



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 08:49 PM EDT

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

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>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

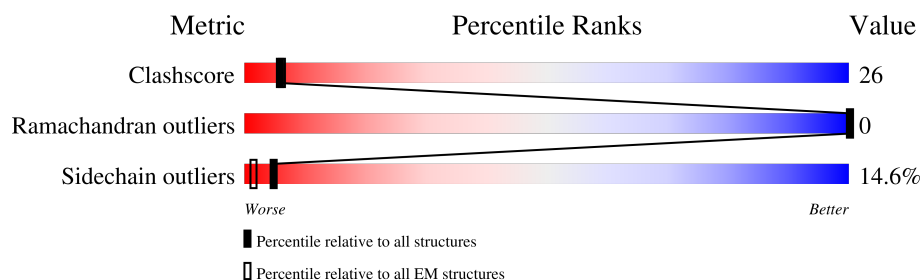
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 ≥ 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> |
| 1 | 2 | 8 | <div> <div>12%</div> <div>62%</div> <div>25%</div> <div>12%</div> </div> |
| 1 | 2A | 8 | <div> <div>62%</div> <div>12%</div> <div>62%</div> <div>25%</div> </div> |
| 1 | 3 | 8 | <div> <div>38%</div> <div>50%</div> <div>50%</div> </div> |
| 1 | 3A | 8 | <div> <div>62%</div> <div>25%</div> <div>75%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 1 | D | 8 | |
| 1 | DA | 8 | |
| 1 | DB | 8 | |
| 1 | E | 8 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 1 | LA | 8 | |
| 1 | LB | 8 | |
| 1 | M | 8 | |
| 1 | MA | 8 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 1 | TB | 8 | |
| 1 | U | 8 | |
| 1 | UA | 8 | |
| 1 | V | 8 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 1 | g | 8 | |
| 1 | gA | 8 | |
| 1 | h | 8 | |
| 1 | hA | 8 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 1 | sA | 8 | |
| 1 | t | 8 | |
| 1 | tA | 8 | |
| 1 | u | 8 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | - |
| 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 | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 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 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | Y | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | Z | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | j | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | k | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | l | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | m | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | D | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | n | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | o | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | p | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | q | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | r | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | s | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | t | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | E | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | u | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | v | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | w | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | x | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | y | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|---------|-------|
| 1 | z | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 0 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | F | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 1 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 2 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 3 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 4 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 5 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 6 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 7 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | G | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 8 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | 9 | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | AA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | BA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | CA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | DA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | EA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | H | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | FA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | GA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |

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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 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | aA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | bA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | cA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | dA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | eA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | fA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | gA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | c | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | hA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | iA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | jA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | kA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | lA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | mA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | nA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | d | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | oA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | pA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | qA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |
| 1 | rA | 8 | Total 84 | C 60 | N 11 | O 13 | 0 | 0 |

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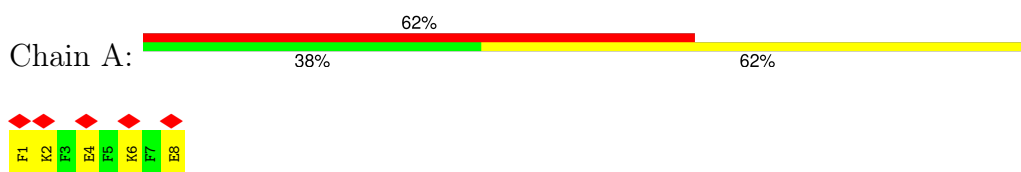
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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 1 | TB | 8 | Total | C | N | O | 0 | 0 |
| | | | 84 | 60 | 11 | 13 | | |

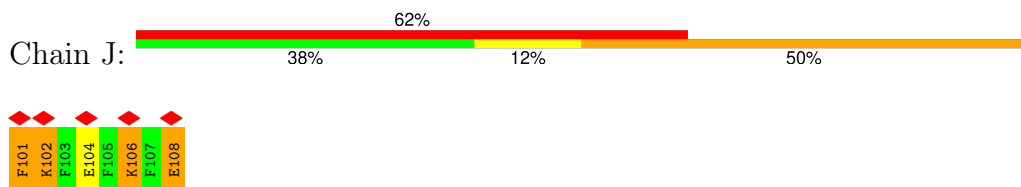
3 Residue-property plots [i](#)

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.

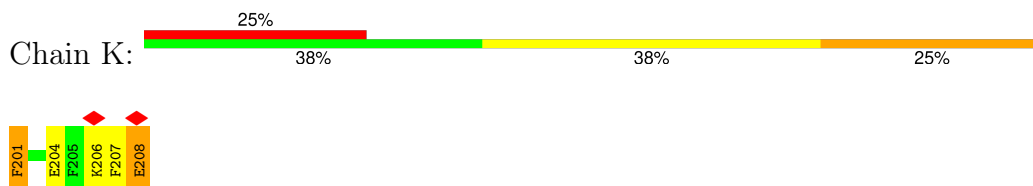
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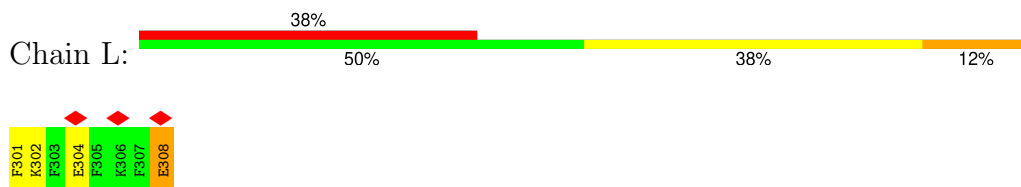
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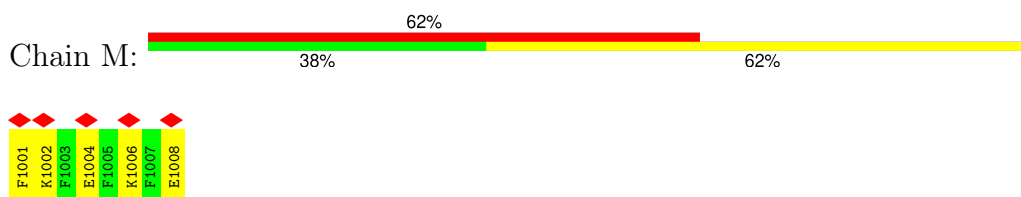
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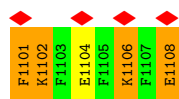
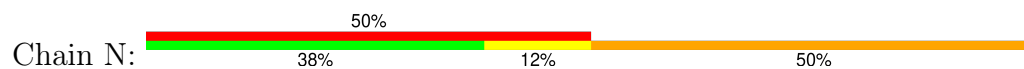
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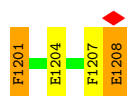
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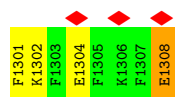
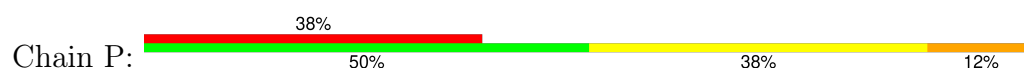
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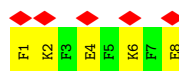
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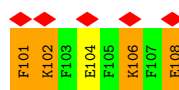
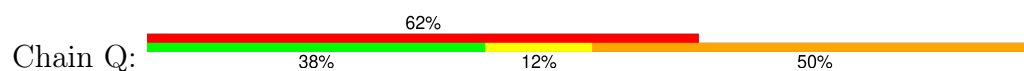
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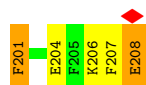
● Molecule 1: KFE8 peptide



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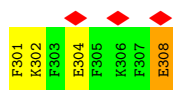


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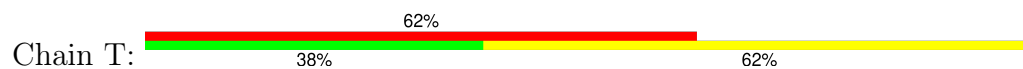


● Molecule 1: KFE8 peptide





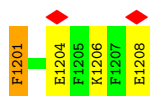
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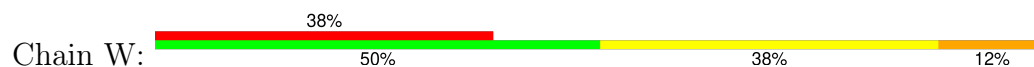
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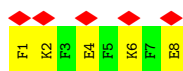
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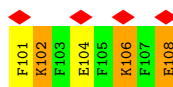
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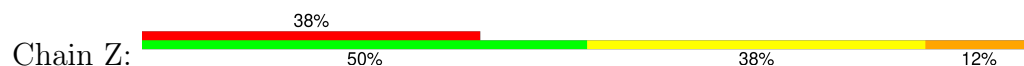
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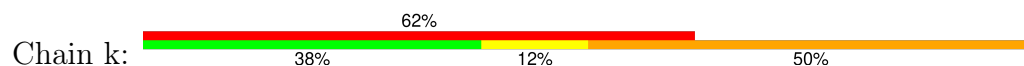
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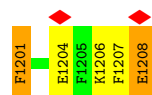
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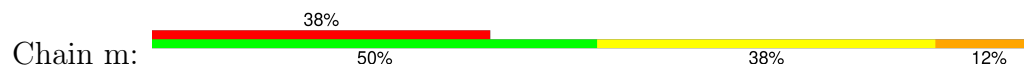
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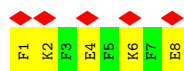


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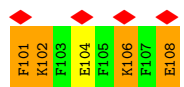
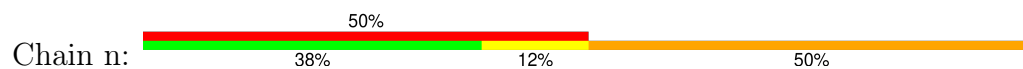


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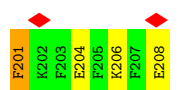




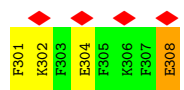
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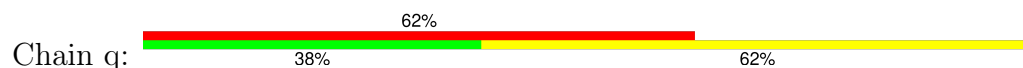
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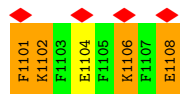
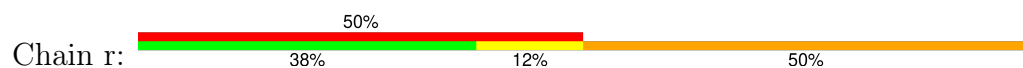
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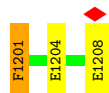
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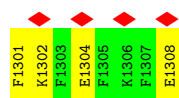
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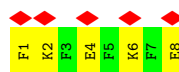
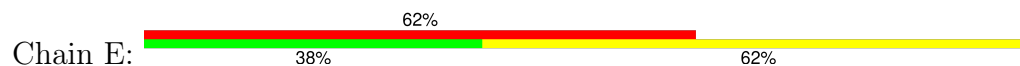
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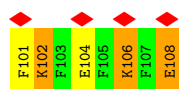
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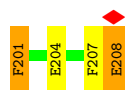
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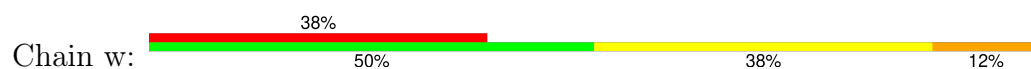
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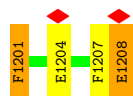


