



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 12:57 PM BST

PDB ID : 4PTJ
Title : Ensemble model for Escherichia coli dihydrofolate reductase at 277K
Authors : Keedy, D.A.; van den Bedem, H.; Sivak, D.A.; Petsko, G.A.; Ringe, D.; Wilson, M.A.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.05 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

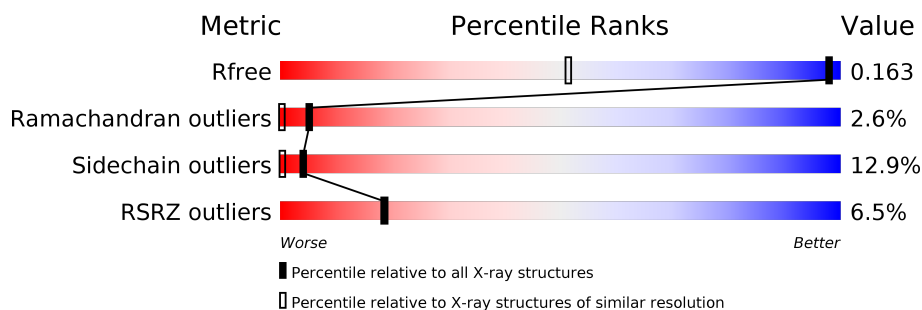
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1202 (1.10-1.02) |
| Ramachandran outliers | 138981 | 1204 (1.10-1.02) |
| Sidechain outliers | 138945 | 1202 (1.10-1.02) |
| RSRZ outliers | 127900 | 1178 (1.10-1.02) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1-A | 159 | <div> <div>6%</div> <div>82%</div> <div>15%</div> <div>..</div> </div> |
| 1 | 10-A | 159 | <div> <div>6%</div> <div>81%</div> <div>15%</div> <div>..</div> </div> |
| 1 | 100-A | 159 | <div> <div>6%</div> <div>83%</div> <div>13%</div> <div>.</div> </div> |
| 1 | 101-A | 159 | <div> <div>6%</div> <div>81%</div> <div>14%</div> <div>..</div> </div> |
| 1 | 102-A | 159 | <div> <div>6%</div> <div>87%</div> <div>8%</div> <div>..</div> </div> |
| 1 | 103-A | 159 | <div> <div>6%</div> <div>84%</div> <div>10%</div> <div>..</div> </div> |
| 1 | 104-A | 159 | <div> <div>6%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 105-A | 159 | |
| 1 | 106-A | 159 | |
| 1 | 107-A | 159 | |
| 1 | 108-A | 159 | |
| 1 | 109-A | 159 | |
| 1 | 11-A | 159 | |
| 1 | 110-A | 159 | |
| 1 | 111-A | 159 | |
| 1 | 112-A | 159 | |
| 1 | 113-A | 159 | |
| 1 | 114-A | 159 | |
| 1 | 115-A | 159 | |
| 1 | 116-A | 159 | |
| 1 | 117-A | 159 | |
| 1 | 118-A | 159 | |
| 1 | 119-A | 159 | |
| 1 | 12-A | 159 | |
| 1 | 120-A | 159 | |
| 1 | 121-A | 159 | |
| 1 | 122-A | 159 | |
| 1 | 123-A | 159 | |
| 1 | 124-A | 159 | |
| 1 | 125-A | 159 | |
| 1 | 13-A | 159 | |
| 1 | 14-A | 159 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 15-A | 159 | |
| 1 | 16-A | 159 | |
| 1 | 17-A | 159 | |
| 1 | 18-A | 159 | |
| 1 | 19-A | 159 | |
| 1 | 2-A | 159 | |
| 1 | 20-A | 159 | |
| 1 | 21-A | 159 | |
| 1 | 22-A | 159 | |
| 1 | 23-A | 159 | |
| 1 | 24-A | 159 | |
| 1 | 25-A | 159 | |
| 1 | 26-A | 159 | |
| 1 | 27-A | 159 | |
| 1 | 28-A | 159 | |
| 1 | 29-A | 159 | |
| 1 | 3-A | 159 | |
| 1 | 30-A | 159 | |
| 1 | 31-A | 159 | |
| 1 | 32-A | 159 | |
| 1 | 33-A | 159 | |
| 1 | 34-A | 159 | |
| 1 | 35-A | 159 | |
| 1 | 36-A | 159 | |
| 1 | 37-A | 159 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 38-A | 159 | |
| 1 | 39-A | 159 | |
| 1 | 4-A | 159 | |
| 1 | 40-A | 159 | |
| 1 | 41-A | 159 | |
| 1 | 42-A | 159 | |
| 1 | 43-A | 159 | |
| 1 | 44-A | 159 | |
| 1 | 45-A | 159 | |
| 1 | 46-A | 159 | |
| 1 | 47-A | 159 | |
| 1 | 48-A | 159 | |
| 1 | 49-A | 159 | |
| 1 | 5-A | 159 | |
| 1 | 50-A | 159 | |
| 1 | 51-A | 159 | |
| 1 | 52-A | 159 | |
| 1 | 53-A | 159 | |
| 1 | 54-A | 159 | |
| 1 | 55-A | 159 | |
| 1 | 56-A | 159 | |
| 1 | 57-A | 159 | |
| 1 | 58-A | 159 | |
| 1 | 59-A | 159 | |
| 1 | 6-A | 159 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 60-A | 159 | |
| 1 | 61-A | 159 | |
| 1 | 62-A | 159 | |
| 1 | 63-A | 159 | |
| 1 | 64-A | 159 | |
| 1 | 65-A | 159 | |
| 1 | 66-A | 159 | |
| 1 | 67-A | 159 | |
| 1 | 68-A | 159 | |
| 1 | 69-A | 159 | |
| 1 | 7-A | 159 | |
| 1 | 70-A | 159 | |
| 1 | 71-A | 159 | |
| 1 | 72-A | 159 | |
| 1 | 73-A | 159 | |
| 1 | 74-A | 159 | |
| 1 | 75-A | 159 | |
| 1 | 76-A | 159 | |
| 1 | 77-A | 159 | |
| 1 | 78-A | 159 | |
| 1 | 79-A | 159 | |
| 1 | 8-A | 159 | |
| 1 | 80-A | 159 | |
| 1 | 81-A | 159 | |
| 1 | 82-A | 159 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 83-A | 159 | |
| 1 | 84-A | 159 | |
| 1 | 85-A | 159 | |
| 1 | 86-A | 159 | |
| 1 | 87-A | 159 | |
| 1 | 88-A | 159 | |
| 1 | 89-A | 159 | |
| 1 | 9-A | 159 | |
| 1 | 90-A | 159 | |
| 1 | 91-A | 159 | |
| 1 | 92-A | 159 | |
| 1 | 93-A | 159 | |
| 1 | 94-A | 159 | |
| 1 | 95-A | 159 | |
| 1 | 96-A | 159 | |
| 1 | 97-A | 159 | |
| 1 | 98-A | 159 | |
| 1 | 99-A | 159 | |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 339833 atoms, of which 157875 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydrofolate reductase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 1-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 2-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 3-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 4-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 5-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 6-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 7-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 8-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 9-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 10-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 11-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 12-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 13-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 14-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 15-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 16-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 17-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 18-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 19-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 20-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 21-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 22-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 23-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 24-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 25-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 26-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 27-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 28-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 29-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 30-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 31-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 32-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 33-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 34-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 35-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 36-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 37-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 38-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 39-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 40-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 41-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 42-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 43-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 44-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 45-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 46-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 47-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 48-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 49-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 50-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 51-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 52-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 53-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 54-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 55-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 56-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 57-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 58-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 59-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 60-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 61-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 62-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 63-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 64-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 65-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 66-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 67-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 68-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 69-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 70-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 71-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 72-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 73-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 74-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 75-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 76-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 77-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 78-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 79-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 80-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 81-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 82-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 83-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 84-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 85-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 86-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 87-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 88-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 89-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 90-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 91-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 92-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 93-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 94-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 95-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 96-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 97-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 98-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 99-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 100-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

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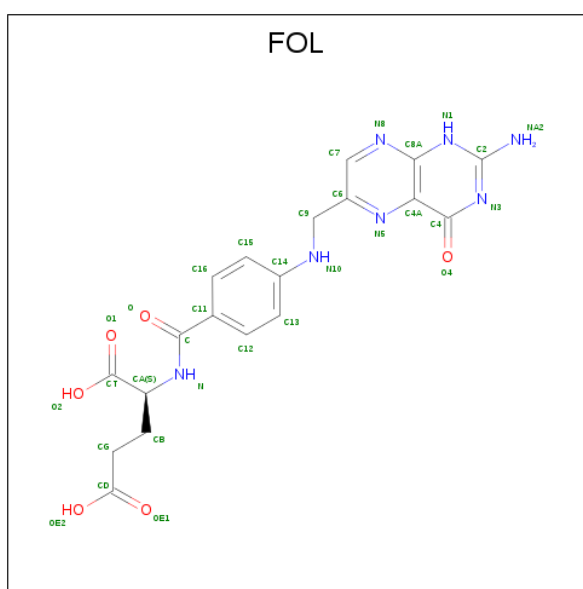
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 101-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 102-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 103-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 104-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 105-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 106-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 107-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 108-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 109-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 110-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 111-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 112-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 113-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 114-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 115-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 116-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 117-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 118-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 119-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 120-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 121-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 122-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 123-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 124-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 125-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 1-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 2-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 3-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 4-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 5-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 6-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 7-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 8-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 9-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 10-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 11-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 12-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 13-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 14-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 15-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 16-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 17-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 18-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 19-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 20-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 21-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 22-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 23-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 24-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 25-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 26-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 27-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 28-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 29-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 30-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 31-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 32-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 33-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 34-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 35-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 36-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 37-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 38-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 39-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 40-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 41-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 42-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 43-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 44-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 45-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 46-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 47-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 48-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 49-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 50-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 51-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 52-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 53-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 54-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 55-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 56-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 57-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 58-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 59-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 60-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 61-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 62-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 63-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 64-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 65-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 66-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 67-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 68-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 69-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 70-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 71-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 72-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 73-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 74-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 75-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 76-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 77-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 78-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 79-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 80-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 81-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 82-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 83-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 84-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 85-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 86-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 87-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 88-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 89-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 90-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 91-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 92-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 93-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 94-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 95-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 96-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 97-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 98-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 99-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 100-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 101-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 102-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 103-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 104-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 105-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 106-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 107-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 108-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 109-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 110-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 111-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 112-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2 | 113-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 114-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 115-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 116-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 117-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 118-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 119-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 120-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 121-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 122-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 123-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 124-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 125-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|---------|
| 3 | 1-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 2-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 3-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 4-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 5-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 6-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 7-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 8-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 9-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 10-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 11-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 12-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 13-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |
| 3 | 14-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 73 | 21 | 25 | 7 | 17 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 15-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 16-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 17-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 18-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 19-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 20-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 21-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 22-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 23-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 24-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 25-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 26-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 27-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 28-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 29-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 30-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 31-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 32-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 33-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 34-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 35-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 36-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 37-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 38-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 39-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 40-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 41-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 42-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 43-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 44-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 45-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 46-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 47-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 48-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 49-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 50-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 51-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 52-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 53-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 54-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 55-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 56-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 57-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 58-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 59-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 60-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 61-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 62-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 63-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 64-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 65-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 66-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 67-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 68-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 69-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 70-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 71-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 72-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 73-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 74-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 75-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 76-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 77-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 78-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 79-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 80-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 81-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 82-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 83-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 84-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 85-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 86-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 87-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 88-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 89-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 90-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 91-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 92-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 93-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 94-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 95-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 96-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 97-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 98-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 99-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 100-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 101-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 102-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 103-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 104-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 105-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 106-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 107-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 108-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 109-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 110-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 111-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 112-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 113-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 114-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 115-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 116-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 117-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 118-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 119-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 120-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 121-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 122-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 123-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 124-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 125-A | 1 | Total 73 | C 21 | H 25 | N 7 | O 17 | P 3 | 0 | 0 |

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | 122-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 110-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 37-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 80-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 94-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 60-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 123-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 44-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 50-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 104-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 12-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 114-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |
| 4 | 19-A | 2 | Total | Mn | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | 73-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 1-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 53-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 25-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 32-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 93-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 77-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 58-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 57-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 29-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 101-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 3-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 11-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 84-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 98-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 108-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 16-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 65-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 117-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 41-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 5-A | 2 | Total 2 | Mn 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | 8-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 21-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 109-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 102-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 113-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 36-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 81-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 97-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 61-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 48-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 124-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 45-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 35-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 105-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 7-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 15-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 88-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 18-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 72-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 52-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 26-A | 2 | Total 2 | Mn 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | 120-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 118-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 89-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 31-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 82-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 92-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 76-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 46-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 56-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 106-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 10-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 85-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 39-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 91-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 66-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 79-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 55-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 22-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 103-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 112-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 86-A | 2 | Total 2 | Mn 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | 96-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 62-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 49-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 125-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 42-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 119-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 34-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 14-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 63-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 68-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 71-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 27-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 121-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 111-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 30-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 83-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 95-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 2-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 9-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 75-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 47-A | 2 | Total 2 | Mn 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | 51-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 107-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 13-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 115-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 74-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 24-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 4-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 38-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 33-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 116-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 90-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 67-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 78-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 59-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 54-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 23-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 28-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 100-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 87-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 99-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 6-A | 2 | Total 2 | Mn 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | 43-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 17-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 64-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 69-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 70-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 40-A | 2 | Total 2 | Mn 2 | 0 | 0 |
| 4 | 20-A | 2 | Total 2 | Mn 2 | 0 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 1-A | 89 | Total 89 | O 89 | 0 | 0 |
| 5 | 2-A | 91 | Total 91 | O 91 | 0 | 0 |
| 5 | 3-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 4-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 5-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 6-A | 112 | Total 112 | O 112 | 0 | 0 |
| 5 | 7-A | 107 | Total 107 | O 107 | 0 | 0 |
| 5 | 8-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 9-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 10-A | 90 | Total 90 | O 90 | 0 | 0 |
| 5 | 11-A | 110 | Total 110 | O 110 | 0 | 0 |
| 5 | 12-A | 102 | Total 102 | O 102 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 13-A | 117 | Total 117 | O 117 | 0 | 0 |
| 5 | 14-A | 116 | Total 116 | O 116 | 0 | 0 |
| 5 | 15-A | 113 | Total 113 | O 113 | 0 | 0 |
| 5 | 16-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 17-A | 95 | Total 95 | O 95 | 0 | 0 |
| 5 | 18-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 19-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 20-A | 100 | Total 100 | O 100 | 0 | 0 |
| 5 | 21-A | 103 | Total 103 | O 103 | 0 | 0 |
| 5 | 22-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 23-A | 110 | Total 110 | O 110 | 0 | 0 |
| 5 | 24-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 25-A | 106 | Total 106 | O 106 | 0 | 0 |
| 5 | 26-A | 112 | Total 112 | O 112 | 0 | 0 |
| 5 | 27-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 28-A | 100 | Total 100 | O 100 | 0 | 0 |
| 5 | 29-A | 95 | Total 95 | O 95 | 0 | 0 |
| 5 | 30-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 31-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 32-A | 106 | Total 106 | O 106 | 0 | 0 |
| 5 | 33-A | 105 | Total 105 | O 105 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 34-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 35-A | 100 | Total 100 | O 100 | 0 | 0 |
| 5 | 36-A | 104 | Total 104 | O 104 | 0 | 0 |
| 5 | 37-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 38-A | 119 | Total 119 | O 119 | 0 | 0 |
| 5 | 39-A | 118 | Total 118 | O 118 | 0 | 0 |
| 5 | 40-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 41-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 42-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 43-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 44-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 45-A | 107 | Total 107 | O 107 | 0 | 0 |
| 5 | 46-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 47-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 48-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 49-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 50-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 51-A | 104 | Total 104 | O 104 | 0 | 0 |
| 5 | 52-A | 107 | Total 107 | O 107 | 0 | 0 |
| 5 | 53-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 54-A | 103 | Total 103 | O 103 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 55-A | 106 | Total 106 | O 106 | 0 | 0 |
| 5 | 56-A | 110 | Total 110 | O 110 | 0 | 0 |
| 5 | 57-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 58-A | 116 | Total 116 | O 116 | 0 | 0 |
| 5 | 59-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 60-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 61-A | 109 | Total 109 | O 109 | 0 | 0 |
| 5 | 62-A | 107 | Total 107 | O 107 | 0 | 0 |
| 5 | 63-A | 110 | Total 110 | O 110 | 0 | 0 |
| 5 | 64-A | 102 | Total 102 | O 102 | 0 | 0 |
| 5 | 65-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 66-A | 104 | Total 104 | O 104 | 0 | 0 |
| 5 | 67-A | 99 | Total 99 | O 99 | 0 | 0 |
| 5 | 68-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 69-A | 95 | Total 95 | O 95 | 0 | 0 |
| 5 | 70-A | 103 | Total 103 | O 103 | 0 | 0 |
| 5 | 71-A | 103 | Total 103 | O 103 | 0 | 0 |
| 5 | 72-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 73-A | 108 | Total 108 | O 108 | 0 | 0 |
| 5 | 74-A | 111 | Total 111 | O 111 | 0 | 0 |
| 5 | 75-A | 109 | Total 109 | O 109 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5 | 76-A | 93 | Total O 93 93 | 0 | 0 |
| 5 | 77-A | 87 | Total O 87 87 | 0 | 0 |
| 5 | 78-A | 95 | Total O 95 95 | 0 | 0 |
| 5 | 79-A | 115 | Total O 115 115 | 0 | 0 |
| 5 | 80-A | 109 | Total O 109 109 | 0 | 0 |
| 5 | 81-A | 106 | Total O 106 106 | 0 | 0 |
| 5 | 82-A | 107 | Total O 107 107 | 0 | 0 |
| 5 | 83-A | 116 | Total O 116 116 | 0 | 0 |
| 5 | 84-A | 111 | Total O 111 111 | 0 | 0 |
| 5 | 85-A | 118 | Total O 118 118 | 0 | 0 |
| 5 | 86-A | 109 | Total O 109 109 | 0 | 0 |
| 5 | 87-A | 113 | Total O 113 113 | 0 | 0 |
| 5 | 88-A | 103 | Total O 103 103 | 0 | 0 |
| 5 | 89-A | 109 | Total O 109 109 | 0 | 0 |
| 5 | 90-A | 103 | Total O 103 103 | 0 | 0 |
| 5 | 91-A | 93 | Total O 93 93 | 0 | 0 |
| 5 | 92-A | 98 | Total O 98 98 | 0 | 0 |
| 5 | 93-A | 117 | Total O 117 117 | 0 | 0 |
| 5 | 94-A | 121 | Total O 121 121 | 0 | 0 |
| 5 | 95-A | 111 | Total O 111 111 | 0 | 0 |
| 5 | 96-A | 104 | Total O 104 104 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5 | 97-A | 93 | Total O 93 93 | 0 | 0 |
| 5 | 98-A | 98 | Total O 98 98 | 0 | 0 |
| 5 | 99-A | 99 | Total O 99 99 | 0 | 0 |
| 5 | 100-A | 107 | Total O 107 107 | 0 | 0 |
| 5 | 101-A | 107 | Total O 107 107 | 0 | 0 |
| 5 | 102-A | 100 | Total O 100 100 | 0 | 0 |
| 5 | 103-A | 105 | Total O 105 105 | 0 | 0 |
| 5 | 104-A | 94 | Total O 94 94 | 0 | 0 |
| 5 | 105-A | 90 | Total O 90 90 | 0 | 0 |
| 5 | 106-A | 91 | Total O 91 91 | 0 | 0 |
| 5 | 107-A | 113 | Total O 113 113 | 0 | 0 |
| 5 | 108-A | 108 | Total O 108 108 | 0 | 0 |
| 5 | 109-A | 111 | Total O 111 111 | 0 | 0 |
| 5 | 110-A | 113 | Total O 113 113 | 0 | 0 |
| 5 | 111-A | 109 | Total O 109 109 | 0 | 0 |
| 5 | 112-A | 92 | Total O 92 92 | 0 | 0 |
| 5 | 113-A | 101 | Total O 101 101 | 0 | 0 |
| 5 | 114-A | 103 | Total O 103 103 | 0 | 0 |
| 5 | 115-A | 102 | Total O 102 102 | 0 | 0 |
| 5 | 116-A | 101 | Total O 101 101 | 0 | 0 |
| 5 | 117-A | 95 | Total O 95 95 | 0 | 0 |

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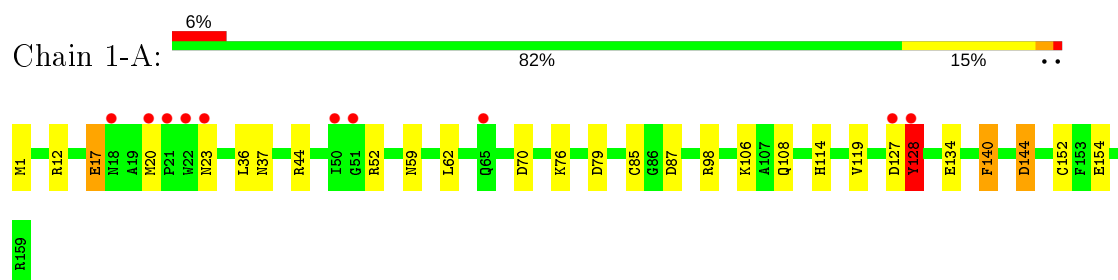
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 118-A | 107 | Total 107 | O 107 | 0 | 0 |
| 5 | 119-A | 106 | Total 106 | O 106 | 0 | 0 |
| 5 | 120-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 121-A | 115 | Total 115 | O 115 | 0 | 0 |
| 5 | 122-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 123-A | 105 | Total 105 | O 105 | 0 | 0 |
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| 5 | 125-A | 102 | Total 102 | O 102 | 0 | 0 |

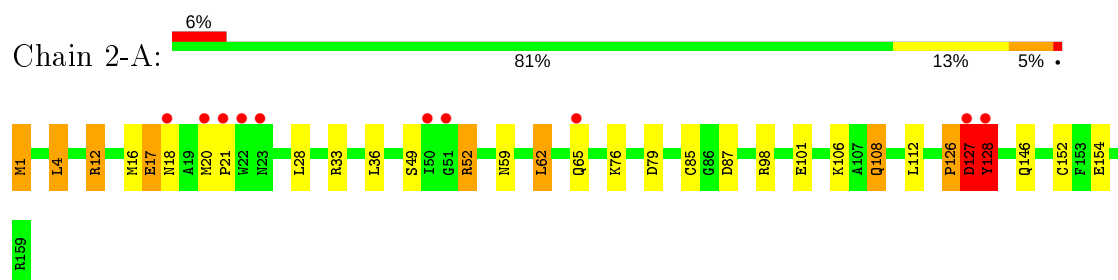
3 Residue-property plots [i](#)

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

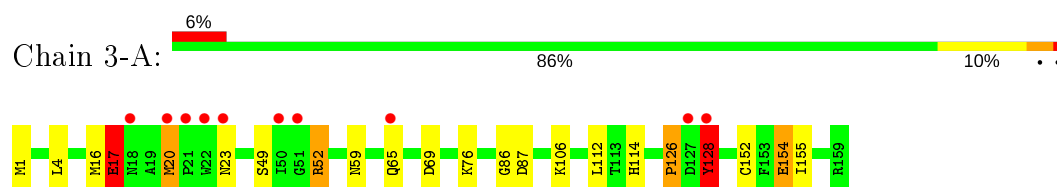
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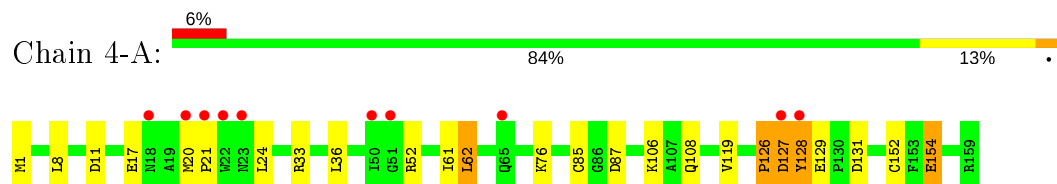
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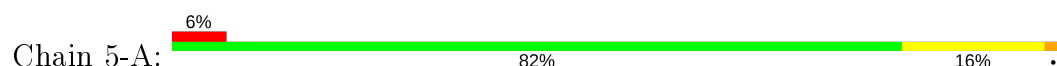
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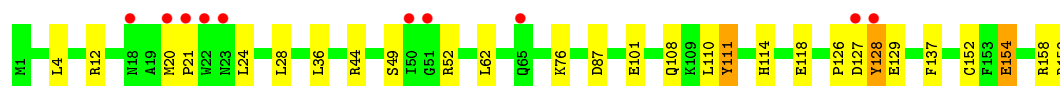


