD2  | 1:MA:106:LYS:HA   | 1.43                     | 0.41              |
| 1:UA:206:LYS:HB3  | 1:cA:304:GLU:HB3  | 2.02                     | 0.41              |
| 1:VA:304:GLU:HB3  | 1:iA:206:LYS:HB3  | 2.03                     | 0.41              |
| 1:dA:1002:LYS:HE2 | 1:dA:1002:LYS:HB2 | 1.70                     | 0.41              |
| 1:L:308:GMA:HG2   | 1:5:1102:LYS:HD3  | 2.03                     | 0.41              |
| 1:Y:208:GMA:N2    | 1:r:1101:5CR:N    | 2.68                     | 0.41              |
| 1:CA:1106:LYS:HA  | 1:CA:1106:LYS:HD2 | 1.43                     | 0.41              |
| 1:H:3:PHE:CZ      | 1:h:7:PHE:HZ      | 2.38                     | 0.41              |
| 1:IA:1003:PHE:CZ  | 1:JB:1007:PHE:HZ  | 2.38                     | 0.41              |
| 1:NA:206:LYS:HB2  | 1:NA:206:LYS:HE2  | 1.77                     | 0.41              |
| 1:f:4:GLU:O       | 1:GB:105:PHE:HA   | 2.21                     | 0.41              |
| 1:k:1101:5CR:N    | 1:NA:208:GMA:N2   | 2.69                     | 0.40              |
| 1:r:1106:LYS:HA   | 1:r:1106:LYS:HD2  | 1.43                     | 0.40              |
| 1:Q:101:5CR:N     | 1:DA:1208:GMA:N2  | 2.69                     | 0.40              |
| 1:o:206:LYS:HB2   | 1:o:206:LYS:HE2   | 1.77                     | 0.40              |
| 1:U:1106:LYS:HA   | 1:U:1106:LYS:HD2  | 1.43                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:jA:307:PHE:HE1  | 1:wA:201:5CR:CZ   | 2.34                     | 0.40              |
| 1:tA:1204:GLU:HB3 | 1:8A:1306:LYS:HB3 | 2.02                     | 0.40              |
| 1:BB:305:PHE:HE1  | 1:OB:203:PHE:CE1  | 2.39                     | 0.40              |
| 1:Q:102:LYS:HD3   | 1:EA:1308:GMA:HG2 | 2.04                     | 0.40              |
| 1:d:6:LYS:HE2     | 1:d:6:LYS:HB2     | 1.70                     | 0.40              |
| 1:CB:1002:LYS:HB2 | 1:CB:1002:LYS:HE2 | 1.70                     | 0.40              |
| 1:FB:1305:PHE:HE1 | 1:SB:1203:PHE:CE1 | 2.39                     | 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%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 0A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 1     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 1A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 2     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 2A    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 3     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 3A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 4     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 4A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 5     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 5A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 6     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 6A    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed  | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------|----------|---------|----------|-------------|-----|
| 1   | 7     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 7A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 8     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 8A    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | 9     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | 9A    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | A     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | AA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | AB    | 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   | BB    | 6/8 (75%) | 6 (100%) | 0       | 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   | CB    | 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%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | DB    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 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   | EB    | 6/8 (75%) | 6 (100%) | 0       | 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   | FB    | 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%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | GB    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 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   | HB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | I     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed  | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------|----------|---------|----------|-------------|-----|
| 1   | IA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | IB    | 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   | JB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | K     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | KA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | KB    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | L     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | LA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | LB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | M     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | MA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | MB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | N     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | NA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | NB    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | O     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | OA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | OB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | P     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | PA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | PB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | Q     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | QA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | QB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | R     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | RA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | RB    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | S     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | SA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed  | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------|----------|---------|----------|-------------|-----|
| 1   | SB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | T     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | TA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | TB    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | U     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | UA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | V     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | VA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | W     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | WA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | X     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | XA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | Y     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | YA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | Z     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | ZA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | a     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | aA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | b     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | bA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | c     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | cA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | d     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | dA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | e     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | eA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | f     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | fA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | g     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | gA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | h     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed  | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------|----------|---------|----------|-------------|-----|
| 1   | hA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | i     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | iA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | j     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | jA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | k     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | kA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | l     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | lA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | m     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | mA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | n     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | nA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | o     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | oA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | p     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | pA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | q     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | qA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | r     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | rA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | s     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | sA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | t     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | tA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | u     | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | uA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |
| 1   | v     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | vA    | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | w     | 6/8 (75%) | 5 (83%)  | 1 (17%) | 0        | 100         | 100 |
| 1   | wA    | 6/8 (75%) | 6 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | x     | 6/8 (75%)      | 5 (83%)   | 1 (17%) | 0        | 100         | 100 |
| 1   | xA    | 6/8 (75%)      | 6 (100%)  | 0       | 0        | 100         | 100 |
| 1   | y     | 6/8 (75%)      | 6 (100%)  | 0       | 0        | 100         | 100 |
| 1   | yA    | 6/8 (75%)      | 6 (100%)  | 0       | 0        | 100         | 100 |
| 1   | z     | 6/8 (75%)      | 5 (83%)   | 1 (17%) | 0        | 100         | 100 |
| 1   | zA    | 6/8 (75%)      | 5 (83%)   | 1 (17%) | 0        | 100         | 100 |
| All | All   | 864/1152 (75%) | 792 (92%) | 72 (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%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 0A    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 1     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | 1A    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 2     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 2A    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 3     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 3A    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 4     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 4A    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 5     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | 5A    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | 6     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 6A    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | 7     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |

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| Mol | Chain | Analysed   | Rotameric | Outliers | Percentiles |     |
|-----|-------|------------|-----------|----------|-------------|-----|
| 1   | 7A    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 8     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | 8A    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 9     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | 9A    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | A     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | AA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | AB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | B     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | BA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | BB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | C     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | CA    | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | CB    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | D     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | DA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | DB    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | E     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | EA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | EB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | F     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | FA    | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | FB    | 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   | GB    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | H     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | HA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | HB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | I     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | IA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed   | Rotameric | Outliers | Percentiles |     |
|-----|-------|------------|-----------|----------|-------------|-----|
| 1   | IB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | J     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | JA    | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | JB    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | K     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | KA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | KB    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | L     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | LA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | LB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | M     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | MA    | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | MB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | N     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | NA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | NB    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | O     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | OA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | OB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | P     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | PA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | PB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | QA    | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | QB    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | R     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | RA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | RB    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | S     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | SA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | SB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed   | Rotameric | Outliers | Percentiles |     |
|-----|-------|------------|-----------|----------|-------------|-----|
| 1   | T     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | TA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | TB    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | U     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | UA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | V     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | VA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | W     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | WA    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | X     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | XA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | Y     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | YA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | Z     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | ZA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | a     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | aA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | b     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | bA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | c     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | cA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | d     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | dA    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | e     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | eA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | f     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | fA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | g     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | gA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | h     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | hA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |

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| Mol | Chain | Analysed   | Rotameric | Outliers | Percentiles |     |
|-----|-------|------------|-----------|----------|-------------|-----|
| 1   | i     | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | iA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | j     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | jA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | k     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | kA    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | l     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | lA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | m     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | mA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | n     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | nA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | o     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | oA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | p     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | pA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | q     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | qA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | r     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | rA    | 6/6 (100%) | 3 (50%)   | 3 (50%)  | 0           | 0   |
| 1   | s     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | sA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | t     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | tA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | u     | 6/6 (100%) | 4 (67%)   | 2 (33%)  | 0           | 0   |
| 1   | uA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | v     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | vA    | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | w     | 6/6 (100%) | 5 (83%)   | 1 (17%)  | 2           | 9   |
| 1   | wA    | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |
| 1   | x     | 6/6 (100%) | 6 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |     |
|-----|-------|----------------|-----------|-----------|-------------|-----|
| 1   | xA    | 6/6 (100%)     | 6 (100%)  | 0         | 100         | 100 |
| 1   | y     | 6/6 (100%)     | 4 (67%)   | 2 (33%)   | 0           | 0   |
| 1   | yA    | 6/6 (100%)     | 3 (50%)   | 3 (50%)   | 0           | 0   |
| 1   | z     | 6/6 (100%)     | 6 (100%)  | 0         | 100         | 100 |
| 1   | zA    | 6/6 (100%)     | 5 (83%)   | 1 (17%)   | 2           | 9   |
| All | All   | 864/864 (100%) | 738 (85%) | 126 (15%) | 5           | 12  |

All (126) 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   | N     | 1102 | LYS  |
| 1   | N     | 1106 | LYS  |
| 1   | P     | 1302 | LYS  |
| 1   | Q     | 102  | LYS  |
| 1   | Q     | 106  | LYS  |
| 1   | S     | 302  | LYS  |
| 1   | U     | 1102 | LYS  |
| 1   | U     | 1106 | LYS  |
| 1   | W     | 1302 | LYS  |
| 1   | X     | 102  | LYS  |
| 1   | X     | 106  | LYS  |
| 1   | Z     | 302  | LYS  |
| 1   | k     | 1102 | LYS  |
| 1   | k     | 1106 | LYS  |
| 1   | m     | 1302 | LYS  |
| 1   | n     | 102  | LYS  |
| 1   | n     | 106  | LYS  |
| 1   | p     | 302  | LYS  |
| 1   | r     | 1102 | LYS  |
| 1   | r     | 1106 | LYS  |
| 1   | t     | 1302 | LYS  |
| 1   | u     | 102  | LYS  |
| 1   | u     | 106  | LYS  |
| 1   | w     | 302  | LYS  |
| 1   | y     | 1102 | LYS  |
| 1   | y     | 1106 | LYS  |
| 1   | 0     | 1302 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 102  | LYS  |
| 1   | 1     | 106  | LYS  |
| 1   | 3     | 302  | LYS  |
| 1   | 5     | 1102 | LYS  |
| 1   | 5     | 1106 | LYS  |
| 1   | 7     | 1302 | LYS  |
| 1   | 8     | 102  | LYS  |
| 1   | 8     | 106  | LYS  |
| 1   | AA    | 302  | LYS  |
| 1   | CA    | 1102 | LYS  |
| 1   | CA    | 1106 | LYS  |
| 1   | EA    | 1302 | LYS  |
| 1   | FA    | 102  | LYS  |
| 1   | FA    | 106  | LYS  |
| 1   | HA    | 302  | LYS  |
| 1   | JA    | 1102 | LYS  |
| 1   | JA    | 1106 | LYS  |
| 1   | LA    | 1302 | LYS  |
| 1   | MA    | 102  | LYS  |
| 1   | MA    | 106  | LYS  |
| 1   | OA    | 302  | LYS  |
| 1   | QA    | 1102 | LYS  |
| 1   | QA    | 1106 | LYS  |
| 1   | SA    | 1302 | LYS  |
| 1   | a     | 2    | LYS  |
| 1   | a     | 4    | GLU  |
| 1   | a     | 6    | LYS  |
| 1   | TA    | 104  | GLU  |
| 1   | WA    | 1002 | LYS  |
| 1   | WA    | 1004 | GLU  |
| 1   | WA    | 1006 | LYS  |
| 1   | XA    | 1104 | GLU  |
| 1   | b     | 2    | LYS  |
| 1   | b     | 4    | GLU  |
| 1   | b     | 6    | LYS  |
| 1   | aA    | 104  | GLU  |
| 1   | dA    | 1002 | LYS  |
| 1   | dA    | 1004 | GLU  |
| 1   | dA    | 1006 | LYS  |
| 1   | eA    | 1104 | GLU  |
| 1   | c     | 2    | LYS  |
| 1   | c     | 4    | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | c     | 6    | LYS  |
| 1   | hA    | 104  | GLU  |
| 1   | kA    | 1002 | LYS  |
| 1   | kA    | 1004 | GLU  |
| 1   | kA    | 1006 | LYS  |
| 1   | lA    | 1104 | GLU  |
| 1   | d     | 2    | LYS  |
| 1   | d     | 4    | GLU  |
| 1   | d     | 6    | LYS  |
| 1   | oA    | 104  | GLU  |
| 1   | rA    | 1002 | LYS  |
| 1   | rA    | 1004 | GLU  |
| 1   | rA    | 1006 | LYS  |
| 1   | sA    | 1104 | GLU  |
| 1   | e     | 2    | LYS  |
| 1   | e     | 4    | GLU  |
| 1   | e     | 6    | LYS  |
| 1   | vA    | 104  | GLU  |
| 1   | yA    | 1002 | LYS  |
| 1   | yA    | 1004 | GLU  |
| 1   | yA    | 1006 | LYS  |
| 1   | zA    | 1104 | GLU  |
| 1   | f     | 2    | LYS  |
| 1   | f     | 4    | GLU  |
| 1   | f     | 6    | LYS  |
| 1   | 2A    | 104  | GLU  |
| 1   | 5A    | 1002 | LYS  |
| 1   | 5A    | 1004 | GLU  |
| 1   | 5A    | 1006 | LYS  |
| 1   | 6A    | 1104 | GLU  |
| 1   | g     | 2    | LYS  |
| 1   | g     | 4    | GLU  |
| 1   | g     | 6    | LYS  |
| 1   | 9A    | 104  | GLU  |
| 1   | CB    | 1002 | LYS  |
| 1   | CB    | 1004 | GLU  |
| 1   | CB    | 1006 | LYS  |
| 1   | DB    | 1104 | GLU  |
| 1   | h     | 2    | LYS  |
| 1   | h     | 4    | GLU  |
| 1   | h     | 6    | LYS  |
| 1   | GB    | 104  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | JB    | 1002 | LYS  |
| 1   | JB    | 1004 | GLU  |
| 1   | JB    | 1006 | LYS  |
| 1   | KB    | 1104 | GLU  |
| 1   | i     | 2    | LYS  |
| 1   | i     | 4    | GLU  |
| 1   | i     | 6    | LYS  |
| 1   | NB    | 104  | GLU  |
| 1   | QB    | 1002 | LYS  |
| 1   | QB    | 1004 | GLU  |
| 1   | QB    | 1006 | LYS  |
| 1   | RB    | 1104 | 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 ⓘ