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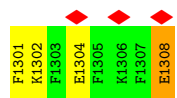
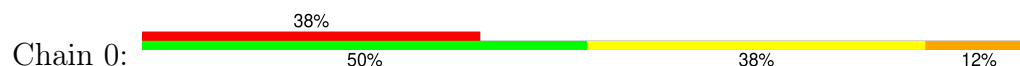




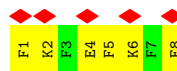
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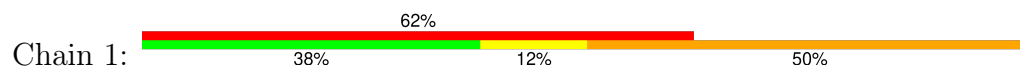
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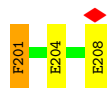
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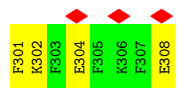
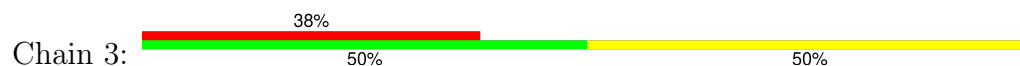
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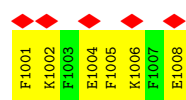
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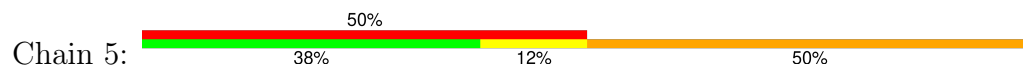
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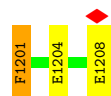
- Molecule 1: KFE8 peptide



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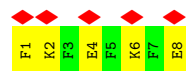
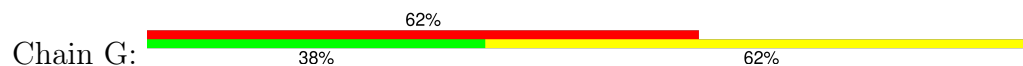
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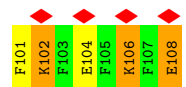
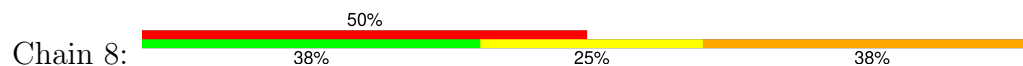
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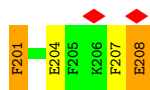


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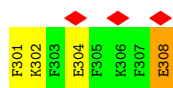
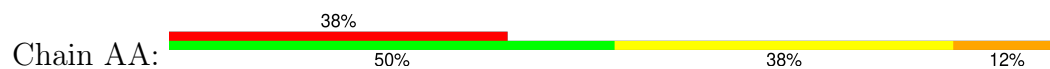


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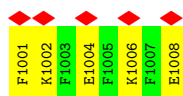




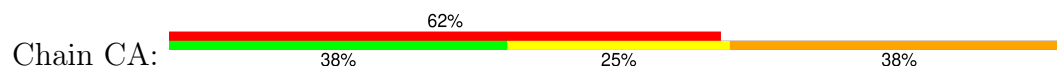
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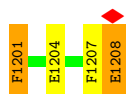
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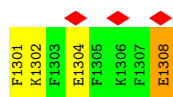
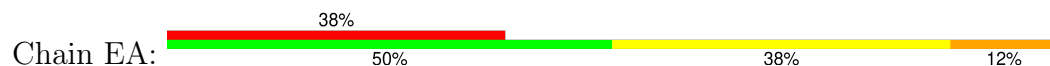
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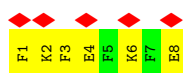
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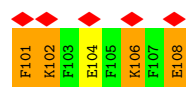
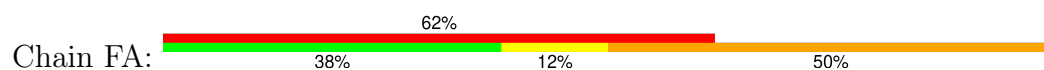
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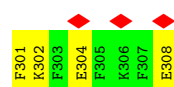
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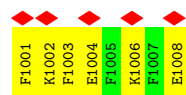
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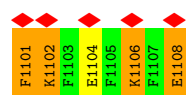
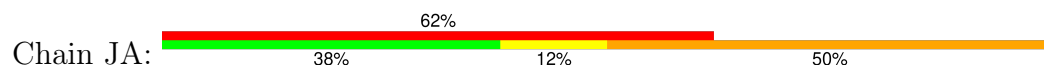
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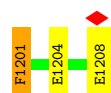
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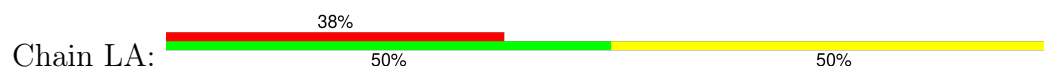
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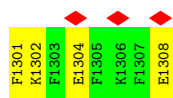


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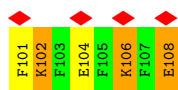




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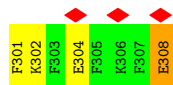
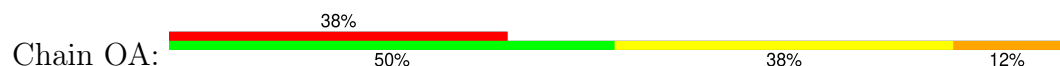
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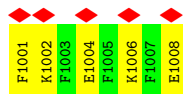
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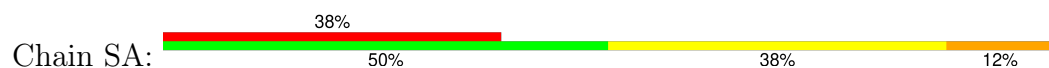
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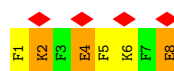
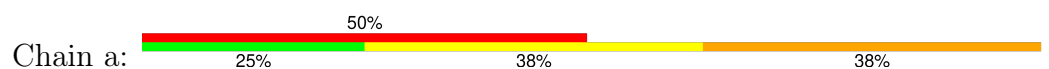
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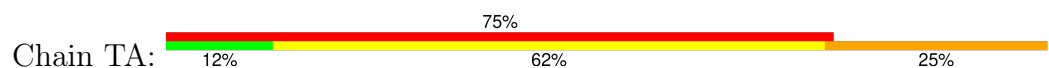
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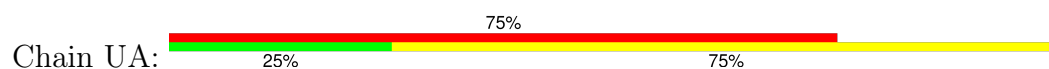
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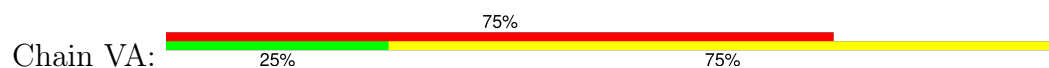
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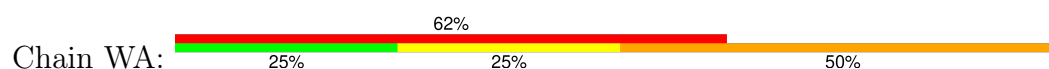
- Molecule 1: KFE8 peptide



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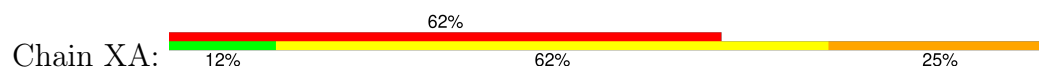


- Molecule 1: KFE8 peptide

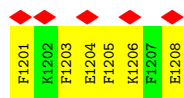




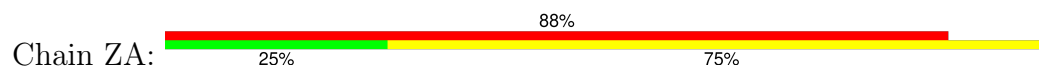
- Molecule 1: KFE8 peptide



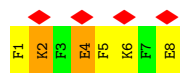
- Molecule 1: KFE8 peptide



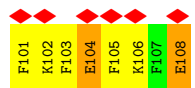
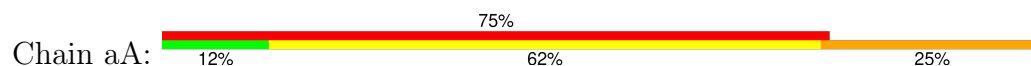
- Molecule 1: KFE8 peptide



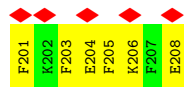
- Molecule 1: KFE8 peptide



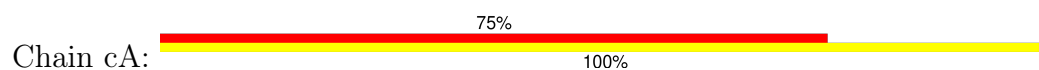
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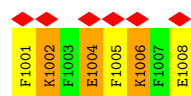
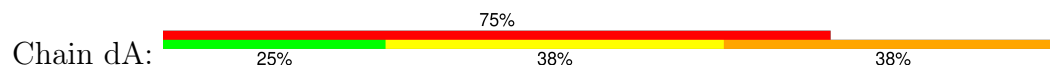
- Molecule 1: KFE8 peptide



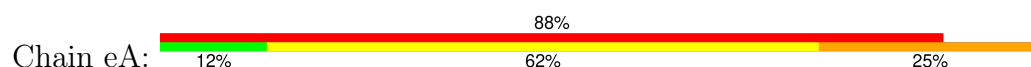
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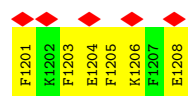
- Molecule 1: KFE8 peptide



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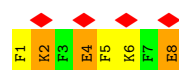
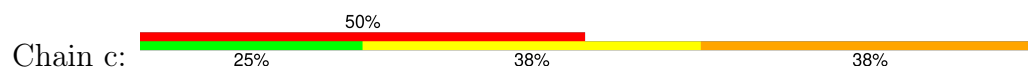
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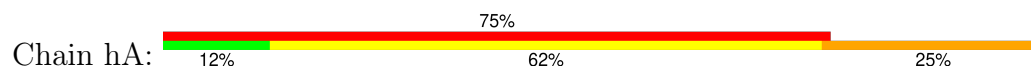
- Molecule 1: KFE8 peptide



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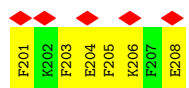


- Molecule 1: KFE8 peptide

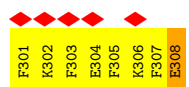
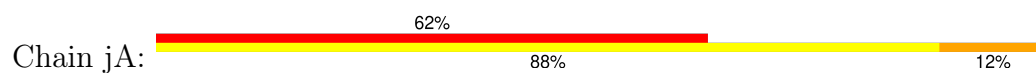




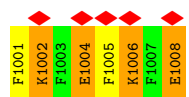
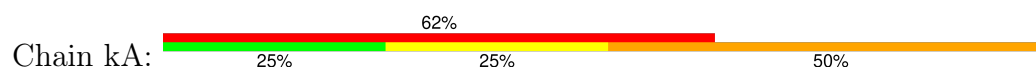
- Molecule 1: KFE8 peptide