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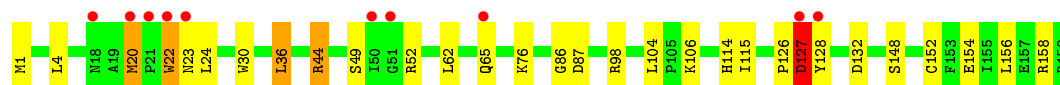
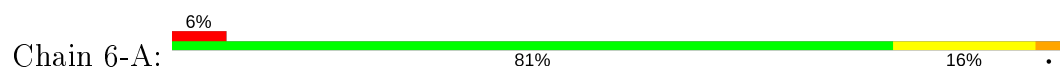


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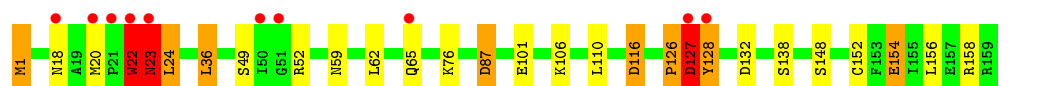
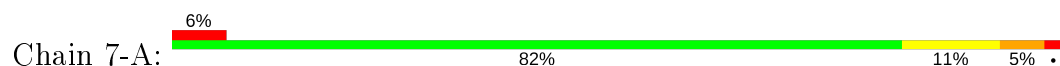




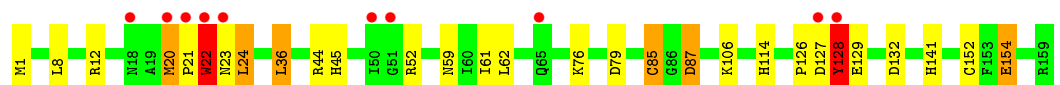
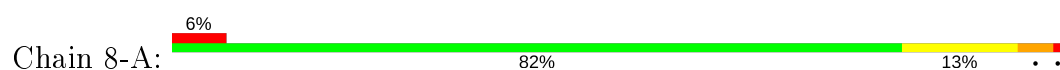
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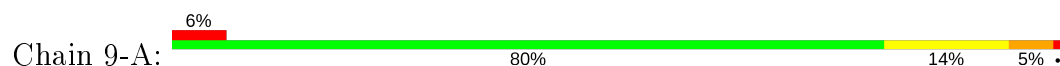
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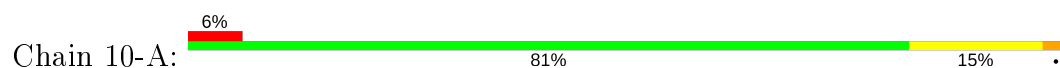
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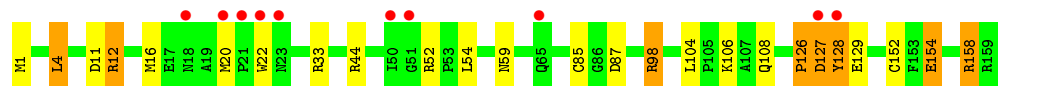
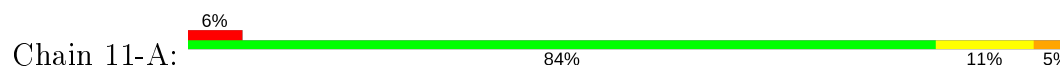
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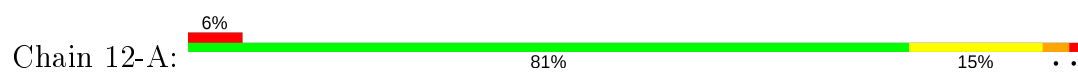
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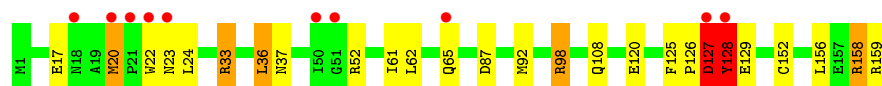
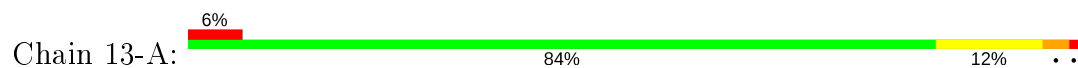
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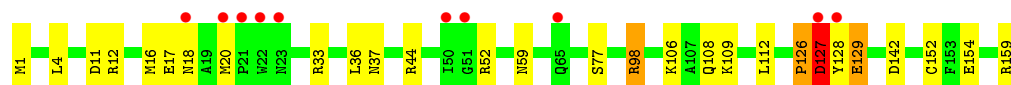
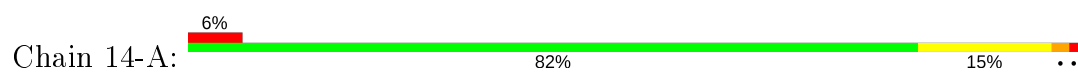
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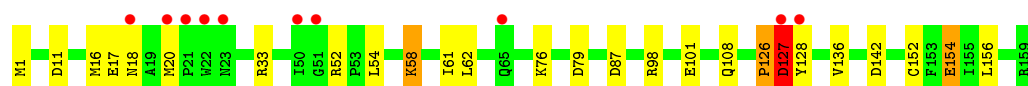
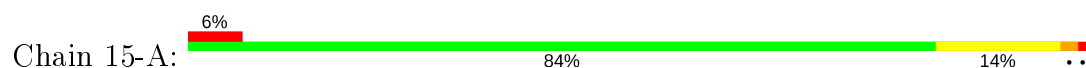
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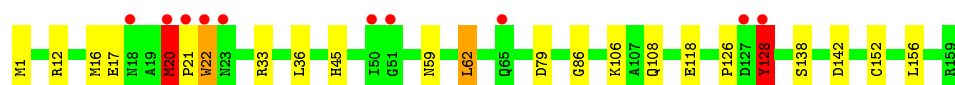
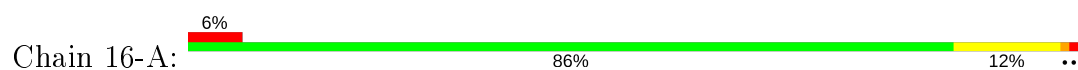
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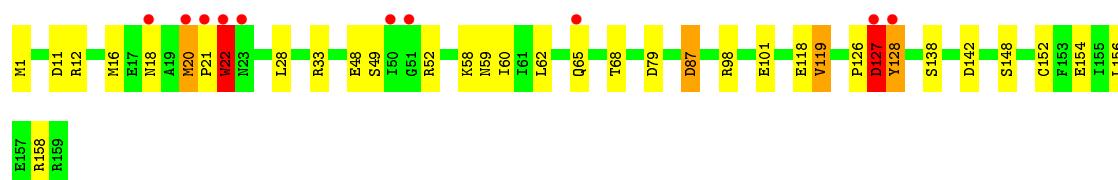
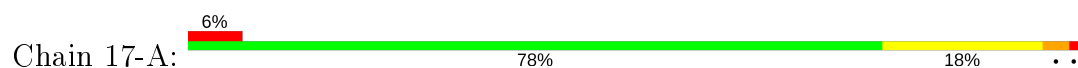
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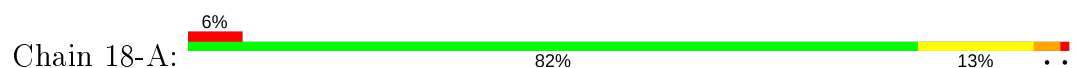
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- Molecule 1: Dihydrofolate reductase

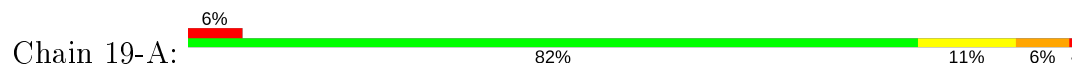


- Molecule 1: Dihydrofolate reductase





- Molecule 1: Dihydrofolate reductase



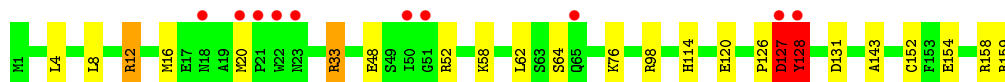
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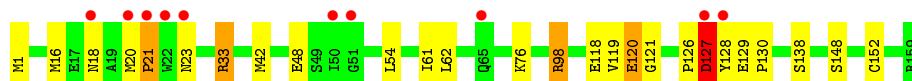
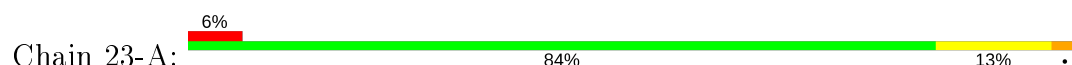
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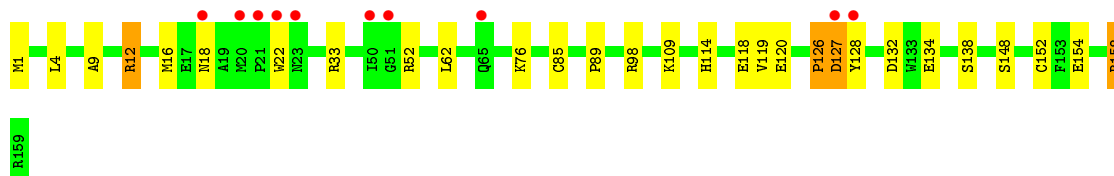
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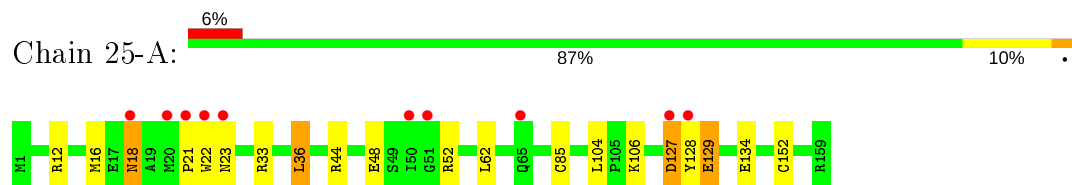
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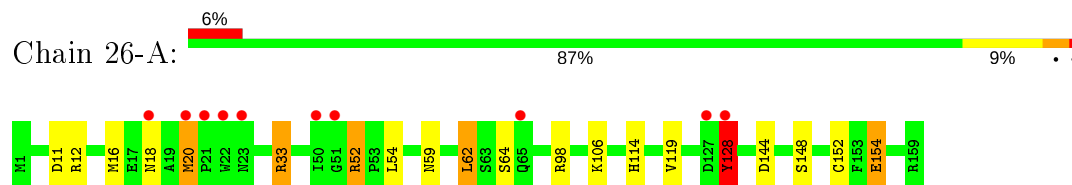
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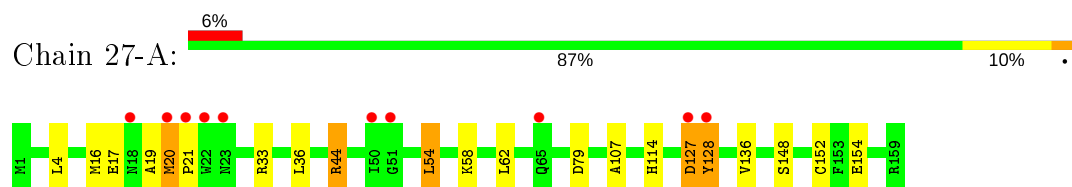
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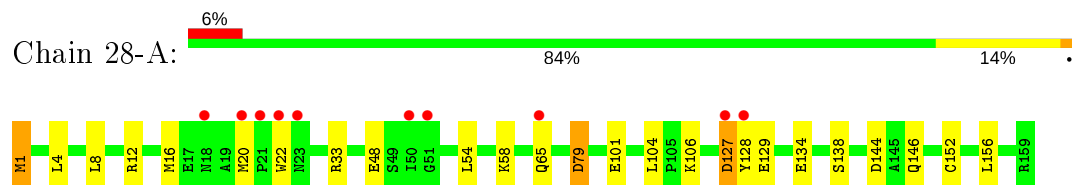
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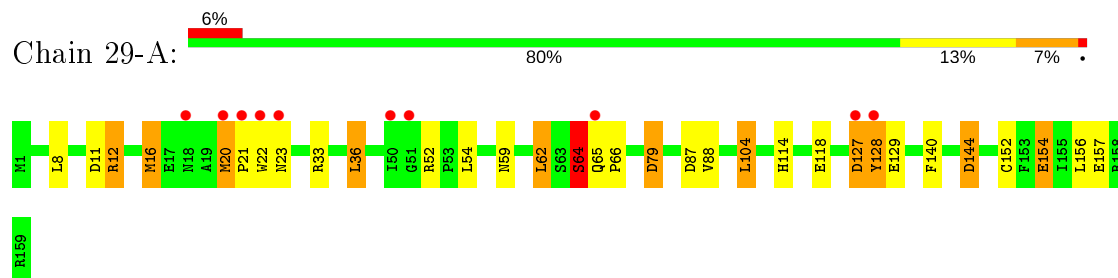
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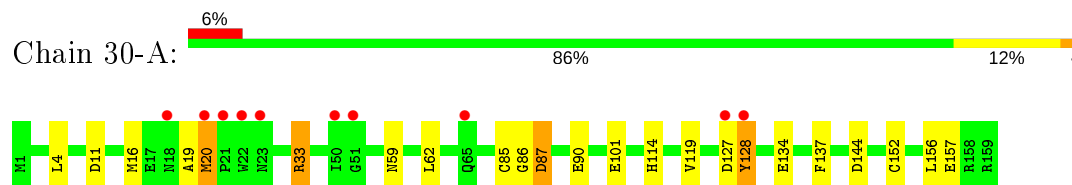
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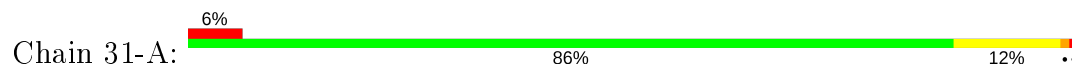
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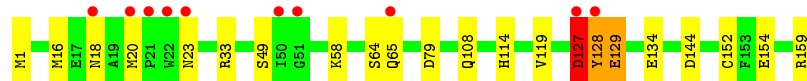


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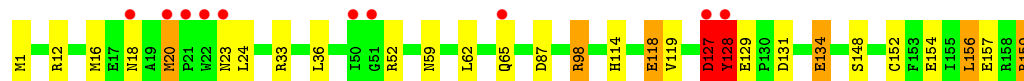
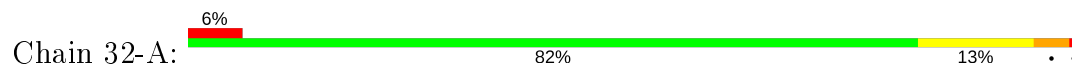


- Molecule 1: Dihydrofolate reductase

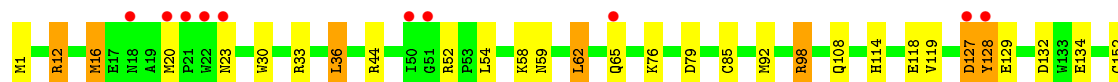
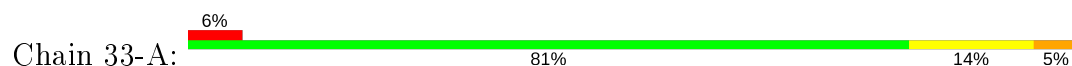




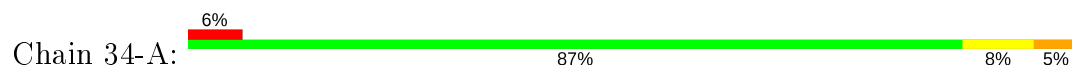
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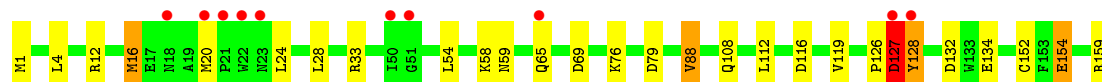
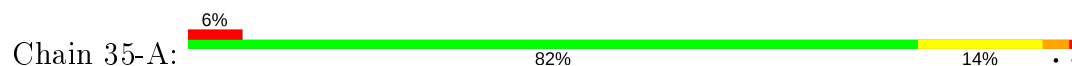
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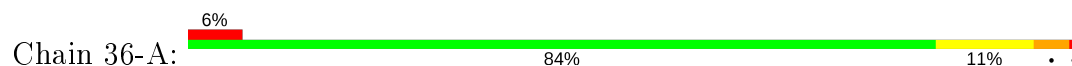
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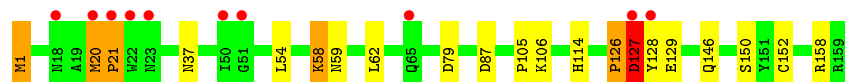
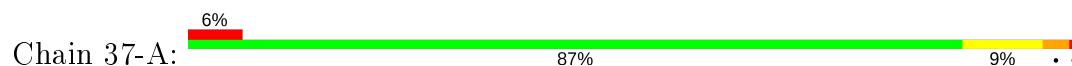
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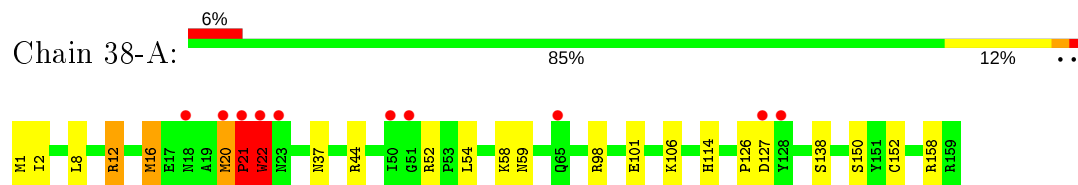
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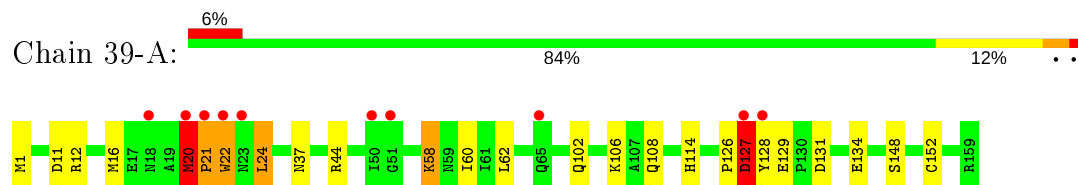
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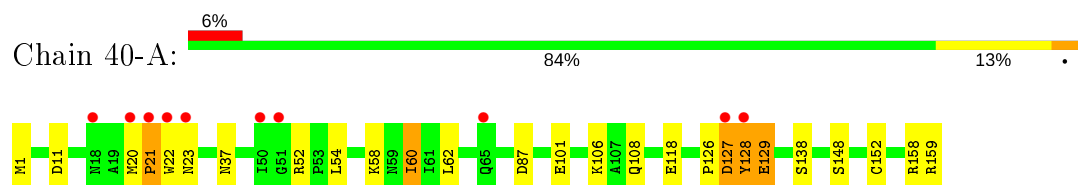
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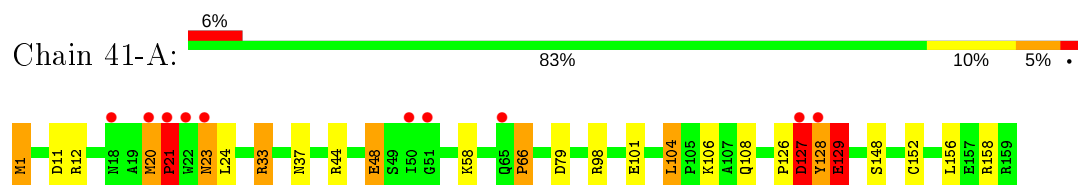
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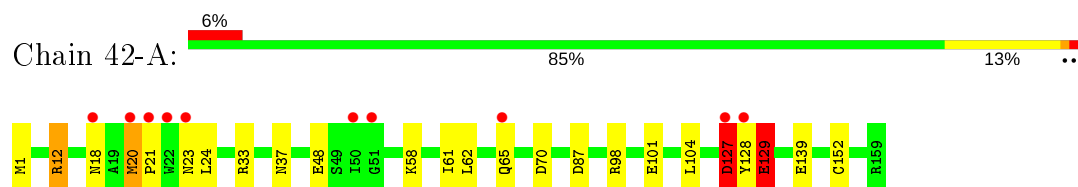
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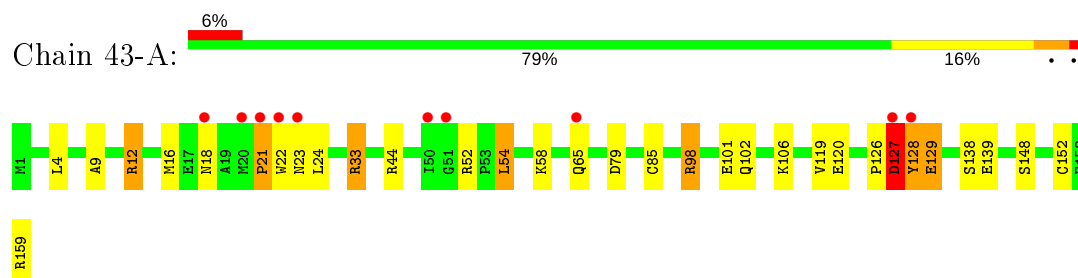
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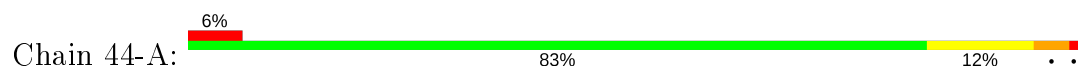
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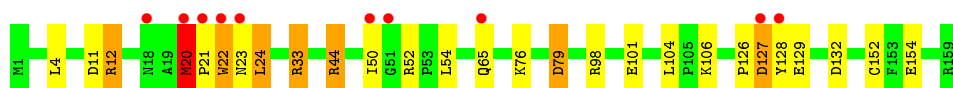


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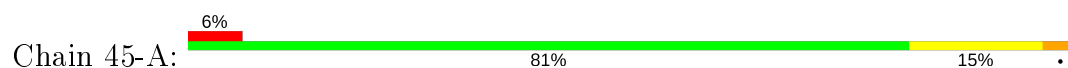