288 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   | 5CR  | 1A    | 1301 | 1    | 13,14,15     | 1.27 | 1 (7%)      | 16,17,19    | 0.94 | 1 (6%)      |
| 1   | GMA  | BA    | 1008 | 1    | 9,9,9        | 1.18 | 1 (11%)     | 10,11,11    | 1.26 | 0           |
| 1   | GMA  | 1A    | 1308 | 1    | 9,9,9        | 1.19 | 1 (11%)     | 10,11,11    | 1.33 | 0           |
| 1   | GMA  | zA    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)     | 10,11,11    | 1.19 | 0           |
| 1   | 5CR  | y     | 1101 | 1    | 13,14,15     | 1.29 | 1 (7%)      | 16,17,19    | 1.47 | 2 (12%)     |
| 1   | 5CR  | 2     | 201  | 1    | 13,14,15     | 1.32 | 2 (15%)     | 16,17,19    | 1.33 | 3 (18%)     |
| 1   | 5CR  | dA    | 1001 | 1    | 13,14,15     | 1.34 | 2 (15%)     | 16,17,19    | 1.71 | 3 (18%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | GMA  | v     | 208  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | O     | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | N     | 1108 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.25 | 1 (10%)  |
| 1   | GMA  | fA    | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.12 | 0        |
| 1   | 5CR  | l     | 1201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | iA    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | bA    | 201  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | 9A    | 101  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | GMA  | ZA    | 1308 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | GMA  | JB    | 1008 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | A     | 8    | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | nA    | 1301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | F     | 8    | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | 5CR  | CB    | 1001 | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | nA    | 1308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | GMA  | Y     | 208  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | GMA  | l     | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | 5CR  | JB    | 1001 | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | 5CR  | J     | 101  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | m     | 1301 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.16 | 2 (12%)  |
| 1   | 5CR  | fA    | 1201 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.11 | 1 (6%)   |
| 1   | 5CR  | NA    | 201  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | 5CR  | 7     | 1301 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | MB    | 1301 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | uA    | 1301 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 0.92 | 1 (6%)   |
| 1   | GMA  | FA    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.25 | 1 (10%)  |
| 1   | GMA  | dA    | 1008 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | DA    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.29 | 2 (20%)  |
| 1   | 5CR  | c     | 1    | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.69 | 3 (18%)  |
| 1   | 5CR  | FB    | 1301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | F     | 1    | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | GMA  | t     | 1308 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | QB    | 1001 | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | JA    | 1108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | GMA  | 4A    | 308  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.31 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | IB    | 301  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | yA    | 1008 | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.17 | 0        |
| 1   | 5CR  | C     | 1    | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | 6     | 1201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | XA    | 1108 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | GMA  | 1     | 108  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 1 (10%)  |
| 1   | 5CR  | Y     | 201  | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | 5CR  | D     | 1    | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | GMA  | P     | 1308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | u     | 108  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | GMA  | 2     | 208  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | 5CR  | zA    | 1101 | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | 5CR  | 4A    | 301  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | lA    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | GMA  | 7A    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | SB    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.13 | 0        |
| 1   | GMA  | GB    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | HB    | 201  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | MA    | 101  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | xA    | 301  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 0.95 | 1 (6%)   |
| 1   | 5CR  | a     | 1    | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | 5CR  | q     | 1001 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | pA    | 201  | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | JA    | 1101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | PA    | 1001 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.58 | 2 (12%)  |
| 1   | GMA  | M     | 1008 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | WA    | 1008 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | cA    | 308  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | 5CR  | LA    | 1301 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | UA    | 201  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | 4     | 1008 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | GMA  | NB    | 108  | 1    | 9,9,9        | 1.17 | 1 (11%)  | 10,11,11    | 1.18 | 0        |
| 1   | 5CR  | jA    | 301  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | 5CR  | e     | 1    | 1    | 13,14,15     | 1.36 | 2 (15%)  | 16,17,19    | 1.69 | 3 (18%)  |
| 1   | 5CR  | x     | 1001 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | GMA  | KA    | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | GMA  | aA    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.22 | 0        |
| 1   | GMA  | d     | 8    | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | DB    | 1108 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | GMA  | TB    | 1308 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | 5CR  | FA    | 101  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | GMA  | q     | 1008 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | a     | 8    | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | K     | 208  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | rA    | 1008 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | I     | 8    | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | 5CR  | BA    | 1001 | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | 5CR  | tA    | 1201 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | 3A    | 201  | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.11 | 1 (6%)   |
| 1   | 5CR  | K     | 201  | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | GMA  | Z     | 308  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | hA    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | 5CR  | PB    | 301  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | k     | 1101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | g     | 1    | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | 6A    | 1101 | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | 6A    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | 5CR  | EA    | 1301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | S     | 301  | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | GMA  | NA    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.29 | 2 (20%)  |
| 1   | GMA  | IA    | 1008 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | T     | 1008 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | 5CR  | GB    | 101  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.06 | 1 (6%)   |
| 1   | GMA  | LA    | 1308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | 3A    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | IB    | 308  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.35 | 0        |
| 1   | GMA  | o     | 208  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | 5CR  | b     | 1    | 1    | 13,14,15     | 1.33 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | 5CR  | QA    | 1101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | NB    | 101  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | GMA  | EB    | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | AA    | 301  | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | VA    | 301  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 0.92 | 1 (6%)   |
| 1   | 5CR  | M     | 1001 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | 5CR  | aA    | 101  | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | D     | 8    | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | UA    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | QA    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | 5CR  | n     | 101  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | N     | 1101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | z     | 1201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.32 | 2 (12%)  |
| 1   | 5CR  | 3     | 301  | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | GMA  | LB    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | eA    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.21 | 0        |
| 1   | 5CR  | DB    | 1101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | 5CR  | hA    | 101  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | GMA  | Q     | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | 5CR  | 9     | 201  | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | GMA  | J     | 108  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | 5CR  | sA    | 1101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | 5CR  | 2A    | 101  | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | RB    | 1108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.18 | 0        |
| 1   | 5CR  | IA    | 1001 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | i     | 1    | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.69 | 3 (18%)  |
| 1   | 5CR  | KB    | 1101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.06 | 1 (6%)   |
| 1   | 5CR  | eA    | 1101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | PA    | 1008 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | 5CR  | W     | 1301 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | 7A    | 1201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | Q     | 101  | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.48 | 2 (12%)  |
| 1   | GMA  | C     | 8    | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | 5CR  | OA    | 301  | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | RA    | 1201 | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | H     | 8    | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | 5A    | 1008 | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | wA    | 201  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.13 | 1 (6%)   |
| 1   | GMA  | BB    | 308  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | GMA  | G     | 8    | 1    | 9,9,9        | 1.17 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | AB    | 208  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | t     | 1301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | GMA  | 6     | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | GMA  | RA    | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.29 | 2 (20%)  |
| 1   | GMA  | CA    | 1108 | 1    | 9,9,9        | 1.17 | 1 (11%)  | 10,11,11    | 1.22 | 0        |
| 1   | GMA  | jA    | 308  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.35 | 0        |
| 1   | GMA  | HB    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | VA    | 308  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | 5CR  | I     | 1    | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.58 | 2 (12%)  |
| 1   | GMA  | 2A    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.18 | 0        |
| 1   | 5CR  | TB    | 1301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | GMA  | U     | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | 5CR  | O     | 1201 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | GMA  | L     | 308  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | 5CR  | 0     | 1301 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | GMA  | h     | 8    | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | GMA  | f     | 8    | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | AA    | 308  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | CB    | 1008 | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | SA    | 1301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | GMA  | n     | 108  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.24 | 1 (10%)  |
| 1   | GMA  | SA    | 1308 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | OB    | 201  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | EA    | 1308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | 5CR  | X     | 101  | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | yA    | 1001 | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | L     | 301  | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | 5CR  | XA    | 1101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | GMA  | S     | 308  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | p     | 308  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.24 | 0        |
| 1   | GMA  | TA    | 108  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | GMA  | xA    | 308  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5CR  | kA    | 1001 | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | cA    | 301  | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.92 | 1 (6%)   |
| 1   | 5CR  | iA    | 201  | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | 0A    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | w     | 301  | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | DA    | 1201 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.32 | 3 (18%)  |
| 1   | 5CR  | R     | 201  | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 2 (12%)  |
| 1   | 5CR  | p     | 301  | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | 5CR  | d     | 1    | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | E     | 8    | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | 8     | 108  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | GMA  | OA    | 308  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | c     | 8    | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | b     | 8    | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.17 | 0        |
| 1   | GMA  | oA    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | GMA  | sA    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | GMA  | QB    | 1008 | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | uA    | 1308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | 5CR  | v     | 201  | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.33 | 2 (12%)  |
| 1   | 5CR  | RB    | 1101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | GMA  | 7     | 1308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | CA    | 1101 | 1    | 13,14,15     | 1.31 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | mA    | 1201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | 0     | 1308 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.24 | 0        |
| 1   | GMA  | vA    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.19 | 0        |
| 1   | 5CR  | 5     | 1101 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | gA    | 1301 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | 0A    | 1201 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | SB    | 1201 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | KB    | 1108 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |
| 1   | 5CR  | oA    | 101  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.07 | 1 (6%)   |
| 1   | 5CR  | 8A    | 1301 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | x     | 1008 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | mA    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | MA    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.24 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | GMA  | qA    | 308  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | 5CR  | P     | 1301 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.17 | 2 (12%)  |
| 1   | GMA  | tA    | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | BB    | 301  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 0.94 | 1 (6%)   |
| 1   | 5CR  | 4     | 1001 | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | TA    | 101  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.08 | 1 (6%)   |
| 1   | GMA  | GA    | 208  | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.28 | 2 (20%)  |
| 1   | GMA  | r     | 1108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 1 (10%)  |
| 1   | 5CR  | 1     | 101  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | qA    | 301  | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 0.92 | 1 (6%)   |
| 1   | 5CR  | EB    | 1201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | 8     | 101  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.47 | 2 (12%)  |
| 1   | 5CR  | U     | 1101 | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.48 | 2 (12%)  |
| 1   | 5CR  | E     | 1    | 1    | 13,14,15     | 1.28 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | rA    | 1001 | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | GMA  | PB    | 308  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |
| 1   | 5CR  | YA    | 1201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | 5CR  | G     | 1    | 1    | 13,14,15     | 1.27 | 1 (7%)   | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | GMA  | R     | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.28 | 1 (10%)  |
| 1   | GMA  | W     | 1308 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | 5CR  | o     | 201  | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | X     | 108  | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | GMA  | w     | 308  | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.24 | 0        |
| 1   | 5CR  | B     | 1    | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | 5CR  | GA    | 201  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | m     | 1308 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | wA    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | V     | 1201 | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | y     | 1108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | GMA  | z     | 1208 | 1    | 9,9,9        | 1.22 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | GMA  | gA    | 1308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | GMA  | YA    | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | Z     | 301  | 1    | 13,14,15     | 1.31 | 2 (15%)  | 16,17,19    | 1.16 | 2 (12%)  |
| 1   | 5CR  | AB    | 201  | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | 9A    | 108  | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.20 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | GMA  | 8A    | 1308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.32 | 0        |
| 1   | 5CR  | WA    | 1001 | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | 5CR  | r     | 1101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | A     | 1    | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | 5CR  | T     | 1001 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.57 | 2 (12%)  |
| 1   | GMA  | V     | 1208 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | GMA  | j     | 1008 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.27 | 0        |
| 1   | GMA  | 9     | 208  | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.29 | 2 (20%)  |
| 1   | GMA  | g     | 8    | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |
| 1   | GMA  | OB    | 208  | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.14 | 0        |
| 1   | 5CR  | KA    | 1201 | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.33 | 3 (18%)  |
| 1   | GMA  | k     | 1108 | 1    | 9,9,9        | 1.18 | 1 (11%)  | 10,11,11    | 1.23 | 0        |
| 1   | 5CR  | LB    | 1201 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.12 | 1 (6%)   |
| 1   | GMA  | HA    | 308  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | 5CR  | vA    | 101  | 1    | 13,14,15     | 1.28 | 1 (7%)   | 16,17,19    | 1.09 | 1 (6%)   |
| 1   | 5CR  | 5A    | 1001 | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | 5CR  | ZA    | 1301 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 0.93 | 1 (6%)   |
| 1   | GMA  | i     | 8    | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.17 | 0        |
| 1   | 5CR  | lA    | 1101 | 1    | 13,14,15     | 1.29 | 1 (7%)   | 16,17,19    | 1.09 | 1 (6%)   |
| 1   | GMA  | B     | 8    | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.26 | 0        |
| 1   | GMA  | bA    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.13 | 0        |
| 1   | GMA  | kA    | 1008 | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | 5CR  | H     | 1    | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | GMA  | 3     | 308  | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.25 | 0        |
| 1   | GMA  | 5     | 1108 | 1    | 9,9,9        | 1.17 | 1 (11%)  | 10,11,11    | 1.23 | 1 (10%)  |
| 1   | 5CR  | s     | 1201 | 1    | 13,14,15     | 1.30 | 2 (15%)  | 16,17,19    | 1.34 | 3 (18%)  |
| 1   | 5CR  | u     | 101  | 1    | 13,14,15     | 1.30 | 1 (7%)   | 16,17,19    | 1.46 | 2 (12%)  |
| 1   | 5CR  | HA    | 301  | 1    | 13,14,15     | 1.27 | 2 (15%)  | 16,17,19    | 1.18 | 2 (12%)  |
| 1   | GMA  | pA    | 208  | 1    | 9,9,9        | 1.23 | 1 (11%)  | 10,11,11    | 1.15 | 0        |
| 1   | GMA  | MB    | 1308 | 1    | 9,9,9        | 1.20 | 1 (11%)  | 10,11,11    | 1.34 | 0        |
| 1   | 5CR  | h     | 1    | 1    | 13,14,15     | 1.35 | 2 (15%)  | 16,17,19    | 1.70 | 3 (18%)  |
| 1   | 5CR  | j     | 1001 | 1    | 13,14,15     | 1.29 | 2 (15%)  | 16,17,19    | 1.56 | 2 (12%)  |
| 1   | 5CR  | f     | 1    | 1    | 13,14,15     | 1.34 | 2 (15%)  | 16,17,19    | 1.71 | 3 (18%)  |
| 1   | GMA  | s     | 1208 | 1    | 9,9,9        | 1.21 | 1 (11%)  | 10,11,11    | 1.27 | 1 (10%)  |
| 1   | GMA  | FB    | 1308 | 1    | 9,9,9        | 1.19 | 1 (11%)  | 10,11,11    | 1.33 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | GMA  | e     | 8   | 1    | 9,9,9        | 1.24 | 1 (11%)  | 10,11,11    | 1.16 | 0        |

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   | 5CR  | 1A    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | BA    | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 1A    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | zA    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | y     | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 2     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | dA    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | v     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | O     | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | N     | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | fA    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | l     | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | iA    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | bA    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 9A    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | ZA    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | JB    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | A     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | nA    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | F     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | CB    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | nA    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | Y     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | l     | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | JB    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | J     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | m     | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | fA    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | NA    | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 7     | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 5CR  | MB    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | uA    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | FA    | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | dA    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | DA    | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | c     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | FB    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | F     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | t     | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | QB    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | JA    | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | 4A    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | IB    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | yA    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | C     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 6     | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | XA    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | 1     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | Y     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | D     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | P     | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | u     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | 2     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | zA    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 4A    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | lA    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | 7A    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | SB    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | GB    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | HB    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | MA    | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | xA    | 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  | q     | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | pA    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | JA    | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | PA    | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | GMA  | M     | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | WA    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | cA    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | LA    | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | UA    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 4     | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | NB    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | jA    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | e     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | x     | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | KA    | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | aA    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | d     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | DB    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | TB    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | FA    | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | q     | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | a     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | K     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | rA    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | I     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | BA    | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | tA    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 3A    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | K     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | Z     | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | hA    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | PB    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | k     | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | g     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 6A    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 6A    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | EA    | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | S     | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | NA    | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | IA    | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | T     | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | GB    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | GMA  | LA    | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 3A    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | IB    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | o     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | b     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | QA    | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | NB    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | EB    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | AA    | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | VA    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | M     | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | aA    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | D     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | UA    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | QA    | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | n     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | N     | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | z     | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 3     | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | LB    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | eA    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | DB    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | hA    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | Q     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | 9     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | J     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | sA    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 2A    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | RB    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | IA    | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | i     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | KB    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | eA    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | PA    | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | W     | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 7A    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | Q     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | C     | 8    | 1    | -       | 1/9/9/9   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 5CR  | OA    | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | RA    | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | H     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 5A    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | wA    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | BB    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | G     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | AB    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | t     | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 6     | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | RA    | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | CA    | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | jA    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | HB    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | VA    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | I     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 2A    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | TB    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | U     | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | O     | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | L     | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | 0     | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | h     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | f     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | AA    | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | CB    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | SA    | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | n     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | SA    | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | OB    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | EA    | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | X     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | yA    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | L     | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | XA    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | S     | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | p     | 308  | 1    | -       | 1/9/9/9   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | GMA  | TA    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | xA    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | kA    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | cA    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | iA    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 0A    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | w     | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | DA    | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | R     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | p     | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | d     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | E     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 8     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | OA    | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | c     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | b     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | oA    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | sA    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | QB    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | uA    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | v     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | RB    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 7     | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | CA    | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | mA    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 0     | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | vA    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | 5     | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | gA    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 0A    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | SB    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | KB    | 1108 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | oA    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 8A    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | x     | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | mA    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | MA    | 108  | 1    | -       | 2/9/9/9   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | GMA  | qA    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | P     | 1301 | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | tA    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | BB    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 4     | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | TA    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | GA    | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | r     | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | 1     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | qA    | 301  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | EB    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 8     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | U     | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | E     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | rA    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | PB    | 308  | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | YA    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | G     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | R     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | W     | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | o     | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | X     | 108  | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | w     | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | B     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | GA    | 201  | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | m     | 1308 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | wA    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | V     | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | y     | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | GMA  | z     | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | gA    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | YA    | 1208 | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | Z     | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | AB    | 201  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 9A    | 108  | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | 8A    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | WA    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 5CR  | r     | 1101 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | A     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | T     | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | V     | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | j     | 1008 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 9     | 208  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | g     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | GMA  | OB    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | 5CR  | KA    | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | k     | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | LB    | 1201 | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | GMA  | HA    | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | 5CR  | vA    | 101  | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | 5A    | 1001 | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | ZA    | 1301 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | GMA  | i     | 8    | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | lA    | 1101 | 1    | -       | 1/9/10/12 | 0/1/1/1 |
| 1   | GMA  | B     | 8    | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | bA    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | kA    | 1008 | 1    | -       | 8/9/9/9   | -       |
| 1   | 5CR  | H     | 1    | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | GMA  | 3     | 308  | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | 5     | 1108 | 1    | -       | 2/9/9/9   | -       |
| 1   | 5CR  | s     | 1201 | 1    | -       | 4/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | u     | 101  | 1    | -       | 2/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | HA    | 301  | 1    | -       | 3/9/10/12 | 0/1/1/1 |
| 1   | GMA  | pA    | 208  | 1    | -       | 4/9/9/9   | -       |
| 1   | GMA  | MB    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | 5CR  | h     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | j     | 1001 | 1    | -       | 0/9/10/12 | 0/1/1/1 |
| 1   | 5CR  | f     | 1    | 1    | -       | 6/9/10/12 | 0/1/1/1 |
| 1   | GMA  | s     | 1208 | 1    | -       | 1/9/9/9   | -       |
| 1   | GMA  | FB    | 1308 | 1    | -       | 0/9/9/9   | -       |
| 1   | GMA  | e     | 8    | 1    | -       | 8/9/9/9   | -       |