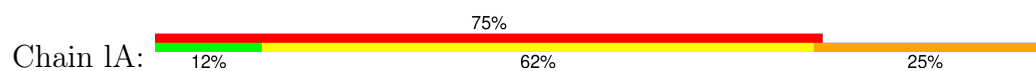
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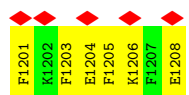
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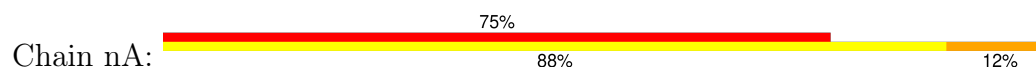
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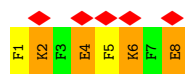
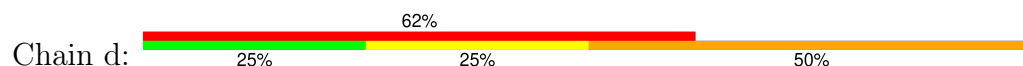
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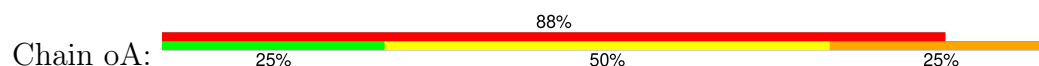
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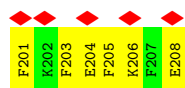
• Molecule 1: KFE8 peptide



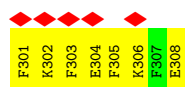
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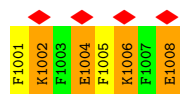
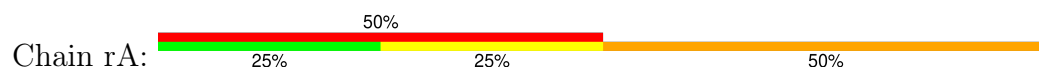
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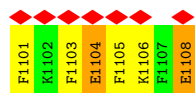
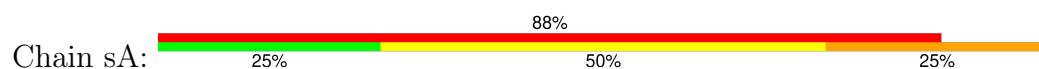
• Molecule 1: KFE8 peptide



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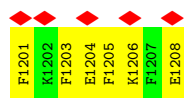


• Molecule 1: KFE8 peptide



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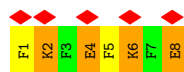




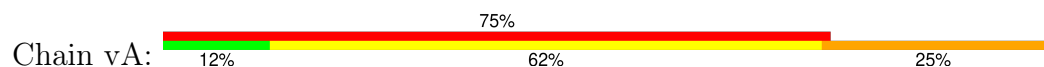
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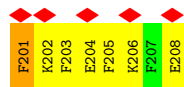
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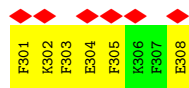
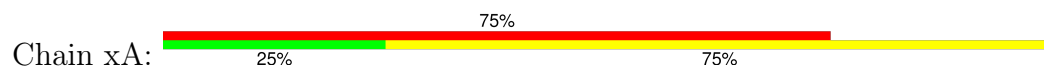
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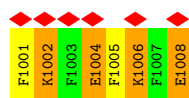
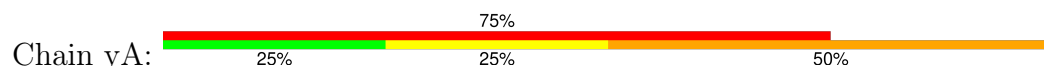
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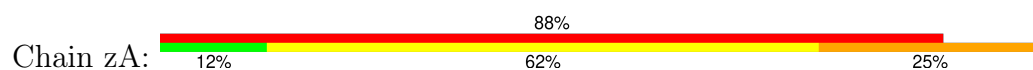
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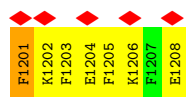
- Molecule 1: KFE8 peptide



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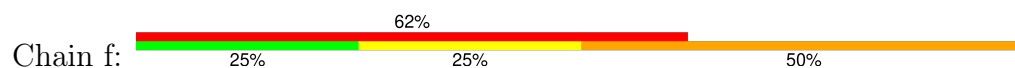
- Molecule 1: KFE8 peptide



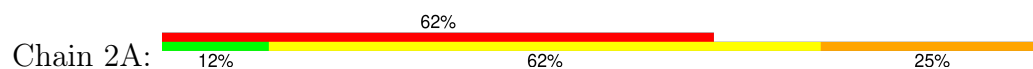
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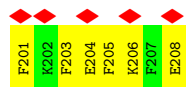
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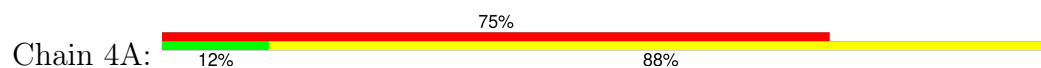
- Molecule 1: KFE8 peptide



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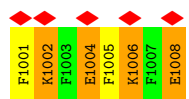
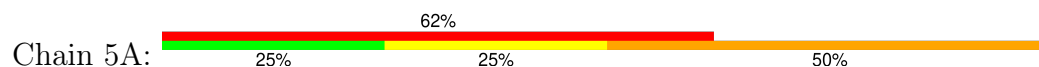


- Molecule 1: KFE8 peptide

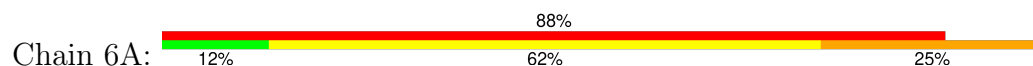




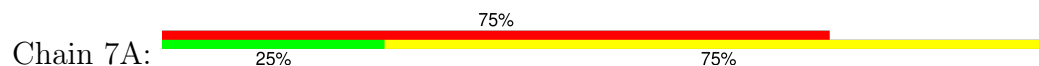
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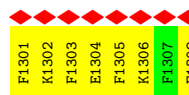
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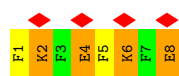
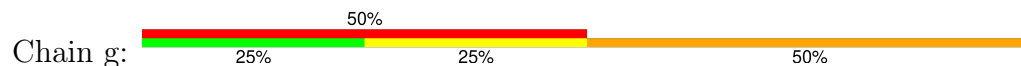
- Molecule 1: KFE8 peptide



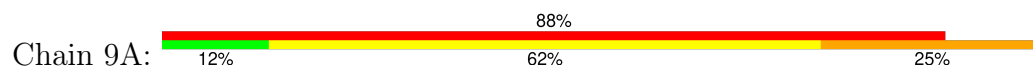
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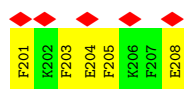
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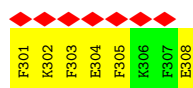
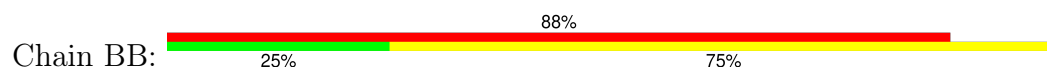
- Molecule 1: KFE8 peptide



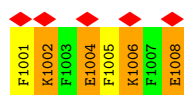
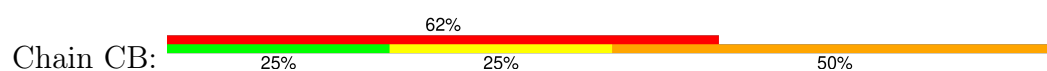
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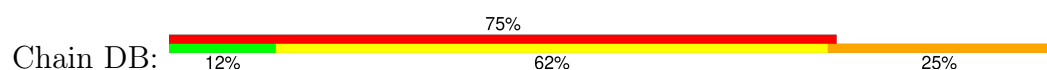
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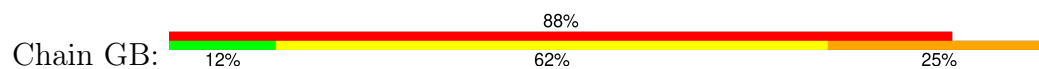


- Molecule 1: KFE8 peptide





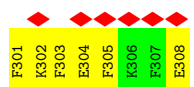
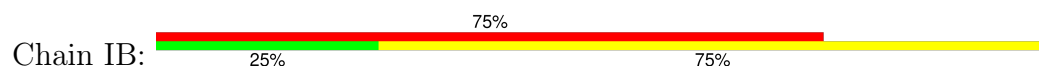
- Molecule 1: KFE8 peptide



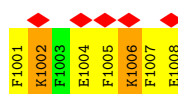
- Molecule 1: KFE8 peptide



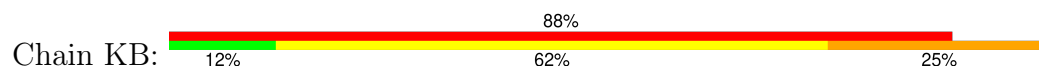
- Molecule 1: KFE8 peptide



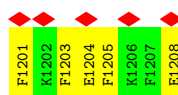
- Molecule 1: KFE8 peptide



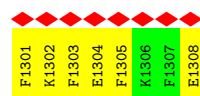
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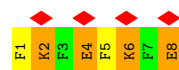
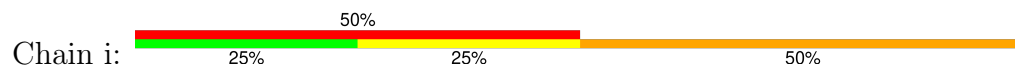
- Molecule 1: KFE8 peptide



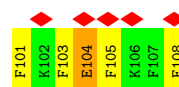
- Molecule 1: KFE8 peptide



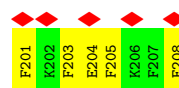
- Molecule 1: KFE8 peptide



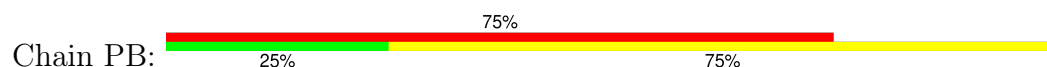
- Molecule 1: KFE8 peptide



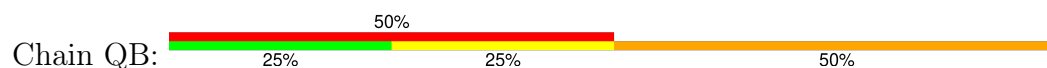
- Molecule 1: KFE8 peptide



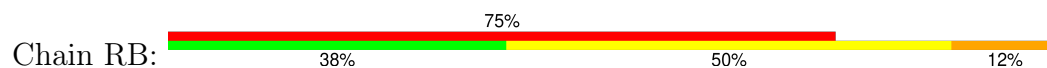
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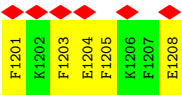
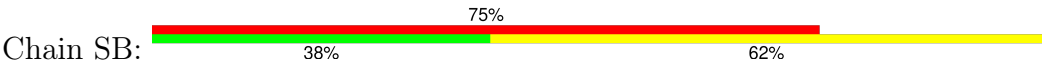


- Molecule 1: KFE8 peptide

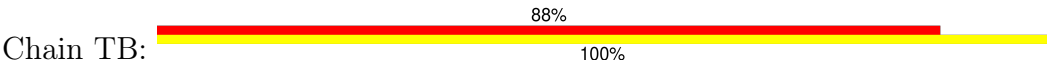




● Molecule 1: KFE8 peptide



● Molecule 1: KFE8 peptide



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 | 7 |
| 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 | 7 |
| 1 | 3 | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | 7 | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |

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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 | 7 |
| 1 | A | 6/6 (100%) | 6 (100%) | 0 | 100 | 100 |
| 1 | AA | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | E | 6/6 (100%) | 6 (100%) | 0 | 100 | 100 |
| 1 | EA | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | H | 6/6 (100%) | 6 (100%) | 0 | 100 | 100 |
| 1 | HA | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | L | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 1 | LA | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | O | 6/6 (100%) | 6 (100%) | 0 | 100 | 100 |
| 1 | OA | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 1 | OB | 6/6 (100%) | 6 (100%) | 0 | 100 | 100 |
| 1 | P | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | S | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 1 | SA | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 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 | 7 |
| 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 | 7 |
| 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 | 7 |
| 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 | 7 |
| 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 | 7 |
| 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 | 7 |