- Molecule 1: Dihydrofolate reductase

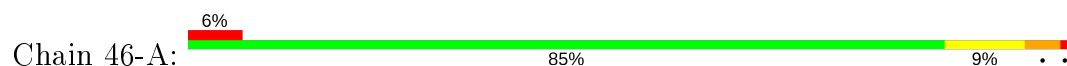




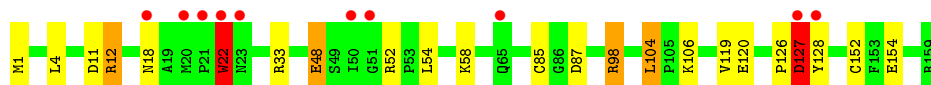
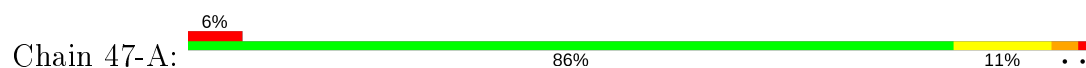
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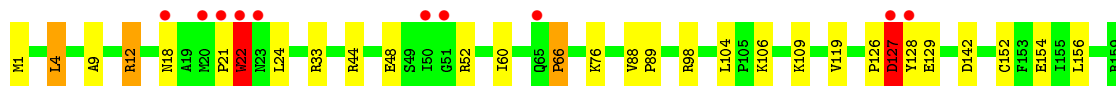
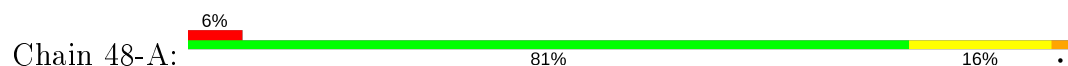
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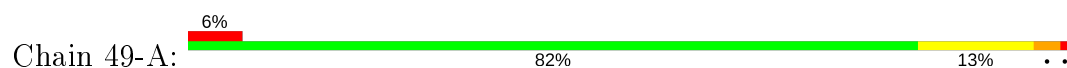
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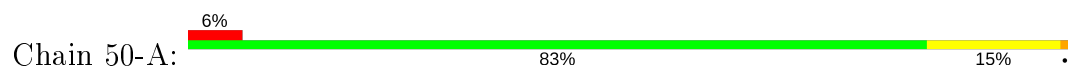
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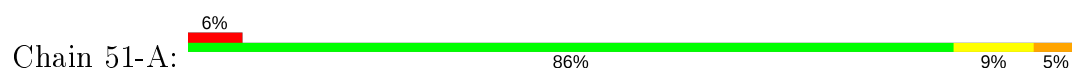
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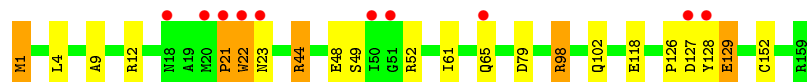
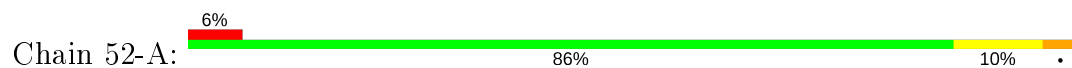
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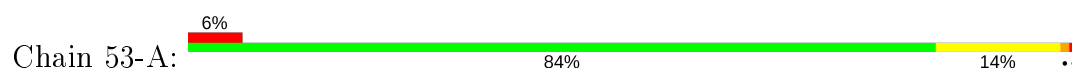
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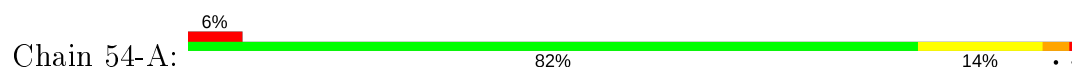
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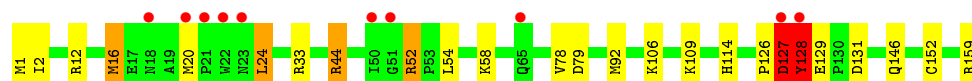
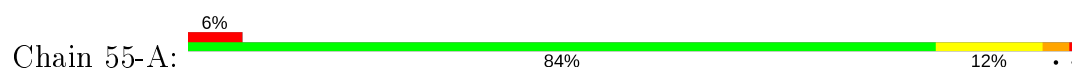
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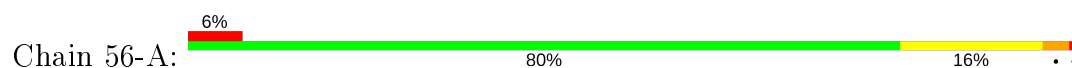
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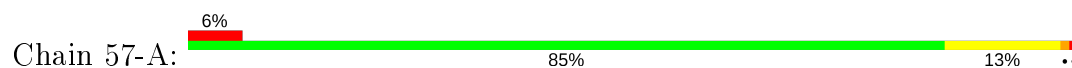
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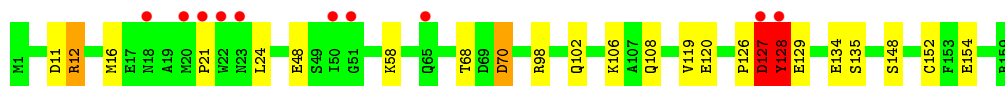


- Molecule 1: Dihydrofolate reductase

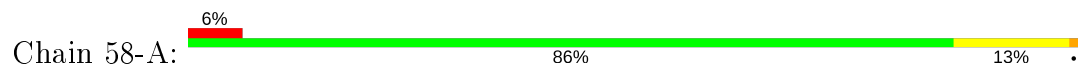


- Molecule 1: Dihydrofolate reductase

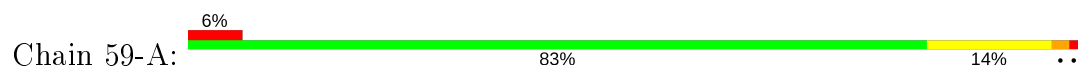




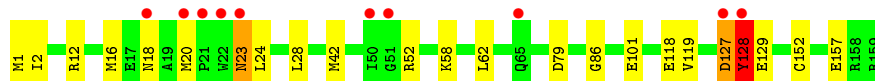
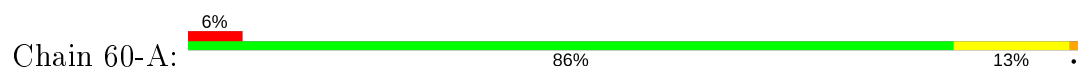
- Molecule 1: Dihydrofolate reductase



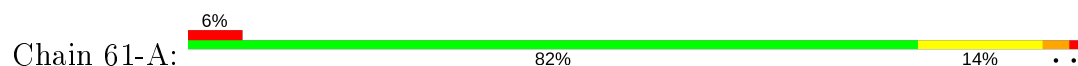
- Molecule 1: Dihydrofolate reductase



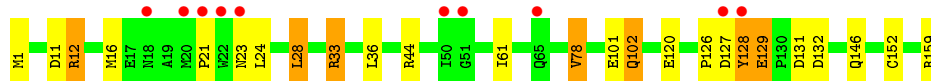
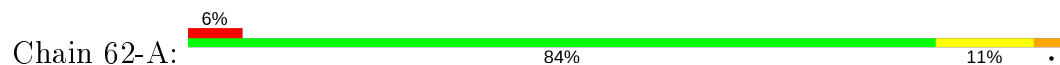
- Molecule 1: Dihydrofolate reductase



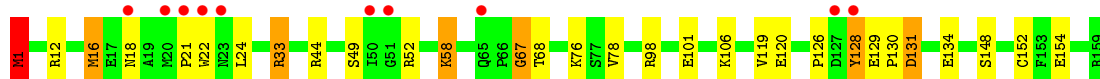
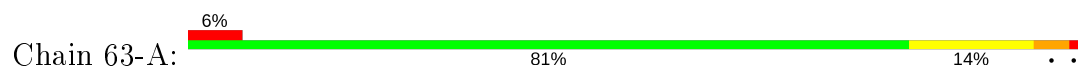
- Molecule 1: Dihydrofolate reductase



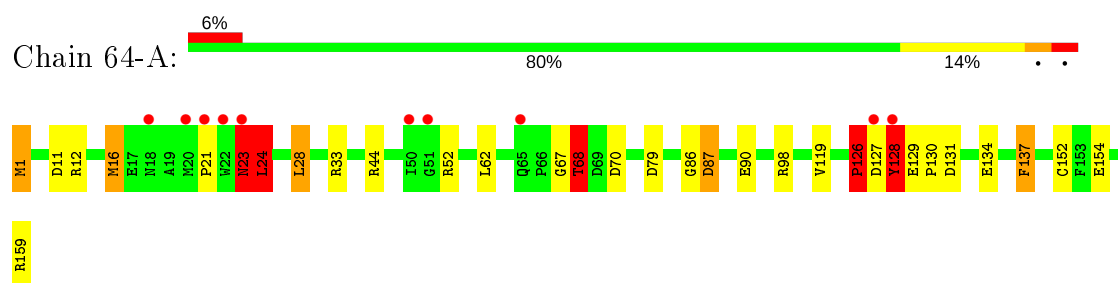
- Molecule 1: Dihydrofolate reductase



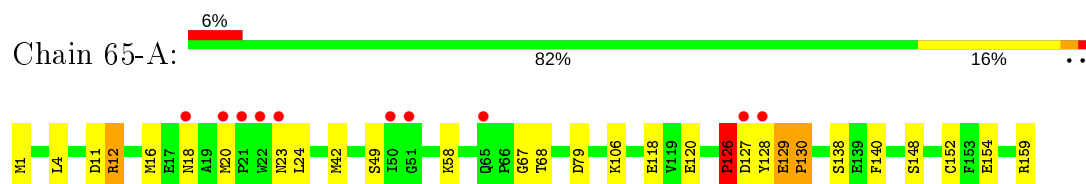
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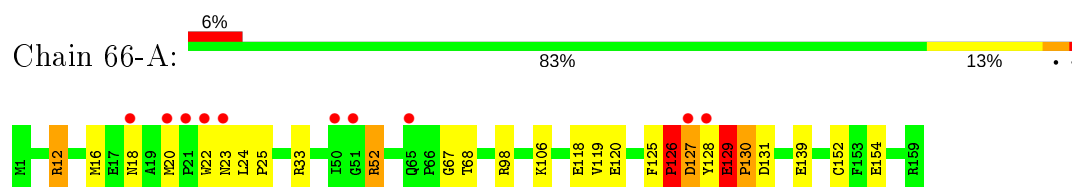
- Molecule 1: Dihydrofolate reductase



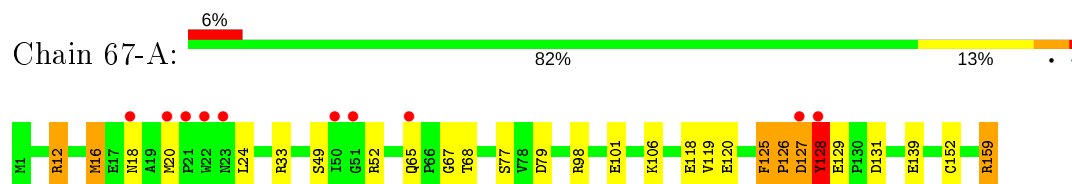
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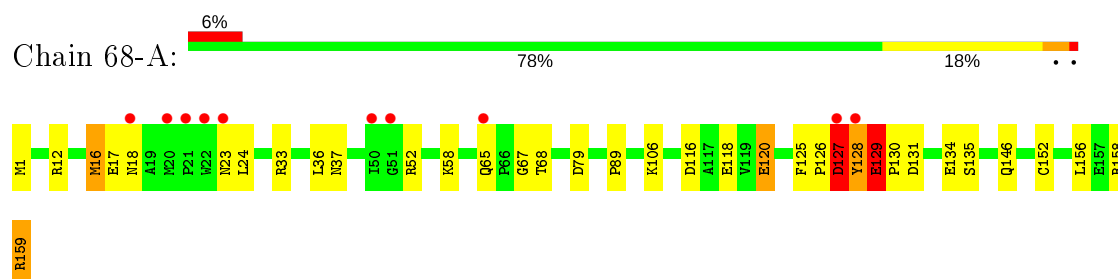
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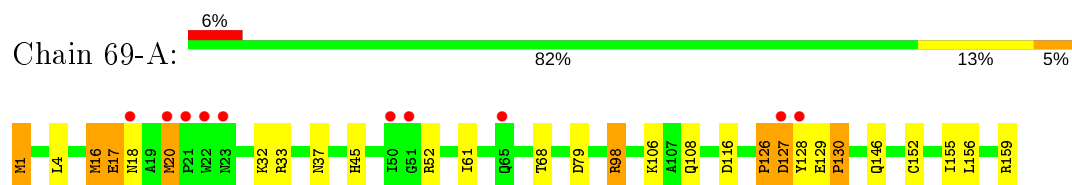
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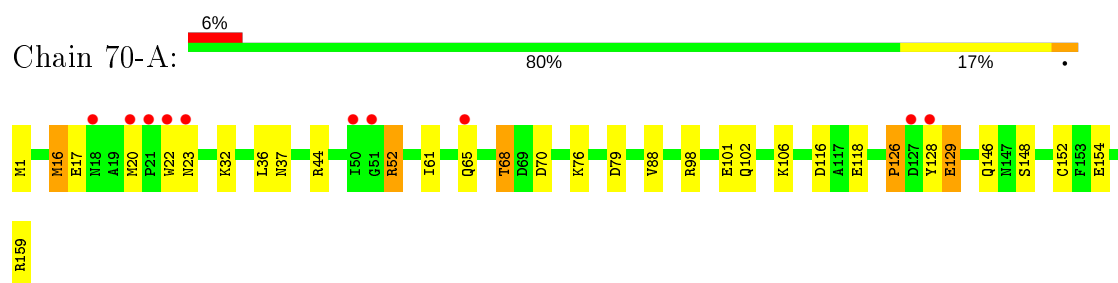
- Molecule 1: Dihydrofolate reductase



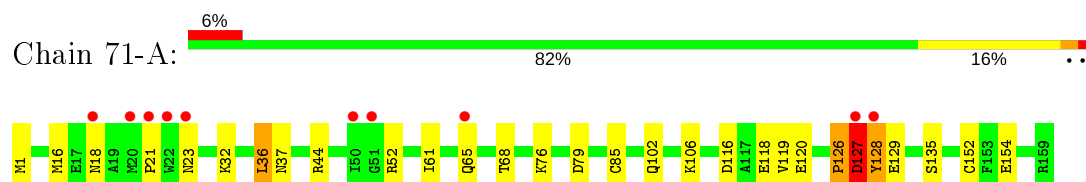
- Molecule 1: Dihydrofolate reductase



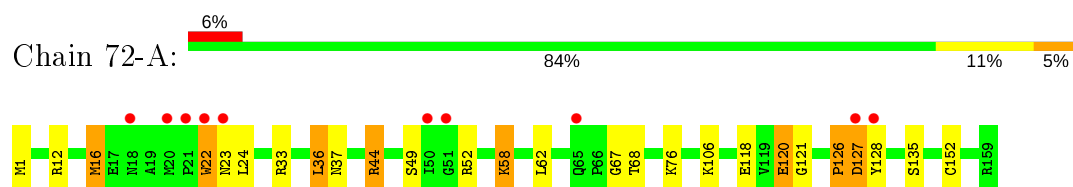
- Molecule 1: Dihydrofolate reductase



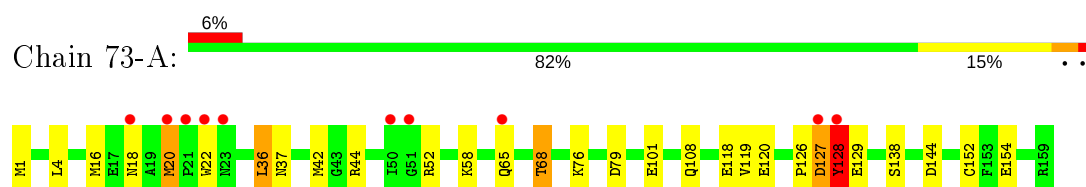
- Molecule 1: Dihydrofolate reductase



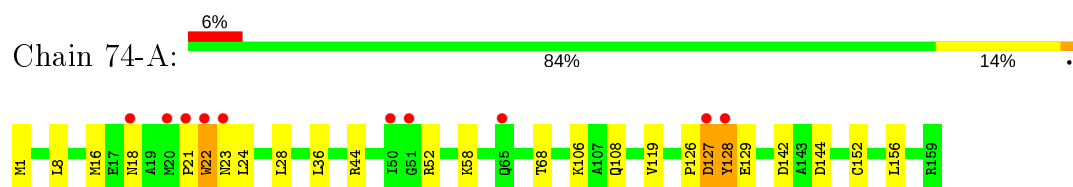
- Molecule 1: Dihydrofolate reductase



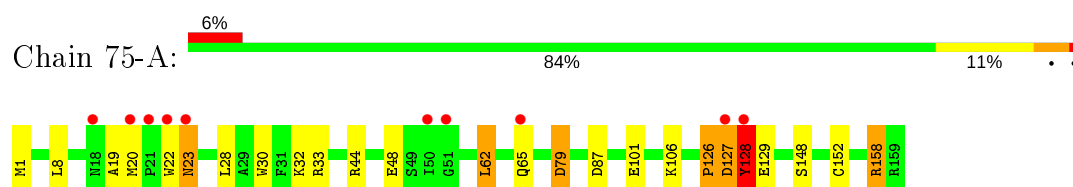
- Molecule 1: Dihydrofolate reductase



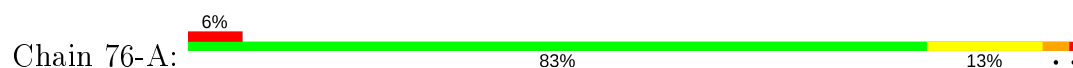
- Molecule 1: Dihydrofolate reductase

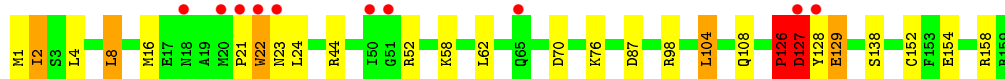


- Molecule 1: Dihydrofolate reductase

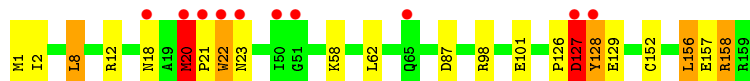
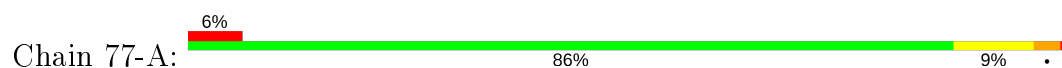


- Molecule 1: Dihydrofolate reductase

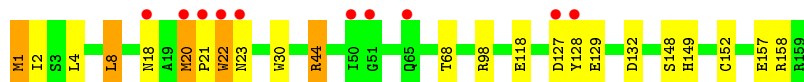
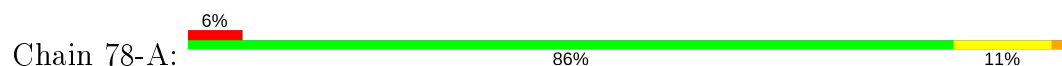




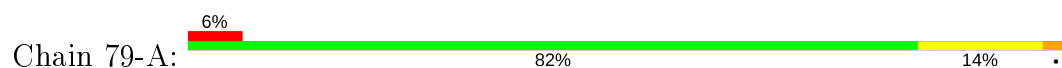
- Molecule 1: Dihydrofolate reductase



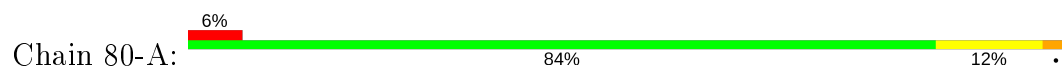
- Molecule 1: Dihydrofolate reductase



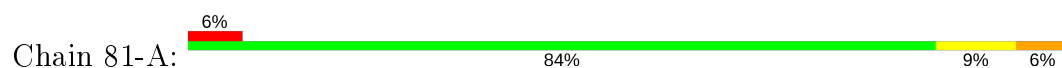
- Molecule 1: Dihydrofolate reductase



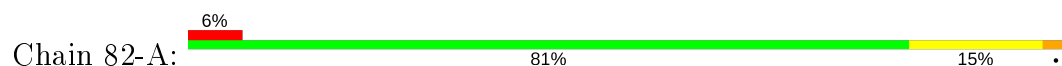
- Molecule 1: Dihydrofolate reductase



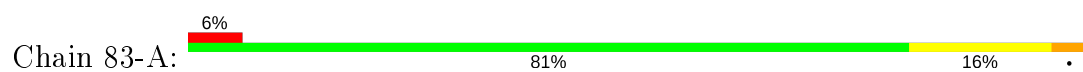
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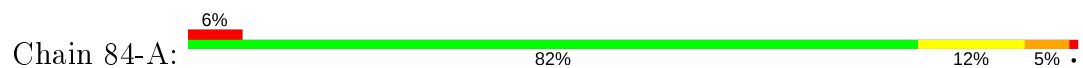
- Molecule 1: Dihydrofolate reductase



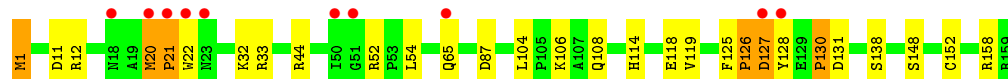
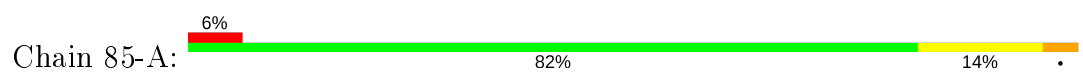
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



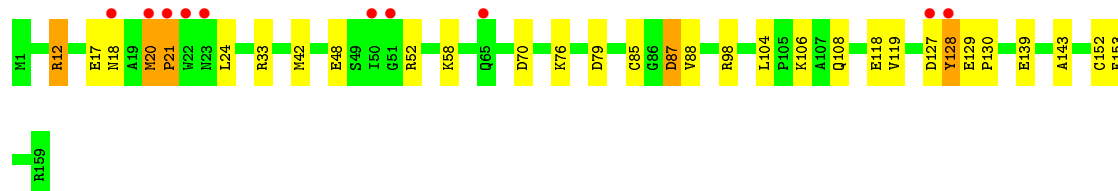
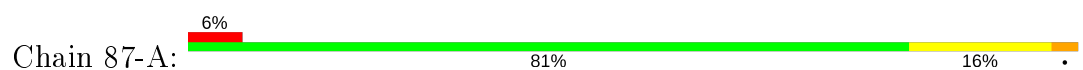
- Molecule 1: Dihydrofolate reductase



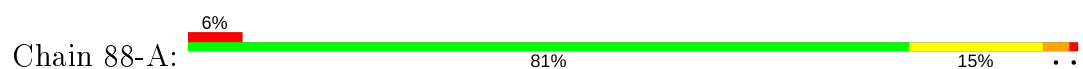
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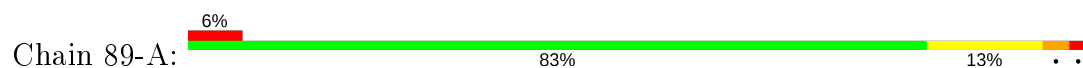
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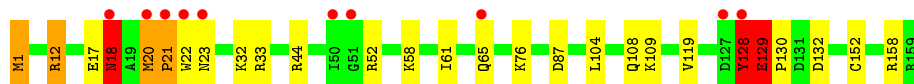


- Molecule 1: Dihydrofolate reductase

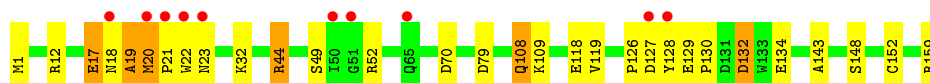
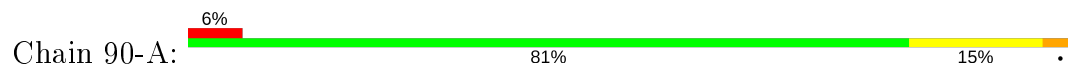


- Molecule 1: Dihydrofolate reductase

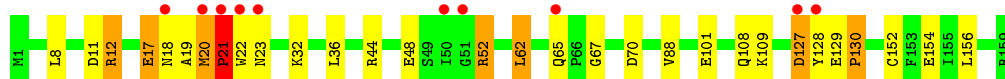
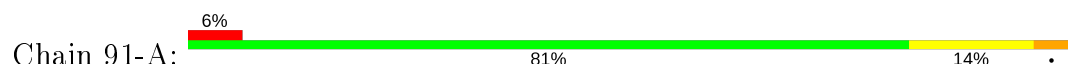




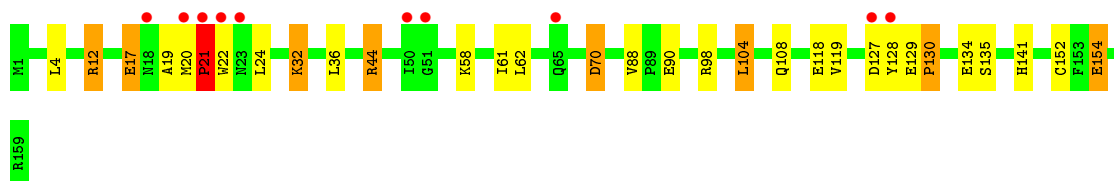
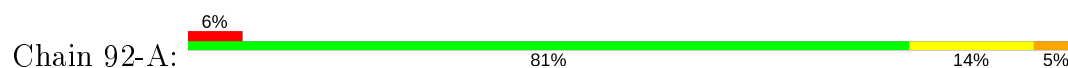
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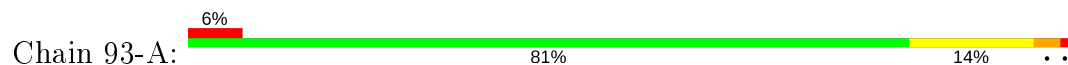
- Molecule 1: Dihydrofolate reductase