All (353) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | d     | 1    | 5CR  | CAL-N | 3.73 | 1.46        | 1.34     |
| 1   | e     | 1    | 5CR  | CAL-N | 3.72 | 1.46        | 1.34     |
| 1   | rA    | 1001 | 5CR  | CAL-N | 3.72 | 1.46        | 1.34     |
| 1   | yA    | 1001 | 5CR  | CAL-N | 3.71 | 1.46        | 1.34     |
| 1   | i     | 1    | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | h     | 1    | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | QB    | 1001 | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | WA    | 1001 | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | a     | 1    | 5CR  | CAL-N | 3.70 | 1.46        | 1.34     |
| 1   | 5A    | 1001 | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | g     | 1    | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | JB    | 1001 | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | CB    | 1001 | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | f     | 1    | 5CR  | CAL-N | 3.69 | 1.46        | 1.34     |
| 1   | c     | 1    | 5CR  | CAL-N | 3.68 | 1.46        | 1.34     |
| 1   | kA    | 1001 | 5CR  | CAL-N | 3.68 | 1.46        | 1.34     |
| 1   | dA    | 1001 | 5CR  | CAL-N | 3.67 | 1.46        | 1.34     |
| 1   | b     | 1    | 5CR  | CAL-N | 3.66 | 1.46        | 1.34     |
| 1   | X     | 101  | 5CR  | CAL-N | 3.47 | 1.45        | 1.34     |
| 1   | k     | 1101 | 5CR  | CAL-N | 3.46 | 1.45        | 1.34     |
| 1   | 5     | 1101 | 5CR  | CAL-N | 3.45 | 1.45        | 1.34     |
| 1   | CA    | 1101 | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | hA    | 101  | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | l     | 101  | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | FA    | 101  | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | JA    | 1101 | 5CR  | CAL-N | 3.44 | 1.45        | 1.34     |
| 1   | n     | 101  | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | r     | 1101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | u     | 101  | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | QA    | 1101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | LB    | 1201 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | HB    | 201  | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | y     | 1101 | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | 9A    | 101  | 5CR  | CAL-N | 3.43 | 1.45        | 1.34     |
| 1   | N     | 1101 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | tA    | 1201 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | OB    | 201  | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | KB    | 1101 | 5CR  | CAL-N | 3.42 | 1.45        | 1.34     |
| 1   | DB    | 1101 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | MA    | 101  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | pA    | 201  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | U     | 1101 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | 0A    | 1201 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | 8     | 101  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | IB    | 301  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | VA    | 301  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | lA    | 1101 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | qA    | 301  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | MB    | 1301 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | GB    | 101  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | SB    | 1201 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | RB    | 1101 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | Q     | 101  | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | uA    | 1301 | 5CR  | CAL-N | 3.41 | 1.45        | 1.34     |
| 1   | UA    | 201  | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | YA    | 1201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | iA    | 201  | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | mA    | 1201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | oA    | 101  | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | wA    | 201  | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | J     | 101  | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | NB    | 101  | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | fA    | 1201 | 5CR  | CAL-N | 3.40 | 1.45        | 1.34     |
| 1   | 7A    | 1201 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | ZA    | 1301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | sA    | 1101 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | 4A    | 301  | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | 8A    | 1301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | FB    | 1301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | TB    | 1301 | 5CR  | CAL-N | 3.39 | 1.45        | 1.34     |
| 1   | jA    | 301  | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | bA    | 201  | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | EB    | 1201 | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | 3A    | 201  | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | xA    | 301  | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | 1A    | 1301 | 5CR  | CAL-N | 3.38 | 1.45        | 1.34     |
| 1   | PB    | 301  | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | TA    | 101  | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | cA    | 301  | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | AB    | 201  | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | BB    | 301  | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | vA    | 101  | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | nA    | 1301 | 5CR  | CAL-N | 3.37 | 1.45        | 1.34     |
| 1   | XA    | 1101 | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | 6A    | 1101 | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | eA    | 1101 | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | aA    | 101  | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | gA    | 1301 | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | 2A    | 101  | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | NA    | 201  | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | o     | 201  | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | zA    | 1101 | 5CR  | CAL-N | 3.36 | 1.45        | 1.34     |
| 1   | V     | 1201 | 5CR  | CAL-N | 3.35 | 1.45        | 1.34     |
| 1   | l     | 1201 | 5CR  | CAL-N | 3.35 | 1.45        | 1.34     |
| 1   | RA    | 1201 | 5CR  | CAL-N | 3.35 | 1.45        | 1.34     |
| 1   | R     | 201  | 5CR  | CAL-N | 3.35 | 1.45        | 1.34     |
| 1   | 2     | 201  | 5CR  | CAL-N | 3.35 | 1.45        | 1.34     |
| 1   | Y     | 201  | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | z     | 1201 | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | GA    | 201  | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | DA    | 1201 | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | 9     | 201  | 5CR  | CAL-N | 3.34 | 1.45        | 1.34     |
| 1   | KA    | 1201 | 5CR  | CAL-N | 3.33 | 1.45        | 1.34     |
| 1   | v     | 201  | 5CR  | CAL-N | 3.33 | 1.45        | 1.34     |
| 1   | s     | 1201 | 5CR  | CAL-N | 3.33 | 1.45        | 1.34     |
| 1   | 6     | 1201 | 5CR  | CAL-N | 3.33 | 1.45        | 1.34     |
| 1   | O     | 1201 | 5CR  | CAL-N | 3.32 | 1.45        | 1.34     |
| 1   | K     | 201  | 5CR  | CAL-N | 3.31 | 1.45        | 1.34     |
| 1   | x     | 1001 | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | q     | 1001 | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | 4     | 1001 | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | A     | 1    | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | M     | 1001 | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | F     | 1    | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | C     | 1    | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | E     | 1    | 5CR  | CAL-N | 3.30 | 1.45        | 1.34     |
| 1   | H     | 1    | 5CR  | CAL-N | 3.29 | 1.45        | 1.34     |
| 1   | j     | 1001 | 5CR  | CAL-N | 3.29 | 1.45        | 1.34     |
| 1   | D     | 1    | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | IA    | 1001 | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | PA    | 1001 | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | T     | 1001 | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | 0     | 1301 | 5CR  | CAL-N | 3.28 | 1.44        | 1.34     |
| 1   | B     | 1    | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | Z     | 301  | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | m     | 1301 | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | I     | 1    | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | t     | 1301 | 5CR  | CAL-N | 3.27 | 1.44        | 1.34     |
| 1   | BA    | 1001 | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | w     | 301  | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | p     | 301  | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | S     | 301  | 5CR  | CAL-N | 3.26 | 1.44        | 1.34     |
| 1   | L     | 301  | 5CR  | CAL-N | 3.25 | 1.44        | 1.34     |
| 1   | P     | 1301 | 5CR  | CAL-N | 3.25 | 1.44        | 1.34     |
| 1   | G     | 1    | 5CR  | CAL-N | 3.25 | 1.44        | 1.34     |
| 1   | W     | 1301 | 5CR  | CAL-N | 3.25 | 1.44        | 1.34     |
| 1   | EA    | 1301 | 5CR  | CAL-N | 3.24 | 1.44        | 1.34     |
| 1   | SA    | 1301 | 5CR  | CAL-N | 3.24 | 1.44        | 1.34     |
| 1   | AA    | 301  | 5CR  | CAL-N | 3.23 | 1.44        | 1.34     |
| 1   | 7     | 1301 | 5CR  | CAL-N | 3.23 | 1.44        | 1.34     |
| 1   | 3     | 301  | 5CR  | CAL-N | 3.23 | 1.44        | 1.34     |
| 1   | OA    | 301  | 5CR  | CAL-N | 3.23 | 1.44        | 1.34     |
| 1   | LA    | 1301 | 5CR  | CAL-N | 3.22 | 1.44        | 1.34     |
| 1   | HA    | 301  | 5CR  | CAL-N | 3.20 | 1.44        | 1.34     |
| 1   | KA    | 1208 | GMA  | CD-N2 | 2.34 | 1.38        | 1.32     |
| 1   | 9     | 208  | GMA  | CD-N2 | 2.34 | 1.38        | 1.32     |
| 1   | DA    | 1208 | GMA  | CD-N2 | 2.32 | 1.38        | 1.32     |
| 1   | l     | 1208 | GMA  | CD-N2 | 2.32 | 1.38        | 1.32     |
| 1   | Y     | 208  | GMA  | CD-N2 | 2.32 | 1.38        | 1.32     |
| 1   | NA    | 208  | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | m     | 1308 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | Z     | 308  | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | W     | 1308 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | 6     | 1208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | z     | 1208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | s     | 1208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | V     | 1208 | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | S     | 308  | GMA  | CD-N2 | 2.31 | 1.38        | 1.32     |
| 1   | GA    | 208  | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | e     | 8    | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | RA    | 1208 | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | 5A    | 1008 | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | iA    | 208  | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | 2     | 208  | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | R     | 208  | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | AA    | 308  | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | OA    | 308  | GMA  | CD-N2 | 2.30 | 1.38        | 1.32     |
| 1   | mA    | 1208 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | f     | 8    | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | i     | 8    | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | YA    | 1208 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | yA    | 1008 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | SA    | 1308 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | o     | 208  | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | 7     | 1308 | GMA  | CD-N2 | 2.29 | 1.38        | 1.32     |
| 1   | v     | 208  | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | t     | 1308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | TB    | 1308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | EA    | 1308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | OB    | 208  | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | UA    | 208  | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | wA    | 208  | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | AB    | 208  | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | ZA    | 1308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | jA    | 308  | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | 0A    | 1208 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | FB    | 1308 | GMA  | CD-N2 | 2.28 | 1.38        | 1.32     |
| 1   | HB    | 208  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | nA    | 1308 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | BB    | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | IB    | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | L     | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | VA    | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | xA    | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | w     | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | O     | 1208 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | HA    | 308  | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | LA    | 1308 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | LB    | 1208 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | a     | 8    | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | MB    | 1308 | GMA  | CD-N2 | 2.27 | 1.38        | 1.32     |
| 1   | 3A    | 208  | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | cA    | 308  | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | EB    | 1208 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | kA    | 1008 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | p     | 308  | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | WA    | 1008 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | QB    | 1008 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | gA    | 1308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | P     | 1308 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |
| 1   | 7A    | 1208 | GMA  | CD-N2 | 2.26 | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | 0     | 1308 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | h     | 8    | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | JB    | 1008 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | g     | 8    | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | SB    | 1208 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | PA    | 1008 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | PB    | 308  | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | 3     | 308  | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | 1A    | 1308 | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | K     | 208  | GMA  | CD-N2 | 2.25 | 1.38        | 1.32     |
| 1   | dA    | 1008 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | I     | 8    | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | qA    | 308  | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | CB    | 1008 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | d     | 8    | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | b     | 8    | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | rA    | 1008 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | 8A    | 1308 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | tA    | 1208 | GMA  | CD-N2 | 2.24 | 1.38        | 1.32     |
| 1   | pA    | 208  | GMA  | CD-N2 | 2.23 | 1.38        | 1.32     |
| 1   | uA    | 1308 | GMA  | CD-N2 | 2.23 | 1.38        | 1.32     |
| 1   | c     | 8    | GMA  | CD-N2 | 2.23 | 1.38        | 1.32     |
| 1   | zA    | 1108 | GMA  | CD-N2 | 2.22 | 1.38        | 1.32     |
| 1   | bA    | 208  | GMA  | CD-N2 | 2.22 | 1.38        | 1.32     |
| 1   | 4A    | 308  | GMA  | CD-N2 | 2.22 | 1.38        | 1.32     |
| 1   | fA    | 1208 | GMA  | CD-N2 | 2.22 | 1.38        | 1.32     |
| 1   | vA    | 108  | GMA  | CD-N2 | 2.21 | 1.38        | 1.32     |
| 1   | J     | 108  | GMA  | CD-N2 | 2.21 | 1.38        | 1.32     |
| 1   | 6A    | 1108 | GMA  | CD-N2 | 2.21 | 1.38        | 1.32     |
| 1   | T     | 1008 | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | 9A    | 108  | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | E     | 8    | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | DB    | 1108 | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | N     | 1108 | GMA  | CD-N2 | 2.20 | 1.38        | 1.32     |
| 1   | 2A    | 108  | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | QA    | 1108 | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | B     | 8    | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | r     | 1108 | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | aA    | 108  | GMA  | CD-N2 | 2.19 | 1.38        | 1.32     |
| 1   | n     | 108  | GMA  | CD-N2 | 2.18 | 1.38        | 1.32     |
| 1   | lA    | 1108 | GMA  | CD-N2 | 2.18 | 1.38        | 1.32     |
| 1   | 4     | 1008 | GMA  | CD-N2 | 2.18 | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | XA    | 1108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | eA    | 1108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | hA    | 108  | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | JA    | 1108 | GMA  | CD-N2   | 2.18  | 1.38        | 1.32     |
| 1   | MA    | 108  | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | oA    | 108  | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | FA    | 108  | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | C     | 8    | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | KB    | 1108 | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | sA    | 1108 | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | TA    | 108  | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | M     | 1008 | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | H     | 8    | GMA  | CD-N2   | 2.17  | 1.38        | 1.32     |
| 1   | x     | 1008 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | U     | 1108 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | 3     | 301  | 5CR  | OAB-CAL | -2.16 | 1.18        | 1.23     |
| 1   | Q     | 108  | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | 1     | 108  | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | 8     | 108  | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | j     | 1008 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | RB    | 1108 | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | GB    | 108  | GMA  | CD-N2   | 2.16  | 1.38        | 1.32     |
| 1   | F     | 8    | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | q     | 1008 | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | NB    | 108  | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | 5     | 1108 | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | CA    | 1108 | GMA  | CD-N2   | 2.15  | 1.38        | 1.32     |
| 1   | D     | 8    | GMA  | CD-N2   | 2.14  | 1.38        | 1.32     |
| 1   | IA    | 1008 | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | A     | 8    | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | u     | 108  | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | y     | 1108 | GMA  | CD-N2   | 2.14  | 1.37        | 1.32     |
| 1   | k     | 1108 | GMA  | CD-N2   | 2.13  | 1.37        | 1.32     |
| 1   | 7     | 1301 | 5CR  | OAB-CAL | -2.13 | 1.18        | 1.23     |
| 1   | BA    | 1008 | GMA  | CD-N2   | 2.12  | 1.37        | 1.32     |
| 1   | G     | 8    | GMA  | CD-N2   | 2.12  | 1.37        | 1.32     |
| 1   | 0     | 1301 | 5CR  | OAB-CAL | -2.11 | 1.18        | 1.23     |
| 1   | Z     | 301  | 5CR  | OAB-CAL | -2.11 | 1.18        | 1.23     |
| 1   | OA    | 301  | 5CR  | OAB-CAL | -2.10 | 1.18        | 1.23     |
| 1   | X     | 108  | GMA  | CD-N2   | 2.10  | 1.37        | 1.32     |
| 1   | m     | 1301 | 5CR  | OAB-CAL | -2.09 | 1.18        | 1.23     |
| 1   | SA    | 1301 | 5CR  | OAB-CAL | -2.09 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | g     | 1    | 5CR  | OAB-CAL | -2.09 | 1.18        | 1.23     |
| 1   | t     | 1301 | 5CR  | OAB-CAL | -2.08 | 1.18        | 1.23     |
| 1   | p     | 301  | 5CR  | OAB-CAL | -2.08 | 1.18        | 1.23     |
| 1   | P     | 1301 | 5CR  | OAB-CAL | -2.08 | 1.18        | 1.23     |
| 1   | e     | 1    | 5CR  | OAB-CAL | -2.07 | 1.18        | 1.23     |
| 1   | w     | 301  | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | LA    | 1301 | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | HA    | 301  | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | CB    | 1001 | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | AA    | 301  | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | EA    | 1301 | 5CR  | OAB-CAL | -2.06 | 1.18        | 1.23     |
| 1   | T     | 1001 | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | 2     | 201  | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | Y     | 201  | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | W     | 1301 | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | b     | 1    | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | yA    | 1001 | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | 5A    | 1001 | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | L     | 301  | 5CR  | OAB-CAL | -2.05 | 1.18        | 1.23     |
| 1   | WA    | 1001 | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | dA    | 1001 | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | PA    | 1001 | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | B     | 1    | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | C     | 1    | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | i     | 1    | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | H     | 1    | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | a     | 1    | 5CR  | OAB-CAL | -2.04 | 1.18        | 1.23     |
| 1   | S     | 301  | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | q     | 1001 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | l     | 1201 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | R     | 201  | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | 6     | 1201 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | D     | 1    | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | f     | 1    | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | j     | 1001 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | IA    | 1001 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | rA    | 1001 | 5CR  | OAB-CAL | -2.03 | 1.18        | 1.23     |
| 1   | x     | 1001 | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | E     | 1    | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | c     | 1    | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | kA    | 1001 | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | h     | 1    | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | iA    | 201  | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | 9     | 201  | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | d     | 1    | 5CR  | OAB-CAL | -2.02 | 1.18        | 1.23     |
| 1   | QB    | 1001 | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | V     | 1201 | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | qA    | 301  | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | I     | 1    | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | JB    | 1001 | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | s     | 1201 | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | AB    | 201  | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | pA    | 201  | 5CR  | OAB-CAL | -2.01 | 1.18        | 1.23     |
| 1   | 4     | 1001 | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |
| 1   | fA    | 1201 | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |
| 1   | o     | 201  | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |
| 1   | z     | 1201 | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |
| 1   | 3A    | 201  | 5CR  | OAB-CAL | -2.00 | 1.18        | 1.23     |