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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 | 7 |
| 1 | m | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | p | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | t | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| 1 | w | 6/6 (100%) | 5 (83%) | 1 (17%) | 2 | 7 |
| 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 | 7 |
| All | All | 864/864 (100%) | 738 (85%) | 126 (15%) | 5 | 10 |

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 | Z | 301 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.16 | 2 (12%) |
| 1 | 5CR | 9 | 201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.32 | 3 (18%) |
| 1 | GMA | oA | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | GMA | 8A | 1308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.32 | 0 |
| 1 | GMA | zA | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.19 | 0 |
| 1 | GMA | FB | 1308 | 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%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5CR | x | 1001 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | GMA | I | 8 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.28 | 1 (10%) |
| 1 | GMA | S | 308 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | GMA | f | 8 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | 5CR | FB | 1301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.94 | 1 (6%) |
| 1 | 5CR | K | 201 | 1 | 13,14,15 | 1.31 | 1 (7%) | 16,17,19 | 1.32 | 3 (18%) |
| 1 | GMA | T | 1008 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.27 | 1 (10%) |
| 1 | GMA | W | 1308 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | GMA | OB | 208 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.14 | 0 |
| 1 | 5CR | XA | 1101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.08 | 1 (6%) |
| 1 | 5CR | mA | 1201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | P | 1308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | 5CR | TA | 101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.08 | 1 (6%) |
| 1 | 5CR | QB | 1001 | 1 | 13,14,15 | 1.34 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | 5CR | v | 201 | 1 | 13,14,15 | 1.31 | 1 (7%) | 16,17,19 | 1.33 | 2 (12%) |
| 1 | 5CR | 4 | 1001 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | GMA | iA | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | e | 8 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | 5CR | M | 1001 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.57 | 2 (12%) |
| 1 | 5CR | Y | 201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | 5CR | HA | 301 | 1 | 13,14,15 | 1.27 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | 5CR | KB | 1101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.06 | 1 (6%) |
| 1 | GMA | G | 8 | 1 | 9,9,9 | 1.17 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | 5CR | GA | 201 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | GMA | wA | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.14 | 0 |
| 1 | GMA | TB | 1308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | 5CR | R | 201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.33 | 2 (12%) |
| 1 | GMA | KA | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.28 | 2 (20%) |
| 1 | GMA | 3 | 308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | 5CR | dA | 1001 | 1 | 13,14,15 | 1.34 | 2 (15%) | 16,17,19 | 1.71 | 3 (18%) |
| 1 | 5CR | MA | 101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | 5CR | OA | 301 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | GMA | k | 1108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.23 | 0 |
| 1 | GMA | FA | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.25 | 1 (10%) |
| 1 | GMA | WA | 1008 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.15 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | GMA | pA | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | BB | 308 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.33 | 0 |
| 1 | GMA | n | 108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.24 | 1 (10%) |
| 1 | GMA | H | 8 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | 5CR | y | 1101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |
| 1 | GMA | eA | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.21 | 0 |
| 1 | 5CR | 2 | 201 | 1 | 13,14,15 | 1.32 | 2 (15%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | GMA | mA | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | KB | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | GMA | GB | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | 5CR | MB | 1301 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 0.94 | 1 (6%) |
| 1 | 5CR | DA | 1201 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.32 | 3 (18%) |
| 1 | GMA | V | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.27 | 1 (10%) |
| 1 | GMA | TA | 108 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | GMA | Y | 208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.28 | 2 (20%) |
| 1 | 5CR | G | 1 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.57 | 2 (12%) |
| 1 | GMA | vA | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.19 | 0 |
| 1 | 5CR | 0 | 1301 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | 5CR | c | 1 | 1 | 13,14,15 | 1.34 | 2 (15%) | 16,17,19 | 1.69 | 3 (18%) |
| 1 | 5CR | xA | 301 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 0.95 | 1 (6%) |
| 1 | 5CR | QA | 1101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | GMA | qA | 308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.33 | 0 |
| 1 | 5CR | OB | 201 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | a | 8 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | dA | 1008 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | 5CR | g | 1 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | GMA | GA | 208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.28 | 2 (20%) |
| 1 | GMA | fA | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.12 | 0 |
| 1 | GMA | SA | 1308 | 1 | 9,9,9 | 1.22 | 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 | JB | 1008 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | B | 1 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.57 | 2 (12%) |
| 1 | 5CR | 2A | 101 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | 5CR | CB | 1001 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | GMA | r | 1108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.23 | 1 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5CR | X | 101 | 1 | 13,14,15 | 1.31 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | GMA | CA | 1108 | 1 | 9,9,9 | 1.17 | 1 (11%) | 10,11,11 | 1.22 | 0 |
| 1 | 5CR | V | 1201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | GMA | RA | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.29 | 2 (20%) |
| 1 | GMA | 2A | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.18 | 0 |
| 1 | GMA | HB | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | uA | 1301 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 0.92 | 1 (6%) |
| 1 | 5CR | vA | 101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.09 | 1 (6%) |
| 1 | 5CR | J | 101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |
| 1 | 5CR | YA | 1201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | LB | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | L | 301 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | GMA | m | 1308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | 5CR | a | 1 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.71 | 3 (18%) |
| 1 | GMA | z | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.27 | 1 (10%) |
| 1 | GMA | IA | 1008 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | GMA | NA | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.29 | 2 (20%) |
| 1 | GMA | X | 108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.23 | 0 |
| 1 | 5CR | N | 1101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |
| 1 | GMA | gA | 1308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | GMA | 1A | 1308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.33 | 0 |
| 1 | 5CR | nA | 1301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.93 | 1 (6%) |
| 1 | 5CR | zA | 1101 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.08 | 1 (6%) |
| 1 | 5CR | BB | 301 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 0.94 | 1 (6%) |
| 1 | GMA | x | 1008 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | 5CR | oA | 101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | GMA | b | 8 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.17 | 0 |
| 1 | 5CR | j | 1001 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | GMA | EB | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.14 | 0 |
| 1 | GMA | CB | 1008 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | o | 1308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.24 | 0 |
| 1 | GMA | p | 308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.24 | 0 |
| 1 | GMA | D | 8 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | GMA | QB | 1008 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | 5CR | CA | 1101 | 1 | 13,14,15 | 1.31 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5CR | JA | 1101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | 5CR | r | 1101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | GMA | j | 1008 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | 5CR | cA | 301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.92 | 1 (6%) |
| 1 | 5CR | o | 201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | 5CR | C | 1 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | 5CR | f | 1 | 1 | 13,14,15 | 1.34 | 2 (15%) | 16,17,19 | 1.71 | 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 |
| 1 | 5CR | ZA | 1301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.93 | 1 (6%) |
| 1 | 5CR | jA | 301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.93 | 1 (6%) |
| 1 | 5CR | wA | 201 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.13 | 1 (6%) |
| 1 | 5CR | EB | 1201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | M | 1008 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | 5CR | RB | 1101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | 5CR | kA | 1001 | 1 | 13,14,15 | 1.34 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | 5CR | S | 301 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | 5CR | 6A | 1101 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | GMA | uA | 1308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.33 | 0 |
| 1 | 5CR | O | 1201 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.32 | 3 (18%) |
| 1 | 5CR | p | 301 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | 5CR | AB | 201 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | U | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.24 | 1 (10%) |
| 1 | 5CR | w | 301 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | GMA | t | 1308 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | 5CR | WA | 1001 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.71 | 3 (18%) |
| 1 | GMA | VA | 308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | GMA | ZA | 1308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | GMA | UA | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | J | 108 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.24 | 1 (10%) |
| 1 | GMA | C | 8 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | 5CR | A | 1 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.57 | 2 (12%) |
| 1 | GMA | i | 8 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.17 | 0 |
| 1 | 5CR | 9A | 101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.08 | 1 (6%) |
| 1 | 5CR | 6 | 1201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.33 | 3 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5CR | yA | 1001 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | GMA | l | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.28 | 2 (20%) |
| 1 | GMA | o | 208 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | GMA | tA | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.14 | 0 |
| 1 | GMA | cA | 308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | GMA | yA | 1008 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.17 | 0 |
| 1 | 5CR | H | 1 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | GMA | w | 308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.24 | 0 |
| 1 | GMA | A | 8 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | GMA | kA | 1008 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | DB | 1101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | GMA | AB | 208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | JB | 1001 | 1 | 13,14,15 | 1.34 | 2 (15%) | 16,17,19 | 1.71 | 3 (18%) |
| 1 | 5CR | IB | 301 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 0.93 | 1 (6%) |
| 1 | 5CR | PB | 301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.94 | 1 (6%) |
| 1 | GMA | XA | 1108 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | 5CR | 7 | 1301 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | 5CR | 3A | 201 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.11 | 1 (6%) |
| 1 | GMA | q | 1008 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | 5CR | s | 1201 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.34 | 3 (18%) |
| 1 | 5CR | HB | 201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | NB | 108 | 1 | 9,9,9 | 1.17 | 1 (11%) | 10,11,11 | 1.18 | 0 |
| 1 | 5CR | 3 | 301 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | GMA | RB | 1108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.18 | 0 |
| 1 | 5CR | PA | 1001 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.58 | 2 (12%) |
| 1 | GMA | hA | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.19 | 0 |
| 1 | GMA | l | 108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.23 | 1 (10%) |
| 1 | 5CR | SB | 1201 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | MB | 1308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | GMA | d | 8 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | GMA | PA | 1008 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.28 | 1 (10%) |
| 1 | 5CR | IA | 1001 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | 5CR | e | 1 | 1 | 13,14,15 | 1.36 | 2 (15%) | 16,17,19 | 1.69 | 3 (18%) |
| 1 | 5CR | 0A | 1201 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | 5CR | 8A | 1301 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 0.93 | 1 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5CR | EA | 1301 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | GMA | 7 | 1308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | GMA | 8 | 108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.23 | 0 |
| 1 | GMA | DA | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.29 | 2 (20%) |
| 1 | GMA | lA | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.19 | 0 |
| 1 | 5CR | GB | 101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.06 | 1 (6%) |
| 1 | GMA | 5 | 1108 | 1 | 9,9,9 | 1.17 | 1 (11%) | 10,11,11 | 1.23 | 1 (10%) |
| 1 | GMA | AA | 308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | 5CR | U | 1101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.48 | 2 (12%) |
| 1 | 5CR | 7A | 1201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | SB | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.13 | 0 |
| 1 | GMA | O | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | GMA | sA | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.19 | 0 |
| 1 | 5CR | hA | 101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.08 | 1 (6%) |
| 1 | 5CR | 1 | 101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | GMA | IB | 308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.35 | 0 |
| 1 | 5CR | FA | 101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | 5CR | F | 1 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | 5CR | TB | 1301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.94 | 1 (6%) |
| 1 | GMA | DB | 1108 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | 5CR | t | 1301 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | GMA | Z | 308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | GMA | OA | 308 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | 5CR | d | 1 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | GMA | 0A | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | N | 1108 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.25 | 1 (10%) |
| 1 | 5CR | tA | 1201 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | 5CR | D | 1 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | 5CR | k | 1101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |
| 1 | GMA | 6A | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.19 | 0 |
| 1 | 5CR | 8 | 101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |
| 1 | 5CR | u | 101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | GMA | 7A | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | LA | 1308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | GMA | s | 1208 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.27 | 1 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | GMA | YA | 1208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | 2 | 208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.27 | 1 (10%) |
| 1 | 5CR | 4A | 301 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 0.93 | 1 (6%) |
| 1 | GMA | nA | 1308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.34 | 0 |
| 1 | 5CR | VA | 301 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 0.92 | 1 (6%) |
| 1 | GMA | 4 | 1008 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.28 | 1 (10%) |
| 1 | 5CR | n | 101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.46 | 2 (12%) |
| 1 | GMA | EA | 1308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | 5CR | fA | 1201 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.11 | 1 (6%) |
| 1 | 5CR | BA | 1001 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.57 | 2 (12%) |
| 1 | 5CR | sA | 1101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | 5CR | i | 1 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.69 | 3 (18%) |
| 1 | GMA | L | 308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | GMA | QA | 1108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.24 | 1 (10%) |
| 1 | 5CR | lA | 1101 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.09 | 1 (6%) |
| 1 | 5CR | b | 1 | 1 | 13,14,15 | 1.33 | 2 (15%) | 16,17,19 | 1.71 | 3 (18%) |
| 1 | GMA | Q | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.24 | 1 (10%) |
| 1 | GMA | h | 8 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.14 | 0 |
| 1 | 5CR | I | 1 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.58 | 2 (12%) |
| 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 | 5CR | 5A | 1001 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.71 | 3 (18%) |
| 1 | GMA | PB | 308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.33 | 0 |
| 1 | GMA | bA | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.13 | 0 |
| 1 | 5CR | rA | 1001 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | GMA | MA | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.24 | 0 |
| 1 | 5CR | iA | 201 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | 5CR | h | 1 | 1 | 13,14,15 | 1.35 | 2 (15%) | 16,17,19 | 1.70 | 3 (18%) |
| 1 | GMA | K | 208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | GMA | c | 8 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | GMA | g | 8 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | 5CR | q | 1001 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |
| 1 | 5CR | Q | 101 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.48 | 2 (12%) |
| 1 | 5CR | SA | 1301 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | 5CR | gA | 1301 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 0.94 | 1 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | GMA | F | 8 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | GMA | 3A | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | eA | 1101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | GMA | xA | 308 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.33 | 0 |
| 1 | 5CR | NB | 101 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | GMA | y | 1108 | 1 | 9,9,9 | 1.18 | 1 (11%) | 10,11,11 | 1.23 | 0 |
| 1 | GMA | HA | 308 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.25 | 0 |
| 1 | 5CR | bA | 201 | 1 | 13,14,15 | 1.28 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | v | 208 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | GMA | B | 8 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.26 | 0 |
| 1 | 5CR | l | 1201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | 5CR | qA | 301 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 0.92 | 1 (6%) |
| 1 | GMA | R | 208 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.28 | 1 (10%) |
| 1 | GMA | 9 | 208 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.29 | 2 (20%) |
| 1 | GMA | 5A | 1008 | 1 | 9,9,9 | 1.24 | 1 (11%) | 10,11,11 | 1.16 | 0 |
| 1 | 5CR | m | 1301 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.16 | 2 (12%) |
| 1 | GMA | 6 | 1208 | 1 | 9,9,9 | 1.22 | 1 (11%) | 10,11,11 | 1.27 | 1 (10%) |
| 1 | GMA | 9A | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.20 | 0 |
| 1 | 5CR | RA | 1201 | 1 | 13,14,15 | 1.31 | 1 (7%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | GMA | rA | 1008 | 1 | 9,9,9 | 1.23 | 1 (11%) | 10,11,11 | 1.15 | 0 |
| 1 | 5CR | aA | 101 | 1 | 13,14,15 | 1.27 | 1 (7%) | 16,17,19 | 1.07 | 1 (6%) |
| 1 | 5CR | pA | 201 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | 5CR | UA | 201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | GMA | jA | 308 | 1 | 9,9,9 | 1.20 | 1 (11%) | 10,11,11 | 1.35 | 0 |
| 1 | 5CR | AA | 301 | 1 | 13,14,15 | 1.29 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | 5CR | KA | 1201 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | 5CR | LB | 1201 | 1 | 13,14,15 | 1.29 | 1 (7%) | 16,17,19 | 1.12 | 1 (6%) |
| 1 | 5CR | 5 | 1101 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.47 | 2 (12%) |
| 1 | 5CR | LA | 1301 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.17 | 2 (12%) |
| 1 | 5CR | NA | 201 | 1 | 13,14,15 | 1.30 | 1 (7%) | 16,17,19 | 1.33 | 3 (18%) |
| 1 | 5CR | T | 1001 | 1 | 13,14,15 | 1.30 | 2 (15%) | 16,17,19 | 1.57 | 2 (12%) |
| 1 | GMA | E | 8 | 1 | 9,9,9 | 1.21 | 1 (11%) | 10,11,11 | 1.27 | 0 |
| 1 | GMA | aA | 108 | 1 | 9,9,9 | 1.19 | 1 (11%) | 10,11,11 | 1.22 | 0 |
| 1 | 5CR | W | 1301 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.18 | 2 (12%) |
| 1 | 5CR | z | 1201 | 1 | 13,14,15 | 1.31 | 2 (15%) | 16,17,19 | 1.32 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5CR | E | 1 | 1 | 13,14,15 | 1.28 | 2 (15%) | 16,17,19 | 1.56 | 2 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | 5CR | Z | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 9 | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | oA | 108 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | 8A | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | zA | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | FB | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | P | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | x | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | I | 8 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | S | 308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | f | 8 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | FB | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | K | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | T | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | W | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | OB | 208 | 1 | - | 4/9/9/9 | - |
| 1 | 5CR | XA | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | mA | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | P | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | TA | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | QB | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | 5CR | v | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 4 | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | iA | 208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | e | 8 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | M | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | Y | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | HA | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | KB | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | G | 8 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | GA | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | GMA | wA | 208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | TB | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | R | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | KA | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 3 | 308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | dA | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | 5CR | MA | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | OA | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | k | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | FA | 108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | WA | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | GMA | pA | 208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | BB | 308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | n | 108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | H | 8 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | y | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | eA | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | 2 | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | mA | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | KB | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | GB | 108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | MB | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | DA | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | V | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | TA | 108 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | Y | 208 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | G | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | vA | 108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | 0 | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | c | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | 5CR | xA | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | QA | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | qA | 308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | OB | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | a | 8 | 1 | - | 8/9/9/9 | - |
| 1 | GMA | dA | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | g | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | GMA | GA | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | fA | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | SA | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | u | 108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | JB | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | B | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 2A | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | CB | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | r | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | X | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | CA | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | V | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | RA | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 2A | 108 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | HB | 208 | 1 | - | 4/9/9/9 | - |
| 1 | 5CR | uA | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | vA | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | J | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | YA | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | LB | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | 5CR | L | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | m | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | a | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | z | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | IA | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | NA | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | X | 108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | N | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | gA | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | 1A | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | nA | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | zA | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | BB | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | x | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | oA | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | b | 8 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | j | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | GMA | EB | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | CB | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | GMA | 0 | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | p | 308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | D | 8 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | QB | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | CA | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | JA | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | r | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | j | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | cA | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | o | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | C | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | f | 1 | 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 | ZA | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | jA | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | wA | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | EB | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | M | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | RB | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | kA | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | 5CR | S | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 6A | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | uA | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | O | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | p | 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 | U | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | w | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | t | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | WA | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | VA | 308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | ZA | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | UA | 208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | J | 108 | 1 | - | 2/9/9/9 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | GMA | C | 8 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | A | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | i | 8 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | 9A | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 6 | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | yA | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | l | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | o | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | tA | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | cA | 308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | yA | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | H | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | w | 308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | A | 8 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | kA | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | DB | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | AB | 208 | 1 | - | 4/9/9/9 | - |
| 1 | 5CR | JB | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | 5CR | IB | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | PB | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | XA | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | 7 | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 3A | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | q | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | s | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | HB | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | NB | 108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | 3 | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | RB | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | PA | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | hA | 108 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | 1 | 108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | SB | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | MB | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | d | 8 | 1 | - | 8/9/9/9 | - |
| 1 | GMA | PA | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | IA | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | e | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | 5CR | 0A | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 8A | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | EA | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | 7 | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 8 | 108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | DA | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | lA | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | GB | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | 5 | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | AA | 308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | U | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 7A | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | SB | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | O | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | sA | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | hA | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 1 | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | IB | 308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | FA | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | F | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | TB | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | DB | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | t | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | Z | 308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | OA | 308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | d | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | 0A | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | N | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | tA | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | D | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | k | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | 6A | 1108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | 8 | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | u | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | 7A | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | LA | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | s | 1208 | 1 | - | 1/9/9/9 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | GMA | YA | 1208 | 1 | - | 4/9/9/9 | - |
| 1 | GMA | 2 | 208 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | 4A | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | nA | 1308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | VA | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | 4 | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | n | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | EA | 1308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | fA | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | BA | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | sA | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | i | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | L | 308 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | QA | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | lA | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | b | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | Q | 108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | h | 8 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | I | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 1A | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | BA | 1008 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | 5A | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | PB | 308 | 1 | - | 0/9/9/9 | - |
| 1 | GMA | bA | 208 | 1 | - | 4/9/9/9 | - |
| 1 | 5CR | rA | 1001 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | MA | 108 | 1 | - | 2/9/9/9 | - |
| 1 | 5CR | iA | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | h | 1 | 1 | - | 6/9/10/12 | 0/1/1/1 |
| 1 | GMA | K | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | c | 8 | 1 | - | 8/9/9/9 | - |
| 1 | GMA | g | 8 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | q | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | 5CR | Q | 101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | SA | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | gA | 1301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | F | 8 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 3A | 208 | 1 | - | 4/9/9/9 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | 5CR | eA | 1101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | xA | 308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | NB | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | GMA | y | 1108 | 1 | - | 2/9/9/9 | - |
| 1 | GMA | HA | 308 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | bA | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | v | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | B | 8 | 1 | - | 1/9/9/9 | - |
| 1 | 5CR | l | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | qA | 301 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | R | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 9 | 208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 5A | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | m | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | GMA | 6 | 1208 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | 9A | 108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | RA | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | GMA | rA | 1008 | 1 | - | 8/9/9/9 | - |
| 1 | 5CR | aA | 101 | 1 | - | 1/9/10/12 | 0/1/1/1 |
| 1 | 5CR | pA | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | UA | 201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | GMA | jA | 308 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | AA | 301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | KA | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | LB | 1201 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | 5 | 1101 | 1 | - | 2/9/10/12 | 0/1/1/1 |
| 1 | 5CR | LA | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | NA | 201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | T | 1001 | 1 | - | 0/9/10/12 | 0/1/1/1 |
| 1 | GMA | E | 8 | 1 | - | 1/9/9/9 | - |
| 1 | GMA | aA | 108 | 1 | - | 0/9/9/9 | - |
| 1 | 5CR | W | 1301 | 1 | - | 3/9/10/12 | 0/1/1/1 |
| 1 | 5CR | z | 1201 | 1 | - | 4/9/10/12 | 0/1/1/1 |
| 1 | 5CR | E | 1 | 1 | - | 0/9/10/12 | 0/1/1/1 |