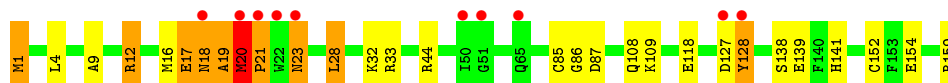
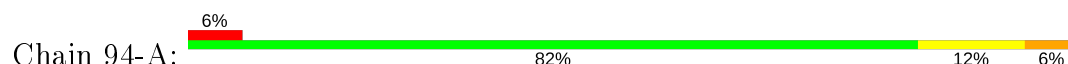
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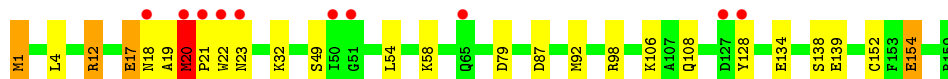
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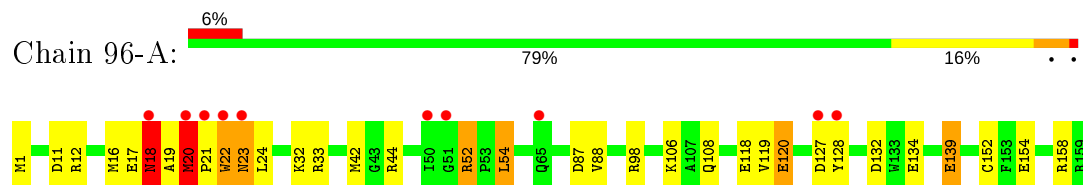
- Molecule 1: Dihydrofolate reductase



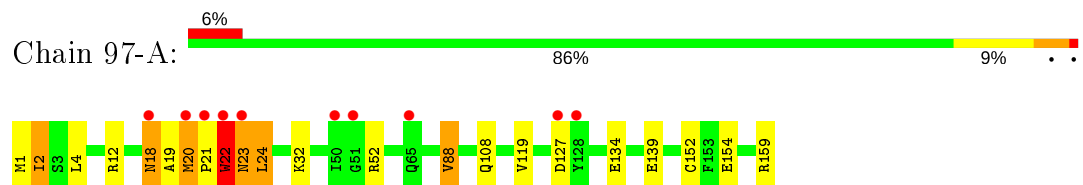
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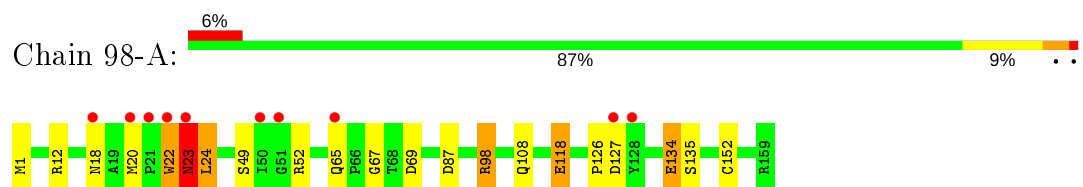
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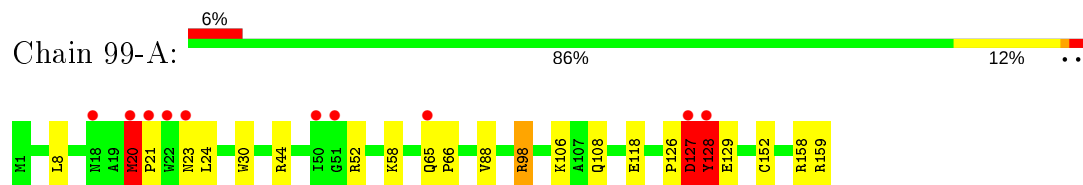
- Molecule 1: Dihydrofolate reductase



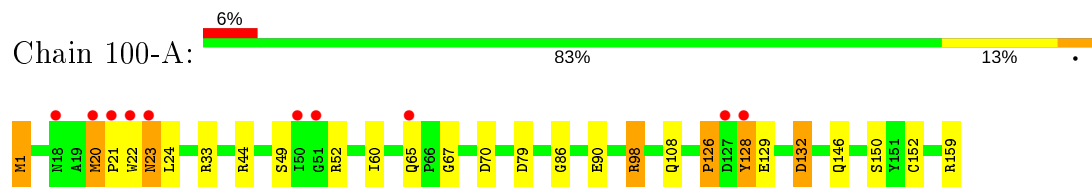
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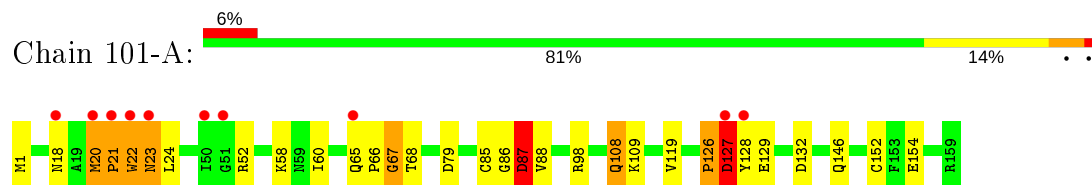
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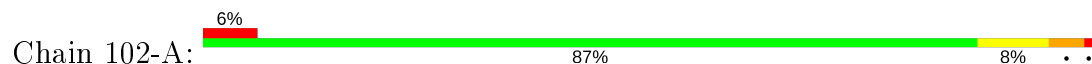
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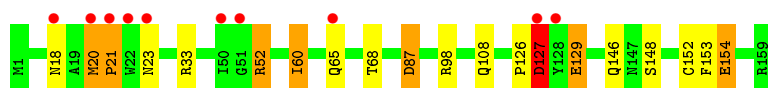


- Molecule 1: Dihydrofolate reductase

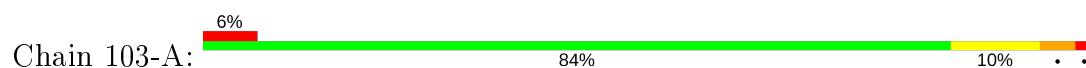


- Molecule 1: Dihydrofolate reductase

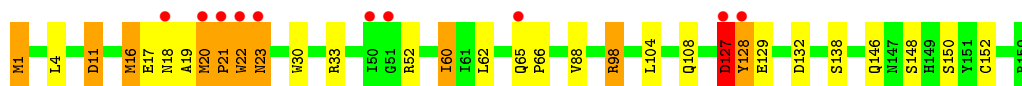
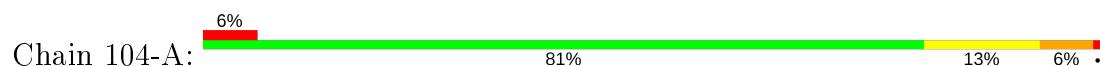




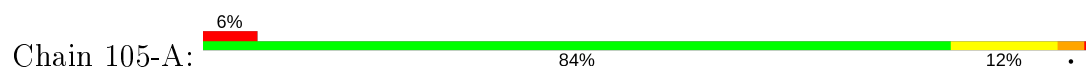
- Molecule 1: Dihydrofolate reductase



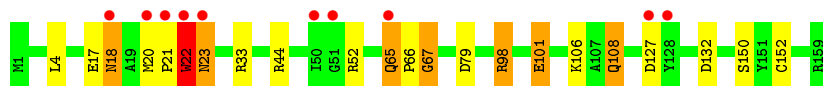
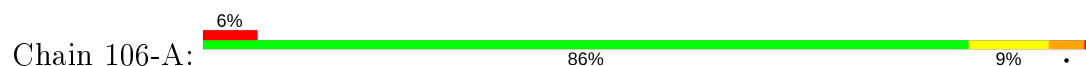
- Molecule 1: Dihydrofolate reductase



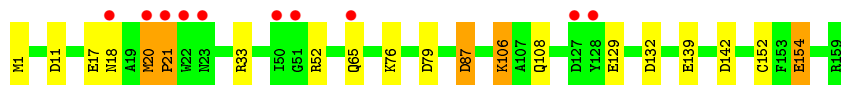
- Molecule 1: Dihydrofolate reductase



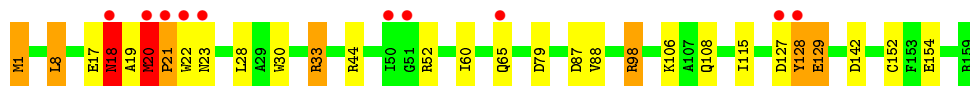
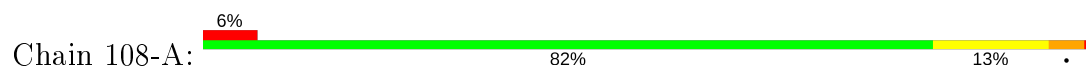
- Molecule 1: Dihydrofolate reductase



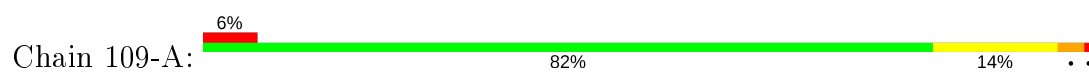
- Molecule 1: Dihydrofolate reductase



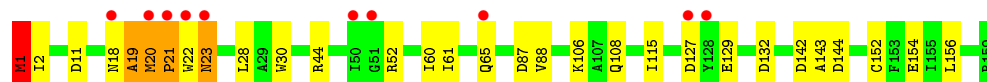
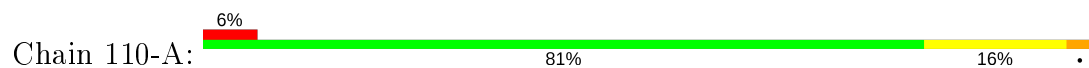
- Molecule 1: Dihydrofolate reductase



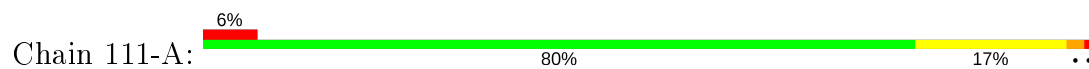
- Molecule 1: Dihydrofolate reductase



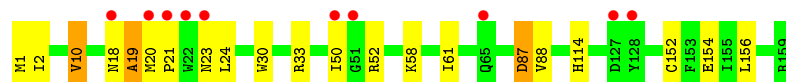
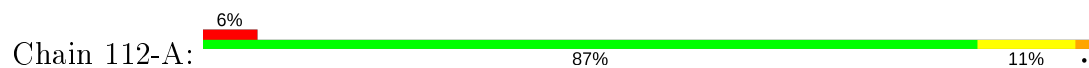
• Molecule 1: Dihydrofolate reductase



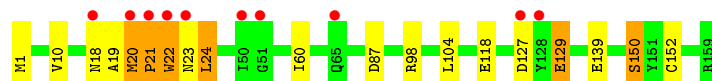
• Molecule 1: Dihydrofolate reductase



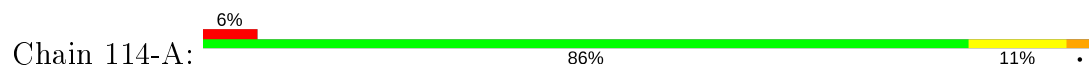
• Molecule 1: Dihydrofolate reductase



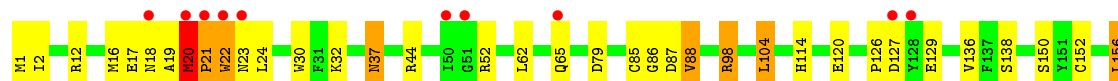
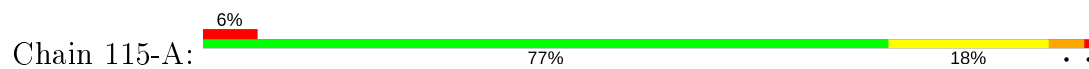
• Molecule 1: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase

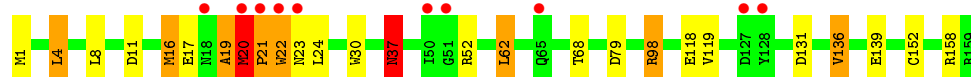
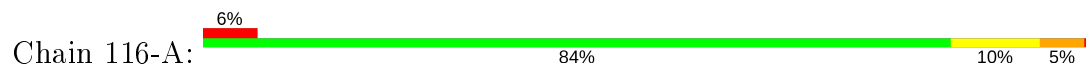


• Molecule 1: Dihydrofolate reductase

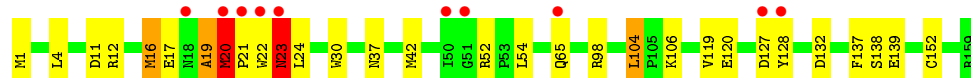
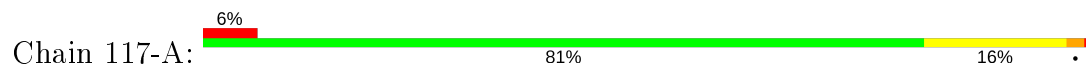




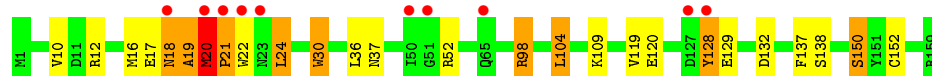
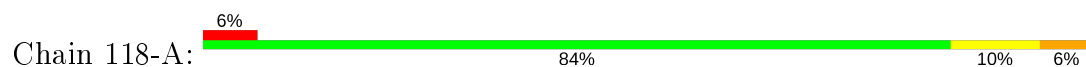
- Molecule 1: Dihydrofolate reductase



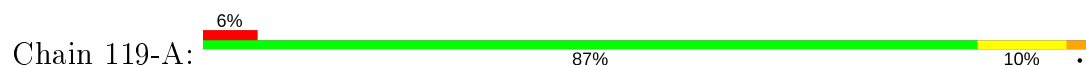
- Molecule 1: Dihydrofolate reductase



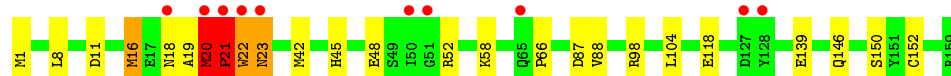
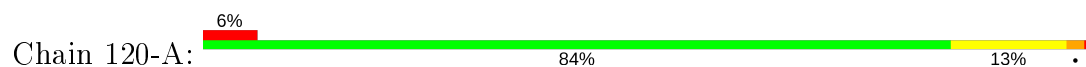
- Molecule 1: Dihydrofolate reductase



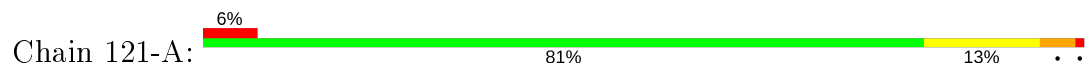
- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

Chain 122-A: 




- Molecule 1: Dihydrofolate reductase

Chain 123-A: 




- Molecule 1: Dihydrofolate reductase

Chain 124-A: 



- Molecule 1: Dihydrofolate reductase

Chain 125-A: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 34.30Å 45.52Å 98.71Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.40 – 1.05 49.36 – 1.05 | Depositor EDS |
| % Data completeness (in resolution range) | 98.2 (49.40-1.05) 96.1 (49.36-1.05) | Depositor EDS |
| R_{merge} | 0.04 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.22 (at 1.05Å) | Xtriage |
| Refinement program | PHENIX 1.8.4-1496 | Depositor |
| R, R_{free} | 0.136 , 0.166 0.142 , 0.163 | Depositor DCC |
| R_{free} test set | 3666 reflections (5.11%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 10.4 | Xtriage |
| Anisotropy | 0.167 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 999.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.97 | EDS |
| Total number of atoms | 339833 | wwPDB-VP |
| Average B, all atoms (Å ²) | 11.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, CSD, NAP, MN