All (304) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | b     | 1    | 5CR  | CAA-CAL-N | 5.24  | 124.81      | 116.12   |
| 1   | f     | 1    | 5CR  | CAA-CAL-N | 5.24  | 124.80      | 116.12   |
| 1   | 5A    | 1001 | 5CR  | CAA-CAL-N | 5.23  | 124.79      | 116.12   |
| 1   | a     | 1    | 5CR  | CAA-CAL-N | 5.23  | 124.79      | 116.12   |
| 1   | WA    | 1001 | 5CR  | CAA-CAL-N | 5.23  | 124.79      | 116.12   |
| 1   | QB    | 1001 | 5CR  | CAA-CAL-N | 5.23  | 124.79      | 116.12   |
| 1   | dA    | 1001 | 5CR  | CAA-CAL-N | 5.22  | 124.78      | 116.12   |
| 1   | CB    | 1001 | 5CR  | CAA-CAL-N | 5.22  | 124.78      | 116.12   |
| 1   | g     | 1    | 5CR  | CAA-CAL-N | 5.22  | 124.77      | 116.12   |
| 1   | JB    | 1001 | 5CR  | CAA-CAL-N | 5.22  | 124.77      | 116.12   |
| 1   | rA    | 1001 | 5CR  | CAA-CAL-N | 5.21  | 124.76      | 116.12   |
| 1   | kA    | 1001 | 5CR  | CAA-CAL-N | 5.21  | 124.75      | 116.12   |
| 1   | d     | 1    | 5CR  | CAA-CAL-N | 5.20  | 124.75      | 116.12   |
| 1   | yA    | 1001 | 5CR  | CAA-CAL-N | 5.19  | 124.73      | 116.12   |
| 1   | i     | 1    | 5CR  | CAA-CAL-N | 5.19  | 124.73      | 116.12   |
| 1   | h     | 1    | 5CR  | CAA-CAL-N | 5.19  | 124.72      | 116.12   |
| 1   | c     | 1    | 5CR  | CAA-CAL-N | 5.18  | 124.70      | 116.12   |
| 1   | e     | 1    | 5CR  | CAA-CAL-N | 5.17  | 124.70      | 116.12   |
| 1   | BA    | 1001 | 5CR  | CG-CB-CA  | -4.72 | 106.79      | 113.51   |
| 1   | I     | 1    | 5CR  | CG-CB-CA  | -4.71 | 106.80      | 113.51   |
| 1   | A     | 1    | 5CR  | CG-CB-CA  | -4.71 | 106.80      | 113.51   |
| 1   | M     | 1001 | 5CR  | CG-CB-CA  | -4.71 | 106.81      | 113.51   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | G     | 1    | 5CR  | CG-CB-CA  | -4.71 | 106.81      | 113.51   |
| 1   | PA    | 1001 | 5CR  | CG-CB-CA  | -4.70 | 106.82      | 113.51   |
| 1   | T     | 1001 | 5CR  | CG-CB-CA  | -4.69 | 106.83      | 113.51   |
| 1   | D     | 1    | 5CR  | CG-CB-CA  | -4.69 | 106.83      | 113.51   |
| 1   | B     | 1    | 5CR  | CG-CB-CA  | -4.69 | 106.84      | 113.51   |
| 1   | q     | 1001 | 5CR  | CG-CB-CA  | -4.69 | 106.84      | 113.51   |
| 1   | H     | 1    | 5CR  | CG-CB-CA  | -4.67 | 106.86      | 113.51   |
| 1   | x     | 1001 | 5CR  | CG-CB-CA  | -4.67 | 106.86      | 113.51   |
| 1   | E     | 1    | 5CR  | CG-CB-CA  | -4.67 | 106.86      | 113.51   |
| 1   | j     | 1001 | 5CR  | CG-CB-CA  | -4.66 | 106.88      | 113.51   |
| 1   | C     | 1    | 5CR  | CG-CB-CA  | -4.66 | 106.88      | 113.51   |
| 1   | IA    | 1001 | 5CR  | CG-CB-CA  | -4.66 | 106.88      | 113.51   |
| 1   | 4     | 1001 | 5CR  | CG-CB-CA  | -4.66 | 106.88      | 113.51   |
| 1   | F     | 1    | 5CR  | CG-CB-CA  | -4.64 | 106.91      | 113.51   |
| 1   | U     | 1101 | 5CR  | CG-CB-CA  | -4.48 | 107.14      | 113.51   |
| 1   | QA    | 1101 | 5CR  | CG-CB-CA  | -4.47 | 107.16      | 113.51   |
| 1   | n     | 101  | 5CR  | CG-CB-CA  | -4.46 | 107.16      | 113.51   |
| 1   | u     | 101  | 5CR  | CG-CB-CA  | -4.46 | 107.17      | 113.51   |
| 1   | Q     | 101  | 5CR  | CG-CB-CA  | -4.45 | 107.17      | 113.51   |
| 1   | CA    | 1101 | 5CR  | CG-CB-CA  | -4.45 | 107.17      | 113.51   |
| 1   | MA    | 101  | 5CR  | CG-CB-CA  | -4.45 | 107.18      | 113.51   |
| 1   | y     | 1101 | 5CR  | CG-CB-CA  | -4.45 | 107.18      | 113.51   |
| 1   | 5     | 1101 | 5CR  | CG-CB-CA  | -4.45 | 107.18      | 113.51   |
| 1   | 8     | 101  | 5CR  | CG-CB-CA  | -4.44 | 107.19      | 113.51   |
| 1   | k     | 1101 | 5CR  | CG-CB-CA  | -4.43 | 107.20      | 113.51   |
| 1   | N     | 1101 | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | l     | 101  | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | FA    | 101  | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | r     | 1101 | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | J     | 101  | 5CR  | CG-CB-CA  | -4.43 | 107.21      | 113.51   |
| 1   | JA    | 1101 | 5CR  | CG-CB-CA  | -4.42 | 107.22      | 113.51   |
| 1   | X     | 101  | 5CR  | CG-CB-CA  | -4.41 | 107.24      | 113.51   |
| 1   | V     | 1201 | 5CR  | CAA-CAL-N | 3.00  | 121.09      | 116.12   |
| 1   | 9     | 201  | 5CR  | CAA-CAL-N | 3.00  | 121.09      | 116.12   |
| 1   | R     | 201  | 5CR  | CAA-CAL-N | 3.00  | 121.09      | 116.12   |
| 1   | NA    | 201  | 5CR  | CAA-CAL-N | 3.00  | 121.09      | 116.12   |
| 1   | Y     | 201  | 5CR  | CAA-CAL-N | 3.00  | 121.09      | 116.12   |
| 1   | DA    | 1201 | 5CR  | CAA-CAL-N | 3.00  | 121.08      | 116.12   |
| 1   | RA    | 1201 | 5CR  | CAA-CAL-N | 2.99  | 121.08      | 116.12   |
| 1   | s     | 1201 | 5CR  | CAA-CAL-N | 2.98  | 121.07      | 116.12   |
| 1   | l     | 1201 | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |
| 1   | o     | 201  | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | KA    | 1201 | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |
| 1   | v     | 201  | 5CR  | CAA-CAL-N | 2.98  | 121.06      | 116.12   |
| 1   | GA    | 201  | 5CR  | CAA-CAL-N | 2.97  | 121.05      | 116.12   |
| 1   | O     | 1201 | 5CR  | CAA-CAL-N | 2.97  | 121.04      | 116.12   |
| 1   | z     | 1201 | 5CR  | CAA-CAL-N | 2.97  | 121.04      | 116.12   |
| 1   | 6     | 1201 | 5CR  | CAA-CAL-N | 2.96  | 121.03      | 116.12   |
| 1   | K     | 201  | 5CR  | CAA-CAL-N | 2.95  | 121.01      | 116.12   |
| 1   | 2     | 201  | 5CR  | CAA-CAL-N | 2.93  | 120.98      | 116.12   |
| 1   | UA    | 201  | 5CR  | CG-CB-CA  | -2.88 | 109.41      | 113.51   |
| 1   | 0A    | 1201 | 5CR  | CG-CB-CA  | -2.87 | 109.42      | 113.51   |
| 1   | iA    | 201  | 5CR  | CG-CB-CA  | -2.87 | 109.43      | 113.51   |
| 1   | YA    | 1201 | 5CR  | CG-CB-CA  | -2.87 | 109.43      | 113.51   |
| 1   | wA    | 201  | 5CR  | CG-CB-CA  | -2.87 | 109.43      | 113.51   |
| 1   | mA    | 1201 | 5CR  | CG-CB-CA  | -2.86 | 109.44      | 113.51   |
| 1   | AB    | 201  | 5CR  | CG-CB-CA  | -2.86 | 109.44      | 113.51   |
| 1   | bA    | 201  | 5CR  | CG-CB-CA  | -2.85 | 109.45      | 113.51   |
| 1   | OB    | 201  | 5CR  | CG-CB-CA  | -2.85 | 109.45      | 113.51   |
| 1   | SB    | 1201 | 5CR  | CG-CB-CA  | -2.85 | 109.46      | 113.51   |
| 1   | fA    | 1201 | 5CR  | CG-CB-CA  | -2.84 | 109.47      | 113.51   |
| 1   | LB    | 1201 | 5CR  | CG-CB-CA  | -2.84 | 109.48      | 113.51   |
| 1   | EB    | 1201 | 5CR  | CG-CB-CA  | -2.84 | 109.48      | 113.51   |
| 1   | pA    | 201  | 5CR  | CG-CB-CA  | -2.82 | 109.49      | 113.51   |
| 1   | 3A    | 201  | 5CR  | CG-CB-CA  | -2.82 | 109.50      | 113.51   |
| 1   | 7A    | 1201 | 5CR  | CG-CB-CA  | -2.82 | 109.50      | 113.51   |
| 1   | tA    | 1201 | 5CR  | CG-CB-CA  | -2.82 | 109.50      | 113.51   |
| 1   | HB    | 201  | 5CR  | CG-CB-CA  | -2.82 | 109.50      | 113.51   |
| 1   | F     | 1    | 5CR  | CAA-CAL-N | 2.70  | 120.60      | 116.12   |
| 1   | I     | 1    | 5CR  | CAA-CAL-N | 2.69  | 120.58      | 116.12   |
| 1   | 4     | 1001 | 5CR  | CAA-CAL-N | 2.69  | 120.57      | 116.12   |
| 1   | G     | 1    | 5CR  | CAA-CAL-N | 2.68  | 120.57      | 116.12   |
| 1   | B     | 1    | 5CR  | CAA-CAL-N | 2.67  | 120.55      | 116.12   |
| 1   | M     | 1001 | 5CR  | CAA-CAL-N | 2.67  | 120.55      | 116.12   |
| 1   | T     | 1001 | 5CR  | CAA-CAL-N | 2.67  | 120.54      | 116.12   |
| 1   | E     | 1    | 5CR  | CAA-CAL-N | 2.67  | 120.54      | 116.12   |
| 1   | A     | 1    | 5CR  | CAA-CAL-N | 2.67  | 120.54      | 116.12   |
| 1   | PA    | 1001 | 5CR  | CAA-CAL-N | 2.67  | 120.54      | 116.12   |
| 1   | j     | 1001 | 5CR  | CAA-CAL-N | 2.66  | 120.52      | 116.12   |
| 1   | x     | 1001 | 5CR  | CAA-CAL-N | 2.66  | 120.52      | 116.12   |
| 1   | BA    | 1001 | 5CR  | CAA-CAL-N | 2.66  | 120.52      | 116.12   |
| 1   | C     | 1    | 5CR  | CAA-CAL-N | 2.65  | 120.51      | 116.12   |
| 1   | D     | 1    | 5CR  | CAA-CAL-N | 2.64  | 120.49      | 116.12   |
| 1   | IA    | 1001 | 5CR  | CAA-CAL-N | 2.64  | 120.49      | 116.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | q     | 1001 | 5CR  | CAA-CAL-N   | 2.63  | 120.48      | 116.12   |
| 1   | H     | 1    | 5CR  | CAA-CAL-N   | 2.60  | 120.44      | 116.12   |
| 1   | vA    | 101  | 5CR  | CAA-CAL-N   | 2.57  | 120.38      | 116.12   |
| 1   | XA    | 1101 | 5CR  | CAA-CAL-N   | 2.57  | 120.37      | 116.12   |
| 1   | lA    | 1101 | 5CR  | CAA-CAL-N   | 2.56  | 120.37      | 116.12   |
| 1   | NB    | 101  | 5CR  | CAA-CAL-N   | 2.56  | 120.36      | 116.12   |
| 1   | RB    | 1101 | 5CR  | CAA-CAL-N   | 2.56  | 120.36      | 116.12   |
| 1   | zA    | 1101 | 5CR  | CAA-CAL-N   | 2.55  | 120.35      | 116.12   |
| 1   | WA    | 1001 | 5CR  | OAB-CAL-N   | -2.55 | 117.48      | 121.98   |
| 1   | oA    | 101  | 5CR  | CAA-CAL-N   | 2.55  | 120.34      | 116.12   |
| 1   | hA    | 101  | 5CR  | CAA-CAL-N   | 2.54  | 120.34      | 116.12   |
| 1   | a     | 1    | 5CR  | OAB-CAL-N   | -2.54 | 117.49      | 121.98   |
| 1   | rA    | 1001 | 5CR  | OAB-CAL-N   | -2.54 | 117.49      | 121.98   |
| 1   | TA    | 101  | 5CR  | CAA-CAL-N   | 2.54  | 120.33      | 116.12   |
| 1   | sA    | 1101 | 5CR  | CAA-CAL-N   | 2.54  | 120.33      | 116.12   |
| 1   | eA    | 1101 | 5CR  | CAA-CAL-N   | 2.54  | 120.32      | 116.12   |
| 1   | 9A    | 101  | 5CR  | CAA-CAL-N   | 2.53  | 120.32      | 116.12   |
| 1   | aA    | 101  | 5CR  | CAA-CAL-N   | 2.53  | 120.32      | 116.12   |
| 1   | DB    | 1101 | 5CR  | CAA-CAL-N   | 2.53  | 120.32      | 116.12   |
| 1   | 6A    | 1101 | 5CR  | CAA-CAL-N   | 2.53  | 120.31      | 116.12   |
| 1   | d     | 1    | 5CR  | OAB-CAL-N   | -2.53 | 117.51      | 121.98   |
| 1   | 2A    | 101  | 5CR  | CAA-CAL-N   | 2.53  | 120.31      | 116.12   |
| 1   | QB    | 1001 | 5CR  | OAB-CAL-N   | -2.51 | 117.54      | 121.98   |
| 1   | e     | 1    | 5CR  | OAB-CAL-N   | -2.51 | 117.55      | 121.98   |
| 1   | yA    | 1001 | 5CR  | OAB-CAL-N   | -2.51 | 117.55      | 121.98   |
| 1   | GB    | 101  | 5CR  | CAA-CAL-N   | 2.50  | 120.27      | 116.12   |
| 1   | 5A    | 1001 | 5CR  | OAB-CAL-N   | -2.50 | 117.56      | 121.98   |
| 1   | b     | 1    | 5CR  | OAB-CAL-CAA | -2.50 | 117.60      | 122.05   |
| 1   | i     | 1    | 5CR  | OAB-CAL-N   | -2.50 | 117.57      | 121.98   |
| 1   | f     | 1    | 5CR  | OAB-CAL-N   | -2.49 | 117.57      | 121.98   |
| 1   | KB    | 1101 | 5CR  | CAA-CAL-N   | 2.49  | 120.25      | 116.12   |
| 1   | dA    | 1001 | 5CR  | OAB-CAL-CAA | -2.49 | 117.62      | 122.05   |
| 1   | JB    | 1001 | 5CR  | OAB-CAL-N   | -2.49 | 117.58      | 121.98   |
| 1   | g     | 1    | 5CR  | OAB-CAL-N   | -2.49 | 117.58      | 121.98   |
| 1   | CB    | 1001 | 5CR  | OAB-CAL-CAA | -2.49 | 117.62      | 122.05   |
| 1   | b     | 1    | 5CR  | OAB-CAL-N   | -2.49 | 117.58      | 121.98   |
| 1   | f     | 1    | 5CR  | OAB-CAL-CAA | -2.49 | 117.63      | 122.05   |
| 1   | h     | 1    | 5CR  | OAB-CAL-N   | -2.49 | 117.59      | 121.98   |
| 1   | kA    | 1001 | 5CR  | OAB-CAL-CAA | -2.48 | 117.64      | 122.05   |
| 1   | CB    | 1001 | 5CR  | OAB-CAL-N   | -2.48 | 117.60      | 121.98   |
| 1   | g     | 1    | 5CR  | OAB-CAL-CAA | -2.48 | 117.64      | 122.05   |
| 1   | dA    | 1001 | 5CR  | OAB-CAL-N   | -2.48 | 117.60      | 121.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | c     | 1    | 5CR  | OAB-CAL-CAA | -2.48 | 117.64      | 122.05   |
| 1   | JB    | 1001 | 5CR  | OAB-CAL-CAA | -2.48 | 117.64      | 122.05   |
| 1   | 5A    | 1001 | 5CR  | OAB-CAL-CAA | -2.48 | 117.65      | 122.05   |
| 1   | kA    | 1001 | 5CR  | OAB-CAL-N   | -2.47 | 117.61      | 121.98   |
| 1   | QB    | 1001 | 5CR  | OAB-CAL-CAA | -2.46 | 117.67      | 122.05   |
| 1   | c     | 1    | 5CR  | OAB-CAL-N   | -2.45 | 117.65      | 121.98   |
| 1   | h     | 1    | 5CR  | OAB-CAL-CAA | -2.45 | 117.69      | 122.05   |
| 1   | i     | 1    | 5CR  | OAB-CAL-CAA | -2.45 | 117.70      | 122.05   |
| 1   | yA    | 1001 | 5CR  | OAB-CAL-CAA | -2.44 | 117.72      | 122.05   |
| 1   | a     | 1    | 5CR  | OAB-CAL-CAA | -2.43 | 117.72      | 122.05   |
| 1   | WA    | 1001 | 5CR  | OAB-CAL-CAA | -2.43 | 117.73      | 122.05   |
| 1   | d     | 1    | 5CR  | OAB-CAL-CAA | -2.42 | 117.75      | 122.05   |
| 1   | rA    | 1001 | 5CR  | OAB-CAL-CAA | -2.42 | 117.75      | 122.05   |
| 1   | e     | 1    | 5CR  | OAB-CAL-CAA | -2.42 | 117.75      | 122.05   |
| 1   | o     | 201  | 5CR  | CG-CB-CA    | -2.35 | 110.17      | 113.51   |
| 1   | s     | 1201 | 5CR  | CG-CB-CA    | -2.35 | 110.17      | 113.51   |
| 1   | 2     | 201  | 5CR  | CG-CB-CA    | -2.32 | 110.21      | 113.51   |
| 1   | 6     | 1201 | 5CR  | CG-CB-CA    | -2.30 | 110.24      | 113.51   |
| 1   | V     | 1201 | 5CR  | CG-CB-CA    | -2.30 | 110.24      | 113.51   |
| 1   | R     | 201  | 5CR  | CG-CB-CA    | -2.30 | 110.25      | 113.51   |
| 1   | l     | 1201 | 5CR  | CG-CB-CA    | -2.29 | 110.25      | 113.51   |
| 1   | Y     | 201  | 5CR  | CG-CB-CA    | -2.29 | 110.25      | 113.51   |
| 1   | 7     | 1301 | 5CR  | CAA-CAL-N   | 2.29  | 119.91      | 116.12   |
| 1   | BB    | 301  | 5CR  | CAA-CAL-N   | 2.29  | 119.91      | 116.12   |
| 1   | z     | 1201 | 5CR  | CG-CB-CA    | -2.29 | 110.26      | 113.51   |
| 1   | xA    | 301  | 5CR  | CAA-CAL-N   | 2.28  | 119.90      | 116.12   |
| 1   | O     | 1201 | 5CR  | CG-CB-CA    | -2.28 | 110.27      | 113.51   |
| 1   | RA    | 1201 | 5CR  | CG-CB-CA    | -2.28 | 110.27      | 113.51   |
| 1   | v     | 201  | 5CR  | CG-CB-CA    | -2.28 | 110.27      | 113.51   |
| 1   | GA    | 201  | 5CR  | CG-CB-CA    | -2.28 | 110.27      | 113.51   |
| 1   | L     | 301  | 5CR  | CAA-CAL-N   | 2.28  | 119.89      | 116.12   |
| 1   | S     | 301  | 5CR  | CAA-CAL-N   | 2.27  | 119.89      | 116.12   |
| 1   | 3     | 301  | 5CR  | CAA-CAL-N   | 2.27  | 119.89      | 116.12   |
| 1   | FB    | 1301 | 5CR  | CAA-CAL-N   | 2.27  | 119.89      | 116.12   |
| 1   | w     | 301  | 5CR  | CAA-CAL-N   | 2.27  | 119.89      | 116.12   |
| 1   | PB    | 301  | 5CR  | CAA-CAL-N   | 2.27  | 119.89      | 116.12   |
| 1   | K     | 201  | 5CR  | CG-CB-CA    | -2.27 | 110.28      | 113.51   |
| 1   | W     | 1301 | 5CR  | CAA-CAL-N   | 2.27  | 119.88      | 116.12   |
| 1   | MB    | 1301 | 5CR  | CAA-CAL-N   | 2.27  | 119.88      | 116.12   |
| 1   | TB    | 1301 | 5CR  | CAA-CAL-N   | 2.27  | 119.88      | 116.12   |
| 1   | LA    | 1301 | 5CR  | CAA-CAL-N   | 2.27  | 119.88      | 116.12   |
| 1   | NA    | 201  | 5CR  | CG-CB-CA    | -2.26 | 110.29      | 113.51   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | HA    | 301  | 5CR  | CAA-CAL-N | 2.26  | 119.87      | 116.12   |
| 1   | gA    | 1301 | 5CR  | CAA-CAL-N | 2.26  | 119.87      | 116.12   |
| 1   | IB    | 301  | 5CR  | CAA-CAL-N | 2.26  | 119.86      | 116.12   |
| 1   | KA    | 1201 | 5CR  | CG-CB-CA  | -2.26 | 110.30      | 113.51   |
| 1   | EA    | 1301 | 5CR  | CAA-CAL-N | 2.26  | 119.86      | 116.12   |
| 1   | 1A    | 1301 | 5CR  | CAA-CAL-N | 2.26  | 119.86      | 116.12   |
| 1   | m     | 1301 | 5CR  | CAA-CAL-N | 2.25  | 119.86      | 116.12   |
| 1   | P     | 1301 | 5CR  | CAA-CAL-N | 2.25  | 119.85      | 116.12   |
| 1   | DA    | 1201 | 5CR  | CG-CB-CA  | -2.25 | 110.31      | 113.51   |
| 1   | 7     | 1301 | 5CR  | O-C-CA    | -2.25 | 118.98      | 124.77   |
| 1   | AA    | 301  | 5CR  | CAA-CAL-N | 2.25  | 119.85      | 116.12   |
| 1   | Z     | 301  | 5CR  | O-C-CA    | -2.25 | 118.99      | 124.77   |
| 1   | 9     | 201  | 5CR  | CG-CB-CA  | -2.25 | 110.31      | 113.51   |
| 1   | 0     | 1301 | 5CR  | O-C-CA    | -2.25 | 118.99      | 124.77   |
| 1   | nA    | 1301 | 5CR  | CAA-CAL-N | 2.25  | 119.84      | 116.12   |
| 1   | w     | 301  | 5CR  | O-C-CA    | -2.24 | 119.00      | 124.77   |
| 1   | p     | 301  | 5CR  | O-C-CA    | -2.24 | 119.00      | 124.77   |
| 1   | cA    | 301  | 5CR  | CAA-CAL-N | 2.24  | 119.84      | 116.12   |
| 1   | OA    | 301  | 5CR  | CAA-CAL-N | 2.24  | 119.84      | 116.12   |
| 1   | SA    | 1301 | 5CR  | CAA-CAL-N | 2.24  | 119.83      | 116.12   |
| 1   | t     | 1301 | 5CR  | O-C-CA    | -2.24 | 119.01      | 124.77   |
| 1   | 0     | 1301 | 5CR  | CAA-CAL-N | 2.24  | 119.83      | 116.12   |
| 1   | uA    | 1301 | 5CR  | CAA-CAL-N | 2.24  | 119.83      | 116.12   |
| 1   | Z     | 301  | 5CR  | CAA-CAL-N | 2.24  | 119.83      | 116.12   |
| 1   | m     | 1301 | 5CR  | O-C-CA    | -2.24 | 119.01      | 124.77   |
| 1   | 3     | 301  | 5CR  | O-C-CA    | -2.24 | 119.01      | 124.77   |
| 1   | jA    | 301  | 5CR  | CAA-CAL-N | 2.24  | 119.83      | 116.12   |
| 1   | t     | 1301 | 5CR  | CAA-CAL-N | 2.23  | 119.82      | 116.12   |
| 1   | ZA    | 1301 | 5CR  | CAA-CAL-N | 2.23  | 119.82      | 116.12   |
| 1   | OA    | 301  | 5CR  | O-C-CA    | -2.23 | 119.03      | 124.77   |
| 1   | HA    | 301  | 5CR  | O-C-CA    | -2.23 | 119.04      | 124.77   |
| 1   | 8A    | 1301 | 5CR  | CAA-CAL-N | 2.23  | 119.81      | 116.12   |
| 1   | p     | 301  | 5CR  | CAA-CAL-N | 2.23  | 119.81      | 116.12   |
| 1   | SA    | 1301 | 5CR  | O-C-CA    | -2.23 | 119.05      | 124.77   |
| 1   | EA    | 1301 | 5CR  | O-C-CA    | -2.23 | 119.05      | 124.77   |
| 1   | LA    | 1301 | 5CR  | O-C-CA    | -2.22 | 119.05      | 124.77   |
| 1   | AA    | 301  | 5CR  | O-C-CA    | -2.22 | 119.05      | 124.77   |
| 1   | 4A    | 301  | 5CR  | CAA-CAL-N | 2.22  | 119.80      | 116.12   |
| 1   | VA    | 301  | 5CR  | CAA-CAL-N | 2.22  | 119.79      | 116.12   |
| 1   | qA    | 301  | 5CR  | CAA-CAL-N | 2.21  | 119.79      | 116.12   |
| 1   | P     | 1301 | 5CR  | O-C-CA    | -2.20 | 119.11      | 124.77   |
| 1   | S     | 301  | 5CR  | O-C-CA    | -2.20 | 119.11      | 124.77   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | W     | 1301 | 5CR  | O-C-CA    | -2.20 | 119.12      | 124.77   |
| 1   | L     | 301  | 5CR  | O-C-CA    | -2.18 | 119.17      | 124.77   |
| 1   | J     | 101  | 5CR  | CAA-CAL-N | 2.17  | 119.72      | 116.12   |
| 1   | k     | 1101 | 5CR  | CAA-CAL-N | 2.16  | 119.69      | 116.12   |
| 1   | N     | 1101 | 5CR  | CAA-CAL-N | 2.15  | 119.69      | 116.12   |
| 1   | X     | 101  | 5CR  | CAA-CAL-N | 2.15  | 119.68      | 116.12   |
| 1   | r     | 1101 | 5CR  | CAA-CAL-N | 2.14  | 119.67      | 116.12   |
| 1   | Q     | 101  | 5CR  | CAA-CAL-N | 2.14  | 119.67      | 116.12   |
| 1   | y     | 1101 | 5CR  | CAA-CAL-N | 2.13  | 119.66      | 116.12   |
| 1   | FA    | 101  | 5CR  | CAA-CAL-N | 2.13  | 119.64      | 116.12   |
| 1   | U     | 1101 | 5CR  | CAA-CAL-N | 2.12  | 119.64      | 116.12   |
| 1   | n     | 101  | 5CR  | CAA-CAL-N | 2.12  | 119.64      | 116.12   |
| 1   | u     | 101  | 5CR  | CAA-CAL-N | 2.12  | 119.64      | 116.12   |
| 1   | CA    | 1101 | 5CR  | CAA-CAL-N | 2.12  | 119.63      | 116.12   |
| 1   | JA    | 1101 | 5CR  | CAA-CAL-N | 2.11  | 119.62      | 116.12   |
| 1   | 5     | 1101 | 5CR  | CAA-CAL-N | 2.11  | 119.62      | 116.12   |
| 1   | 8     | 101  | 5CR  | CAA-CAL-N | 2.11  | 119.62      | 116.12   |
| 1   | MA    | 101  | 5CR  | CAA-CAL-N | 2.11  | 119.61      | 116.12   |
| 1   | QA    | 1101 | 5CR  | CAA-CAL-N | 2.10  | 119.59      | 116.12   |
| 1   | 1     | 101  | 5CR  | CAA-CAL-N | 2.09  | 119.58      | 116.12   |
| 1   | KA    | 1208 | GMA  | O1-CD-CA  | 2.08  | 123.35      | 120.25   |
| 1   | 9     | 208  | GMA  | O1-CD-CA  | 2.08  | 123.35      | 120.25   |
| 1   | GA    | 208  | GMA  | O1-CD-CA  | 2.07  | 123.33      | 120.25   |
| 1   | DA    | 1208 | GMA  | O1-CD-CA  | 2.06  | 123.32      | 120.25   |
| 1   | NA    | 208  | GMA  | O1-CD-CA  | 2.05  | 123.31      | 120.25   |
| 1   | GA    | 201  | 5CR  | O-C-CA    | -2.05 | 119.50      | 124.77   |
| 1   | R     | 208  | GMA  | O1-CD-CA  | 2.05  | 123.30      | 120.25   |
| 1   | RA    | 1208 | GMA  | O1-CD-CA  | 2.05  | 123.30      | 120.25   |
| 1   | NA    | 208  | GMA  | O1-CD-N2  | -2.05 | 119.43      | 123.04   |
| 1   | KA    | 1201 | 5CR  | O-C-CA    | -2.04 | 119.53      | 124.77   |
| 1   | s     | 1208 | GMA  | O1-CD-CA  | 2.04  | 123.28      | 120.25   |
| 1   | s     | 1201 | 5CR  | O-C-CA    | -2.03 | 119.54      | 124.77   |
| 1   | l     | 1208 | GMA  | O1-CD-CA  | 2.03  | 123.28      | 120.25   |
| 1   | RA    | 1208 | GMA  | O1-CD-N2  | -2.03 | 119.46      | 123.04   |
| 1   | o     | 201  | 5CR  | O-C-CA    | -2.03 | 119.55      | 124.77   |
| 1   | n     | 108  | GMA  | O1-CD-CA  | 2.03  | 123.27      | 120.25   |
| 1   | 2     | 201  | 5CR  | O-C-CA    | -2.03 | 119.56      | 124.77   |
| 1   | Y     | 208  | GMA  | O1-CD-N2  | -2.03 | 119.46      | 123.04   |
| 1   | 9     | 208  | GMA  | O1-CD-N2  | -2.03 | 119.47      | 123.04   |
| 1   | JA    | 1108 | GMA  | O1-CD-CA  | 2.02  | 123.26      | 120.25   |
| 1   | RA    | 1201 | 5CR  | O-C-CA    | -2.02 | 119.57      | 124.77   |
| 1   | 5     | 1108 | GMA  | O1-CD-CA  | 2.02  | 123.26      | 120.25   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | FA    | 108  | GMA  | O1-CD-CA | 2.02  | 123.26      | 120.25   |
| 1   | 6     | 1201 | 5CR  | O-C-CA   | -2.02 | 119.57      | 124.77   |
| 1   | U     | 1108 | GMA  | O1-CD-CA | 2.02  | 123.26      | 120.25   |
| 1   | NA    | 201  | 5CR  | O-C-CA   | -2.02 | 119.58      | 124.77   |
| 1   | Q     | 108  | GMA  | O1-CD-CA | 2.02  | 123.26      | 120.25   |
| 1   | r     | 1108 | GMA  | O1-CD-CA | 2.02  | 123.26      | 120.25   |
| 1   | 1     | 108  | GMA  | O1-CD-CA | 2.02  | 123.25      | 120.25   |
| 1   | 6     | 1208 | GMA  | O1-CD-CA | 2.02  | 123.25      | 120.25   |
| 1   | 4     | 1008 | GMA  | O1-CD-CA | 2.02  | 123.25      | 120.25   |
| 1   | V     | 1208 | GMA  | O1-CD-CA | 2.01  | 123.25      | 120.25   |
| 1   | DA    | 1208 | GMA  | O1-CD-N2 | -2.01 | 119.48      | 123.04   |
| 1   | DA    | 1201 | 5CR  | O-C-CA   | -2.01 | 119.59      | 124.77   |
| 1   | N     | 1108 | GMA  | O1-CD-CA | 2.01  | 123.25      | 120.25   |
| 1   | z     | 1208 | GMA  | O1-CD-CA | 2.01  | 123.25      | 120.25   |
| 1   | QA    | 1108 | GMA  | O1-CD-CA | 2.01  | 123.25      | 120.25   |
| 1   | K     | 201  | 5CR  | O-C-CA   | -2.01 | 119.59      | 124.77   |
| 1   | l     | 1208 | GMA  | O1-CD-N2 | -2.01 | 119.49      | 123.04   |
| 1   | PA    | 1008 | GMA  | O1-CD-CA | 2.01  | 123.25      | 120.25   |
| 1   | Y     | 208  | GMA  | O1-CD-CA | 2.01  | 123.24      | 120.25   |
| 1   | O     | 1201 | 5CR  | O-C-CA   | -2.01 | 119.61      | 124.77   |
| 1   | 9     | 201  | 5CR  | O-C-CA   | -2.01 | 119.61      | 124.77   |
| 1   | GA    | 208  | GMA  | O1-CD-N2 | -2.01 | 119.50      | 123.04   |
| 1   | T     | 1008 | GMA  | O1-CD-CA | 2.00  | 123.24      | 120.25   |
| 1   | l     | 1201 | 5CR  | O-C-CA   | -2.00 | 119.61      | 124.77   |
| 1   | J     | 108  | GMA  | O1-CD-CA | 2.00  | 123.23      | 120.25   |
| 1   | 2     | 208  | GMA  | O1-CD-CA | 2.00  | 123.23      | 120.25   |
| 1   | I     | 8    | GMA  | O1-CD-CA | 2.00  | 123.23      | 120.25   |
| 1   | Y     | 201  | 5CR  | O-C-CA   | -2.00 | 119.62      | 124.77   |
| 1   | KA    | 1208 | GMA  | O1-CD-N2 | -2.00 | 119.51      | 123.04   |
| 1   | V     | 1201 | 5CR  | O-C-CA   | -2.00 | 119.62      | 124.77   |