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 | 9 | 201 | 5CR | 1 | 0 |
| 1 | oA | 108 | GMA | 1 | 0 |
| 1 | zA | 1108 | GMA | 1 | 0 |
| 1 | S | 308 | GMA | 7 | 0 |
| 1 | f | 8 | GMA | 1 | 0 |
| 1 | K | 201 | 5CR | 1 | 0 |
| 1 | W | 1308 | GMA | 4 | 0 |
| 1 | P | 1308 | GMA | 6 | 0 |
| 1 | v | 201 | 5CR | 1 | 0 |
| 1 | e | 8 | GMA | 1 | 0 |
| 1 | Y | 201 | 5CR | 1 | 0 |
| 1 | GA | 201 | 5CR | 1 | 0 |
| 1 | R | 201 | 5CR | 1 | 0 |
| 1 | k | 1108 | GMA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | FA | 108 | GMA | 1 | 0 |
| 1 | WA | 1008 | GMA | 1 | 0 |
| 1 | n | 108 | GMA | 1 | 0 |
| 1 | eA | 1108 | GMA | 1 | 0 |
| 1 | 2 | 201 | 5CR | 1 | 0 |
| 1 | KB | 1108 | GMA | 1 | 0 |
| 1 | GB | 108 | GMA | 1 | 0 |
| 1 | DA | 1201 | 5CR | 1 | 0 |
| 1 | TA | 108 | GMA | 1 | 0 |
| 1 | Y | 208 | GMA | 3 | 0 |
| 1 | vA | 108 | GMA | 1 | 0 |
| 1 | a | 8 | GMA | 1 | 0 |
| 1 | SA | 1308 | GMA | 6 | 0 |
| 1 | u | 108 | GMA | 1 | 0 |
| 1 | r | 1108 | GMA | 1 | 0 |
| 1 | CA | 1108 | GMA | 1 | 0 |
| 1 | V | 1201 | 5CR | 1 | 0 |
| 1 | RA | 1208 | GMA | 3 | 0 |
| 1 | 2A | 108 | GMA | 1 | 0 |
| 1 | J | 101 | 5CR | 6 | 0 |
| 1 | m | 1308 | GMA | 6 | 0 |
| 1 | z | 1208 | GMA | 2 | 0 |
| 1 | NA | 208 | GMA | 3 | 0 |
| 1 | X | 108 | GMA | 1 | 0 |
| 1 | N | 1101 | 5CR | 6 | 0 |
| 1 | CB | 1008 | GMA | 1 | 0 |
| 1 | 0 | 1308 | GMA | 7 | 0 |
| 1 | p | 308 | GMA | 4 | 0 |
| 1 | QB | 1008 | GMA | 2 | 0 |
| 1 | JA | 1101 | 5CR | 5 | 0 |
| 1 | r | 1101 | 5CR | 6 | 0 |
| 1 | o | 201 | 5CR | 1 | 0 |
| 1 | JA | 1108 | GMA | 1 | 0 |
| 1 | wA | 201 | 5CR | 1 | 0 |
| 1 | O | 1201 | 5CR | 1 | 0 |
| 1 | U | 1108 | GMA | 1 | 0 |
| 1 | J | 108 | GMA | 1 | 0 |
| 1 | i | 8 | GMA | 2 | 0 |
| 1 | 6 | 1201 | 5CR | 1 | 0 |
| 1 | l | 1208 | GMA | 3 | 0 |
| 1 | yA | 1008 | GMA | 1 | 0 |
| 1 | w | 308 | GMA | 7 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | kA | 1008 | GMA | 1 | 0 |
| 1 | XA | 1108 | GMA | 1 | 0 |
| 1 | s | 1201 | 5CR | 1 | 0 |
| 1 | hA | 108 | GMA | 1 | 0 |
| 1 | l | 108 | GMA | 1 | 0 |
| 1 | d | 8 | GMA | 1 | 0 |
| 1 | 0A | 1201 | 5CR | 1 | 0 |
| 1 | 8 | 108 | GMA | 1 | 0 |
| 1 | DA | 1208 | GMA | 3 | 0 |
| 1 | lA | 1108 | GMA | 1 | 0 |
| 1 | 5 | 1108 | GMA | 1 | 0 |
| 1 | AA | 308 | GMA | 7 | 0 |
| 1 | U | 1101 | 5CR | 5 | 0 |
| 1 | O | 1208 | GMA | 3 | 0 |
| 1 | sA | 1108 | GMA | 1 | 0 |
| 1 | l | 101 | 5CR | 6 | 0 |
| 1 | FA | 101 | 5CR | 6 | 0 |
| 1 | DB | 1108 | GMA | 1 | 0 |
| 1 | Z | 308 | GMA | 7 | 0 |
| 1 | OA | 308 | GMA | 7 | 0 |
| 1 | N | 1108 | GMA | 1 | 0 |
| 1 | k | 1101 | 5CR | 7 | 0 |
| 1 | 6A | 1108 | GMA | 1 | 0 |
| 1 | nA | 1308 | GMA | 1 | 0 |
| 1 | n | 101 | 5CR | 5 | 0 |
| 1 | EA | 1308 | GMA | 7 | 0 |
| 1 | L | 308 | GMA | 7 | 0 |
| 1 | QA | 1108 | GMA | 1 | 0 |
| 1 | Q | 108 | GMA | 1 | 0 |
| 1 | MA | 108 | GMA | 1 | 0 |
| 1 | K | 208 | GMA | 3 | 0 |
| 1 | c | 8 | GMA | 1 | 0 |
| 1 | g | 8 | GMA | 1 | 0 |
| 1 | Q | 101 | 5CR | 6 | 0 |
| 1 | y | 1108 | GMA | 1 | 0 |
| 1 | v | 208 | GMA | 2 | 0 |
| 1 | l | 1201 | 5CR | 1 | 0 |
| 1 | R | 208 | GMA | 2 | 0 |
| 1 | 9 | 208 | GMA | 3 | 0 |
| 1 | 5A | 1008 | GMA | 1 | 0 |
| 1 | 9A | 108 | GMA | 1 | 0 |
| 1 | RA | 1201 | 5CR | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | rA | 1008 | GMA | 1 | 0 |
| 1 | jA | 308 | GMA | 1 | 0 |
| 1 | KA | 1201 | 5CR | 1 | 0 |
| 1 | 5 | 1101 | 5CR | 6 | 0 |
| 1 | NA | 201 | 5CR | 1 | 0 |
| 1 | aA | 108 | GMA | 1 | 0 |
| 1 | z | 1201 | 5CR | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