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 | 1-A | 0.85 | 1/1296 (0.1%) | 1.08 | 6/1762 (0.3%) |
| 1 | 2-A | 0.87 | 3/1296 (0.2%) | 1.20 | 14/1762 (0.8%) |
| 1 | 3-A | 0.85 | 2/1296 (0.2%) | 1.11 | 10/1762 (0.6%) |
| 1 | 4-A | 0.90 | 4/1296 (0.3%) | 1.09 | 11/1762 (0.6%) |
| 1 | 5-A | 0.87 | 4/1296 (0.3%) | 1.16 | 12/1762 (0.7%) |
| 1 | 6-A | 0.87 | 1/1296 (0.1%) | 1.17 | 13/1762 (0.7%) |
| 1 | 7-A | 1.06 | 7/1296 (0.5%) | 1.26 | 16/1762 (0.9%) |
| 1 | 8-A | 0.88 | 0/1296 | 1.18 | 10/1762 (0.6%) |
| 1 | 9-A | 0.97 | 3/1296 (0.2%) | 1.22 | 15/1762 (0.9%) |
| 1 | 10-A | 0.91 | 2/1296 (0.2%) | 1.17 | 15/1762 (0.9%) |
| 1 | 11-A | 0.99 | 6/1296 (0.5%) | 1.19 | 17/1762 (1.0%) |
| 1 | 12-A | 0.88 | 2/1296 (0.2%) | 1.14 | 10/1762 (0.6%) |
| 1 | 13-A | 0.92 | 3/1296 (0.2%) | 1.23 | 12/1762 (0.7%) |
| 1 | 14-A | 0.96 | 3/1296 (0.2%) | 1.25 | 11/1762 (0.6%) |
| 1 | 15-A | 0.91 | 2/1296 (0.2%) | 1.14 | 7/1762 (0.4%) |
| 1 | 16-A | 0.81 | 0/1296 | 1.08 | 4/1762 (0.2%) |
| 1 | 17-A | 0.86 | 3/1296 (0.2%) | 1.20 | 14/1762 (0.8%) |
| 1 | 18-A | 1.00 | 4/1296 (0.3%) | 1.20 | 14/1762 (0.8%) |
| 1 | 19-A | 0.95 | 3/1296 (0.2%) | 1.19 | 11/1762 (0.6%) |
| 1 | 20-A | 0.92 | 5/1296 (0.4%) | 1.13 | 6/1762 (0.3%) |
| 1 | 21-A | 0.86 | 1/1296 (0.1%) | 1.06 | 8/1762 (0.5%) |
| 1 | 22-A | 0.89 | 2/1296 (0.2%) | 1.16 | 10/1762 (0.6%) |
| 1 | 23-A | 0.88 | 3/1296 (0.2%) | 1.08 | 6/1762 (0.3%) |
| 1 | 24-A | 0.96 | 6/1296 (0.5%) | 1.15 | 11/1762 (0.6%) |
| 1 | 25-A | 0.94 | 4/1296 (0.3%) | 1.05 | 3/1762 (0.2%) |
| 1 | 26-A | 0.83 | 2/1296 (0.2%) | 1.13 | 10/1762 (0.6%) |
| 1 | 27-A | 0.91 | 3/1296 (0.2%) | 1.07 | 5/1762 (0.3%) |
| 1 | 28-A | 1.04 | 8/1296 (0.6%) | 1.25 | 17/1762 (1.0%) |
| 1 | 29-A | 1.17 | 8/1296 (0.6%) | 1.21 | 13/1762 (0.7%) |
| 1 | 30-A | 0.85 | 2/1296 (0.2%) | 1.05 | 4/1762 (0.2%) |
| 1 | 31-A | 0.82 | 1/1296 (0.1%) | 1.03 | 7/1762 (0.4%) |
| 1 | 32-A | 0.98 | 4/1296 (0.3%) | 1.23 | 16/1762 (0.9%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 33-A | 0.91 | 5/1296 (0.4%) | 1.14 | 13/1762 (0.7%) |
| 1 | 34-A | 0.94 | 4/1296 (0.3%) | 1.15 | 11/1762 (0.6%) |
| 1 | 35-A | 0.87 | 2/1296 (0.2%) | 1.20 | 14/1762 (0.8%) |
| 1 | 36-A | 0.87 | 3/1296 (0.2%) | 1.12 | 10/1762 (0.6%) |
| 1 | 37-A | 0.91 | 5/1296 (0.4%) | 1.10 | 7/1762 (0.4%) |
| 1 | 38-A | 0.95 | 5/1296 (0.4%) | 1.19 | 10/1762 (0.6%) |
| 1 | 39-A | 0.91 | 1/1296 (0.1%) | 1.06 | 7/1762 (0.4%) |
| 1 | 40-A | 0.84 | 1/1296 (0.1%) | 1.11 | 9/1762 (0.5%) |
| 1 | 41-A | 0.94 | 3/1296 (0.2%) | 1.22 | 16/1762 (0.9%) |
| 1 | 42-A | 0.85 | 1/1296 (0.1%) | 1.21 | 9/1762 (0.5%) |
| 1 | 43-A | 0.97 | 4/1296 (0.3%) | 1.18 | 11/1762 (0.6%) |
| 1 | 44-A | 0.97 | 4/1296 (0.3%) | 1.20 | 13/1762 (0.7%) |
| 1 | 45-A | 1.05 | 9/1296 (0.7%) | 1.13 | 8/1762 (0.5%) |
| 1 | 46-A | 0.92 | 4/1296 (0.3%) | 1.16 | 11/1762 (0.6%) |
| 1 | 47-A | 1.01 | 8/1296 (0.6%) | 1.15 | 8/1762 (0.5%) |
| 1 | 48-A | 0.90 | 2/1296 (0.2%) | 1.16 | 12/1762 (0.7%) |
| 1 | 49-A | 0.98 | 8/1296 (0.6%) | 1.08 | 4/1762 (0.2%) |
| 1 | 50-A | 0.92 | 4/1296 (0.3%) | 1.07 | 9/1762 (0.5%) |
| 1 | 51-A | 0.94 | 3/1296 (0.2%) | 1.16 | 11/1762 (0.6%) |
| 1 | 52-A | 1.00 | 6/1296 (0.5%) | 1.06 | 6/1762 (0.3%) |
| 1 | 53-A | 0.87 | 3/1296 (0.2%) | 1.07 | 10/1762 (0.6%) |
| 1 | 54-A | 1.01 | 6/1296 (0.5%) | 1.15 | 11/1762 (0.6%) |
| 1 | 55-A | 0.96 | 4/1296 (0.3%) | 1.20 | 17/1762 (1.0%) |
| 1 | 56-A | 0.89 | 4/1296 (0.3%) | 1.13 | 10/1762 (0.6%) |
| 1 | 57-A | 0.95 | 3/1296 (0.2%) | 1.20 | 13/1762 (0.7%) |
| 1 | 58-A | 0.95 | 3/1296 (0.2%) | 1.13 | 7/1762 (0.4%) |
| 1 | 59-A | 0.85 | 1/1296 (0.1%) | 1.10 | 9/1762 (0.5%) |
| 1 | 60-A | 0.87 | 0/1296 | 1.12 | 7/1762 (0.4%) |
| 1 | 61-A | 0.98 | 7/1296 (0.5%) | 1.15 | 11/1762 (0.6%) |
| 1 | 62-A | 0.94 | 3/1296 (0.2%) | 1.14 | 7/1762 (0.4%) |
| 1 | 63-A | 1.05 | 4/1296 (0.3%) | 1.23 | 16/1762 (0.9%) |
| 1 | 64-A | 1.32 | 8/1296 (0.6%) | 1.36 | 22/1762 (1.2%) |
| 1 | 65-A | 0.90 | 2/1296 (0.2%) | 1.09 | 7/1762 (0.4%) |
| 1 | 66-A | 1.03 | 3/1296 (0.2%) | 1.23 | 12/1762 (0.7%) |
| 1 | 67-A | 0.91 | 4/1296 (0.3%) | 1.17 | 15/1762 (0.9%) |
| 1 | 68-A | 1.01 | 7/1296 (0.5%) | 1.30 | 15/1762 (0.9%) |
| 1 | 69-A | 0.90 | 1/1296 (0.1%) | 1.13 | 8/1762 (0.5%) |
| 1 | 70-A | 0.89 | 1/1296 (0.1%) | 1.23 | 17/1762 (1.0%) |
| 1 | 71-A | 0.93 | 5/1296 (0.4%) | 1.06 | 5/1762 (0.3%) |
| 1 | 72-A | 0.93 | 4/1296 (0.3%) | 1.22 | 13/1762 (0.7%) |
| 1 | 73-A | 0.94 | 3/1296 (0.2%) | 1.16 | 12/1762 (0.7%) |
| 1 | 74-A | 0.94 | 3/1296 (0.2%) | 1.08 | 5/1762 (0.3%) |
| 1 | 75-A | 0.94 | 1/1296 (0.1%) | 1.15 | 7/1762 (0.4%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 76-A | 0.95 | 3/1296 (0.2%) | 1.20 | 13/1762 (0.7%) |
| 1 | 77-A | 0.99 | 5/1296 (0.4%) | 1.16 | 10/1762 (0.6%) |
| 1 | 78-A | 0.94 | 2/1296 (0.2%) | 1.17 | 11/1762 (0.6%) |
| 1 | 79-A | 1.09 | 5/1296 (0.4%) | 1.17 | 8/1762 (0.5%) |
| 1 | 80-A | 0.91 | 2/1296 (0.2%) | 1.15 | 11/1762 (0.6%) |
| 1 | 81-A | 0.95 | 4/1296 (0.3%) | 1.21 | 15/1762 (0.9%) |
| 1 | 82-A | 1.05 | 8/1296 (0.6%) | 1.16 | 14/1762 (0.8%) |
| 1 | 83-A | 0.97 | 6/1296 (0.5%) | 1.22 | 14/1762 (0.8%) |
| 1 | 84-A | 0.98 | 6/1296 (0.5%) | 1.19 | 15/1762 (0.9%) |
| 1 | 85-A | 0.85 | 0/1296 | 1.25 | 13/1762 (0.7%) |
| 1 | 86-A | 0.93 | 3/1296 (0.2%) | 1.11 | 6/1762 (0.3%) |
| 1 | 87-A | 0.89 | 2/1296 (0.2%) | 1.10 | 6/1762 (0.3%) |
| 1 | 88-A | 0.92 | 0/1296 | 1.22 | 13/1762 (0.7%) |
| 1 | 89-A | 0.93 | 3/1296 (0.2%) | 1.14 | 9/1762 (0.5%) |
| 1 | 90-A | 0.88 | 1/1296 (0.1%) | 1.15 | 13/1762 (0.7%) |
| 1 | 91-A | 0.99 | 3/1296 (0.2%) | 1.18 | 13/1762 (0.7%) |
| 1 | 92-A | 0.96 | 4/1296 (0.3%) | 1.24 | 13/1762 (0.7%) |
| 1 | 93-A | 1.02 | 7/1296 (0.5%) | 1.28 | 14/1762 (0.8%) |
| 1 | 94-A | 0.93 | 4/1296 (0.3%) | 1.17 | 11/1762 (0.6%) |
| 1 | 95-A | 0.99 | 6/1296 (0.5%) | 1.14 | 9/1762 (0.5%) |
| 1 | 96-A | 1.01 | 4/1296 (0.3%) | 1.32 | 17/1762 (1.0%) |
| 1 | 97-A | 0.89 | 3/1296 (0.2%) | 1.13 | 12/1762 (0.7%) |
| 1 | 98-A | 1.00 | 6/1296 (0.5%) | 1.22 | 13/1762 (0.7%) |
| 1 | 99-A | 0.88 | 3/1296 (0.2%) | 1.12 | 12/1762 (0.7%) |
| 1 | 100-A | 0.89 | 1/1296 (0.1%) | 1.17 | 11/1762 (0.6%) |
| 1 | 101-A | 0.94 | 4/1296 (0.3%) | 1.15 | 11/1762 (0.6%) |
| 1 | 102-A | 0.95 | 5/1296 (0.4%) | 1.19 | 13/1762 (0.7%) |
| 1 | 103-A | 0.92 | 2/1296 (0.2%) | 1.13 | 11/1762 (0.6%) |
| 1 | 104-A | 0.97 | 6/1296 (0.5%) | 1.24 | 14/1762 (0.8%) |
| 1 | 105-A | 0.88 | 3/1296 (0.2%) | 1.09 | 8/1762 (0.5%) |
| 1 | 106-A | 0.93 | 4/1296 (0.3%) | 1.15 | 8/1762 (0.5%) |
| 1 | 107-A | 0.96 | 4/1296 (0.3%) | 1.17 | 11/1762 (0.6%) |
| 1 | 108-A | 1.05 | 5/1296 (0.4%) | 1.17 | 16/1762 (0.9%) |
| 1 | 109-A | 1.04 | 5/1296 (0.4%) | 1.23 | 11/1762 (0.6%) |
| 1 | 110-A | 1.30 | 5/1296 (0.4%) | 1.16 | 9/1762 (0.5%) |
| 1 | 111-A | 1.34 | 5/1296 (0.4%) | 1.16 | 11/1762 (0.6%) |
| 1 | 112-A | 1.36 | 3/1296 (0.2%) | 1.16 | 8/1762 (0.5%) |
| 1 | 113-A | 0.95 | 6/1296 (0.5%) | 1.06 | 6/1762 (0.3%) |
| 1 | 114-A | 0.88 | 0/1296 | 1.11 | 8/1762 (0.5%) |
| 1 | 115-A | 0.93 | 5/1296 (0.4%) | 1.22 | 14/1762 (0.8%) |
| 1 | 116-A | 0.93 | 3/1296 (0.2%) | 1.17 | 11/1762 (0.6%) |
| 1 | 117-A | 0.99 | 4/1296 (0.3%) | 1.12 | 12/1762 (0.7%) |
| 1 | 118-A | 0.96 | 4/1296 (0.3%) | 1.18 | 9/1762 (0.5%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 119-A | 1.00 | 5/1296 (0.4%) | 1.14 | 9/1762 (0.5%) |
| 1 | 120-A | 0.96 | 3/1296 (0.2%) | 1.10 | 7/1762 (0.4%) |
| 1 | 121-A | 1.01 | 5/1296 (0.4%) | 1.15 | 12/1762 (0.7%) |
| 1 | 122-A | 0.97 | 5/1296 (0.4%) | 1.22 | 11/1762 (0.6%) |
| 1 | 123-A | 0.94 | 5/1296 (0.4%) | 1.11 | 7/1762 (0.4%) |
| 1 | 124-A | 0.98 | 5/1296 (0.4%) | 1.15 | 12/1762 (0.7%) |
| 1 | 125-A | 1.10 | 5/1296 (0.4%) | 1.12 | 12/1762 (0.7%) |
| All | All | 0.96 | 461/162000 (0.3%) | 1.16 | 1350/220250 (0.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 1-A | 0 | 1 |
| 1 | 2-A | 0 | 3 |
| 1 | 3-A | 0 | 3 |
| 1 | 4-A | 0 | 3 |
| 1 | 5-A | 0 | 2 |
| 1 | 6-A | 0 | 2 |
| 1 | 7-A | 0 | 5 |
| 1 | 8-A | 0 | 4 |
| 1 | 9-A | 0 | 4 |
| 1 | 10-A | 0 | 4 |
| 1 | 11-A | 0 | 3 |
| 1 | 12-A | 0 | 3 |
| 1 | 13-A | 0 | 3 |
| 1 | 14-A | 0 | 2 |
| 1 | 15-A | 0 | 3 |
| 1 | 16-A | 0 | 4 |
| 1 | 17-A | 0 | 4 |
| 1 | 18-A | 0 | 2 |
| 1 | 19-A | 0 | 2 |
| 1 | 21-A | 0 | 1 |
| 1 | 22-A | 0 | 3 |
| 1 | 23-A | 0 | 3 |
| 1 | 24-A | 0 | 2 |
| 1 | 26-A | 0 | 1 |
| 1 | 27-A | 0 | 1 |
| 1 | 29-A | 0 | 2 |
| 1 | 30-A | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 31-A | 0 | 2 |
| 1 | 32-A | 0 | 2 |
| 1 | 33-A | 0 | 1 |
| 1 | 36-A | 0 | 2 |
| 1 | 38-A | 0 | 1 |
| 1 | 39-A | 0 | 3 |
| 1 | 40-A | 0 | 2 |
| 1 | 41-A | 0 | 3 |
| 1 | 42-A | 0 | 1 |
| 1 | 43-A | 0 | 3 |
| 1 | 44-A | 0 | 2 |
| 1 | 45-A | 0 | 1 |
| 1 | 46-A | 0 | 2 |
| 1 | 47-A | 0 | 2 |
| 1 | 48-A | 0 | 1 |
| 1 | 49-A | 0 | 2 |
| 1 | 50-A | 0 | 2 |
| 1 | 52-A | 0 | 2 |
| 1 | 54-A | 0 | 4 |
| 1 | 55-A | 0 | 2 |
| 1 | 56-A | 0 | 2 |
| 1 | 57-A | 0 | 2 |
| 1 | 58-A | 0 | 2 |
| 1 | 59-A | 0 | 1 |
| 1 | 60-A | 0 | 1 |
| 1 | 61-A | 0 | 1 |
| 1 | 62-A | 0 | 1 |
| 1 | 63-A | 0 | 3 |
| 1 | 64-A | 0 | 3 |
| 1 | 65-A | 0 | 2 |
| 1 | 66-A | 0 | 6 |
| 1 | 67-A | 0 | 2 |
| 1 | 68-A | 0 | 3 |
| 1 | 69-A | 0 | 3 |
| 1 | 70-A | 0 | 2 |
| 1 | 71-A | 0 | 2 |
| 1 | 72-A | 0 | 1 |
| 1 | 73-A | 0 | 3 |
| 1 | 74-A | 0 | 1 |
| 1 | 75-A | 0 | 4 |
| 1 | 76-A | 0 | 3 |
| 1 | 77-A | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 78-A | 0 | 2 |
| 1 | 79-A | 0 | 1 |
| 1 | 81-A | 0 | 1 |
| 1 | 82-A | 0 | 1 |
| 1 | 83-A | 0 | 2 |
| 1 | 84-A | 0 | 1 |
| 1 | 85-A | 0 | 1 |
| 1 | 86-A | 0 | 1 |
| 1 | 87-A | 0 | 3 |
| 1 | 88-A | 0 | 2 |
| 1 | 89-A | 0 | 2 |
| 1 | 90-A | 0 | 3 |
| 1 | 91-A | 0 | 3 |
| 1 | 92-A | 0 | 2 |
| 1 | 93-A | 0 | 4 |
| 1 | 94-A | 0 | 3 |
| 1 | 95-A | 0 | 2 |
| 1 | 96-A | 0 | 4 |
| 1 | 98-A | 0 | 2 |
| 1 | 99-A | 0 | 2 |
| 1 | 100-A | 0 | 3 |
| 1 | 101-A | 0 | 4 |
| 1 | 102-A | 0 | 4 |
| 1 | 103-A | 0 | 2 |
| 1 | 104-A | 0 | 2 |
| 1 | 105-A | 0 | 1 |
| 1 | 106-A | 0 | 1 |
| 1 | 107-A | 0 | 1 |
| 1 | 108-A | 0 | 3 |
| 1 | 109-A | 0 | 3 |
| 1 | 110-A | 0 | 3 |
| 1 | 111-A | 0 | 3 |
| 1 | 112-A | 0 | 3 |
| 1 | 113-A | 0 | 1 |
| 1 | 114-A | 0 | 4 |
| 1 | 115-A | 0 | 3 |
| 1 | 116-A | 0 | 2 |
| 1 | 117-A | 0 | 2 |
| 1 | 118-A | 0 | 3 |
| 1 | 119-A | 0 | 1 |
| 1 | 120-A | 0 | 2 |
| 1 | 121-A | 0 | 5 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 122-A | 0 | 1 |
| 1 | 123-A | 0 | 2 |
| 1 | 124-A | 0 | 2 |
| 1 | 125-A | 0 | 2 |
| All | All | 0 | 267 |