There are no chirality outliers.

All (702) 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   | N     | 1101 | 5CR  | C-CA-N-CAL |
| 1   | N     | 1101 | 5CR  | N-CA-CB-CG |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | O     | 1201 | 5CR  | N-CA-CB-CG |
| 1   | P     | 1301 | 5CR  | N-CA-CB-CG |
| 1   | P     | 1301 | 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 |
| 1   | S     | 301  | 5CR  | N-CA-CB-CG |
| 1   | S     | 301  | 5CR  | C-CA-CB-CG |
| 1   | U     | 1101 | 5CR  | C-CA-N-CAL |
| 1   | U     | 1101 | 5CR  | N-CA-CB-CG |
| 1   | V     | 1201 | 5CR  | N-CA-CB-CG |
| 1   | W     | 1301 | 5CR  | N-CA-CB-CG |
| 1   | W     | 1301 | 5CR  | C-CA-CB-CG |
| 1   | X     | 101  | 5CR  | C-CA-N-CAL |
| 1   | X     | 101  | 5CR  | N-CA-CB-CG |
| 1   | Y     | 201  | 5CR  | N-CA-CB-CG |
| 1   | Z     | 301  | 5CR  | N-CA-CB-CG |
| 1   | Z     | 301  | 5CR  | C-CA-CB-CG |
| 1   | k     | 1101 | 5CR  | C-CA-N-CAL |
| 1   | k     | 1101 | 5CR  | N-CA-CB-CG |
| 1   | l     | 1201 | 5CR  | N-CA-CB-CG |
| 1   | m     | 1301 | 5CR  | N-CA-CB-CG |
| 1   | m     | 1301 | 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   | r     | 1101 | 5CR  | C-CA-N-CAL |
| 1   | r     | 1101 | 5CR  | N-CA-CB-CG |
| 1   | s     | 1201 | 5CR  | N-CA-CB-CG |
| 1   | t     | 1301 | 5CR  | N-CA-CB-CG |
| 1   | t     | 1301 | 5CR  | C-CA-CB-CG |
| 1   | u     | 101  | 5CR  | C-CA-N-CAL |
| 1   | u     | 101  | 5CR  | N-CA-CB-CG |
| 1   | v     | 201  | 5CR  | N-CA-CB-CG |
| 1   | w     | 301  | 5CR  | N-CA-CB-CG |
| 1   | w     | 301  | 5CR  | C-CA-CB-CG |
| 1   | y     | 1101 | 5CR  | C-CA-N-CAL |
| 1   | y     | 1101 | 5CR  | N-CA-CB-CG |
| 1   | z     | 1201 | 5CR  | N-CA-CB-CG |
| 1   | 0     | 1301 | 5CR  | N-CA-CB-CG |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | 0     | 1301 | 5CR  | C-CA-CB-CG |
| 1   | 1     | 101  | 5CR  | C-CA-N-CAL |
| 1   | 1     | 101  | 5CR  | N-CA-CB-CG |
| 1   | 2     | 201  | 5CR  | N-CA-CB-CG |
| 1   | 3     | 301  | 5CR  | N-CA-CB-CG |
| 1   | 3     | 301  | 5CR  | C-CA-CB-CG |
| 1   | 5     | 1101 | 5CR  | C-CA-N-CAL |
| 1   | 5     | 1101 | 5CR  | N-CA-CB-CG |
| 1   | 6     | 1201 | 5CR  | N-CA-CB-CG |
| 1   | 7     | 1301 | 5CR  | N-CA-CB-CG |
| 1   | 7     | 1301 | 5CR  | C-CA-CB-CG |
| 1   | 8     | 101  | 5CR  | C-CA-N-CAL |
| 1   | 8     | 101  | 5CR  | N-CA-CB-CG |
| 1   | 9     | 201  | 5CR  | N-CA-CB-CG |
| 1   | AA    | 301  | 5CR  | N-CA-CB-CG |
| 1   | AA    | 301  | 5CR  | C-CA-CB-CG |
| 1   | CA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | CA    | 1101 | 5CR  | N-CA-CB-CG |
| 1   | DA    | 1201 | 5CR  | N-CA-CB-CG |
| 1   | EA    | 1301 | 5CR  | N-CA-CB-CG |
| 1   | EA    | 1301 | 5CR  | C-CA-CB-CG |
| 1   | FA    | 101  | 5CR  | C-CA-N-CAL |
| 1   | FA    | 101  | 5CR  | N-CA-CB-CG |
| 1   | GA    | 201  | 5CR  | N-CA-CB-CG |
| 1   | HA    | 301  | 5CR  | N-CA-CB-CG |
| 1   | HA    | 301  | 5CR  | C-CA-CB-CG |
| 1   | JA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | JA    | 1101 | 5CR  | N-CA-CB-CG |
| 1   | KA    | 1201 | 5CR  | N-CA-CB-CG |
| 1   | LA    | 1301 | 5CR  | N-CA-CB-CG |
| 1   | LA    | 1301 | 5CR  | C-CA-CB-CG |
| 1   | MA    | 101  | 5CR  | C-CA-N-CAL |
| 1   | MA    | 101  | 5CR  | N-CA-CB-CG |
| 1   | NA    | 201  | 5CR  | N-CA-CB-CG |
| 1   | OA    | 301  | 5CR  | N-CA-CB-CG |
| 1   | OA    | 301  | 5CR  | C-CA-CB-CG |
| 1   | QA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | QA    | 1101 | 5CR  | N-CA-CB-CG |
| 1   | RA    | 1201 | 5CR  | N-CA-CB-CG |
| 1   | SA    | 1301 | 5CR  | N-CA-CB-CG |
| 1   | SA    | 1301 | 5CR  | C-CA-CB-CG |
| 1   | a     | 1    | 5CR  | C-CA-CB-CG |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | UA    | 201  | 5CR  | C-CA-N-CAL |
| 1   | WA    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | YA    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | b     | 1    | 5CR  | C-CA-CB-CG |
| 1   | bA    | 201  | 5CR  | C-CA-N-CAL |
| 1   | dA    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | fA    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | c     | 1    | 5CR  | C-CA-CB-CG |
| 1   | iA    | 201  | 5CR  | C-CA-N-CAL |
| 1   | kA    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | mA    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | d     | 1    | 5CR  | C-CA-CB-CG |
| 1   | pA    | 201  | 5CR  | C-CA-N-CAL |
| 1   | rA    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | tA    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | e     | 1    | 5CR  | C-CA-CB-CG |
| 1   | wA    | 201  | 5CR  | C-CA-N-CAL |
| 1   | yA    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | 0A    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | f     | 1    | 5CR  | C-CA-CB-CG |
| 1   | 3A    | 201  | 5CR  | C-CA-N-CAL |
| 1   | 5A    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | 7A    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | g     | 1    | 5CR  | C-CA-CB-CG |
| 1   | AB    | 201  | 5CR  | C-CA-N-CAL |
| 1   | CB    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | EB    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | h     | 1    | 5CR  | C-CA-CB-CG |
| 1   | HB    | 201  | 5CR  | C-CA-N-CAL |
| 1   | JB    | 1001 | 5CR  | C-CA-CB-CG |
| 1   | LB    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | OB    | 201  | 5CR  | C-CA-N-CAL |
| 1   | SB    | 1201 | 5CR  | C-CA-N-CAL |
| 1   | A     | 8    | GMA  | N-CA-CD-N2 |
| 1   | M     | 1008 | GMA  | N-CA-CD-N2 |
| 1   | B     | 8    | GMA  | N-CA-CD-N2 |
| 1   | T     | 1008 | GMA  | N-CA-CD-N2 |
| 1   | C     | 8    | GMA  | N-CA-CD-N2 |
| 1   | j     | 1008 | GMA  | N-CA-CD-N2 |
| 1   | D     | 8    | GMA  | N-CA-CD-N2 |
| 1   | q     | 1008 | GMA  | N-CA-CD-N2 |
| 1   | E     | 8    | GMA  | N-CA-CD-N2 |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | x     | 1008 | GMA  | N-CA-CD-N2  |
| 1   | F     | 8    | GMA  | N-CA-CD-N2  |
| 1   | 4     | 1008 | GMA  | N-CA-CD-N2  |
| 1   | G     | 8    | GMA  | N-CA-CD-N2  |
| 1   | BA    | 1008 | GMA  | N-CA-CD-N2  |
| 1   | H     | 8    | GMA  | N-CA-CD-N2  |
| 1   | IA    | 1008 | GMA  | N-CA-CD-N2  |
| 1   | I     | 8    | GMA  | N-CA-CD-N2  |
| 1   | PA    | 1008 | GMA  | N-CA-CD-N2  |
| 1   | a     | 8    | GMA  | N-CA-CB-CG  |
| 1   | a     | 8    | GMA  | CD-CA-CB-CG |
| 1   | UA    | 208  | GMA  | N-CA-CB-CG  |
| 1   | UA    | 208  | GMA  | CD-CA-CB-CG |
| 1   | WA    | 1008 | GMA  | N-CA-CB-CG  |
| 1   | WA    | 1008 | GMA  | CD-CA-CB-CG |
| 1   | YA    | 1208 | GMA  | N-CA-CB-CG  |
| 1   | YA    | 1208 | GMA  | CD-CA-CB-CG |
| 1   | b     | 8    | GMA  | N-CA-CB-CG  |
| 1   | b     | 8    | GMA  | CD-CA-CB-CG |
| 1   | bA    | 208  | GMA  | N-CA-CB-CG  |
| 1   | bA    | 208  | GMA  | CD-CA-CB-CG |
| 1   | dA    | 1008 | GMA  | N-CA-CB-CG  |
| 1   | dA    | 1008 | GMA  | CD-CA-CB-CG |
| 1   | fA    | 1208 | GMA  | N-CA-CB-CG  |
| 1   | fA    | 1208 | GMA  | CD-CA-CB-CG |
| 1   | c     | 8    | GMA  | N-CA-CB-CG  |
| 1   | c     | 8    | GMA  | CD-CA-CB-CG |
| 1   | iA    | 208  | GMA  | N-CA-CB-CG  |
| 1   | iA    | 208  | GMA  | CD-CA-CB-CG |
| 1   | kA    | 1008 | GMA  | N-CA-CB-CG  |
| 1   | kA    | 1008 | GMA  | CD-CA-CB-CG |
| 1   | mA    | 1208 | GMA  | N-CA-CB-CG  |
| 1   | mA    | 1208 | GMA  | CD-CA-CB-CG |
| 1   | d     | 8    | GMA  | N-CA-CB-CG  |
| 1   | d     | 8    | GMA  | CD-CA-CB-CG |
| 1   | pA    | 208  | GMA  | N-CA-CB-CG  |
| 1   | pA    | 208  | GMA  | CD-CA-CB-CG |
| 1   | rA    | 1008 | GMA  | N-CA-CB-CG  |
| 1   | rA    | 1008 | GMA  | CD-CA-CB-CG |
| 1   | tA    | 1208 | GMA  | N-CA-CB-CG  |
| 1   | tA    | 1208 | GMA  | CD-CA-CB-CG |
| 1   | e     | 8    | GMA  | N-CA-CB-CG  |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | e     | 8    | GMA  | CD-CA-CB-CG  |
| 1   | wA    | 208  | GMA  | N-CA-CB-CG   |
| 1   | wA    | 208  | GMA  | CD-CA-CB-CG  |
| 1   | yA    | 1008 | GMA  | N-CA-CB-CG   |
| 1   | yA    | 1008 | GMA  | CD-CA-CB-CG  |
| 1   | 0A    | 1208 | GMA  | N-CA-CB-CG   |
| 1   | 0A    | 1208 | GMA  | CD-CA-CB-CG  |
| 1   | f     | 8    | GMA  | N-CA-CB-CG   |
| 1   | f     | 8    | GMA  | CD-CA-CB-CG  |
| 1   | 3A    | 208  | GMA  | N-CA-CB-CG   |
| 1   | 3A    | 208  | GMA  | CD-CA-CB-CG  |
| 1   | 5A    | 1008 | GMA  | N-CA-CB-CG   |
| 1   | 5A    | 1008 | GMA  | CD-CA-CB-CG  |
| 1   | 7A    | 1208 | GMA  | N-CA-CB-CG   |
| 1   | 7A    | 1208 | GMA  | CD-CA-CB-CG  |
| 1   | g     | 8    | GMA  | N-CA-CB-CG   |
| 1   | g     | 8    | GMA  | CD-CA-CB-CG  |
| 1   | AB    | 208  | GMA  | N-CA-CB-CG   |
| 1   | AB    | 208  | GMA  | CD-CA-CB-CG  |
| 1   | CB    | 1008 | GMA  | N-CA-CB-CG   |
| 1   | CB    | 1008 | GMA  | CD-CA-CB-CG  |
| 1   | EB    | 1208 | GMA  | N-CA-CB-CG   |
| 1   | EB    | 1208 | GMA  | CD-CA-CB-CG  |
| 1   | h     | 8    | GMA  | N-CA-CB-CG   |
| 1   | h     | 8    | GMA  | CD-CA-CB-CG  |
| 1   | HB    | 208  | GMA  | N-CA-CB-CG   |
| 1   | HB    | 208  | GMA  | CD-CA-CB-CG  |
| 1   | JB    | 1008 | GMA  | N-CA-CB-CG   |
| 1   | JB    | 1008 | GMA  | CD-CA-CB-CG  |
| 1   | LB    | 1208 | GMA  | N-CA-CB-CG   |
| 1   | LB    | 1208 | GMA  | CD-CA-CB-CG  |
| 1   | i     | 8    | GMA  | N-CA-CB-CG   |
| 1   | i     | 8    | GMA  | CD-CA-CB-CG  |
| 1   | OB    | 208  | GMA  | N-CA-CB-CG   |
| 1   | OB    | 208  | GMA  | CD-CA-CB-CG  |
| 1   | QB    | 1008 | GMA  | N-CA-CB-CG   |
| 1   | QB    | 1008 | GMA  | CD-CA-CB-CG  |
| 1   | SB    | 1208 | GMA  | N-CA-CB-CG   |
| 1   | SB    | 1208 | GMA  | CD-CA-CB-CG  |
| 1   | K     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | K     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | O     | 1201 | 5CR  | CAA-CAL-N-CA |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | O     | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | R     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | R     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | V     | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | V     | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | Y     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | Y     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | l     | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | l     | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | o     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | o     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | s     | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | s     | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | v     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | v     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | z     | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | z     | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | 2     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | 2     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | 6     | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | 6     | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | 9     | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | 9     | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | DA    | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | DA    | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | GA    | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | GA    | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | KA    | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | KA    | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | NA    | 201  | 5CR  | CAA-CAL-N-CA |
| 1   | NA    | 201  | 5CR  | OAB-CAL-N-CA |
| 1   | RA    | 1201 | 5CR  | CAA-CAL-N-CA |
| 1   | RA    | 1201 | 5CR  | OAB-CAL-N-CA |
| 1   | a     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | a     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | WA    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | WA    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | b     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | b     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | dA    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | dA    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | c     | 1    | 5CR  | CAA-CAL-N-CA |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | c     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | kA    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | kA    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | d     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | d     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | rA    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | rA    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | e     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | e     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | yA    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | yA    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | f     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | f     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | 5A    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | 5A    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | g     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | g     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | CB    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | CB    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | h     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | h     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | JB    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | JB    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | i     | 1    | 5CR  | CAA-CAL-N-CA |
| 1   | i     | 1    | 5CR  | OAB-CAL-N-CA |
| 1   | QB    | 1001 | 5CR  | CAA-CAL-N-CA |
| 1   | QB    | 1001 | 5CR  | OAB-CAL-N-CA |
| 1   | L     | 308  | GMA  | CA-CB-CG-C   |
| 1   | P     | 1308 | GMA  | CA-CB-CG-C   |
| 1   | S     | 308  | GMA  | CA-CB-CG-C   |
| 1   | W     | 1308 | GMA  | CA-CB-CG-C   |
| 1   | Z     | 308  | GMA  | CA-CB-CG-C   |
| 1   | m     | 1308 | GMA  | CA-CB-CG-C   |
| 1   | p     | 308  | GMA  | CA-CB-CG-C   |
| 1   | t     | 1308 | GMA  | CA-CB-CG-C   |
| 1   | w     | 308  | GMA  | CA-CB-CG-C   |
| 1   | 0     | 1308 | GMA  | CA-CB-CG-C   |
| 1   | 3     | 308  | GMA  | CA-CB-CG-C   |
| 1   | 7     | 1308 | GMA  | CA-CB-CG-C   |
| 1   | AA    | 308  | GMA  | CA-CB-CG-C   |
| 1   | EA    | 1308 | GMA  | CA-CB-CG-C   |
| 1   | HA    | 308  | GMA  | CA-CB-CG-C   |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | LA    | 1308 | GMA  | CA-CB-CG-C   |
| 1   | OA    | 308  | GMA  | CA-CB-CG-C   |
| 1   | SA    | 1308 | GMA  | CA-CB-CG-C   |
| 1   | K     | 208  | GMA  | CA-CB-CG-C   |
| 1   | O     | 1208 | GMA  | CA-CB-CG-C   |
| 1   | R     | 208  | GMA  | CA-CB-CG-C   |
| 1   | V     | 1208 | GMA  | CA-CB-CG-C   |
| 1   | Y     | 208  | GMA  | CA-CB-CG-C   |
| 1   | l     | 1208 | GMA  | CA-CB-CG-C   |
| 1   | o     | 208  | GMA  | CA-CB-CG-C   |
| 1   | s     | 1208 | GMA  | CA-CB-CG-C   |
| 1   | v     | 208  | GMA  | CA-CB-CG-C   |
| 1   | z     | 1208 | GMA  | CA-CB-CG-C   |
| 1   | 2     | 208  | GMA  | CA-CB-CG-C   |
| 1   | 6     | 1208 | GMA  | CA-CB-CG-C   |
| 1   | 9     | 208  | GMA  | CA-CB-CG-C   |
| 1   | DA    | 1208 | GMA  | CA-CB-CG-C   |
| 1   | GA    | 208  | GMA  | CA-CB-CG-C   |
| 1   | KA    | 1208 | GMA  | CA-CB-CG-C   |
| 1   | NA    | 208  | GMA  | CA-CB-CG-C   |
| 1   | RA    | 1208 | GMA  | CA-CB-CG-C   |
| 1   | L     | 301  | 5CR  | C-CA-N-CAL   |
| 1   | P     | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | S     | 301  | 5CR  | C-CA-N-CAL   |
| 1   | W     | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | Z     | 301  | 5CR  | C-CA-N-CAL   |
| 1   | m     | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | p     | 301  | 5CR  | C-CA-N-CAL   |
| 1   | t     | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | w     | 301  | 5CR  | C-CA-N-CAL   |
| 1   | 0     | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | 3     | 301  | 5CR  | C-CA-N-CAL   |
| 1   | 7     | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | AA    | 301  | 5CR  | C-CA-N-CAL   |
| 1   | EA    | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | HA    | 301  | 5CR  | C-CA-N-CAL   |
| 1   | LA    | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | OA    | 301  | 5CR  | C-CA-N-CAL   |
| 1   | SA    | 1301 | 5CR  | C-CA-N-CAL   |
| 1   | nA    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | jA    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | cA    | 301  | 5CR  | CA-CB-CG-CD2 |