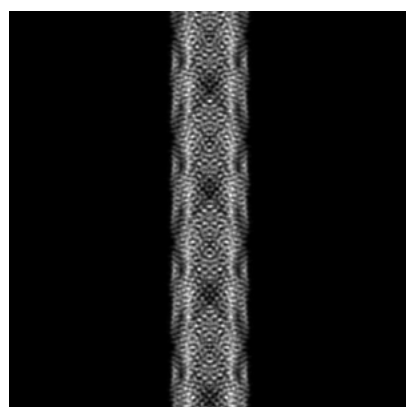
6 Map visualisation [i](#)

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

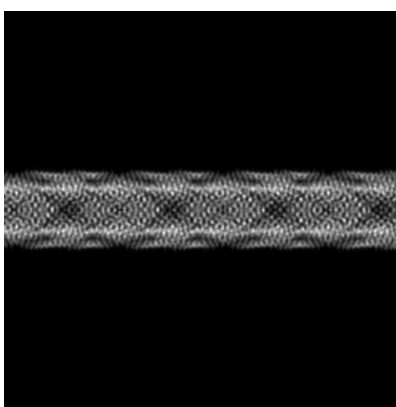
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

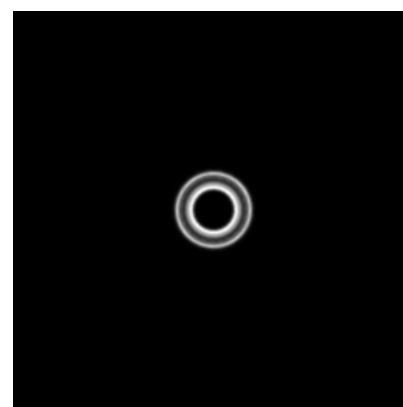
6.1.1 Primary map



X



Y

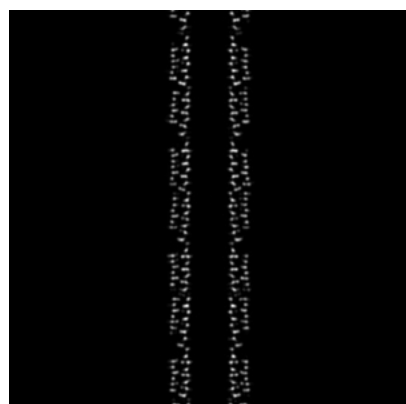


Z

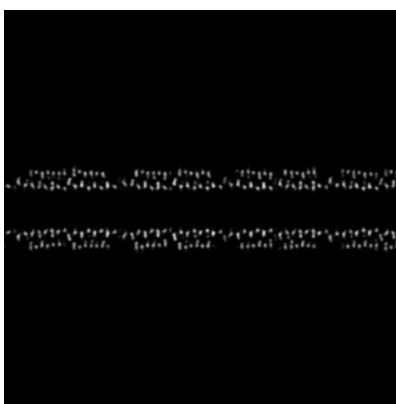
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

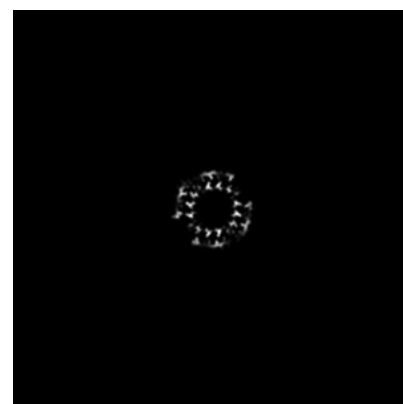
6.2.1 Primary map



X Index: 160



Y Index: 160

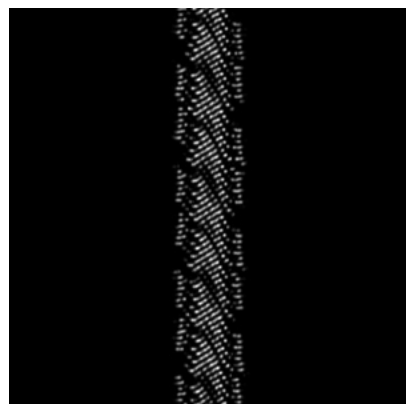


Z Index: 160

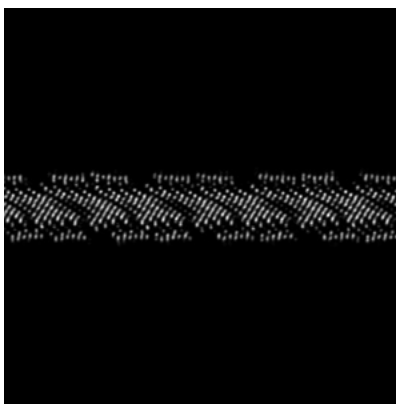
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

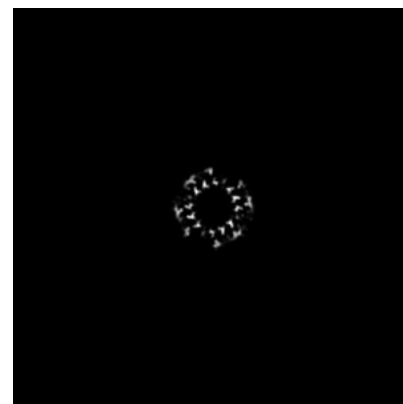
6.3.1 Primary map



X Index: 177



Y Index: 143

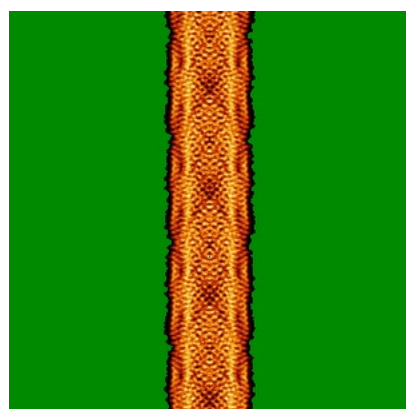


Z Index: 61

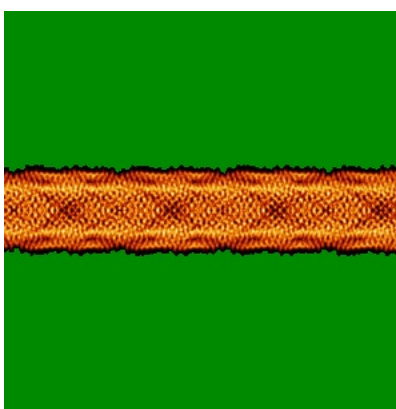
The images above show the largest variance slices of the map in three orthogonal directions.