All (461) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | 111-A | 30 | TRP | CB-CG | 35.12 | 2.13 | 1.50 |
| 1 | 112-A | 30 | TRP | CB-CG | 34.17 | 2.11 | 1.50 |
| 1 | 110-A | 30 | TRP | CB-CG | 28.63 | 2.01 | 1.50 |
| 1 | 64-A | 154 | GLU | CB-CG | 21.19 | 1.92 | 1.52 |
| 1 | 125-A | 30 | TRP | CB-CG | 20.27 | 1.86 | 1.50 |
| 1 | 64-A | 154 | GLU | CG-CD | 19.48 | 1.81 | 1.51 |
| 1 | 108-A | 30 | TRP | CB-CG | -17.10 | 1.19 | 1.50 |
| 1 | 79-A | 22 | TRP | CB-CG | -16.73 | 1.20 | 1.50 |
| 1 | 29-A | 154 | GLU | CB-CG | 16.32 | 1.83 | 1.52 |
| 1 | 117-A | 30 | TRP | CB-CG | 16.06 | 1.79 | 1.50 |
| 1 | 63-A | 154 | GLU | CB-CG | 14.67 | 1.80 | 1.52 |
| 1 | 52-A | 9 | ALA | CA-CB | -13.67 | 1.23 | 1.52 |
| 1 | 9-A | 85 | CYS | CB-SG | -13.48 | 1.59 | 1.82 |
| 1 | 124-A | 30 | TRP | CB-CG | 13.29 | 1.74 | 1.50 |
| 1 | 64-A | 154 | GLU | CD-OE2 | 13.23 | 1.40 | 1.25 |
| 1 | 29-A | 154 | GLU | CG-CD | 12.88 | 1.71 | 1.51 |
| 1 | 15-A | 154 | GLU | CB-CG | 12.47 | 1.75 | 1.52 |
| 1 | 54-A | 85 | CYS | CB-SG | 12.42 | 2.03 | 1.82 |
| 1 | 91-A | 101 | GLU | CB-CG | 12.11 | 1.75 | 1.52 |
| 1 | 66-A | 154 | GLU | CG-CD | 11.90 | 1.69 | 1.51 |
| 1 | 18-A | 101 | GLU | CB-CG | 11.68 | 1.74 | 1.52 |
| 1 | 28-A | 12 | ARG | CG-CD | 11.50 | 1.80 | 1.51 |
| 1 | 28-A | 12 | ARG | CB-CG | 11.41 | 1.83 | 1.52 |
| 1 | 51-A | 154 | GLU | CG-CD | -11.38 | 1.34 | 1.51 |
| 1 | 123-A | 30 | TRP | CB-CG | 11.05 | 1.70 | 1.50 |
| 1 | 119-A | 22 | TRP | CB-CG | -10.65 | 1.31 | 1.50 |
| 1 | 7-A | 154 | GLU | CG-CD | 10.51 | 1.67 | 1.51 |
| 1 | 11-A | 126 | PRO | C-O | 10.49 | 1.44 | 1.23 |
| 1 | 98-A | 24 | LEU | N-CA | 10.45 | 1.67 | 1.46 |
| 1 | 61-A | 78 | VAL | CB-CG1 | -10.39 | 1.31 | 1.52 |
| 1 | 121-A | 21 | PRO | CB-CG | 10.37 | 2.01 | 1.50 |
| 1 | 78-A | 30 | TRP | CB-CG | -10.37 | 1.31 | 1.50 |
| 1 | 4-A | 154 | GLU | CD-OE2 | 10.34 | 1.37 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 29-A | 154 | GLU | CD-OE2 | 10.28 | 1.36 | 1.25 |
| 1 | 11-A | 98 | ARG | CG-CD | 10.27 | 1.77 | 1.51 |
| 1 | 66-A | 154 | GLU | CB-CG | 10.10 | 1.71 | 1.52 |
| 1 | 77-A | 101 | GLU | CB-CG | 10.05 | 1.71 | 1.52 |
| 1 | 29-A | 12 | ARG | CB-CG | 9.88 | 1.79 | 1.52 |
| 1 | 110-A | 60 | ILE | CB-CG2 | -9.87 | 1.22 | 1.52 |
| 1 | 58-A | 78 | VAL | CB-CG1 | -9.82 | 1.32 | 1.52 |
| 1 | 71-A | 102 | GLN | CG-CD | 9.59 | 1.73 | 1.51 |
| 1 | 68-A | 16 | MET | CB-CG | 9.53 | 1.81 | 1.51 |
| 1 | 112-A | 30 | TRP | CG-CD1 | 9.49 | 1.50 | 1.36 |
| 1 | 76-A | 22 | TRP | CB-CG | 9.48 | 1.67 | 1.50 |
| 1 | 74-A | 22 | TRP | CB-CG | -9.47 | 1.33 | 1.50 |
| 1 | 29-A | 12 | ARG | CG-CD | 9.44 | 1.75 | 1.51 |
| 1 | 95-A | 12 | ARG | CB-CG | 9.41 | 1.77 | 1.52 |
| 1 | 78-A | 22 | TRP | CB-CG | -9.37 | 1.33 | 1.50 |
| 1 | 49-A | 129 | GLU | CB-CG | 9.32 | 1.69 | 1.52 |
| 1 | 19-A | 85 | CYS | CB-SG | -9.31 | 1.66 | 1.82 |
| 1 | 25-A | 129 | GLU | CB-CG | 9.26 | 1.69 | 1.52 |
| 1 | 118-A | 30 | TRP | CB-CG | 9.19 | 1.66 | 1.50 |
| 1 | 49-A | 129 | GLU | CG-CD | 9.16 | 1.65 | 1.51 |
| 1 | 63-A | 154 | GLU | CG-CD | 9.10 | 1.65 | 1.51 |
| 1 | 95-A | 12 | ARG | CG-CD | 9.08 | 1.74 | 1.51 |
| 1 | 19-A | 22 | TRP | CB-CG | -9.02 | 1.34 | 1.50 |
| 1 | 82-A | 22 | TRP | CB-CG | -8.96 | 1.34 | 1.50 |
| 1 | 38-A | 16 | MET | CG-SD | 8.88 | 2.04 | 1.81 |
| 1 | 101-A | 85 | CYS | CB-SG | -8.82 | 1.67 | 1.82 |
| 1 | 111-A | 30 | TRP | CG-CD1 | 8.80 | 1.49 | 1.36 |
| 1 | 57-A | 127 | ASP | CA-CB | 8.73 | 1.73 | 1.53 |
| 1 | 46-A | 22 | TRP | CB-CG | 8.70 | 1.66 | 1.50 |
| 1 | 110-A | 30 | TRP | CG-CD1 | 8.70 | 1.49 | 1.36 |
| 1 | 94-A | 85 | CYS | CB-SG | 8.70 | 1.97 | 1.82 |
| 1 | 103-A | 60 | ILE | CB-CG2 | -8.69 | 1.25 | 1.52 |
| 1 | 121-A | 85 | CYS | CB-SG | -8.69 | 1.67 | 1.82 |
| 1 | 47-A | 85 | CYS | CB-SG | 8.68 | 1.97 | 1.82 |
| 1 | 45-A | 154 | GLU | CB-CG | 8.63 | 1.68 | 1.52 |
| 1 | 92-A | 98 | ARG | CG-CD | 8.57 | 1.73 | 1.51 |
| 1 | 14-A | 37 | ASN | CB-CG | 8.50 | 1.70 | 1.51 |
| 1 | 101-A | 20 | MET | CB-CG | 8.49 | 1.78 | 1.51 |
| 1 | 120-A | 20 | MET | CG-SD | 8.44 | 2.03 | 1.81 |
| 1 | 50-A | 9 | ALA | CA-CB | -8.38 | 1.34 | 1.52 |
| 1 | 7-A | 154 | GLU | CD-OE2 | 8.38 | 1.34 | 1.25 |
| 1 | 64-A | 134 | GLU | CG-CD | 8.37 | 1.64 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 96-A | 18 | ASN | N-CA | 8.35 | 1.63 | 1.46 |
| 1 | 10-A | 154 | GLU | CG-CD | -8.34 | 1.39 | 1.51 |
| 1 | 125-A | 22 | TRP | CB-CG | 8.31 | 1.65 | 1.50 |
| 1 | 109-A | 154 | GLU | CB-CG | -8.29 | 1.36 | 1.52 |
| 1 | 13-A | 125 | PHE | CA-C | 8.29 | 1.74 | 1.52 |
| 1 | 83-A | 85 | CYS | CB-SG | -8.27 | 1.68 | 1.82 |
| 1 | 87-A | 85 | CYS | CB-SG | 8.27 | 1.96 | 1.82 |
| 1 | 64-A | 126 | PRO | CA-C | 8.15 | 1.69 | 1.52 |
| 1 | 53-A | 85 | CYS | CB-SG | -8.15 | 1.68 | 1.82 |
| 1 | 50-A | 118 | GLU | CB-CG | 8.14 | 1.67 | 1.52 |
| 1 | 68-A | 16 | MET | CG-SD | 8.13 | 2.02 | 1.81 |
| 1 | 109-A | 129 | GLU | CB-CG | 8.13 | 1.67 | 1.52 |
| 1 | 64-A | 134 | GLU | CB-CG | 8.12 | 1.67 | 1.52 |
| 1 | 38-A | 22 | TRP | CB-CG | 8.12 | 1.64 | 1.50 |
| 1 | 19-A | 154 | GLU | CB-CG | -8.08 | 1.36 | 1.52 |
| 1 | 95-A | 154 | GLU | CG-CD | -8.07 | 1.39 | 1.51 |
| 1 | 32-A | 118 | GLU | CB-CG | 8.07 | 1.67 | 1.52 |
| 1 | 39-A | 16 | MET | CB-CG | 8.02 | 1.77 | 1.51 |
| 1 | 65-A | 154 | GLU | CB-CG | 8.01 | 1.67 | 1.52 |
| 1 | 93-A | 98 | ARG | CG-CD | 8.00 | 1.72 | 1.51 |
| 1 | 84-A | 154 | GLU | CG-CD | 7.90 | 1.63 | 1.51 |
| 1 | 96-A | 22 | TRP | CB-CG | 7.90 | 1.64 | 1.50 |
| 1 | 34-A | 128 | TYR | N-CA | 7.88 | 1.62 | 1.46 |
| 1 | 95-A | 154 | GLU | CD-OE2 | -7.84 | 1.17 | 1.25 |
| 1 | 24-A | 154 | GLU | CB-CG | -7.81 | 1.37 | 1.52 |
| 1 | 54-A | 48 | GLU | CB-CG | 7.79 | 1.67 | 1.52 |
| 1 | 57-A | 120 | GLU | CB-CG | -7.78 | 1.37 | 1.52 |
| 1 | 79-A | 85 | CYS | CB-SG | -7.77 | 1.69 | 1.82 |
| 1 | 80-A | 158 | ARG | CB-CG | -7.72 | 1.31 | 1.52 |
| 1 | 117-A | 20 | MET | CG-SD | -7.72 | 1.61 | 1.81 |
| 1 | 79-A | 129 | GLU | CB-CG | 7.72 | 1.66 | 1.52 |
| 1 | 43-A | 85 | CYS | CB-SG | -7.68 | 1.69 | 1.82 |
| 1 | 17-A | 128 | TYR | CD1-CE1 | -7.68 | 1.27 | 1.39 |
| 1 | 12-A | 85 | CYS | CB-SG | 7.66 | 1.95 | 1.82 |
| 1 | 18-A | 22 | TRP | CB-CG | -7.64 | 1.36 | 1.50 |
| 1 | 33-A | 85 | CYS | CB-SG | -7.64 | 1.69 | 1.82 |
| 1 | 110-A | 2 | ILE | N-CA | 7.60 | 1.61 | 1.46 |
| 1 | 18-A | 154 | GLU | CB-CG | -7.58 | 1.37 | 1.52 |
| 1 | 87-A | 12 | ARG | CG-CD | 7.54 | 1.70 | 1.51 |
| 1 | 47-A | 22 | TRP | CB-CG | 7.53 | 1.63 | 1.50 |
| 1 | 48-A | 22 | TRP | CA-C | 7.51 | 1.72 | 1.52 |
| 1 | 57-A | 128 | TYR | CB-CG | 7.46 | 1.62 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 86-A | 158 | ARG | CB-CG | -7.46 | 1.32 | 1.52 |
| 1 | 11-A | 158 | ARG | CG-CD | 7.45 | 1.70 | 1.51 |
| 1 | 86-A | 12 | ARG | CG-CD | 7.42 | 1.70 | 1.51 |
| 1 | 119-A | 150 | SER | CB-OG | 7.38 | 1.51 | 1.42 |
| 1 | 44-A | 154 | GLU | CG-CD | 7.36 | 1.62 | 1.51 |
| 1 | 71-A | 85 | CYS | CB-SG | 7.35 | 1.94 | 1.82 |
| 1 | 98-A | 98 | ARG | CG-CD | -7.33 | 1.33 | 1.51 |
| 1 | 82-A | 135 | SER | CB-OG | -7.31 | 1.32 | 1.42 |
| 1 | 41-A | 37 | ASN | CB-CG | 7.30 | 1.67 | 1.51 |
| 1 | 82-A | 127 | ASP | CA-CB | 7.29 | 1.70 | 1.53 |
| 1 | 116-A | 30 | TRP | CB-CG | 7.26 | 1.63 | 1.50 |
| 1 | 109-A | 129 | GLU | CG-CD | 7.25 | 1.62 | 1.51 |
| 1 | 46-A | 154 | GLU | CD-OE1 | -7.24 | 1.17 | 1.25 |
| 1 | 65-A | 154 | GLU | CG-CD | 7.21 | 1.62 | 1.51 |
| 1 | 24-A | 98 | ARG | CG-CD | -7.21 | 1.33 | 1.51 |
| 1 | 56-A | 85 | CYS | CB-SG | 7.20 | 1.94 | 1.82 |
| 1 | 83-A | 129 | GLU | CB-CG | 7.17 | 1.65 | 1.52 |
| 1 | 84-A | 126 | PRO | CG-CD | 7.17 | 1.74 | 1.50 |
| 1 | 13-A | 20 | MET | CB-CG | 7.17 | 1.74 | 1.51 |
| 1 | 116-A | 37 | ASN | CB-CG | 7.16 | 1.67 | 1.51 |
| 1 | 32-A | 134 | GLU | CB-CG | 7.16 | 1.65 | 1.52 |
| 1 | 30-A | 85 | CYS | CB-SG | -7.16 | 1.70 | 1.82 |
| 1 | 54-A | 22 | TRP | CB-CG | 7.13 | 1.63 | 1.50 |
| 1 | 108-A | 30 | TRP | CG-CD1 | -7.10 | 1.26 | 1.36 |
| 1 | 93-A | 58 | LYS | CD-CE | 7.06 | 1.69 | 1.51 |
| 1 | 5-A | 154 | GLU | CB-CG | 7.02 | 1.65 | 1.52 |
| 1 | 97-A | 18 | ASN | CB-CG | -7.02 | 1.34 | 1.51 |
| 1 | 64-A | 154 | GLU | CA-CB | 7.01 | 1.69 | 1.53 |
| 1 | 115-A | 30 | TRP | CB-CG | 7.01 | 1.62 | 1.50 |
| 1 | 111-A | 30 | TRP | CD2-CE2 | 6.97 | 1.49 | 1.41 |
| 1 | 118-A | 30 | TRP | CG-CD1 | 6.97 | 1.46 | 1.36 |
| 1 | 55-A | 127 | ASP | CB-CG | -6.95 | 1.37 | 1.51 |
| 1 | 14-A | 154 | GLU | CB-CG | 6.92 | 1.65 | 1.52 |
| 1 | 82-A | 135 | SER | CA-CB | 6.92 | 1.63 | 1.52 |
| 1 | 45-A | 22 | TRP | CB-CG | 6.92 | 1.62 | 1.50 |
| 1 | 122-A | 19 | ALA | CA-CB | 6.91 | 1.67 | 1.52 |
| 1 | 7-A | 22 | TRP | CB-CG | 6.90 | 1.62 | 1.50 |
| 1 | 25-A | 129 | GLU | CG-CD | 6.89 | 1.62 | 1.51 |
| 1 | 73-A | 22 | TRP | CB-CG | -6.88 | 1.37 | 1.50 |
| 1 | 116-A | 20 | MET | CB-CG | 6.87 | 1.73 | 1.51 |
| 1 | 5-A | 154 | GLU | CG-CD | 6.84 | 1.62 | 1.51 |
| 1 | 89-A | 20 | MET | CG-SD | 6.84 | 1.99 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 93-A | 20 | MET | CG-SD | 6.83 | 1.99 | 1.81 |
| 1 | 121-A | 98 | ARG | CG-CD | 6.83 | 1.69 | 1.51 |
| 1 | 45-A | 22 | TRP | CG-CD1 | 6.83 | 1.46 | 1.36 |
| 1 | 104-A | 98 | ARG | CG-CD | 6.82 | 1.69 | 1.51 |
| 1 | 86-A | 12 | ARG | CB-CG | 6.80 | 1.71 | 1.52 |
| 1 | 108-A | 88 | VAL | CB-CG1 | -6.80 | 1.38 | 1.52 |
| 1 | 41-A | 12 | ARG | CG-CD | 6.80 | 1.69 | 1.51 |
| 1 | 67-A | 101 | GLU | CG-CD | 6.78 | 1.62 | 1.51 |
| 1 | 52-A | 22 | TRP | CB-CG | 6.78 | 1.62 | 1.50 |
| 1 | 77-A | 101 | GLU | CG-CD | 6.76 | 1.62 | 1.51 |
| 1 | 56-A | 16 | MET | CB-CG | 6.75 | 1.73 | 1.51 |
| 1 | 26-A | 154 | GLU | CB-CG | 6.74 | 1.65 | 1.52 |
| 1 | 27-A | 58 | LYS | CB-CG | 6.72 | 1.70 | 1.52 |
| 1 | 74-A | 128 | TYR | CB-CG | 6.72 | 1.61 | 1.51 |
| 1 | 51-A | 22 | TRP | CG-CD1 | -6.69 | 1.27 | 1.36 |
| 1 | 122-A | 120 | GLU | CB-CG | 6.69 | 1.64 | 1.52 |
| 1 | 98-A | 24 | LEU | CA-C | 6.66 | 1.70 | 1.52 |
| 1 | 67-A | 128 | TYR | CB-CG | 6.65 | 1.61 | 1.51 |
| 1 | 44-A | 154 | GLU | CD-OE2 | 6.63 | 1.32 | 1.25 |
| 1 | 123-A | 10 | VAL | CB-CG2 | -6.63 | 1.39 | 1.52 |
| 1 | 117-A | 20 | MET | CB-CG | -6.63 | 1.30 | 1.51 |
| 1 | 43-A | 9 | ALA | CA-CB | -6.59 | 1.38 | 1.52 |
| 1 | 100-A | 98 | ARG | CG-CD | -6.59 | 1.35 | 1.51 |
| 1 | 56-A | 108 | GLN | CB-CG | 6.58 | 1.70 | 1.52 |
| 1 | 47-A | 48 | GLU | CB-CG | -6.56 | 1.39 | 1.52 |
| 1 | 49-A | 58 | LYS | CB-CG | 6.54 | 1.70 | 1.52 |
| 1 | 10-A | 98 | ARG | CG-CD | 6.53 | 1.68 | 1.51 |
| 1 | 80-A | 44 | ARG | CG-CD | 6.53 | 1.68 | 1.51 |
| 1 | 124-A | 21 | PRO | CB-CG | 6.53 | 1.82 | 1.50 |
| 1 | 46-A | 85 | CYS | CB-SG | -6.53 | 1.71 | 1.82 |
| 1 | 7-A | 36 | LEU | CG-CD2 | -6.53 | 1.27 | 1.51 |
| 1 | 24-A | 9 | ALA | CA-CB | -6.52 | 1.38 | 1.52 |
| 1 | 68-A | 17 | GLU | CG-CD | 6.51 | 1.61 | 1.51 |
| 1 | 71-A | 154 | GLU | CG-CD | -6.50 | 1.42 | 1.51 |
| 1 | 33-A | 154 | GLU | CD-OE1 | 6.49 | 1.32 | 1.25 |
| 1 | 70-A | 154 | GLU | CG-CD | 6.49 | 1.61 | 1.51 |
| 1 | 84-A | 126 | PRO | CA-C | 6.49 | 1.65 | 1.52 |
| 1 | 32-A | 98 | ARG | CG-CD | -6.46 | 1.35 | 1.51 |
| 1 | 3-A | 154 | GLU | CG-CD | -6.44 | 1.42 | 1.51 |
| 1 | 7-A | 127 | ASP | N-CA | 6.43 | 1.59 | 1.46 |
| 1 | 122-A | 151 | TYR | CD2-CE2 | -6.41 | 1.29 | 1.39 |
| 1 | 47-A | 120 | GLU | CB-CG | -6.39 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 38-A | 158 | ARG | CG-CD | 6.38 | 1.68 | 1.51 |
| 1 | 63-A | 154 | GLU | CD-OE2 | 6.37 | 1.32 | 1.25 |
| 1 | 46-A | 119 | VAL | CB-CG2 | -6.37 | 1.39 | 1.52 |
| 1 | 53-A | 118 | GLU | CG-CD | 6.37 | 1.61 | 1.51 |
| 1 | 29-A | 64 | SER | CA-CB | 6.36 | 1.62 | 1.52 |
| 1 | 53-A | 12 | ARG | CG-CD | 6.34 | 1.67 | 1.51 |
| 1 | 82-A | 127 | ASP | N-CA | 6.33 | 1.59 | 1.46 |
| 1 | 49-A | 154 | GLU | CG-CD | -6.32 | 1.42 | 1.51 |
| 1 | 89-A | 12 | ARG | CG-CD | -6.32 | 1.36 | 1.51 |
| 1 | 120-A | 88 | VAL | CB-CG2 | -6.31 | 1.39 | 1.52 |
| 1 | 37-A | 126 | PRO | C-O | -6.31 | 1.10 | 1.23 |
| 1 | 4-A | 85 | CYS | CB-SG | -6.30 | 1.71 | 1.82 |
| 1 | 59-A | 16 | MET | CB-CG | -6.29 | 1.31 | 1.51 |
| 1 | 73-A | 101 | GLU | CG-CD | 6.28 | 1.61 | 1.51 |
| 1 | 20-A | 120 | GLU | CB-CG | 6.28 | 1.64 | 1.52 |
| 1 | 99-A | 88 | VAL | CB-CG2 | -6.28 | 1.39 | 1.52 |
| 1 | 18-A | 127 | ASP | N-CA | 6.27 | 1.58 | 1.46 |
| 1 | 33-A | 30 | TRP | CG-CD1 | 6.27 | 1.45 | 1.36 |
| 1 | 40-A | 52 | ARG | CB-CG | 6.26 | 1.69 | 1.52 |
| 1 | 98-A | 23 | ASN | N-CA | 6.25 | 1.58 | 1.46 |
| 1 | 102-A | 129 | GLU | CB-CG | 6.25 | 1.64 | 1.52 |
| 1 | 104-A | 60 | ILE | CB-CG2 | -6.24 | 1.33 | 1.52 |
| 1 | 115-A | 20 | MET | CB-CG | 6.23 | 1.71 | 1.51 |
| 1 | 117-A | 127 | ASP | CB-CG | 6.23 | 1.64 | 1.51 |
| 1 | 2-A | 101 | GLU | CB-CG | 6.23 | 1.64 | 1.52 |
| 1 | 83-A | 154 | GLU | CG-CD | 6.22 | 1.61 | 1.51 |
| 1 | 104-A | 128 | TYR | CD2-CE2 | -6.22 | 1.30 | 1.39 |
| 1 | 72-A | 44 | ARG | CG-CD | -6.21 | 1.36 | 1.51 |
| 1 | 90-A | 44 | ARG | CB-CG | 6.20 | 1.69 | 1.52 |