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| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 1   | qA    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | uA    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | xA    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | 1A    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | FB    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | PB    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | gA    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | BB    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | IB    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | TB    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | VA    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | ZA    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | 4A    | 301  | 5CR  | CA-CB-CG-CD2 |
| 1   | 8A    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | MB    | 1301 | 5CR  | CA-CB-CG-CD2 |
| 1   | PB    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | cA    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | gA    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | xA    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | 4A    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | 8A    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | BB    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | FB    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | IB    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | MB    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | VA    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | ZA    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | jA    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | nA    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | qA    | 301  | 5CR  | CA-CB-CG-CD1 |
| 1   | uA    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | 1A    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | TB    | 1301 | 5CR  | CA-CB-CG-CD1 |
| 1   | i     | 1    | 5CR  | C-CA-CB-CG   |
| 1   | QB    | 1001 | 5CR  | C-CA-CB-CG   |
| 1   | a     | 1    | 5CR  | CB-CA-N-CAL  |
| 1   | VA    | 301  | 5CR  | CB-CA-N-CAL  |
| 1   | WA    | 1001 | 5CR  | CB-CA-N-CAL  |
| 1   | ZA    | 1301 | 5CR  | CB-CA-N-CAL  |
| 1   | b     | 1    | 5CR  | CB-CA-N-CAL  |
| 1   | cA    | 301  | 5CR  | CB-CA-N-CAL  |
| 1   | dA    | 1001 | 5CR  | CB-CA-N-CAL  |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | gA    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | c     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | jA    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | kA    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | nA    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | d     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | qA    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | rA    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | uA    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | e     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | xA    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | yA    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | 1A    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | f     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | 4A    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | 5A    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | 8A    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | g     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | BB    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | CB    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | FB    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | h     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | IB    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | MB    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | i     | 1    | 5CR  | CB-CA-N-CAL |
| 1   | PB    | 301  | 5CR  | CB-CA-N-CAL |
| 1   | QB    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | TB    | 1301 | 5CR  | CB-CA-N-CAL |
| 1   | J     | 108  | GMA  | N-CA-CB-CG  |
| 1   | N     | 1108 | GMA  | N-CA-CB-CG  |
| 1   | Q     | 108  | GMA  | N-CA-CB-CG  |
| 1   | U     | 1108 | GMA  | N-CA-CB-CG  |
| 1   | X     | 108  | GMA  | N-CA-CB-CG  |
| 1   | k     | 1108 | GMA  | N-CA-CB-CG  |
| 1   | n     | 108  | GMA  | N-CA-CB-CG  |
| 1   | r     | 1108 | GMA  | N-CA-CB-CG  |
| 1   | u     | 108  | GMA  | N-CA-CB-CG  |
| 1   | y     | 1108 | GMA  | N-CA-CB-CG  |
| 1   | 1     | 108  | GMA  | N-CA-CB-CG  |
| 1   | 5     | 1108 | GMA  | N-CA-CB-CG  |
| 1   | 8     | 108  | GMA  | N-CA-CB-CG  |
| 1   | CA    | 1108 | GMA  | N-CA-CB-CG  |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | FA    | 108  | GMA  | N-CA-CB-CG  |
| 1   | JA    | 1108 | GMA  | N-CA-CB-CG  |
| 1   | MA    | 108  | GMA  | N-CA-CB-CG  |
| 1   | QA    | 1108 | GMA  | N-CA-CB-CG  |
| 1   | a     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | a     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | WA    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | WA    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | b     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | b     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | dA    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | dA    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | c     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | c     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | kA    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | kA    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | d     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | d     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | rA    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | rA    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | e     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | e     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | yA    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | yA    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | f     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | f     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | 5A    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | 5A    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | g     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | g     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | CB    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | CB    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | h     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | h     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | JB    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | JB    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | i     | 8    | GMA  | CB-CA-CD-O1 |
| 1   | i     | 8    | GMA  | CB-CA-CD-N2 |
| 1   | QB    | 1008 | GMA  | CB-CA-CD-O1 |
| 1   | QB    | 1008 | GMA  | CB-CA-CD-N2 |
| 1   | J     | 108  | GMA  | CD-CA-CB-CG |
| 1   | N     | 1108 | GMA  | CD-CA-CB-CG |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | Q     | 108  | GMA  | CD-CA-CB-CG |
| 1   | U     | 1108 | GMA  | CD-CA-CB-CG |
| 1   | X     | 108  | GMA  | CD-CA-CB-CG |
| 1   | k     | 1108 | GMA  | CD-CA-CB-CG |
| 1   | n     | 108  | GMA  | CD-CA-CB-CG |
| 1   | r     | 1108 | GMA  | CD-CA-CB-CG |
| 1   | y     | 1108 | GMA  | CD-CA-CB-CG |
| 1   | 1     | 108  | GMA  | CD-CA-CB-CG |
| 1   | 5     | 1108 | GMA  | CD-CA-CB-CG |
| 1   | 8     | 108  | GMA  | CD-CA-CB-CG |
| 1   | CA    | 1108 | GMA  | CD-CA-CB-CG |
| 1   | FA    | 108  | GMA  | CD-CA-CB-CG |
| 1   | JA    | 1108 | GMA  | CD-CA-CB-CG |
| 1   | MA    | 108  | GMA  | CD-CA-CB-CG |
| 1   | QA    | 1108 | GMA  | CD-CA-CB-CG |
| 1   | u     | 108  | GMA  | CD-CA-CB-CG |
| 1   | a     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | WA    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | b     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | dA    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | c     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | kA    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | d     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | rA    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | e     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | yA    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | f     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | 5A    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | g     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | CB    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | h     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | JB    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | i     | 1    | 5CR  | N-CA-CB-CG  |
| 1   | QB    | 1001 | 5CR  | N-CA-CB-CG  |
| 1   | a     | 1    | 5CR  | C-CA-N-CAL  |
| 1   | TA    | 101  | 5CR  | C-CA-N-CAL  |
| 1   | VA    | 301  | 5CR  | C-CA-N-CAL  |
| 1   | WA    | 1001 | 5CR  | C-CA-N-CAL  |
| 1   | XA    | 1101 | 5CR  | C-CA-N-CAL  |
| 1   | ZA    | 1301 | 5CR  | C-CA-N-CAL  |
| 1   | b     | 1    | 5CR  | C-CA-N-CAL  |
| 1   | aA    | 101  | 5CR  | C-CA-N-CAL  |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | cA    | 301  | 5CR  | C-CA-N-CAL |
| 1   | dA    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | eA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | gA    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | c     | 1    | 5CR  | C-CA-N-CAL |
| 1   | hA    | 101  | 5CR  | C-CA-N-CAL |
| 1   | jA    | 301  | 5CR  | C-CA-N-CAL |
| 1   | kA    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | lA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | nA    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | d     | 1    | 5CR  | C-CA-N-CAL |
| 1   | oA    | 101  | 5CR  | C-CA-N-CAL |
| 1   | qA    | 301  | 5CR  | C-CA-N-CAL |
| 1   | rA    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | sA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | uA    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | e     | 1    | 5CR  | C-CA-N-CAL |
| 1   | vA    | 101  | 5CR  | C-CA-N-CAL |
| 1   | xA    | 301  | 5CR  | C-CA-N-CAL |
| 1   | yA    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | zA    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | 1A    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | f     | 1    | 5CR  | C-CA-N-CAL |
| 1   | 2A    | 101  | 5CR  | C-CA-N-CAL |
| 1   | 4A    | 301  | 5CR  | C-CA-N-CAL |
| 1   | 5A    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | 6A    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | 8A    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | g     | 1    | 5CR  | C-CA-N-CAL |
| 1   | 9A    | 101  | 5CR  | C-CA-N-CAL |
| 1   | BB    | 301  | 5CR  | C-CA-N-CAL |
| 1   | CB    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | DB    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | FB    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | h     | 1    | 5CR  | C-CA-N-CAL |
| 1   | GB    | 101  | 5CR  | C-CA-N-CAL |
| 1   | IB    | 301  | 5CR  | C-CA-N-CAL |
| 1   | JB    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | KB    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | MB    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | i     | 1    | 5CR  | C-CA-N-CAL |
| 1   | NB    | 101  | 5CR  | C-CA-N-CAL |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 1   | PB    | 301  | 5CR  | C-CA-N-CAL |
| 1   | QB    | 1001 | 5CR  | C-CA-N-CAL |
| 1   | RB    | 1101 | 5CR  | C-CA-N-CAL |
| 1   | TB    | 1301 | 5CR  | C-CA-N-CAL |
| 1   | a     | 8    | GMA  | CA-CB-CG-C |
| 1   | WA    | 1008 | GMA  | CA-CB-CG-C |
| 1   | b     | 8    | GMA  | CA-CB-CG-C |
| 1   | dA    | 1008 | GMA  | CA-CB-CG-C |
| 1   | c     | 8    | GMA  | CA-CB-CG-C |
| 1   | kA    | 1008 | GMA  | CA-CB-CG-C |
| 1   | d     | 8    | GMA  | CA-CB-CG-C |
| 1   | rA    | 1008 | GMA  | CA-CB-CG-C |
| 1   | e     | 8    | GMA  | CA-CB-CG-C |
| 1   | yA    | 1008 | GMA  | CA-CB-CG-C |
| 1   | f     | 8    | GMA  | CA-CB-CG-C |
| 1   | 5A    | 1008 | GMA  | CA-CB-CG-C |
| 1   | g     | 8    | GMA  | CA-CB-CG-C |
| 1   | CB    | 1008 | GMA  | CA-CB-CG-C |
| 1   | h     | 8    | GMA  | CA-CB-CG-C |
| 1   | JB    | 1008 | GMA  | CA-CB-CG-C |
| 1   | i     | 8    | GMA  | CA-CB-CG-C |
| 1   | QB    | 1008 | GMA  | CA-CB-CG-C |
| 1   | a     | 8    | GMA  | N-CA-CD-O1 |
| 1   | WA    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | b     | 8    | GMA  | N-CA-CD-O1 |
| 1   | dA    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | c     | 8    | GMA  | N-CA-CD-O1 |
| 1   | kA    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | d     | 8    | GMA  | N-CA-CD-O1 |
| 1   | rA    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | e     | 8    | GMA  | N-CA-CD-O1 |
| 1   | yA    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | f     | 8    | GMA  | N-CA-CD-O1 |
| 1   | 5A    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | g     | 8    | GMA  | N-CA-CD-O1 |
| 1   | CB    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | h     | 8    | GMA  | N-CA-CD-O1 |
| 1   | JB    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | i     | 8    | GMA  | N-CA-CD-O1 |
| 1   | QB    | 1008 | GMA  | N-CA-CD-O1 |
| 1   | K     | 201  | 5CR  | C-CA-CB-CG |
| 1   | O     | 1201 | 5CR  | C-CA-CB-CG |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | R     | 201  | 5CR  | C-CA-CB-CG  |
| 1   | V     | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | Y     | 201  | 5CR  | C-CA-CB-CG  |
| 1   | l     | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | o     | 201  | 5CR  | C-CA-CB-CG  |
| 1   | s     | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | v     | 201  | 5CR  | C-CA-CB-CG  |
| 1   | z     | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | 2     | 201  | 5CR  | C-CA-CB-CG  |
| 1   | 6     | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | 9     | 201  | 5CR  | C-CA-CB-CG  |
| 1   | DA    | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | GA    | 201  | 5CR  | C-CA-CB-CG  |
| 1   | KA    | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | NA    | 201  | 5CR  | C-CA-CB-CG  |
| 1   | RA    | 1201 | 5CR  | C-CA-CB-CG  |
| 1   | UA    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | YA    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | bA    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | fA    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | iA    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | mA    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | pA    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | tA    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | wA    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | 0A    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | 3A    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | 7A    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | AB    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | EB    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | HB    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | JB    | 1001 | 5CR  | CB-CA-N-CAL |
| 1   | LB    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | OB    | 201  | 5CR  | CB-CA-N-CAL |
| 1   | SB    | 1201 | 5CR  | CB-CA-N-CAL |
| 1   | WA    | 1008 | GMA  | O-C-CG-CB   |
| 1   | dA    | 1008 | GMA  | O-C-CG-CB   |
| 1   | f     | 8    | GMA  | O-C-CG-CB   |
| 1   | 5A    | 1008 | GMA  | O-C-CG-CB   |
| 1   | g     | 8    | GMA  | O-C-CG-CB   |
| 1   | CB    | 1008 | GMA  | O-C-CG-CB   |
| 1   | h     | 8    | GMA  | O-C-CG-CB   |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | JB    | 1008 | GMA  | O-C-CG-CB   |
| 1   | i     | 8    | GMA  | O-C-CG-CB   |
| 1   | QB    | 1008 | GMA  | O-C-CG-CB   |
| 1   | a     | 8    | GMA  | O-C-CG-CB   |
| 1   | yA    | 1008 | GMA  | O-C-CG-CB   |
| 1   | a     | 8    | GMA  | OXT-C-CG-CB |
| 1   | WA    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | b     | 8    | GMA  | O-C-CG-CB   |
| 1   | b     | 8    | GMA  | OXT-C-CG-CB |
| 1   | dA    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | c     | 8    | GMA  | O-C-CG-CB   |
| 1   | c     | 8    | GMA  | OXT-C-CG-CB |
| 1   | kA    | 1008 | GMA  | O-C-CG-CB   |
| 1   | kA    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | d     | 8    | GMA  | O-C-CG-CB   |
| 1   | d     | 8    | GMA  | OXT-C-CG-CB |
| 1   | rA    | 1008 | GMA  | O-C-CG-CB   |
| 1   | rA    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | e     | 8    | GMA  | O-C-CG-CB   |
| 1   | yA    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | 5A    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | g     | 8    | GMA  | OXT-C-CG-CB |
| 1   | CB    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | h     | 8    | GMA  | OXT-C-CG-CB |
| 1   | JB    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | i     | 8    | GMA  | OXT-C-CG-CB |
| 1   | QB    | 1008 | GMA  | OXT-C-CG-CB |
| 1   | e     | 8    | GMA  | OXT-C-CG-CB |
| 1   | f     | 8    | GMA  | OXT-C-CG-CB |
| 1   | bA    | 208  | GMA  | OXT-C-CG-CB |
| 1   | fA    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | pA    | 208  | GMA  | OXT-C-CG-CB |
| 1   | tA    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | wA    | 208  | GMA  | OXT-C-CG-CB |
| 1   | 0A    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | HB    | 208  | GMA  | OXT-C-CG-CB |
| 1   | iA    | 208  | GMA  | OXT-C-CG-CB |
| 1   | mA    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | 3A    | 208  | GMA  | OXT-C-CG-CB |
| 1   | LB    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | YA    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | 7A    | 1208 | GMA  | OXT-C-CG-CB |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 1   | UA    | 208  | GMA  | OXT-C-CG-CB |
| 1   | AB    | 208  | GMA  | OXT-C-CG-CB |
| 1   | EB    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | OB    | 208  | GMA  | OXT-C-CG-CB |
| 1   | SB    | 1208 | GMA  | OXT-C-CG-CB |
| 1   | UA    | 208  | GMA  | O-C-CG-CB   |
| 1   | YA    | 1208 | GMA  | O-C-CG-CB   |
| 1   | bA    | 208  | GMA  | O-C-CG-CB   |
| 1   | mA    | 1208 | GMA  | O-C-CG-CB   |
| 1   | pA    | 208  | GMA  | O-C-CG-CB   |
| 1   | tA    | 1208 | GMA  | O-C-CG-CB   |
| 1   | 7A    | 1208 | GMA  | O-C-CG-CB   |
| 1   | EB    | 1208 | GMA  | O-C-CG-CB   |
| 1   | LB    | 1208 | GMA  | O-C-CG-CB   |
| 1   | OB    | 208  | GMA  | O-C-CG-CB   |
| 1   | SB    | 1208 | GMA  | O-C-CG-CB   |
| 1   | wA    | 208  | GMA  | O-C-CG-CB   |
| 1   | 3A    | 208  | GMA  | O-C-CG-CB   |
| 1   | fA    | 1208 | GMA  | O-C-CG-CB   |
| 1   | iA    | 208  | GMA  | O-C-CG-CB   |
| 1   | 0A    | 1208 | GMA  | O-C-CG-CB   |
| 1   | AB    | 208  | GMA  | O-C-CG-CB   |
| 1   | HB    | 208  | GMA  | O-C-CG-CB   |

There are no ring outliers.