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

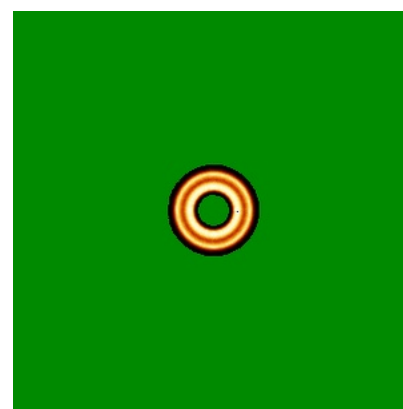
6.4.1 Primary map



X



Y

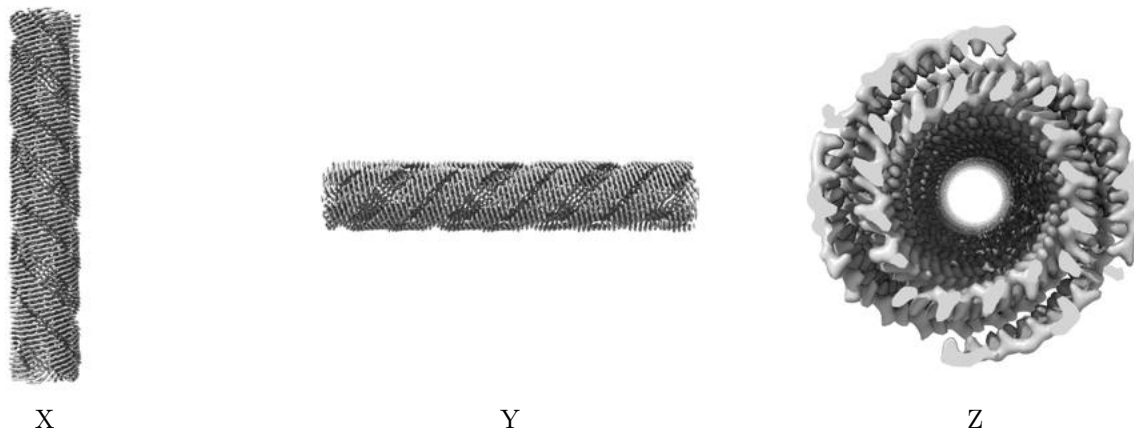


Z

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.

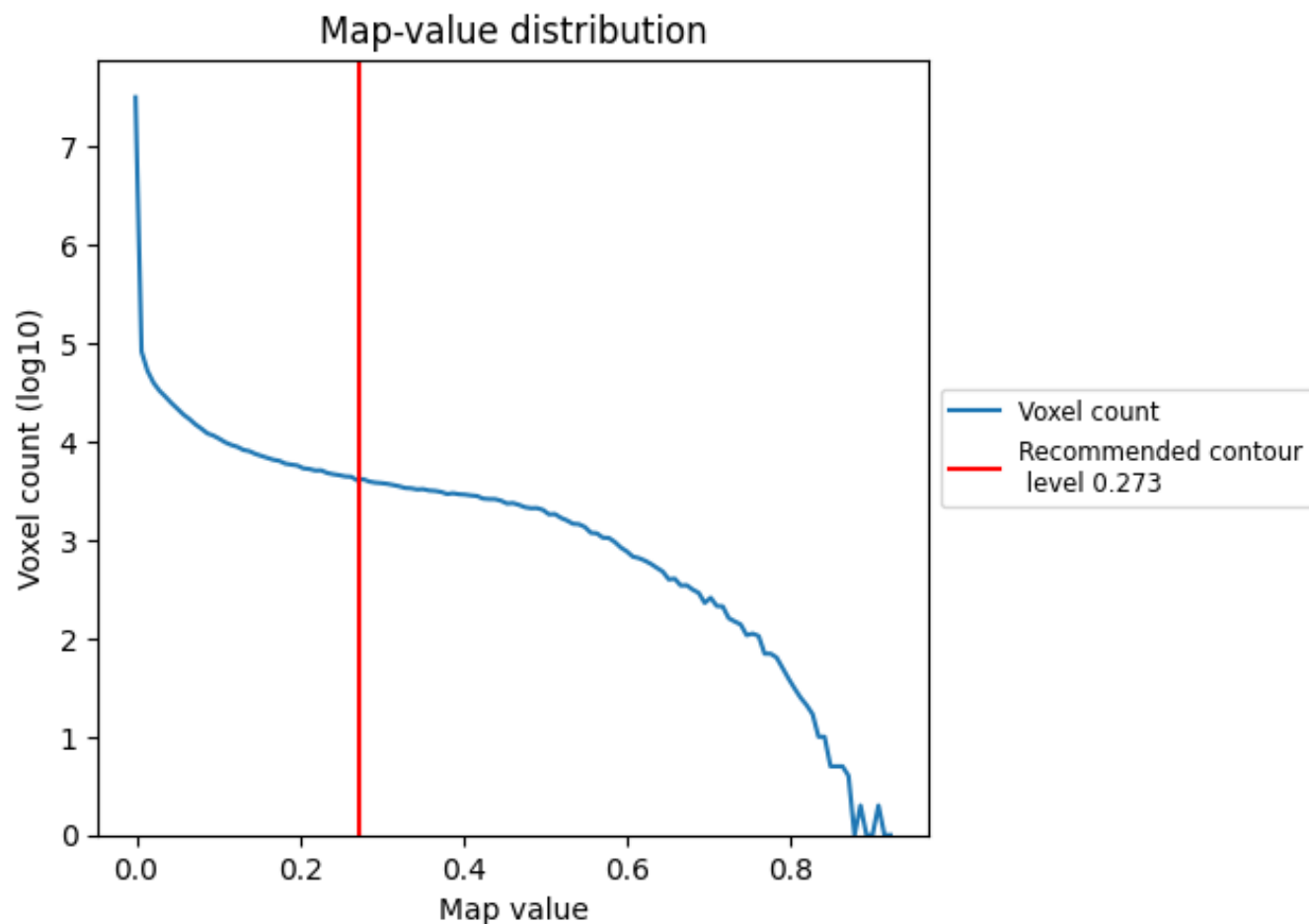
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

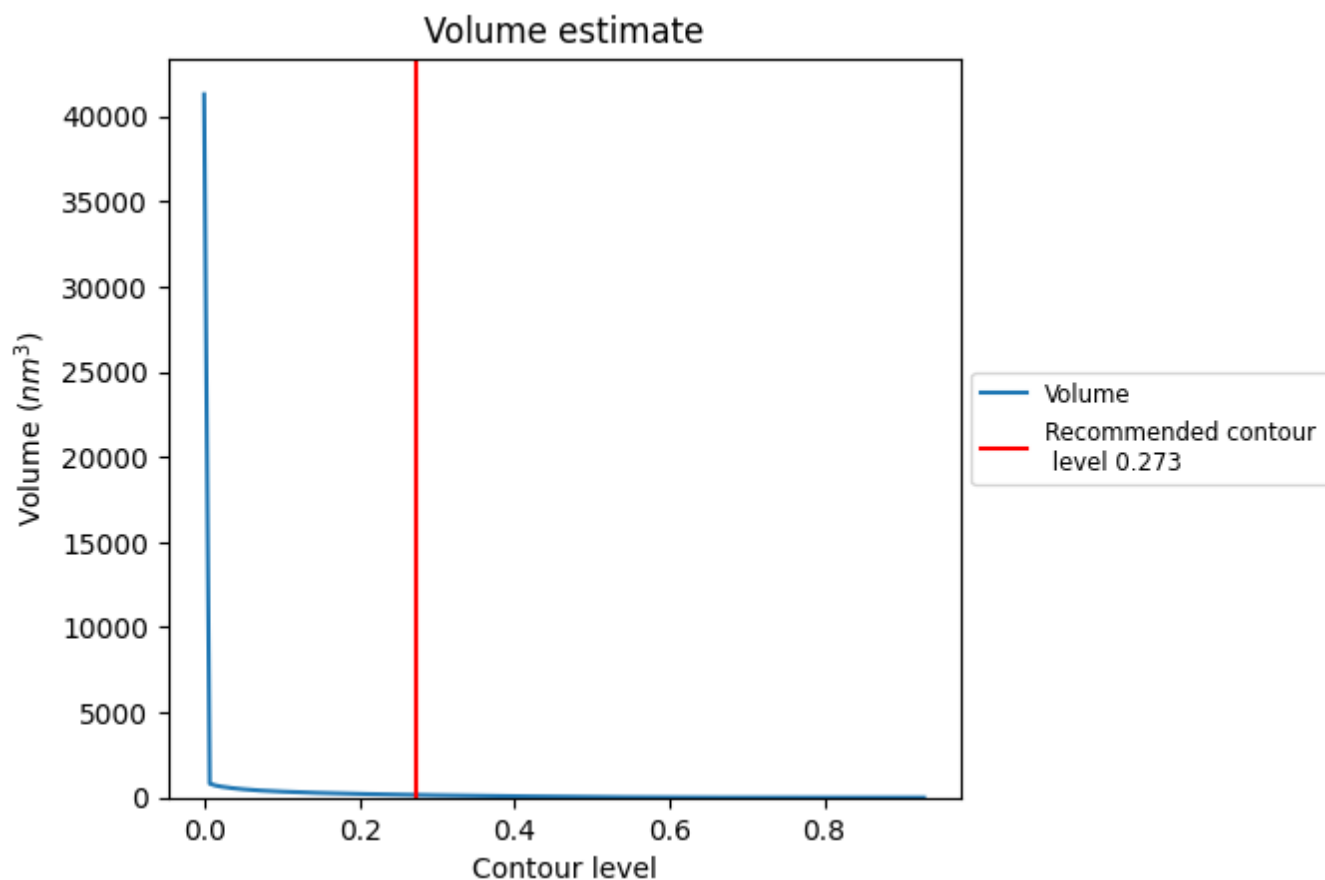
This section contains the results of statistical analysis of the map.

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.