| 1 | 9-A | 98 | ARG | CG-CD | 6.19 | 1.67 | 1.51 |
| 1 | 89-A | 1 | MET | CB-CG | 6.19 | 1.71 | 1.51 |
| 1 | 7-A | 127 | ASP | CB-CG | 6.19 | 1.64 | 1.51 |
| 1 | 102-A | 129 | GLU | CG-CD | 6.19 | 1.61 | 1.51 |
| 1 | 99-A | 126 | PRO | CA-C | 6.18 | 1.65 | 1.52 |
| 1 | 28-A | 22 | TRP | CB-CG | 6.17 | 1.61 | 1.50 |
| 1 | 47-A | 22 | TRP | CG-CD1 | -6.16 | 1.28 | 1.36 |
| 1 | 24-A | 154 | GLU | CD-OE2 | -6.15 | 1.18 | 1.25 |
| 1 | 38-A | 44 | ARG | CG-CD | 6.15 | 1.67 | 1.51 |
| 1 | 68-A | 120 | GLU | CB-CG | 6.15 | 1.63 | 1.52 |
| 1 | 36-A | 17 | GLU | CG-CD | 6.14 | 1.61 | 1.51 |
| 1 | 113-A | 22 | TRP | CB-CG | 6.14 | 1.61 | 1.50 |
| 1 | 20-A | 48 | GLU | CB-CG | 6.13 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 56-A | 154 | GLU | CG-CD | -6.12 | 1.42 | 1.51 |
| 1 | 23-A | 20 | MET | CG-SD | 6.12 | 1.97 | 1.81 |
| 1 | 28-A | 20 | MET | CB-CG | 6.12 | 1.71 | 1.51 |
| 1 | 55-A | 129 | GLU | CB-CG | -6.11 | 1.40 | 1.52 |
| 1 | 121-A | 20 | MET | CG-SD | -6.10 | 1.65 | 1.81 |
| 1 | 52-A | 44 | ARG | CG-CD | -6.09 | 1.36 | 1.51 |
| 1 | 66-A | 12 | ARG | CG-CD | 6.09 | 1.67 | 1.51 |
| 1 | 36-A | 17 | GLU | CB-CG | 6.09 | 1.63 | 1.52 |
| 1 | 20-A | 22 | TRP | CB-CG | 6.06 | 1.61 | 1.50 |
| 1 | 68-A | 126 | PRO | CA-C | -6.05 | 1.40 | 1.52 |
| 1 | 71-A | 119 | VAL | CB-CG2 | 6.04 | 1.65 | 1.52 |
| 1 | 61-A | 11 | ASP | CB-CG | -6.04 | 1.39 | 1.51 |
| 1 | 74-A | 128 | TYR | CD2-CE2 | 6.02 | 1.48 | 1.39 |
| 1 | 75-A | 101 | GLU | CB-CG | -6.02 | 1.40 | 1.52 |
| 1 | 106-A | 98 | ARG | CB-CG | 6.02 | 1.68 | 1.52 |
| 1 | 37-A | 127 | ASP | CB-CG | 6.01 | 1.64 | 1.51 |
| 1 | 72-A | 127 | ASP | CB-CG | 6.01 | 1.64 | 1.51 |
| 1 | 31-A | 127 | ASP | C-O | 6.01 | 1.34 | 1.23 |
| 1 | 123-A | 101 | GLU | CB-CG | 6.00 | 1.63 | 1.52 |
| 1 | 36-A | 108 | GLN | CB-CG | -5.98 | 1.36 | 1.52 |
| 1 | 43-A | 12 | ARG | CB-CG | 5.97 | 1.68 | 1.52 |
| 1 | 45-A | 78 | VAL | CB-CG2 | -5.97 | 1.40 | 1.52 |
| 1 | 93-A | 22 | TRP | CB-CG | 5.95 | 1.60 | 1.50 |
| 1 | 62-A | 78 | VAL | CB-CG1 | -5.93 | 1.40 | 1.52 |
| 1 | 113-A | 150 | SER | CB-OG | -5.93 | 1.34 | 1.42 |
| 1 | 79-A | 158 | ARG | CB-CG | -5.92 | 1.36 | 1.52 |
| 1 | 84-A | 128 | TYR | CB-CG | 5.92 | 1.60 | 1.51 |
| 1 | 41-A | 20 | MET | CG-SD | 5.92 | 1.96 | 1.81 |
| 1 | 22-A | 154 | GLU | CD-OE1 | 5.91 | 1.32 | 1.25 |
| 1 | 67-A | 101 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | 61-A | 85 | CYS | CB-SG | -5.90 | 1.72 | 1.81 |
| 1 | 123-A | 21 | PRO | CA-C | 5.88 | 1.64 | 1.52 |
| 1 | 94-A | 20 | MET | CG-SD | -5.88 | 1.65 | 1.81 |
| 1 | 54-A | 154 | GLU | CD-OE1 | 5.86 | 1.32 | 1.25 |
| 1 | 101-A | 128 | TYR | CD2-CE2 | 5.86 | 1.48 | 1.39 |
| 1 | 69-A | 17 | GLU | CB-CG | 5.84 | 1.63 | 1.52 |
| 1 | 83-A | 44 | ARG | CG-CD | 5.84 | 1.66 | 1.51 |
| 1 | 50-A | 154 | GLU | CG-CD | -5.83 | 1.43 | 1.51 |
| 1 | 118-A | 10 | VAL | CB-CG2 | -5.82 | 1.40 | 1.52 |
| 1 | 98-A | 118 | GLU | CG-CD | 5.82 | 1.60 | 1.51 |
| 1 | 77-A | 157 | GLU | CG-CD | 5.81 | 1.60 | 1.51 |
| 1 | 17-A | 154 | GLU | CD-OE1 | -5.81 | 1.19 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 124-A | 18 | ASN | N-CA | 5.80 | 1.57 | 1.46 |
| 1 | 82-A | 33 | ARG | CG-CD | 5.80 | 1.66 | 1.51 |
| 1 | 115-A | 85 | CYS | CB-SG | -5.80 | 1.72 | 1.81 |
| 1 | 24-A | 85 | CYS | CB-SG | -5.80 | 1.72 | 1.81 |
| 1 | 34-A | 128 | TYR | CB-CG | 5.79 | 1.60 | 1.51 |
| 1 | 44-A | 22 | TRP | CA-CB | 5.79 | 1.66 | 1.53 |
| 1 | 124-A | 20 | MET | CB-CG | 5.79 | 1.69 | 1.51 |
| 1 | 45-A | 151 | TYR | CD2-CE2 | -5.79 | 1.30 | 1.39 |
| 1 | 125-A | 136 | VAL | CB-CG1 | 5.78 | 1.65 | 1.52 |
| 1 | 81-A | 20 | MET | CB-CG | 5.77 | 1.69 | 1.51 |
| 1 | 107-A | 87 | ASP | CB-CG | 5.76 | 1.63 | 1.51 |
| 1 | 2-A | 101 | GLU | CG-CD | 5.76 | 1.60 | 1.51 |
| 1 | 105-A | 34 | ASN | CB-CG | 5.75 | 1.64 | 1.51 |
| 1 | 102-A | 154 | GLU | CB-CG | -5.75 | 1.41 | 1.52 |
| 1 | 23-A | 127 | ASP | N-CA | 5.74 | 1.57 | 1.46 |
| 1 | 98-A | 134 | GLU | CB-CG | 5.74 | 1.63 | 1.52 |
| 1 | 99-A | 98 | ARG | CG-CD | -5.73 | 1.37 | 1.51 |
| 1 | 52-A | 129 | GLU | CB-CG | -5.73 | 1.41 | 1.52 |
| 1 | 79-A | 129 | GLU | CG-CD | 5.72 | 1.60 | 1.51 |
| 1 | 32-A | 128 | TYR | CE1-CZ | -5.72 | 1.31 | 1.38 |
| 1 | 125-A | 129 | GLU | CB-CG | 5.72 | 1.63 | 1.52 |
| 1 | 25-A | 85 | CYS | CB-SG | 5.71 | 1.92 | 1.82 |
| 1 | 6-A | 49 | SER | CA-CB | 5.71 | 1.61 | 1.52 |
| 1 | 107-A | 154 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | 47-A | 98 | ARG | CB-CG | 5.70 | 1.68 | 1.52 |
| 1 | 29-A | 22 | TRP | CB-CG | -5.70 | 1.40 | 1.50 |
| 1 | 81-A | 158 | ARG | CB-CG | 5.68 | 1.67 | 1.52 |
| 1 | 71-A | 128 | TYR | CD2-CE2 | -5.68 | 1.30 | 1.39 |
| 1 | 122-A | 10 | VAL | CB-CG2 | -5.68 | 1.41 | 1.52 |
| 1 | 111-A | 101 | GLU | CG-CD | 5.68 | 1.60 | 1.51 |
| 1 | 93-A | 20 | MET | CB-CG | 5.67 | 1.69 | 1.51 |
| 1 | 113-A | 139 | GLU | CB-CG | 5.65 | 1.62 | 1.52 |
| 1 | 105-A | 85 | CYS | CB-SG | -5.63 | 1.72 | 1.81 |
| 1 | 91-A | 12 | ARG | CZ-NH2 | -5.63 | 1.25 | 1.33 |
| 1 | 4-A | 129 | GLU | CB-CG | 5.62 | 1.62 | 1.52 |
| 1 | 93-A | 21 | PRO | CA-C | 5.61 | 1.64 | 1.52 |
| 1 | 123-A | 18 | ASN | N-CA | 5.61 | 1.57 | 1.46 |
| 1 | 61-A | 12 | ARG | CG-CD | -5.60 | 1.38 | 1.51 |
| 1 | 51-A | 118 | GLU | CB-CG | 5.58 | 1.62 | 1.52 |
| 1 | 27-A | 107 | ALA | CA-CB | -5.57 | 1.40 | 1.52 |
| 1 | 47-A | 127 | ASP | N-CA | 5.57 | 1.57 | 1.46 |
| 1 | 101-A | 88 | VAL | CB-CG2 | -5.57 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 104-A | 1 | MET | CB-CG | 5.57 | 1.69 | 1.51 |
| 1 | 73-A | 128 | TYR | CD2-CE2 | -5.56 | 1.31 | 1.39 |
| 1 | 11-A | 126 | PRO | CA-C | 5.55 | 1.64 | 1.52 |
| 1 | 108-A | 60 | ILE | CB-CG2 | -5.55 | 1.35 | 1.52 |
| 1 | 35-A | 134 | GLU | CB-CG | -5.55 | 1.41 | 1.52 |
| 1 | 72-A | 58 | LYS | CB-CG | 5.54 | 1.67 | 1.52 |
| 1 | 58-A | 30 | TRP | CB-CG | -5.54 | 1.40 | 1.50 |
| 1 | 54-A | 22 | TRP | CG-CD1 | 5.54 | 1.44 | 1.36 |
| 1 | 95-A | 138 | SER | CB-OG | -5.54 | 1.35 | 1.42 |
| 1 | 13-A | 20 | MET | CG-SD | 5.53 | 1.95 | 1.81 |
| 1 | 108-A | 18 | ASN | N-CA | 5.53 | 1.57 | 1.46 |
| 1 | 96-A | 139 | GLU | CB-CG | 5.52 | 1.62 | 1.52 |
| 1 | 84-A | 127 | ASP | N-CA | 5.52 | 1.57 | 1.46 |
| 1 | 81-A | 101 | GLU | CB-CG | -5.51 | 1.41 | 1.52 |
| 1 | 45-A | 118 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 1 | 63-A | 134 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 1 | 92-A | 154 | GLU | CD-OE2 | 5.50 | 1.31 | 1.25 |
| 1 | 21-A | 154 | GLU | CG-CD | 5.49 | 1.60 | 1.51 |
| 1 | 118-A | 21 | PRO | CA-C | 5.49 | 1.63 | 1.52 |
| 1 | 49-A | 127 | ASP | CA-C | 5.49 | 1.67 | 1.52 |
| 1 | 5-A | 129 | GLU | CB-CG | 5.49 | 1.62 | 1.52 |
| 1 | 26-A | 154 | GLU | CG-CD | 5.49 | 1.60 | 1.51 |
| 1 | 92-A | 129 | GLU | CG-CD | -5.49 | 1.43 | 1.51 |
| 1 | 113-A | 10 | VAL | CB-CG2 | -5.49 | 1.41 | 1.52 |
| 1 | 102-A | 20 | MET | N-CA | 5.48 | 1.57 | 1.46 |
| 1 | 94-A | 19 | ALA | CA-C | 5.47 | 1.67 | 1.52 |
| 1 | 115-A | 129 | GLU | CB-CG | -5.46 | 1.41 | 1.52 |
| 1 | 102-A | 127 | ASP | CB-CG | 5.46 | 1.63 | 1.51 |
| 1 | 34-A | 58 | LYS | CB-CG | 5.45 | 1.67 | 1.52 |
| 1 | 82-A | 154 | GLU | CB-CG | 5.45 | 1.62 | 1.52 |
| 1 | 45-A | 129 | GLU | N-CA | 5.45 | 1.57 | 1.46 |
| 1 | 20-A | 127 | ASP | N-CA | 5.45 | 1.57 | 1.46 |
| 1 | 64-A | 128 | TYR | CD1-CE1 | -5.44 | 1.31 | 1.39 |
| 1 | 11-A | 85 | CYS | CB-SG | 5.44 | 1.91 | 1.82 |
| 1 | 104-A | 88 | VAL | CB-CG2 | -5.44 | 1.41 | 1.52 |
| 1 | 30-A | 33 | ARG | CG-CD | 5.43 | 1.65 | 1.51 |
| 1 | 27-A | 44 | ARG | CG-CD | -5.42 | 1.38 | 1.51 |
| 1 | 55-A | 79 | ASP | CB-CG | 5.41 | 1.63 | 1.51 |
| 1 | 113-A | 139 | GLU | CG-CD | 5.41 | 1.60 | 1.51 |
| 1 | 83-A | 20 | MET | CB-CG | 5.41 | 1.68 | 1.51 |
| 1 | 91-A | 20 | MET | CG-SD | 5.39 | 1.95 | 1.81 |
| 1 | 119-A | 154 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 28-A | 48 | GLU | CG-CD | -5.38 | 1.43 | 1.51 |
| 1 | 28-A | 1 | MET | CG-SD | 5.37 | 1.95 | 1.81 |
| 1 | 107-A | 154 | GLU | CG-CD | 5.37 | 1.60 | 1.51 |
| 1 | 54-A | 58 | LYS | CB-CG | 5.36 | 1.67 | 1.52 |
| 1 | 37-A | 79 | ASP | CB-CG | 5.35 | 1.62 | 1.51 |
| 1 | 113-A | 129 | GLU | CB-CG | 5.35 | 1.62 | 1.52 |
| 1 | 45-A | 118 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | 50-A | 127 | ASP | N-CA | 5.33 | 1.57 | 1.46 |
| 1 | 3-A | 17 | GLU | CG-CD | -5.33 | 1.44 | 1.51 |
| 1 | 44-A | 12 | ARG | CG-CD | 5.33 | 1.65 | 1.51 |
| 1 | 97-A | 88 | VAL | CB-CG2 | -5.32 | 1.41 | 1.52 |
| 1 | 52-A | 102 | GLN | CB-CG | 5.32 | 1.67 | 1.52 |
| 1 | 4-A | 17 | GLU | CG-CD | 5.32 | 1.59 | 1.51 |
| 1 | 95-A | 58 | LYS | CD-CE | 5.32 | 1.64 | 1.51 |
| 1 | 49-A | 154 | GLU | CD-OE2 | -5.32 | 1.19 | 1.25 |
| 1 | 17-A | 101 | GLU | CB-CG | 5.31 | 1.62 | 1.52 |
| 1 | 93-A | 76 | LYS | CE-NZ | -5.31 | 1.35 | 1.49 |
| 1 | 111-A | 19 | ALA | N-CA | 5.31 | 1.56 | 1.46 |
| 1 | 61-A | 108 | GLN | CB-CG | 5.31 | 1.66 | 1.52 |
| 1 | 76-A | 58 | LYS | CG-CD | 5.31 | 1.70 | 1.52 |
| 1 | 24-A | 127 | ASP | N-CA | 5.31 | 1.56 | 1.46 |
| 1 | 42-A | 129 | GLU | N-CA | 5.30 | 1.56 | 1.46 |
| 1 | 34-A | 134 | GLU | CD-OE1 | -5.30 | 1.19 | 1.25 |
| 1 | 22-A | 48 | GLU | CB-CG | -5.29 | 1.42 | 1.52 |
| 1 | 77-A | 158 | ARG | CB-CG | 5.28 | 1.66 | 1.52 |
| 1 | 103-A | 98 | ARG | CB-CG | 5.28 | 1.66 | 1.52 |
| 1 | 5-A | 128 | TYR | C-O | -5.28 | 1.13 | 1.23 |
| 1 | 11-A | 154 | GLU | CB-CG | -5.27 | 1.42 | 1.52 |
| 1 | 119-A | 1 | MET | CB-CG | 5.26 | 1.68 | 1.51 |
| 1 | 92-A | 32 | LYS | CB-CG | 5.24 | 1.66 | 1.52 |
| 1 | 33-A | 154 | GLU | CD-OE2 | 5.23 | 1.31 | 1.25 |
| 1 | 45-A | 20 | MET | CG-SD | 5.23 | 1.94 | 1.81 |
| 1 | 122-A | 17 | GLU | CB-CG | 5.22 | 1.62 | 1.52 |
| 1 | 55-A | 58 | LYS | CD-CE | 5.22 | 1.64 | 1.51 |
| 1 | 47-A | 12 | ARG | CG-CD | 5.21 | 1.65 | 1.51 |
| 1 | 106-A | 20 | MET | CG-SD | 5.21 | 1.94 | 1.81 |
| 1 | 20-A | 129 | GLU | CB-CG | 5.21 | 1.62 | 1.52 |
| 1 | 62-A | 102 | GLN | CB-CG | 5.19 | 1.66 | 1.52 |
| 1 | 119-A | 11 | ASP | CB-CG | -5.19 | 1.40 | 1.51 |
| 1 | 28-A | 127 | ASP | CB-CG | 5.19 | 1.62 | 1.51 |
| 1 | 115-A | 88 | VAL | CB-CG1 | -5.18 | 1.42 | 1.52 |
| 1 | 104-A | 98 | ARG | CB-CG | 5.18 | 1.66 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 43-A | 139 | GLU | CB-CG | 5.18 | 1.61 | 1.52 |
| 1 | 96-A | 108 | GLN | CB-CG | 5.18 | 1.66 | 1.52 |
| 1 | 1-A | 85 | CYS | CB-SG | 5.17 | 1.91 | 1.82 |
| 1 | 14-A | 129 | GLU | CB-CG | 5.17 | 1.61 | 1.52 |
| 1 | 37-A | 126 | PRO | CA-C | 5.17 | 1.63 | 1.52 |
| 1 | 107-A | 106 | LYS | CB-CG | 5.17 | 1.66 | 1.52 |
| 1 | 106-A | 108 | GLN | CB-CG | -5.17 | 1.38 | 1.52 |
| 1 | 23-A | 120 | GLU | CB-CG | 5.16 | 1.61 | 1.52 |
| 1 | 62-A | 101 | GLU | CG-CD | 5.16 | 1.59 | 1.51 |
| 1 | 97-A | 154 | GLU | CG-CD | -5.16 | 1.44 | 1.51 |
| 1 | 38-A | 16 | MET | CB-CG | 5.16 | 1.67 | 1.51 |
| 1 | 15-A | 154 | GLU | CD-OE2 | 5.15 | 1.31 | 1.25 |
| 1 | 28-A | 129 | GLU | CB-CG | 5.14 | 1.61 | 1.52 |
| 1 | 106-A | 101 | GLU | CG-CD | -5.14 | 1.44 | 1.51 |
| 1 | 2-A | 85 | CYS | CB-SG | 5.13 | 1.91 | 1.82 |
| 1 | 61-A | 98 | ARG | CB-CG | -5.13 | 1.38 | 1.52 |
| 1 | 84-A | 17 | GLU | CB-CG | 5.13 | 1.61 | 1.52 |
| 1 | 49-A | 101 | GLU | CB-CG | -5.12 | 1.42 | 1.52 |
| 1 | 33-A | 154 | GLU | CG-CD | 5.12 | 1.59 | 1.51 |
| 1 | 81-A | 20 | MET | N-CA | 5.12 | 1.56 | 1.46 |
| 1 | 82-A | 154 | GLU | CG-CD | 5.12 | 1.59 | 1.51 |
| 1 | 112-A | 19 | ALA | CA-CB | 5.11 | 1.63 | 1.52 |
| 1 | 121-A | 134 | GLU | CB-CG | 5.11 | 1.61 | 1.52 |
| 1 | 61-A | 127 | ASP | CB-CG | 5.11 | 1.62 | 1.51 |
| 1 | 77-A | 22 | TRP | CB-CG | -5.11 | 1.41 | 1.50 |
| 1 | 125-A | 18 | ASN | N-CA | 5.11 | 1.56 | 1.46 |
| 1 | 35-A | 127 | ASP | CA-C | 5.11 | 1.66 | 1.52 |
| 1 | 48-A | 9 | ALA | CA-CB | -5.10 | 1.41 | 1.52 |
| 1 | 49-A | 22 | TRP | CB-CG | 5.09 | 1.59 | 1.50 |
| 1 | 109-A | 150 | SER | CB-OG | 5.08 | 1.48 | 1.42 |
| 1 | 25-A | 134 | GLU | CG-CD | -5.07 | 1.44 | 1.51 |
| 1 | 110-A | 1 | MET | N-CA | 5.06 | 1.56 | 1.46 |
| 1 | 68-A | 37 | ASN | CB-CG | 5.06 | 1.62 | 1.51 |
| 1 | 7-A | 127 | ASP | CA-C | 5.05 | 1.66 | 1.52 |
| 1 | 9-A | 37 | ASN | CB-CG | 5.04 | 1.62 | 1.51 |
| 1 | 58-A | 20 | MET | CB-CG | 5.04 | 1.67 | 1.51 |
| 1 | 109-A | 44 | ARG | CG-CD | 5.04 | 1.64 | 1.51 |
| 1 | 76-A | 52 | ARG | CB-CG | 5.04 | 1.66 | 1.52 |
| 1 | 12-A | 127 | ASP | C-O | -5.04 | 1.13 | 1.23 |
| 1 | 94-A | 9 | ALA | CA-CB | -5.04 | 1.41 | 1.52 |
| 1 | 67-A | 101 | GLU | CB-CG | 5.03 | 1.61 | 1.52 |
| 1 | 29-A | 127 | ASP | CB-CG | -5.03 | 1.41 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | 105-A | 1 | MET | CB-CG | 5.02 | 1.67 | 1.51 |
| 1 | 83-A | 129 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |
| 1 | 52-A | 48 | GLU | CB-CG | 5.01 | 1.61 | 1.52 |
| 1 | 37-A | 58 | LYS | CB-CG | 5.01 | 1.66 | 1.52 |
| 1 | 120-A | 11 | ASP | CB-CG | 5.01 | 1.62 | 1.51 |
| 1 | 124-A | 18 | ASN | CB-CG | -5.01 | 1.39 | 1.51 |
| 1 | 72-A | 22 | TRP | CB-CG | -5.00 | 1.41 | 1.50 |
| 1 | 68-A | 159 | ARG | CB-CG | -5.00 | 1.39 | 1.52 |