105 monomers are involved in 177 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | zA    | 1108 | GMA  | 1       | 0            |
| 1   | 2     | 201  | 5CR  | 1       | 0            |
| 1   | v     | 208  | GMA  | 2       | 0            |
| 1   | O     | 1208 | GMA  | 3       | 0            |
| 1   | N     | 1108 | GMA  | 1       | 0            |
| 1   | l     | 1201 | 5CR  | 1       | 0            |
| 1   | nA    | 1308 | GMA  | 1       | 0            |
| 1   | Y     | 208  | GMA  | 3       | 0            |
| 1   | l     | 1208 | GMA  | 3       | 0            |
| 1   | J     | 101  | 5CR  | 6       | 0            |
| 1   | NA    | 201  | 5CR  | 1       | 0            |
| 1   | FA    | 108  | GMA  | 1       | 0            |
| 1   | DA    | 1208 | GMA  | 3       | 0            |
| 1   | JA    | 1108 | GMA  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | yA    | 1008 | GMA  | 1       | 0            |
| 1   | 6     | 1201 | 5CR  | 1       | 0            |
| 1   | XA    | 1108 | GMA  | 1       | 0            |
| 1   | 1     | 108  | GMA  | 1       | 0            |
| 1   | Y     | 201  | 5CR  | 1       | 0            |
| 1   | P     | 1308 | GMA  | 6       | 0            |
| 1   | u     | 108  | GMA  | 1       | 0            |
| 1   | lA    | 1108 | GMA  | 1       | 0            |
| 1   | GB    | 108  | GMA  | 1       | 0            |
| 1   | JA    | 1101 | 5CR  | 5       | 0            |
| 1   | WA    | 1008 | GMA  | 1       | 0            |
| 1   | aA    | 108  | GMA  | 1       | 0            |
| 1   | d     | 8    | GMA  | 1       | 0            |
| 1   | DB    | 1108 | GMA  | 1       | 0            |
| 1   | FA    | 101  | 5CR  | 6       | 0            |
| 1   | a     | 8    | GMA  | 1       | 0            |
| 1   | K     | 208  | GMA  | 3       | 0            |
| 1   | rA    | 1008 | GMA  | 1       | 0            |
| 1   | K     | 201  | 5CR  | 1       | 0            |
| 1   | Z     | 308  | GMA  | 7       | 0            |
| 1   | hA    | 108  | GMA  | 1       | 0            |
| 1   | k     | 1101 | 5CR  | 7       | 0            |
| 1   | 6A    | 1108 | GMA  | 1       | 0            |
| 1   | NA    | 208  | GMA  | 3       | 0            |
| 1   | QA    | 1108 | GMA  | 1       | 0            |
| 1   | n     | 101  | 5CR  | 5       | 0            |
| 1   | N     | 1101 | 5CR  | 6       | 0            |
| 1   | z     | 1201 | 5CR  | 1       | 0            |
| 1   | eA    | 1108 | GMA  | 1       | 0            |
| 1   | Q     | 108  | GMA  | 1       | 0            |
| 1   | 9     | 201  | 5CR  | 1       | 0            |
| 1   | J     | 108  | GMA  | 1       | 0            |
| 1   | Q     | 101  | 5CR  | 6       | 0            |
| 1   | RA    | 1201 | 5CR  | 1       | 0            |
| 1   | 5A    | 1008 | GMA  | 1       | 0            |
| 1   | wA    | 201  | 5CR  | 1       | 0            |
| 1   | RA    | 1208 | GMA  | 3       | 0            |
| 1   | CA    | 1108 | GMA  | 1       | 0            |
| 1   | jA    | 308  | GMA  | 1       | 0            |
| 1   | 2A    | 108  | GMA  | 1       | 0            |
| 1   | U     | 1108 | GMA  | 1       | 0            |
| 1   | O     | 1201 | 5CR  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | L     | 308  | GMA  | 7       | 0            |
| 1   | f     | 8    | GMA  | 1       | 0            |
| 1   | AA    | 308  | GMA  | 7       | 0            |
| 1   | CB    | 1008 | GMA  | 1       | 0            |
| 1   | n     | 108  | GMA  | 1       | 0            |
| 1   | SA    | 1308 | GMA  | 6       | 0            |
| 1   | EA    | 1308 | GMA  | 7       | 0            |
| 1   | S     | 308  | GMA  | 7       | 0            |
| 1   | p     | 308  | GMA  | 4       | 0            |
| 1   | TA    | 108  | GMA  | 1       | 0            |
| 1   | DA    | 1201 | 5CR  | 1       | 0            |
| 1   | R     | 201  | 5CR  | 1       | 0            |
| 1   | 8     | 108  | GMA  | 1       | 0            |
| 1   | OA    | 308  | GMA  | 7       | 0            |
| 1   | c     | 8    | GMA  | 1       | 0            |
| 1   | oA    | 108  | GMA  | 1       | 0            |
| 1   | sA    | 1108 | GMA  | 1       | 0            |
| 1   | QB    | 1008 | GMA  | 2       | 0            |
| 1   | v     | 201  | 5CR  | 1       | 0            |
| 1   | 0     | 1308 | GMA  | 7       | 0            |
| 1   | vA    | 108  | GMA  | 1       | 0            |
| 1   | 5     | 1101 | 5CR  | 6       | 0            |
| 1   | 0A    | 1201 | 5CR  | 1       | 0            |
| 1   | KB    | 1108 | GMA  | 1       | 0            |
| 1   | MA    | 108  | GMA  | 1       | 0            |
| 1   | r     | 1108 | GMA  | 1       | 0            |
| 1   | 1     | 101  | 5CR  | 6       | 0            |
| 1   | U     | 1101 | 5CR  | 5       | 0            |
| 1   | R     | 208  | GMA  | 2       | 0            |
| 1   | W     | 1308 | GMA  | 4       | 0            |
| 1   | o     | 201  | 5CR  | 1       | 0            |
| 1   | X     | 108  | GMA  | 1       | 0            |
| 1   | w     | 308  | GMA  | 7       | 0            |
| 1   | GA    | 201  | 5CR  | 1       | 0            |
| 1   | m     | 1308 | GMA  | 6       | 0            |
| 1   | V     | 1201 | 5CR  | 1       | 0            |
| 1   | y     | 1108 | GMA  | 1       | 0            |
| 1   | z     | 1208 | GMA  | 2       | 0            |
| 1   | 9A    | 108  | GMA  | 1       | 0            |
| 1   | r     | 1101 | 5CR  | 6       | 0            |
| 1   | 9     | 208  | GMA  | 3       | 0            |
| 1   | g     | 8    | GMA  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | KA    | 1201 | 5CR  | 1       | 0            |
| 1   | k     | 1108 | GMA  | 1       | 0            |
| 1   | i     | 8    | GMA  | 2       | 0            |
| 1   | kA    | 1008 | GMA  | 1       | 0            |
| 1   | 5     | 1108 | GMA  | 1       | 0            |
| 1   | s     | 1201 | 5CR  | 1       | 0            |
| 1   | e     | 8    | GMA  | 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.

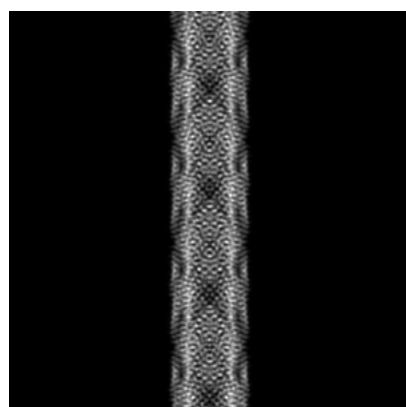
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23486. These allow visual inspection of the internal detail of the map and identification of artifacts.

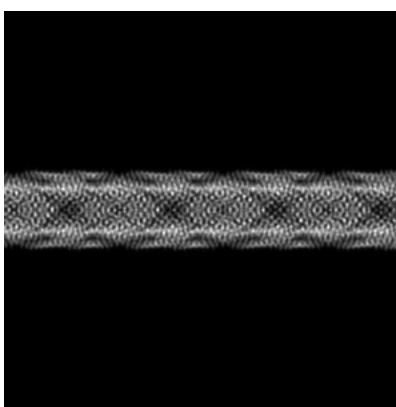
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

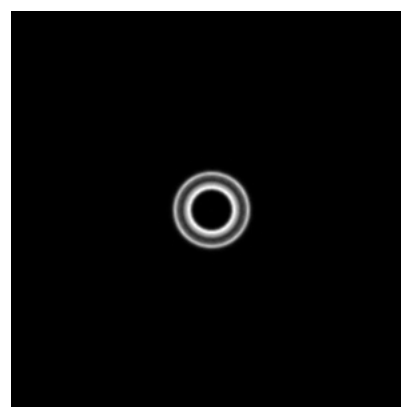
#### 6.1.1 Primary map



X



Y

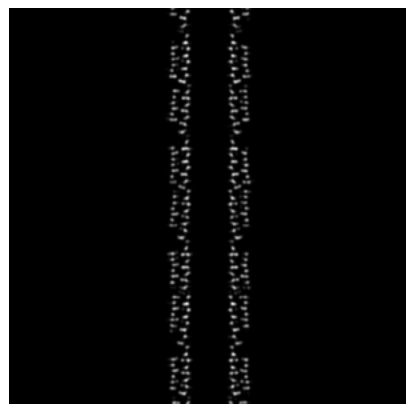


Z

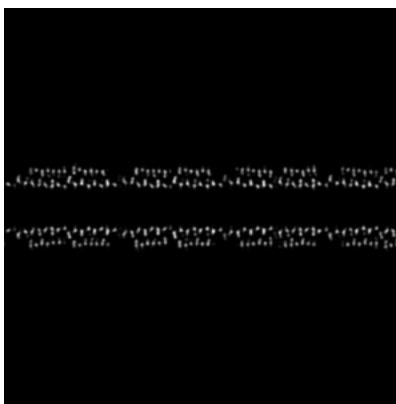
The images above show the map projected in three orthogonal directions.

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

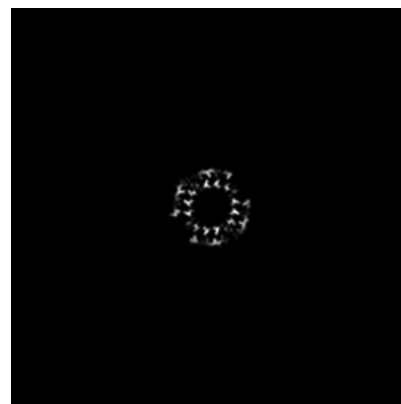
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

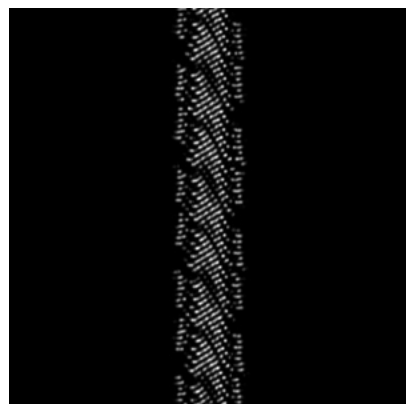


Z Index: 160

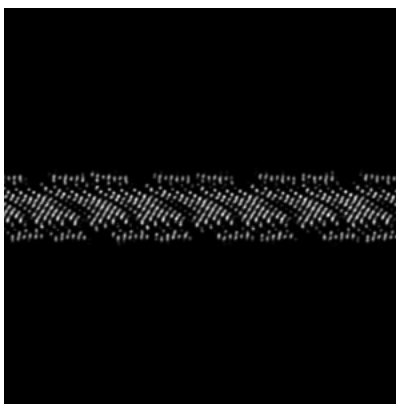
The images above show central slices of the map in three orthogonal directions.

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

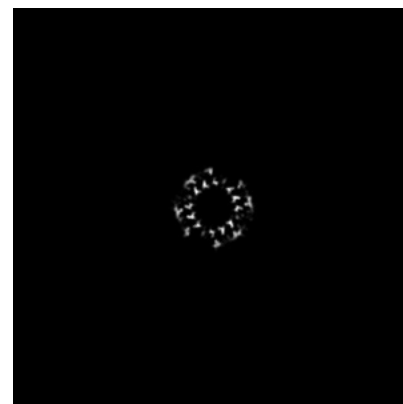
### 6.3.1 Primary map



X Index: 177



Y Index: 143

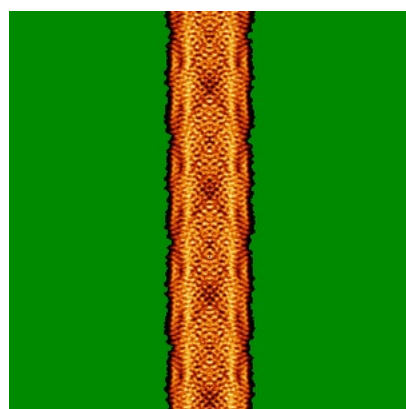


Z Index: 61

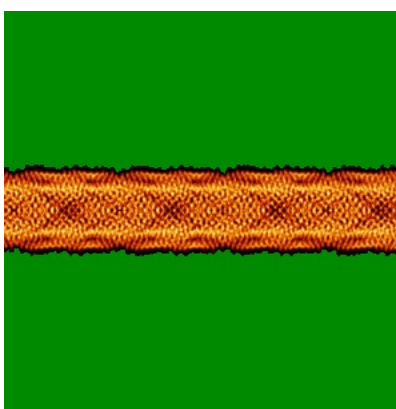
The images above show the largest variance slices of the map in three orthogonal directions.

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

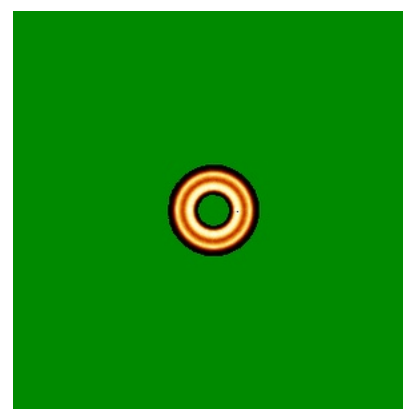
### 6.4.1 Primary map



X



Y

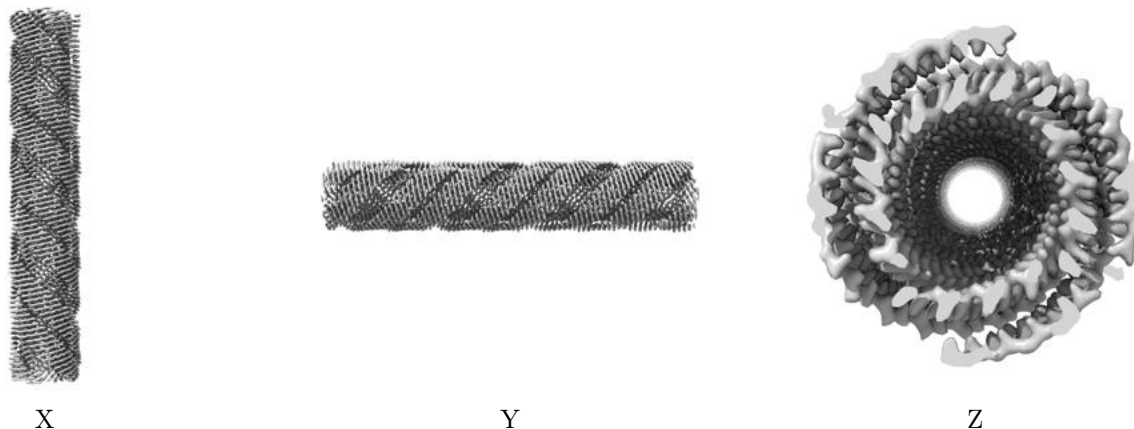


Z

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

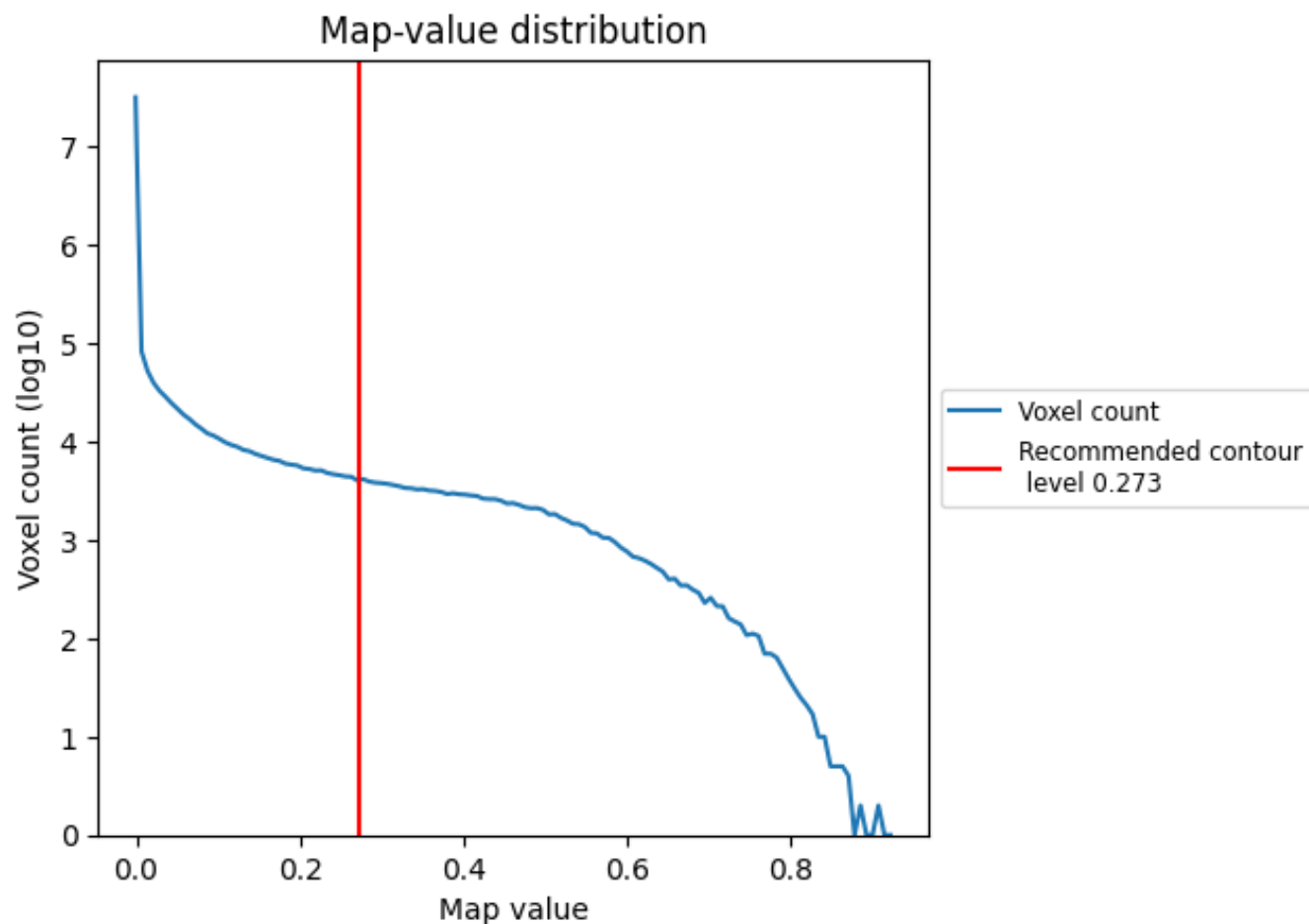
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

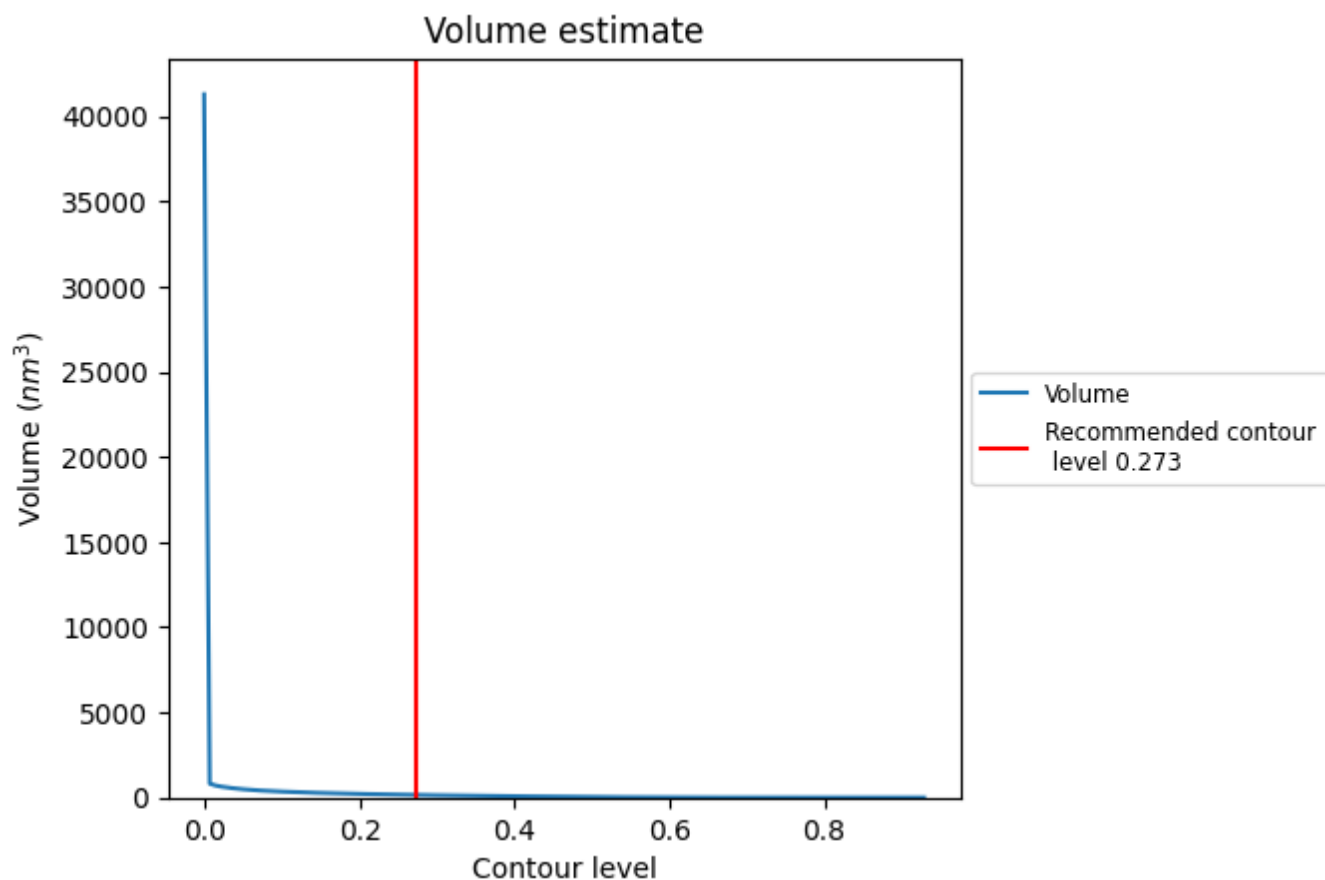
This section contains the results of statistical analysis of the map.