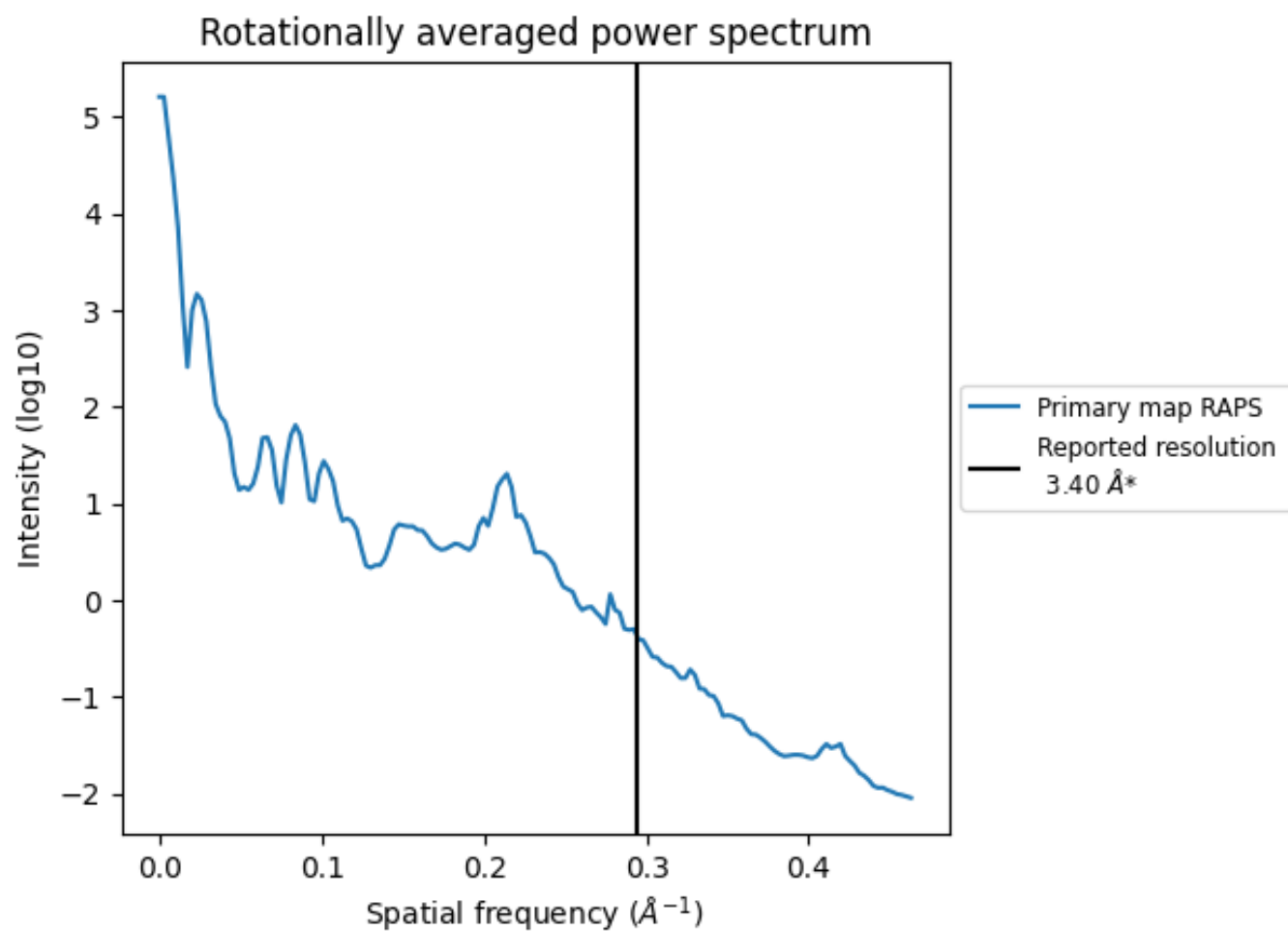
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 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⁻¹

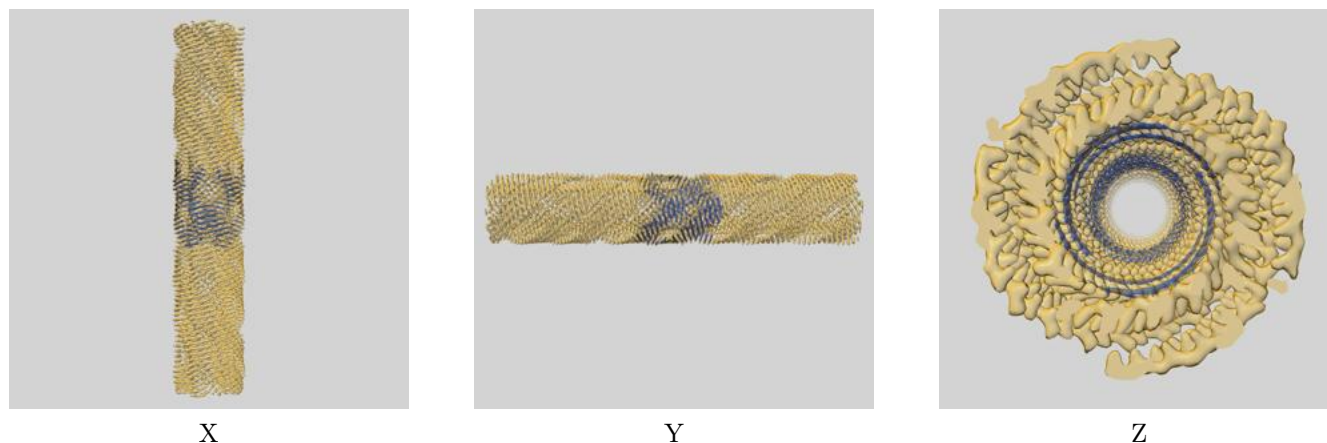
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

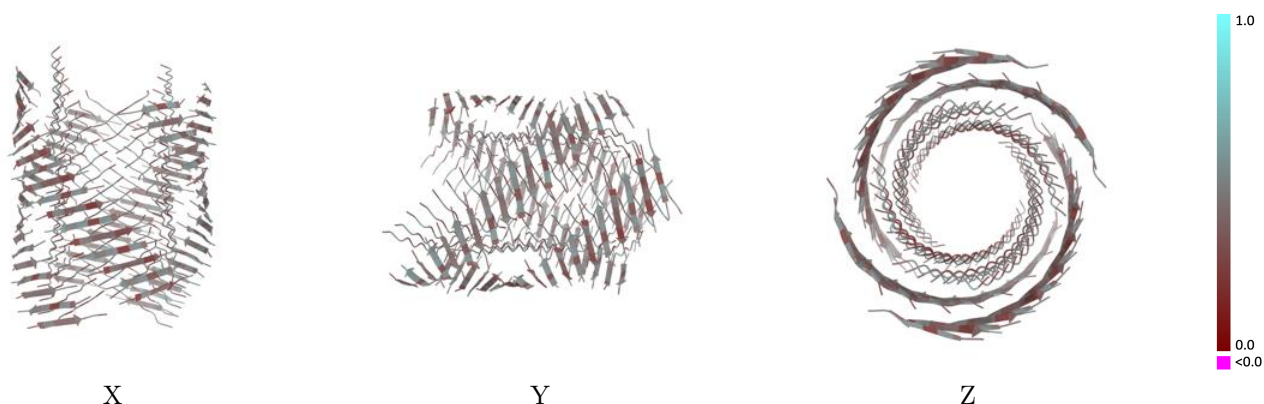
This section contains information regarding the fit between EMDB map EMD-23486 and PDB model 7LQH. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



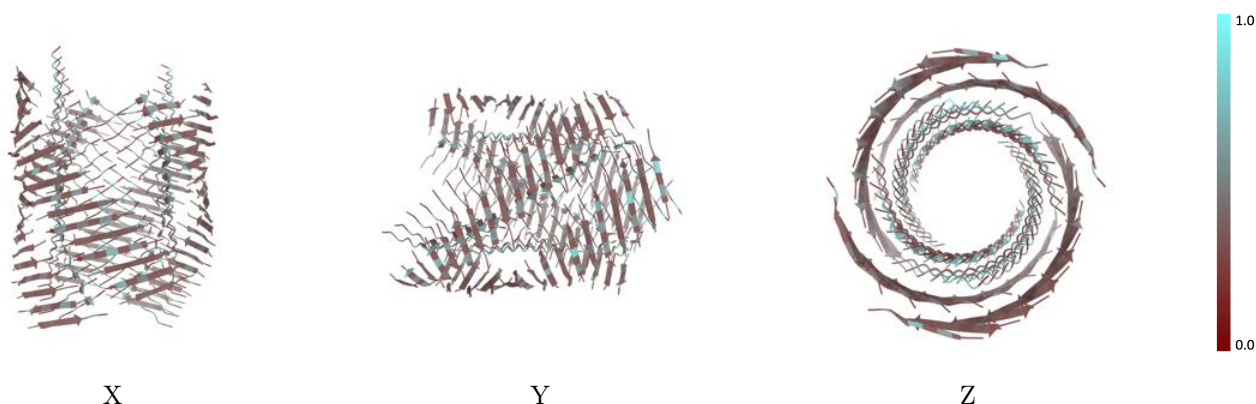
The images above show the 3D surface view of the map at the recommended contour level 0.273 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



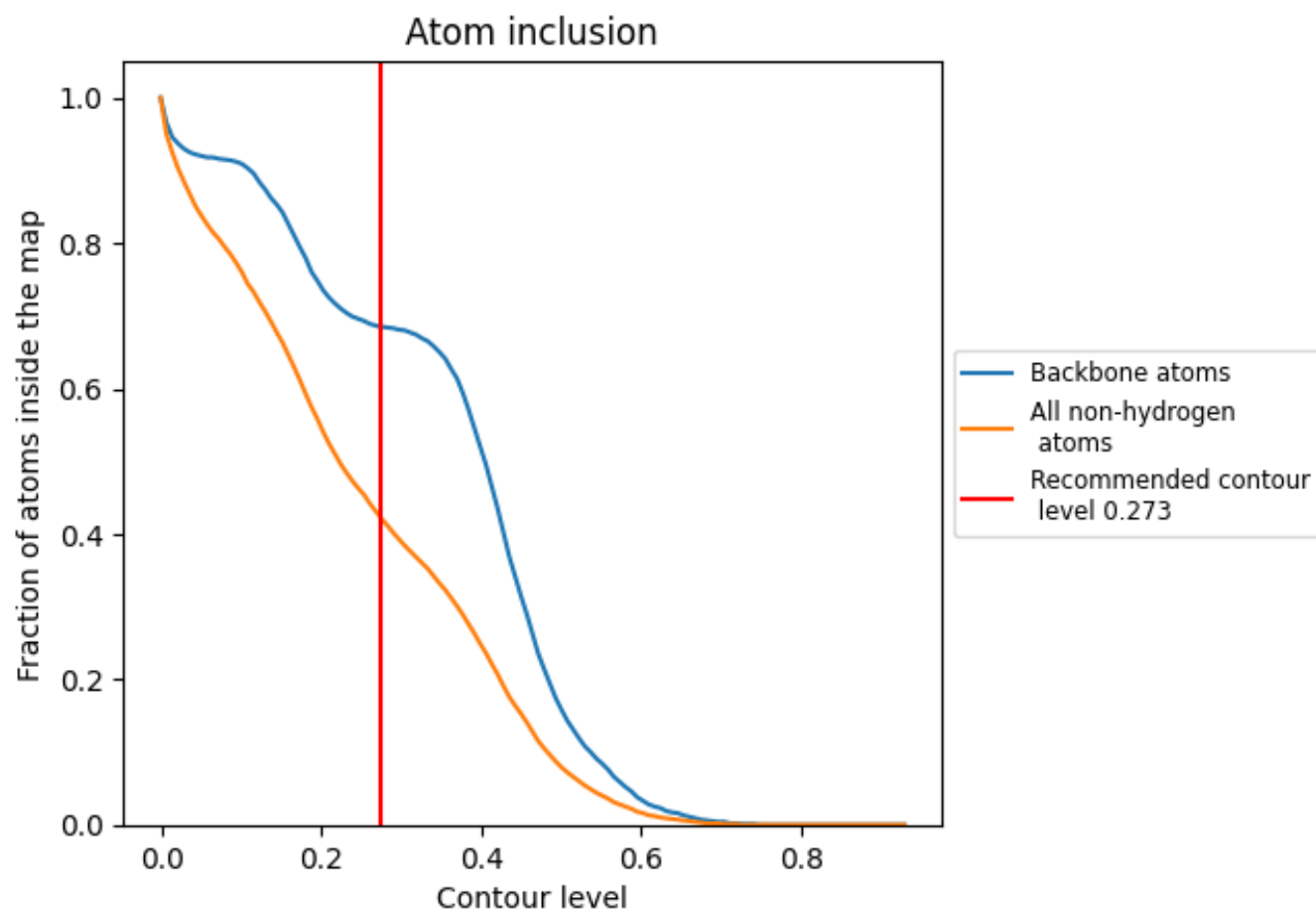
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.273).







































































9.4 Atom inclusion ⓘ



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 |