### 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.

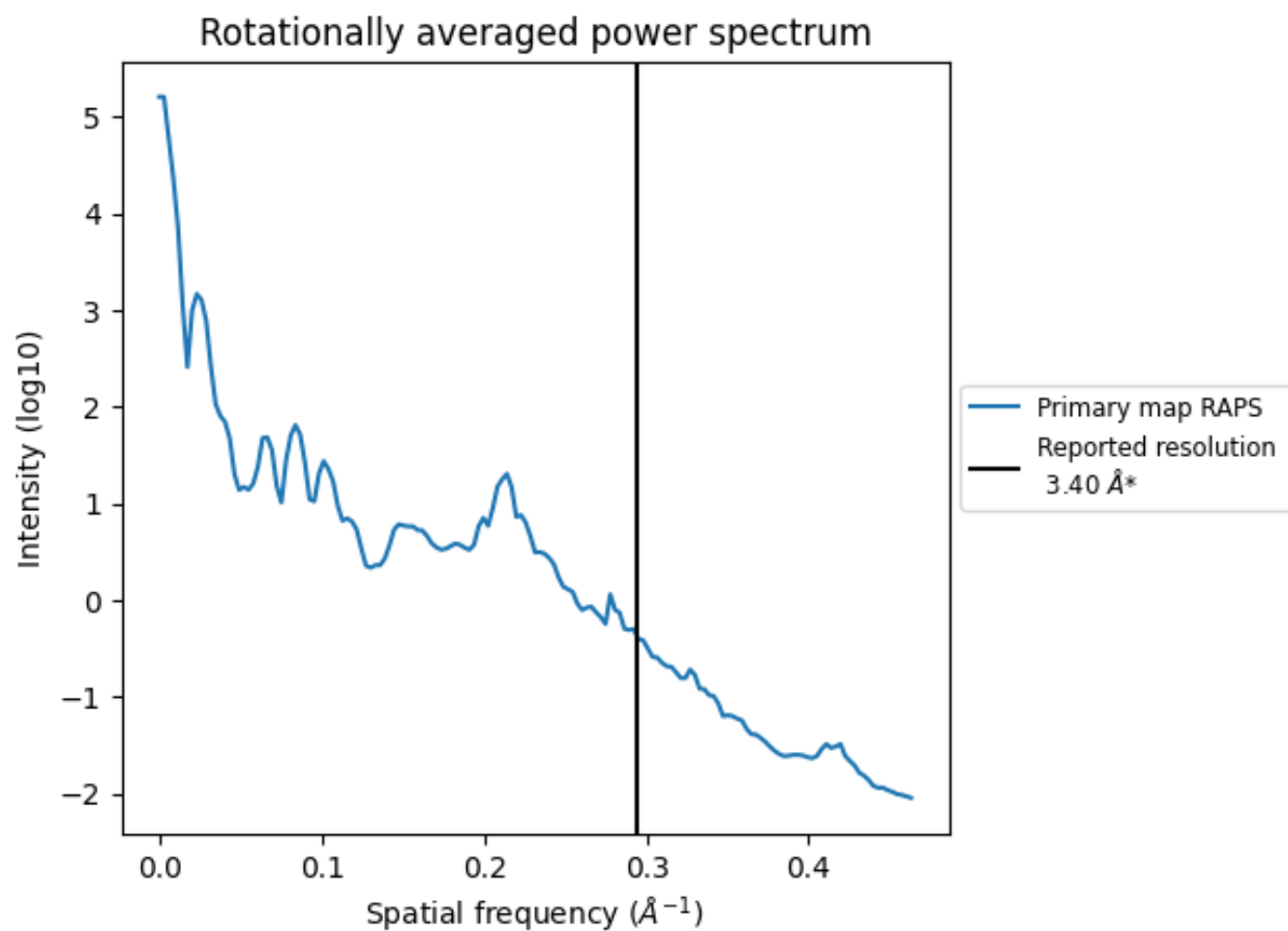
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153  $\text{nm}^3$ ; this corresponds to an approximate mass of 138 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>

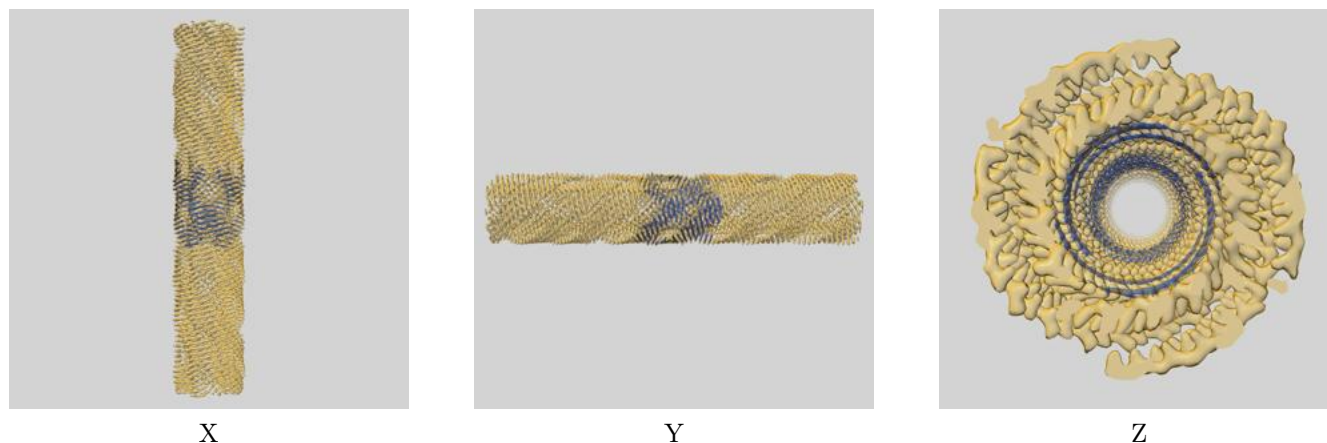
## 8 Fourier-Shell correlation

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

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

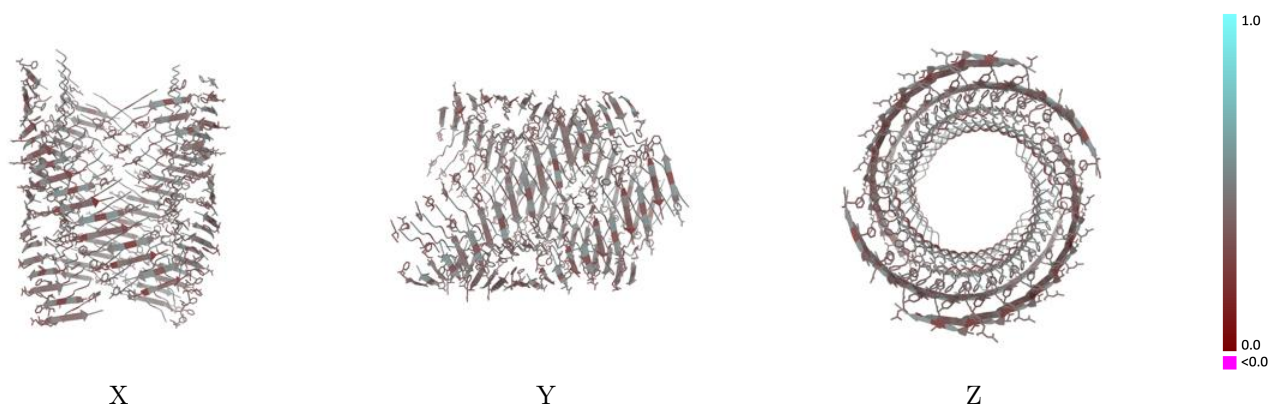
This section contains information regarding the fit between EMDB map EMD-23486 and PDB model 7LQH. Per-residue inclusion information can be found in section 3 on page 18.

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



The images above show the 3D surface view of the map at the recommended contour level 0.273 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](#)

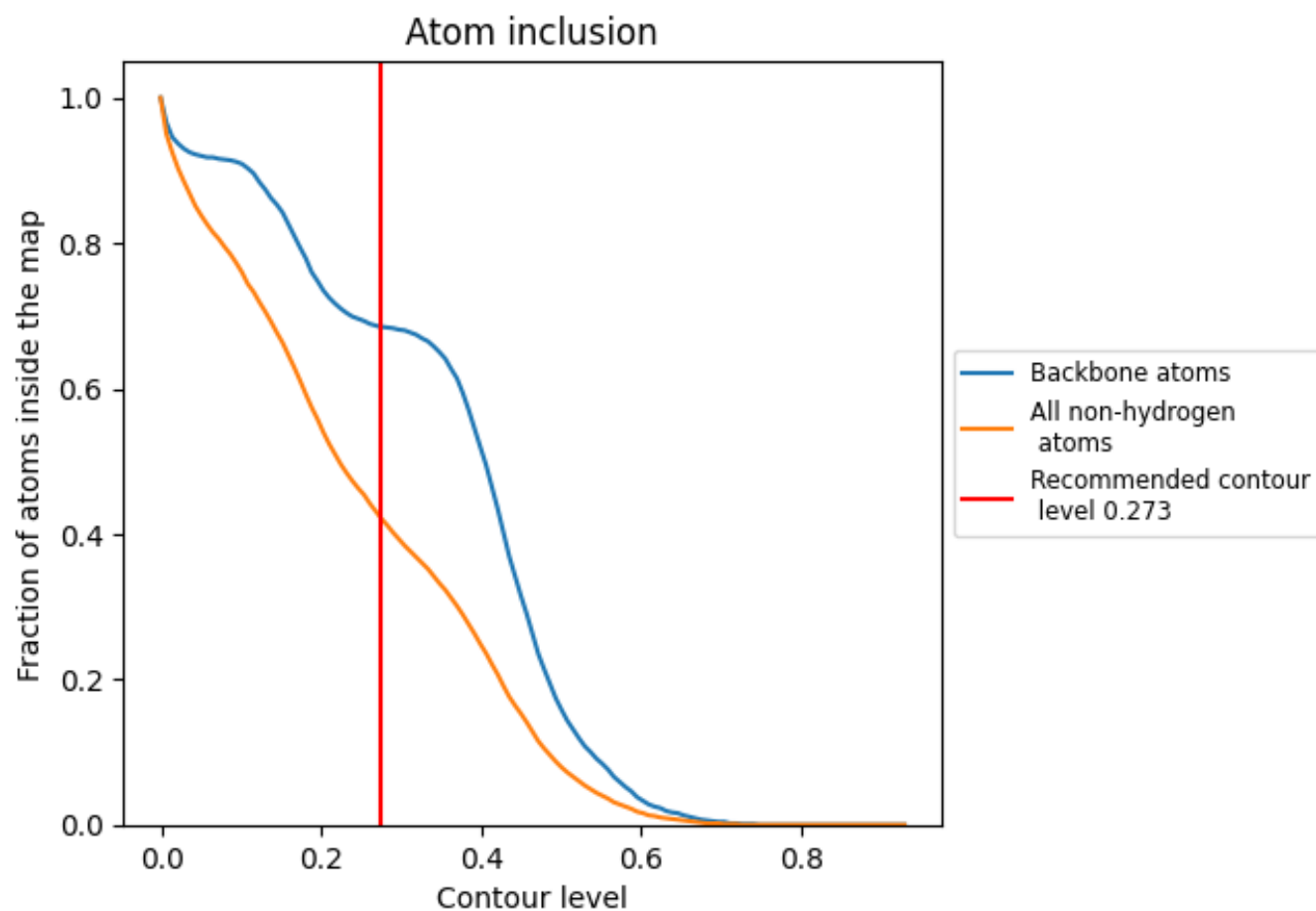


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 42% 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 (0.273) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4240   |  0.4250   |
| 0     |  0.4760   |  0.4280   |
| 0A    |  0.3810   |  0.4720   |
| 1     |  0.4640   |  0.4080   |
| 1A    |  0.3570   |  0.3700   |
| 2     |  0.5120   |  0.4480   |
| 2A    |  0.3810   |  0.4170   |
| 3     |  0.5000   |  0.4400   |
| 3A    |  0.4170   |  0.4720   |
| 4     |  0.4290   |  0.4290   |
| 4A    |  0.3690   |  0.3700   |
| 5     |  0.4410   |  0.4020   |
| 5A    |  0.3930   |  0.4440   |
| 6     |  0.5120   |  0.4570   |
| 6A    |  0.3570  |  0.4020  |
| 7     |  0.4880 |  0.4310 |
| 7A    |  0.3810 |  0.4510 |
| 8     |  0.4640 |  0.4030 |
| 8A    |  0.3330 |  0.3940 |
| 9     |  0.5000 |  0.4580 |
| 9A    |  0.3570 |  0.4260 |
| A     |  0.4170 |  0.4240 |
| AA    |  0.5240 |  0.4250 |
| AB    |  0.4170 |  0.4470 |
| B     |  0.4290 |  0.4130 |
| BA    |  0.4050 |  0.3970 |
| BB    |  0.3690 |  0.3980 |
| C     |  0.4290 |  0.4190 |
| CA    |  0.4170 |  0.3950 |
| CB    |  0.3810 |  0.4370 |
| D     |  0.4170 |  0.4170 |
| DA    |  0.5590 |  0.4420 |
| DB    |  0.3690 |  0.4080 |
| E     |  0.4290 |  0.4240 |
| EA    |  0.5000 |  0.4400 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| EB    |  0.3930   |  0.4530   |
| F     |  0.4170   |  0.4240   |
| FA    |  0.4410   |  0.4000   |
| FB    |  0.3570   |  0.3740   |
| G     |  0.4640   |  0.4260   |
| GA    |  0.5240   |  0.4540   |
| GB    |  0.3570   |  0.4140   |
| H     |  0.4290   |  0.4210   |
| HA    |  0.5120   |  0.4470   |
| HB    |  0.4290   |  0.4600   |
| I     |  0.4290   |  0.4190   |
| IA    |  0.4290   |  0.4200   |
| IB    |  0.3810   |  0.3890   |
| J     |  0.4170   |  0.4060   |
| JA    |  0.4410   |  0.3990   |
| JB    |  0.3930   |  0.4170   |
| K     |  0.5000   |  0.4440   |
| KA    |  0.4760  |  0.4550  |
| KB    |  0.3570 |  0.4110 |
| L     |  0.5000 |  0.4440 |
| LA    |  0.5000 |  0.4420 |
| LB    |  0.4170 |  0.4380 |
| M     |  0.4290 |  0.4120 |
| MA    |  0.4410 |  0.3900 |
| MB    |  0.3330 |  0.3890 |
| N     |  0.4520 |  0.3940 |
| NA    |  0.5240 |  0.4590 |
| NB    |  0.3810 |  0.4100 |
| O     |  0.4880 |  0.4430 |
| OA    |  0.5000 |  0.4220 |
| OB    |  0.4050 |  0.4590 |
| P     |  0.5000 |  0.4450 |
| PA    |  0.4170 |  0.4180 |
| PB    |  0.3810 |  0.4000 |
| Q     |  0.4410 |  0.4040 |
| QA    |  0.4170 |  0.3850 |
| QB    |  0.4170 |  0.4390 |
| R     |  0.4760 |  0.4560 |
| RA    |  0.4880 |  0.4450 |
| RB    |  0.3570 |  0.3950 |
| S     |  0.4760 |  0.4340 |
| SA    |  0.5240 |  0.4480 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| SB    |  0.3810   |  0.4610   |
| T     |  0.4410   |  0.4230   |
| TA    |  0.3690   |  0.4300   |
| TB    |  0.3570   |  0.3750   |
| U     |  0.4290   |  0.4010   |
| UA    |  0.3810   |  0.4770   |
| V     |  0.5000   |  0.4470   |
| VA    |  0.3810   |  0.3840   |
| W     |  0.4880   |  0.4290   |
| WA    |  0.3810   |  0.4290   |
| X     |  0.4410   |  0.3970   |
| XA    |  0.3930   |  0.4050   |
| Y     |  0.5000   |  0.4430   |
| YA    |  0.4050   |  0.4580   |
| Z     |  0.5120   |  0.4230   |
| ZA    |  0.3570   |  0.3800   |
| a     |  0.3930   |  0.4520   |
| aA    |  0.3810   |  0.4130   |
| b     |  0.4050  |  0.4480  |
| bA    |  0.4290 |  0.4580 |
| c     |  0.4290 |  0.4450 |
| cA    |  0.3810 |  0.3910 |
| d     |  0.4170 |  0.4490 |
| dA    |  0.3570 |  0.4400 |
| e     |  0.3810 |  0.4410 |
| eA    |  0.3570 |  0.4220 |
| f     |  0.3810 |  0.4550 |
| fA    |  0.3810 |  0.4560 |
| g     |  0.4170 |  0.4590 |
| gA    |  0.3450 |  0.3690 |
| h     |  0.4290 |  0.4500 |
| hA    |  0.3690 |  0.4140 |
| i     |  0.4410 |  0.4660 |
| iA    |  0.4170 |  0.4540 |
| j     |  0.4290 |  0.4170 |
| jA    |  0.3930 |  0.3680 |
| k     |  0.4050 |  0.3840 |
| kA    |  0.3810 |  0.4440 |
| l     |  0.5000 |  0.4560 |
| lA    |  0.3810 |  0.3960 |
| m     |  0.5120 |  0.4470 |
| mA    |  0.3690 |  0.4550 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| n     |  0.4290   |  0.4070   |
| nA    |  0.3810   |  0.3840   |
| o     |  0.5000   |  0.4560   |
| oA    |  0.3570   |  0.4040   |
| p     |  0.5120   |  0.4470   |
| pA    |  0.4170   |  0.4580   |
| q     |  0.4170   |  0.4150   |
| qA    |  0.3930   |  0.3860   |
| r     |  0.4410   |  0.3930   |
| rA    |  0.3930   |  0.4360   |
| s     |  0.5000   |  0.4430   |
| sA    |  0.3570   |  0.4020   |
| t     |  0.4640   |  0.4350   |
| tA    |  0.3690   |  0.4600   |
| u     |  0.4410   |  0.3940   |
| uA    |  0.3330   |  0.3710   |
| v     |  0.5000   |  0.4390   |
| vA    |  0.3690   |  0.4240   |
| w     |  0.5360  |  0.4180  |
| wA    |  0.3810 |  0.4590 |
| x     |  0.4290 |  0.4060 |
| xA    |  0.3810 |  0.3930 |
| y     |  0.4520 |  0.3930 |
| yA    |  0.3570 |  0.4460 |
| z     |  0.4640 |  0.4490 |
| zA    |  0.3450 |  0.4120 |