All (1350) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 68-A | 16 | MET | CG-SD-CE | -21.11 | 66.42 | 100.20 |
| 1 | 64-A | 12 | ARG | NE-CZ-NH2 | 20.89 | 130.75 | 120.30 |
| 1 | 85-A | 125 | PHE | C-N-CD | -19.27 | 78.22 | 120.60 |
| 1 | 98-A | 12 | ARG | NE-CZ-NH2 | -17.49 | 111.56 | 120.30 |
| 1 | 19-A | 52 | ARG | NE-CZ-NH1 | -15.53 | 112.53 | 120.30 |
| 1 | 70-A | 16 | MET | CG-SD-CE | 15.03 | 124.25 | 100.20 |
| 1 | 41-A | 44 | ARG | NE-CZ-NH1 | 14.55 | 127.58 | 120.30 |
| 1 | 42-A | 20 | MET | C-N-CD | -14.42 | 88.87 | 120.60 |
| 1 | 5-A | 158 | ARG | NE-CZ-NH2 | -14.05 | 113.27 | 120.30 |
| 1 | 41-A | 44 | ARG | NE-CZ-NH2 | -13.56 | 113.52 | 120.30 |
| 1 | 28-A | 12 | ARG | NE-CZ-NH1 | 13.50 | 127.05 | 120.30 |
| 1 | 72-A | 44 | ARG | NE-CZ-NH1 | 13.28 | 126.94 | 120.30 |
| 1 | 121-A | 12 | ARG | NE-CZ-NH1 | 13.01 | 126.81 | 120.30 |
| 1 | 96-A | 44 | ARG | NE-CZ-NH1 | 12.95 | 126.77 | 120.30 |
| 1 | 38-A | 127 | ASP | CB-CG-OD2 | 12.67 | 129.70 | 118.30 |
| 1 | 81-A | 98 | ARG | NE-CZ-NH1 | 12.63 | 126.61 | 120.30 |
| 1 | 107-A | 20 | MET | CB-CG-SD | -12.52 | 74.85 | 112.40 |
| 1 | 116-A | 20 | MET | CA-CB-CG | 12.21 | 134.06 | 113.30 |
| 1 | 93-A | 12 | ARG | NE-CZ-NH2 | 12.18 | 126.39 | 120.30 |
| 1 | 42-A | 127 | ASP | N-CA-C | 12.14 | 143.78 | 111.00 |
| 1 | 46-A | 127 | ASP | N-CA-C | 12.13 | 143.75 | 111.00 |
| 1 | 109-A | 20 | MET | CG-SD-CE | 12.06 | 119.50 | 100.20 |
| 1 | 88-A | 104 | LEU | CB-CG-CD2 | -11.68 | 91.14 | 111.00 |
| 1 | 20-A | 52 | ARG | NE-CZ-NH1 | -11.68 | 114.46 | 120.30 |
| 1 | 2-A | 62 | LEU | CA-CB-CG | 11.67 | 142.13 | 115.30 |
| 1 | 79-A | 129 | GLU | C-N-CD | 11.66 | 152.90 | 128.40 |
| 1 | 13-A | 98 | ARG | NE-CZ-NH2 | -11.63 | 114.49 | 120.30 |
| 1 | 11-A | 12 | ARG | NE-CZ-NH1 | 11.59 | 126.10 | 120.30 |
| 1 | 102-A | 21 | PRO | N-CA-C | 11.50 | 142.01 | 112.10 |
| 1 | 102-A | 21 | PRO | CA-C-O | -11.45 | 92.72 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | 96-A | 98 | ARG | NE-CZ-NH1 | 11.42 | 126.01 | 120.30 |
| 1 | 10-A | 154 | GLU | OE1-CD-OE2 | 11.30 | 136.87 | 123.30 |
| 1 | 81-A | 98 | ARG | NE-CZ-NH2 | -11.26 | 114.67 | 120.30 |
| 1 | 58-A | 16 | MET | CG-SD-CE | 11.25 | 118.20 | 100.20 |
| 1 | 28-A | 12 | ARG | NE-CZ-NH2 | -10.99 | 114.81 | 120.30 |
| 1 | 10-A | 8 | LEU | CB-CG-CD2 | -10.98 | 92.33 | 111.00 |
| 1 | 44-A | 4 | LEU | CB-CG-CD2 | 10.86 | 129.46 | 111.00 |
| 1 | 70-A | 159 | ARG | NE-CZ-NH2 | -10.86 | 114.87 | 120.30 |
| 1 | 12-A | 125 | PHE | C-N-CD | -10.83 | 96.76 | 120.60 |
| 1 | 96-A | 44 | ARG | NE-CZ-NH2 | -10.83 | 114.89 | 120.30 |
| 1 | 72-A | 44 | ARG | NE-CZ-NH2 | -10.80 | 114.90 | 120.30 |
| 1 | 65-A | 126 | PRO | N-CA-C | 10.79 | 140.16 | 112.10 |
| 1 | 32-A | 127 | ASP | CB-CA-C | -10.70 | 88.99 | 110.40 |
| 1 | 96-A | 11 | ASP | CB-CG-OD2 | 10.64 | 127.88 | 118.30 |
| 1 | 118-A | 20 | MET | CG-SD-CE | 10.60 | 117.17 | 100.20 |
| 1 | 49-A | 127 | ASP | N-CA-C | 10.57 | 139.55 | 111.00 |
| 1 | 122-A | 20 | MET | CG-SD-CE | 10.56 | 117.10 | 100.20 |
| 1 | 87-A | 20 | MET | CG-SD-CE | 10.52 | 117.04 | 100.20 |
| 1 | 35-A | 154 | GLU | OE1-CD-OE2 | 10.51 | 135.91 | 123.30 |
| 1 | 84-A | 125 | PHE | C-N-CD | -10.47 | 97.56 | 120.60 |
| 1 | 66-A | 16 | MET | CG-SD-CE | -10.45 | 83.48 | 100.20 |
| 1 | 14-A | 4 | LEU | CB-CG-CD2 | 10.45 | 128.76 | 111.00 |
| 1 | 64-A | 126 | PRO | N-CA-C | 10.42 | 139.19 | 112.10 |
| 1 | 37-A | 128 | TYR | N-CA-C | -10.42 | 82.87 | 111.00 |
| 1 | 18-A | 98 | ARG | NE-CZ-NH1 | 10.33 | 125.47 | 120.30 |
| 1 | 43-A | 127 | ASP | N-CA-C | 10.31 | 138.84 | 111.00 |
| 1 | 122-A | 12 | ARG | NE-CZ-NH1 | 10.28 | 125.44 | 120.30 |
| 1 | 26-A | 98 | ARG | NE-CZ-NH2 | -10.27 | 115.17 | 120.30 |
| 1 | 37-A | 127 | ASP | CB-CG-OD1 | 10.26 | 127.53 | 118.30 |
| 1 | 9-A | 8 | LEU | CB-CG-CD2 | -10.25 | 93.57 | 111.00 |
| 1 | 88-A | 4 | LEU | CB-CG-CD2 | 10.24 | 128.41 | 111.00 |
| 1 | 14-A | 126 | PRO | N-CA-C | 10.23 | 138.69 | 112.10 |
| 1 | 14-A | 112 | LEU | CB-CG-CD1 | 10.19 | 128.33 | 111.00 |
| 1 | 89-A | 12 | ARG | NE-CZ-NH2 | -10.20 | 115.20 | 120.30 |
| 1 | 83-A | 4 | LEU | CB-CG-CD2 | 10.16 | 128.28 | 111.00 |
| 1 | 81-A | 127 | ASP | N-CA-C | 10.15 | 138.40 | 111.00 |
| 1 | 17-A | 128 | TYR | CB-CG-CD1 | -10.13 | 114.92 | 121.00 |
| 1 | 104-A | 98 | ARG | NE-CZ-NH2 | -10.11 | 115.25 | 120.30 |
| 1 | 66-A | 98 | ARG | NE-CZ-NH2 | -10.07 | 115.26 | 120.30 |
| 1 | 70-A | 126 | PRO | N-CA-C | 10.07 | 138.27 | 112.10 |
| 1 | 94-A | 4 | LEU | CB-CG-CD2 | 10.06 | 128.10 | 111.00 |
| 1 | 32-A | 127 | ASP | CB-CG-OD2 | -10.05 | 109.26 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 104-A | 98 | ARG | NE-CZ-NH1 | 10.05 | 125.32 | 120.30 |
| 1 | 93-A | 12 | ARG | NE-CZ-NH1 | -10.03 | 115.28 | 120.30 |
| 1 | 94-A | 12 | ARG | NE-CZ-NH1 | -10.03 | 115.29 | 120.30 |
| 1 | 51-A | 4 | LEU | CB-CG-CD2 | 10.01 | 128.01 | 111.00 |
| 1 | 100-A | 98 | ARG | NE-CZ-NH2 | 9.98 | 125.29 | 120.30 |
| 1 | 10-A | 87 | ASP | CB-CG-OD1 | 9.98 | 127.28 | 118.30 |
| 1 | 98-A | 23 | ASN | N-CA-C | 9.91 | 137.75 | 111.00 |
| 1 | 115-A | 62 | LEU | CA-CB-CG | -9.80 | 92.75 | 115.30 |
| 1 | 56-A | 16 | MET | CG-SD-CE | -9.80 | 84.53 | 100.20 |
| 1 | 46-A | 22 | TRP | CA-CB-CG | 9.75 | 132.22 | 113.70 |
| 1 | 32-A | 128 | TYR | CA-CB-CG | 9.69 | 131.82 | 113.40 |
| 1 | 28-A | 20 | MET | CB-CG-SD | 9.69 | 141.48 | 112.40 |
| 1 | 71-A | 126 | PRO | N-CA-C | 9.69 | 137.29 | 112.10 |
| 1 | 78-A | 20 | MET | C-N-CD | -9.69 | 99.29 | 120.60 |
| 1 | 35-A | 54 | LEU | CB-CG-CD1 | 9.68 | 127.45 | 111.00 |
| 1 | 99-A | 44 | ARG | NE-CZ-NH2 | -9.65 | 115.48 | 120.30 |
| 1 | 118-A | 104 | LEU | CB-CG-CD2 | 9.64 | 127.39 | 111.00 |
| 1 | 64-A | 23 | ASN | N-CA-C | -9.63 | 84.99 | 111.00 |
| 1 | 119-A | 1 | MET | CG-SD-CE | 9.62 | 115.60 | 100.20 |
| 1 | 122-A | 98 | ARG | NE-CZ-NH2 | -9.61 | 115.50 | 120.30 |
| 1 | 102-A | 21 | PRO | CA-C-N | 9.59 | 138.30 | 117.20 |
| 1 | 112-A | 156 | LEU | CA-CB-CG | 9.58 | 137.34 | 115.30 |
| 1 | 34-A | 12 | ARG | CG-CD-NE | 9.58 | 131.91 | 111.80 |
| 1 | 84-A | 127 | ASP | N-CA-C | 9.56 | 136.81 | 111.00 |
| 1 | 30-A | 4 | LEU | CB-CG-CD2 | 9.55 | 127.24 | 111.00 |
| 1 | 54-A | 20 | MET | CG-SD-CE | 9.55 | 115.48 | 100.20 |
| 1 | 76-A | 22 | TRP | CA-CB-CG | 9.55 | 131.84 | 113.70 |
| 1 | 18-A | 127 | ASP | N-CA-C | 9.49 | 136.62 | 111.00 |
| 1 | 82-A | 44 | ARG | NE-CZ-NH1 | 9.46 | 125.03 | 120.30 |
| 1 | 34-A | 20 | MET | CG-SD-CE | -9.35 | 85.24 | 100.20 |
| 1 | 54-A | 70 | ASP | CB-CG-OD1 | 9.33 | 126.70 | 118.30 |
| 1 | 117-A | 16 | MET | CG-SD-CE | 9.32 | 115.11 | 100.20 |
| 1 | 108-A | 98 | ARG | NE-CZ-NH2 | -9.23 | 115.68 | 120.30 |
| 1 | 36-A | 134 | GLU | CA-CB-CG | 9.23 | 133.71 | 113.40 |
| 1 | 57-A | 12 | ARG | NE-CZ-NH2 | -9.22 | 115.69 | 120.30 |
| 1 | 101-A | 21 | PRO | N-CA-C | 9.22 | 136.08 | 112.10 |
| 1 | 85-A | 11 | ASP | CB-CG-OD2 | 9.20 | 126.58 | 118.30 |
| 1 | 57-A | 128 | TYR | N-CA-C | 9.20 | 135.83 | 111.00 |
| 1 | 89-A | 20 | MET | CB-CG-SD | 9.15 | 139.85 | 112.40 |
| 1 | 90-A | 159 | ARG | NE-CZ-NH1 | 9.13 | 124.87 | 120.30 |
| 1 | 101-A | 98 | ARG | NE-CZ-NH2 | 9.13 | 124.86 | 120.30 |
| 1 | 99-A | 126 | PRO | N-CA-C | 9.13 | 135.83 | 112.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 29-A | 79 | ASP | CB-CG-OD1 | -9.12 | 110.09 | 118.30 |
| 1 | 64-A | 154 | GLU | CA-CB-CG | 9.11 | 133.45 | 113.40 |
| 1 | 15-A | 156 | LEU | CA-CB-CG | 9.08 | 136.18 | 115.30 |
| 1 | 93-A | 20 | MET | CG-SD-CE | -9.08 | 85.68 | 100.20 |
| 1 | 116-A | 98 | ARG | CB-CA-C | 9.01 | 128.41 | 110.40 |
| 1 | 7-A | 62 | LEU | CB-CG-CD2 | 9.00 | 126.30 | 111.00 |
| 1 | 66-A | 127 | ASP | CB-CG-OD2 | 9.00 | 126.40 | 118.30 |
| 1 | 13-A | 33 | ARG | NE-CZ-NH2 | -8.97 | 115.81 | 120.30 |
| 1 | 73-A | 129 | GLU | N-CA-C | -8.96 | 86.81 | 111.00 |
| 1 | 96-A | 98 | ARG | NE-CZ-NH2 | -8.94 | 115.83 | 120.30 |
| 1 | 19-A | 1 | MET | CB-CG-SD | -8.93 | 85.60 | 112.40 |
| 1 | 47-A | 22 | TRP | CA-CB-CG | 8.92 | 130.65 | 113.70 |
| 1 | 2-A | 128 | TYR | N-CA-C | 8.91 | 135.06 | 111.00 |
| 1 | 26-A | 98 | ARG | NE-CZ-NH1 | 8.91 | 124.75 | 120.30 |
| 1 | 124-A | 18 | ASN | N-CA-C | 8.90 | 135.03 | 111.00 |
| 1 | 57-A | 127 | ASP | CB-CG-OD2 | -8.89 | 110.30 | 118.30 |
| 1 | 80-A | 127 | ASP | N-CA-C | 8.88 | 134.97 | 111.00 |
| 1 | 92-A | 12 | ARG | NE-CZ-NH2 | -8.85 | 115.88 | 120.30 |
| 1 | 76-A | 8 | LEU | CA-CB-CG | 8.84 | 135.64 | 115.30 |
| 1 | 63-A | 129 | GLU | N-CA-C | -8.83 | 87.15 | 111.00 |
| 1 | 104-A | 4 | LEU | CB-CG-CD2 | 8.83 | 126.01 | 111.00 |
| 1 | 115-A | 98 | ARG | NE-CZ-NH1 | 8.82 | 124.71 | 120.30 |
| 1 | 96-A | 18 | ASN | N-CA-C | 8.79 | 134.74 | 111.00 |
| 1 | 53-A | 98 | ARG | NE-CZ-NH1 | 8.79 | 124.70 | 120.30 |
| 1 | 22-A | 128 | TYR | N-CA-CB | 8.76 | 126.36 | 110.60 |
| 1 | 18-A | 36 | LEU | CA-CB-CG | 8.74 | 135.40 | 115.30 |
| 1 | 62-A | 33 | ARG | NE-CZ-NH1 | 8.74 | 124.67 | 120.30 |
| 1 | 28-A | 4 | LEU | CB-CG-CD2 | 8.71 | 125.80 | 111.00 |
| 1 | 82-A | 135 | SER | N-CA-CB | -8.68 | 97.48 | 110.50 |
| 1 | 9-A | 158 | ARG | NE-CZ-NH1 | 8.68 | 124.64 | 120.30 |
| 1 | 110-A | 44 | ARG | NE-CZ-NH1 | 8.67 | 124.64 | 120.30 |
| 1 | 26-A | 52 | ARG | NE-CZ-NH1 | -8.66 | 115.97 | 120.30 |
| 1 | 117-A | 20 | MET | CG-SD-CE | -8.66 | 86.34 | 100.20 |
| 1 | 72-A | 16 | MET | CG-SD-CE | -8.65 | 86.36 | 100.20 |
| 1 | 13-A | 20 | MET | CB-CG-SD | 8.64 | 138.33 | 112.40 |
| 1 | 115-A | 20 | MET | CG-SD-CE | 8.63 | 114.00 | 100.20 |
| 1 | 91-A | 127 | ASP | CB-CG-OD1 | -8.62 | 110.54 | 118.30 |
| 1 | 99-A | 159 | ARG | NE-CZ-NH1 | 8.62 | 124.61 | 120.30 |
| 1 | 101-A | 58 | LYS | CD-CE-NZ | 8.60 | 131.48 | 111.70 |
| 1 | 49-A | 116 | ASP | CB-CG-OD2 | 8.59 | 126.03 | 118.30 |
| 1 | 54-A | 70 | ASP | CB-CG-OD2 | -8.59 | 110.57 | 118.30 |
| 1 | 100-A | 44 | ARG | NE-CZ-NH2 | -8.57 | 116.01 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 47-A | 22 | TRP | CB-CG-CD2 | 8.56 | 137.73 | 126.60 |
| 1 | 23-A | 20 | MET | CA-CB-CG | 8.56 | 127.84 | 113.30 |
| 1 | 11-A | 126 | PRO | CA-C-N | -8.51 | 98.47 | 117.20 |
| 1 | 43-A | 98 | ARG | CA-CB-CG | 8.51 | 132.12 | 113.40 |
| 1 | 17-A | 127 | ASP | N-CA-C | 8.50 | 133.96 | 111.00 |
| 1 | 77-A | 98 | ARG | NE-CZ-NH2 | -8.50 | 116.05 | 120.30 |
| 1 | 23-A | 16 | MET | CG-SD-CE | 8.49 | 113.79 | 100.20 |
| 1 | 2-A | 28 | LEU | CA-CB-CG | -8.48 | 95.80 | 115.30 |
| 1 | 8-A | 36 | LEU | CA-CB-CG | 8.47 | 134.78 | 115.30 |
| 1 | 28-A | 12 | ARG | CA-CB-CG | 8.47 | 132.03 | 113.40 |
| 1 | 43-A | 4 | LEU | CB-CG-CD2 | 8.44 | 125.35 | 111.00 |
| 1 | 94-A | 12 | ARG | NE-CZ-NH2 | 8.43 | 124.52 | 120.30 |
| 1 | 75-A | 79 | ASP | CB-CG-OD2 | -8.42 | 110.72 | 118.30 |
| 1 | 123-A | 87 | ASP | CB-CG-OD1 | 8.41 | 125.87 | 118.30 |
| 1 | 95-A | 12 | ARG | NE-CZ-NH2 | 8.39 | 124.49 | 120.30 |
| 1 | 50-A | 28 | LEU | CA-CB-CG | -8.36 | 96.08 | 115.30 |
| 1 | 63-A | 16 | MET | CB-CG-SD | -8.35 | 87.35 | 112.40 |
| 1 | 10-A | 87 | ASP | CB-CG-OD2 | -8.35 | 110.79 | 118.30 |
| 1 | 54-A | 154 | GLU | OE1-CD-OE2 | 8.35 | 133.32 | 123.30 |
| 1 | 13-A | 158 | ARG | NE-CZ-NH2 | -8.33 | 116.13 | 120.30 |
| 1 | 7-A | 24 | LEU | CB-CA-C | 8.33 | 126.02 | 110.20 |
| 1 | 32-A | 159 | ARG | NE-CZ-NH1 | 8.32 | 124.46 | 120.30 |
| 1 | 51-A | 128 | TYR | N-CA-C | -8.32 | 88.53 | 111.00 |
| 1 | 5-A | 154 | GLU | CB-CA-C | -8.30 | 93.79 | 110.40 |
| 1 | 104-A | 62 | LEU | CB-CG-CD1 | 8.30 | 125.12 | 111.00 |
| 1 | 32-A | 128 | TYR | CZ-CE2-CD2 | 8.29 | 127.26 | 119.80 |
| 1 | 17-A | 158 | ARG | NE-CZ-NH2 | -8.29 | 116.16 | 120.30 |
| 1 | 80-A | 98 | ARG | NE-CZ-NH1 | 8.29 | 124.44 | 120.30 |
| 1 | 5-A | 154 | GLU | OE1-CD-OE2 | -8.28 | 113.36 | 123.30 |
| 1 | 100-A | 1 | MET | CG-SD-CE | 8.26 | 113.42 | 100.20 |
| 1 | 60-A | 86 | GLY | N-CA-C | 8.25 | 133.73 | 113.10 |
| 1 | 108-A | 28 | LEU | CA-CB-CG | 8.25 | 134.27 | 115.30 |
| 1 | 57-A | 128 | TYR | CA-CB-CG | 8.25 | 129.07 | 113.40 |
| 1 | 78-A | 98 | ARG | NE-CZ-NH2 | -8.23 | 116.18 | 120.30 |
| 1 | 106-A | 65 | GLN | C-N-CD | -8.23 | 102.50 | 120.60 |
| 1 | 89-A | 129 | GLU | C-N-CD | -8.22 | 102.51 | 120.60 |
| 1 | 121-A | 20 | MET | CA-CB-CG | 8.22 | 127.28 | 113.30 |
| 1 | 22-A | 16 | MET | CA-CB-CG | 8.21 | 127.25 | 113.30 |
| 1 | 35-A | 134 | GLU | CB-CA-C | -8.20 | 93.99 | 110.40 |
| 1 | 101-A | 20 | MET | C-N-CD | -8.20 | 102.55 | 120.60 |
| 1 | 27-A | 154 | GLU | OE1-CD-OE2 | -8.20 | 113.46 | 123.30 |
| 1 | 32-A | 154 | GLU | CA-CB-CG | 8.20 | 131.43 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 98-A | 24 | LEU | N-CA-C | 8.19 | 133.12 | 111.00 |
| 1 | 68-A | 127 | ASP | CB-CG-OD2 | 8.19 | 125.67 | 118.30 |
| 1 | 29-A | 62 | LEU | CB-CG-CD2 | 8.18 | 124.91 | 111.00 |
| 1 | 58-A | 101 | GLU | CB-CA-C | -8.18 | 94.04 | 110.40 |
| 1 | 82-A | 44 | ARG | NE-CZ-NH2 | -8.17 | 116.22 | 120.30 |
| 1 | 95-A | 12 | ARG | NE-CZ-NH1 | -8.15 | 116.22 | 120.30 |
| 1 | 76-A | 4 | LEU | CB-CG-CD2 | 8.15 | 124.86 | 111.00 |
| 1 | 110-A | 44 | ARG | NE-CZ-NH2 | -8.15 | 116.23 | 120.30 |
| 1 | 89-A | 18 | ASN | N-CA-C | 8.13 | 132.95 | 111.00 |
| 1 | 15-A | 154 | GLU | CG-CD-OE1 | -8.12 | 102.06 | 118.30 |
| 1 | 97-A | 23 | ASN | N-CA-C | 8.12 | 132.91 | 111.00 |
| 1 | 59-A | 128 | TYR | CB-CG-CD1 | 8.12 | 125.87 | 121.00 |
| 1 | 68-A | 16 | MET | CB-CG-SD | 8.11 | 136.73 | 112.40 |
| 1 | 88-A | 156 | LEU | CA-CB-CG | -8.10 | 96.67 | 115.30 |
| 1 | 107-A | 20 | MET | C-N-CD | 8.10 | 145.41 | 128.40 |
| 1 | 7-A | 158 | ARG | NE-CZ-NH2 | -8.08 | 116.26 | 120.30 |
| 1 | 43-A | 33 | ARG | NE-CZ-NH2 | -8.08 | 116.26 | 120.30 |
| 1 | 48-A | 127 | ASP | CB-CG-OD2 | 8.07 | 125.56 | 118.30 |
| 1 | 80-A | 156 | LEU | CA-CB-CG | 8.06 | 133.83 | 115.30 |
| 1 | 23-A | 42 | MET | CG-SD-CE | -8.03 | 87.35 | 100.20 |
| 1 | 63-A | 1 | MET | CG-SD-CE | -8.03 | 87.36 | 100.20 |
| 1 | 111-A | 30 | TRP | CA-CB-CG | 8.02 | 128.94 | 113.70 |
| 1 | 103-A | 20 | MET | CA-CB-CG | 8.02 | 126.93 | 113.30 |
| 1 | 12-A | 12 | ARG | NE-CZ-NH1 | 8.00 | 124.30 | 120.30 |
| 1 | 77-A | 8 | LEU | CA-CB-CG | 8.00 | 133.69 | 115.30 |
| 1 | 48-A | 156 | LEU | CA-CB-CG | 7.99 | 133.68 | 115.30 |
| 1 | 70-A | 52 | ARG | NE-CZ-NH2 | 7.99 | 124.30 | 120.30 |
| 1 | 61-A | 127 | ASP | N-CA-CB | -7.98 | 96.23 | 110.60 |
| 1 | 14-A | 98 | ARG | CA-CB-CG | 7.98 | 130.95 | 113.40 |
| 1 | 104-A | 132 | ASP | CB-CG-OD1 | 7.97 | 125.48 | 118.30 |
| 1 | 33-A | 52 | ARG | NE-CZ-NH1 | -7.97 | 116.32 | 120.30 |
| 1 | 47-A | 1 | MET | CG-SD-CE | 7.97 | 112.95 | 100.20 |
| 1 | 107-A | 132 | ASP | CB-CG-OD1 | -7.96 | 111.13 | 118.30 |
| 1 | 27-A | 54 | LEU | CB-CG-CD2 | -7.96 | 97.47 | 111.00 |
| 1 | 91-A | 127 | ASP | CB-CG-OD2 | 7.95 | 125.45 | 118.30 |
| 1 | 109-A | 4 | LEU | CB-CG-CD2 | 7.94 | 124.50 | 111.00 |
| 1 | 36-A | 154 | GLU | CA-CB-CG | 7.92 | 130.83 | 113.40 |
| 1 | 70-A | 98 | ARG | NE-CZ-NH1 | 7.92 | 124.26 | 120.30 |
| 1 | 24-A | 4 | LEU | CB-CG-CD2 | 7.91 | 124.45 | 111.00 |
| 1 | 41-A | 104 | LEU | CA-CB-CG | -7.91 | 97.10 | 115.30 |
| 1 | 64-A | 154 | GLU | OE1-CD-OE2 | -7.91 | 113.81 | 123.30 |
| 1 | 14-A | 16 | MET | CB-CG-SD | 7.91 | 136.13 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 99-A | 159 | ARG | NE-CZ-NH2 | -7.90 | 116.35 | 120.30 |
| 1 | 100-A | 126 | PRO | N-CA-C | 7.90 | 132.63 | 112.10 |
| 1 | 66-A | 129 | GLU | C-N-CD | 7.88 | 144.95 | 128.40 |
| 1 | 1-A | 62 | LEU | CB-CG-CD2 | -7.87 | 97.62 | 111.00 |
| 1 | 69-A | 126 | PRO | N-CA-C | 7.87 | 132.56 | 112.10 |
| 1 | 115-A | 44 | ARG | NE-CZ-NH1 | 7.87 | 124.23 | 120.30 |
| 1 | 55-A | 127 | ASP | CB-CG-OD1 | -7.86 | 111.22 | 118.30 |
| 1 | 63-A | 126 | PRO | N-CA-C | 7.86 | 132.54 | 112.10 |
| 1 | 124-A | 1 | MET | CG-SD-CE | 7.86 | 112.77 | 100.20 |
| 1 | 28-A | 1 | MET | CA-CB-CG | 7.85 | 126.64 | 113.30 |
| 1 | 55-A | 54 | LEU | CB-CG-CD1 | 7.83 | 124.32 | 111.00 |
| 1 | 105-A | 42 | MET | CG-SD-CE | -7.83 | 87.67 | 100.20 |
| 1 | 69-A | 4 | LEU | CB-CG-CD2 | 7.83 | 124.31 | 111.00 |
| 1 | 7-A | 158 | ARG | NE-CZ-NH1 | 7.82 | 124.21 | 120.30 |
| 1 | 76-A | 98 | ARG | NE-CZ-NH2 | -7.81 | 116.39 | 120.30 |
| 1 | 43-A | 33 | ARG | NE-CZ-NH1 | 7.81 | 124.20 | 120.30 |
| 1 | 79-A | 79 | ASP | CB-CG-OD1 | 7.81 | 125.33 | 118.30 |
| 1 | 9-A | 85 | CYS | N-CA-CB | 7.80 | 124.64 | 110.60 |
| 1 | 24-A | 12 | ARG | CG-CD-NE | -7.80 | 95.42 | 111.80 |
| 1 | 80-A | 28 | LEU | CA-CB-CG | 7.80 | 133.24 | 115.30 |
| 1 | 108-A | 20 | MET | CG-SD-CE | -7.78 | 87.75 | 100.20 |
| 1 | 104-A | 65 | GLN | C-N-CD | -7.78 | 103.49 | 120.60 |
| 1 | 16-A | 12 | ARG | NE-CZ-NH1 | 7.76 | 124.18 | 120.30 |
| 1 | 9-A | 127 | ASP | N-CA-C | 7.75 | 131.94 | 111.00 |
| 1 | 83-A | 129 | GLU | C-N-CD | 7.75 | 144.68 | 128.40 |
| 1 | 76-A | 127 | ASP | CB-CG-OD1 | 7.75 | 125.27 | 118.30 |
| 1 | 68-A | 129 | GLU | C-N-CD | 7.74 | 144.66 | 128.40 |
| 1 | 40-A | 159 | ARG | NE-CZ-NH1 | 7.73 | 124.17 | 120.30 |
| 1 | 15-A | 154 | GLU | CG-CD-OE2 | 7.72 | 133.74 | 118.30 |
| 1 | 67-A | 101 | GLU | OE1-CD-OE2 | -7.70 | 114.06 | 123.30 |
| 1 | 63-A | 131 | ASP | CB-CG-OD1 | 7.69 | 125.22 | 118.30 |
| 1 | 93-A | 128 | TYR | CB-CG-CD2 | 7.69 | 125.62 | 121.00 |
| 1 | 81-A | 4 | LEU | CB-CG-CD2 | 7.65 | 124.01 | 111.00 |
| 1 | 54-A | 79 | ASP | CB-CG-OD1 | -7.64 | 111.42 | 118.30 |
| 1 | 63-A | 12 | ARG | NE-CZ-NH2 | 7.64 | 124.12 | 120.30 |
| 1 | 7-A | 127 | ASP | N-CA-C | 7.62 | 131.57 | 111.00 |
| 1 | 79-A | 129 | GLU | C-N-CA | -7.59 | 90.12 | 122.00 |
| 1 | 116-A | 20 | MET | CB-CA-C | 7.59 | 125.58 | 110.40 |
| 1 | 57-A | 127 | ASP | N-CA-CB | -7.58 | 96.96 | 110.60 |
| 1 | 95-A | 4 | LEU | CB-CG-CD2 | -7.57 | 98.13 | 111.00 |
| 1 | 57-A | 127 | ASP | N-CA-C | 7.57 | 131.43 | 111.00 |
| 1 | 72-A | 36 | LEU | CA-CB-CG | 7.56 | 132.70 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 33-A | 52 | ARG | NE-CZ-NH2 | 7.56 | 124.08 | 120.30 |
| 1 | 67-A | 125 | PHE | C-N-CD | 7.55 | 144.25 | 128.40 |
| 1 | 73-A | 44 | ARG | NE-CZ-NH2 | -7.55 | 116.53 | 120.30 |
| 1 | 122-A | 23 | ASN | N-CA-C | 7.54 | 131.37 | 111.00 |
| 1 | 27-A | 127 | ASP | N-CA-C | -7.54 | 90.64 | 111.00 |
| 1 | 53-A | 126 | PRO | N-CA-C | -7.53 | 92.52 | 112.10 |
| 1 | 84-A | 130 | PRO | O-C-N | 7.52 | 134.74 | 122.70 |
| 1 | 41-A | 44 | ARG | CD-NE-CZ | 7.52 | 134.12 | 123.60 |
| 1 | 11-A | 12 | ARG | NE-CZ-NH2 | -7.51 | 116.55 | 120.30 |
| 1 | 36-A | 154 | GLU | OE1-CD-OE2 | 7.50 | 132.30 | 123.30 |
| 1 | 68-A | 12 | ARG | CG-CD-NE | 7.49 | 127.53 | 111.80 |
| 1 | 18-A | 129 | GLU | N-CA-C | 7.49 | 131.21 | 111.00 |
| 1 | 75-A | 79 | ASP | CB-CG-OD1 | 7.49 | 125.04 | 118.30 |
| 1 | 22-A | 98 | ARG | NE-CZ-NH2 | -7.48 | 116.56 | 120.30 |
| 1 | 118-A | 20 | MET | CA-CB-CG | 7.48 | 126.02 | 113.30 |
| 1 | 105-A | 19 | ALA | N-CA-C | 7.47 | 131.18 | 111.00 |
| 1 | 76-A | 104 | LEU | CB-CG-CD1 | 7.47 | 123.69 | 111.00 |
| 1 | 47-A | 104 | LEU | CB-CG-CD2 | 7.46 | 123.69 | 111.00 |
| 1 | 92-A | 44 | ARG | NE-CZ-NH1 | 7.46 | 124.03 | 120.30 |
| 1 | 48-A | 88 | VAL | C-N-CD | 7.46 | 144.06 | 128.40 |
| 1 | 44-A | 20 | MET | C-N-CD | -7.46 | 104.20 | 120.60 |
| 1 | 48-A | 22 | TRP | CA-CB-CG | 7.44 | 127.84 | 113.70 |
| 1 | 14-A | 98 | ARG | NE-CZ-NH1 | 7.43 | 124.02 | 120.30 |
| 1 | 40-A | 159 | ARG | NE-CZ-NH2 | -7.43 | 116.58 | 120.30 |
| 1 | 100-A | 98 | ARG | NE-CZ-NH1 | -7.43 | 116.58 | 120.30 |
| 1 | 86-A | 119 | VAL | CB-CA-C | -7.43 | 97.28 | 111.40 |
| 1 | 93-A | 104 | LEU | CB-CG-CD2 | 7.41 | 123.60 | 111.00 |
| 1 | 111-A | 98 | ARG | NE-CZ-NH2 | -7.41 | 116.60 | 120.30 |
| 1 | 69-A | 20 | MET | CA-CB-CG | -7.39 | 100.74 | 113.30 |
| 1 | 78-A | 4 | LEU | CB-CG-CD2 | 7.39 | 123.56 | 111.00 |
| 1 | 55-A | 128 | TYR | N-CA-C | -7.38 | 91.08 | 111.00 |
| 1 | 97-A | 12 | ARG | NE-CZ-NH1 | -7.36 | 116.62 | 120.30 |
| 1 | 43-A | 127 | ASP | CB-CG-OD2 | 7.36 | 124.92 | 118.30 |
| 1 | 87-A | 12 | ARG | NE-CZ-NH2 | 7.35 | 123.97 | 120.30 |
| 1 | 8-A | 128 | TYR | CB-CA-C | 7.35 | 125.09 | 110.40 |
| 1 | 106-A | 67 | GLY | N-CA-C | 7.35 | 131.47 | 113.10 |
| 1 | 90-A | 108 | GLN | CA-CB-CG | 7.33 | 129.54 | 113.40 |
| 1 | 59-A | 98 | ARG | NE-CZ-NH1 | 7.33 | 123.97 | 120.30 |
| 1 | 96-A | 120 | GLU | N-CA-C | 7.33 | 130.80 | 111.00 |
| 1 | 37-A | 20 | MET | N-CA-C | 7.32 | 130.77 | 111.00 |
| 1 | 90-A | 159 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 1 | 44-A | 22 | TRP | CA-CB-CG | 7.31 | 127.59 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 109-A | 1 | MET | CG-SD-CE | 7.31 | 111.90 | 100.20 |
| 1 | 28-A | 79 | ASP | CB-CA-C | -7.30 | 95.81 | 110.40 |
| 1 | 107-A | 20 | MET | N-CA-C | -7.30 | 91.30 | 111.00 |
| 1 | 69-A | 20 | MET | CG-SD-CE | -7.29 | 88.54 | 100.20 |
| 1 | 14-A | 16 | MET | CG-SD-CE | 7.28 | 111.85 | 100.20 |
| 1 | 93-A | 44 | ARG | NE-CZ-NH2 | -7.27 | 116.66 | 120.30 |
| 1 | 98-A | 24 | LEU | CB-CA-C | -7.27 | 96.38 | 110.20 |
| 1 | 77-A | 156 | LEU | CB-CG-CD1 | 7.27 | 123.35 | 111.00 |
| 1 | 5-A | 159 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 |
| 1 | 22-A | 4 | LEU | CB-CG-CD2 | 7.25 | 123.33 | 111.00 |
| 1 | 81-A | 156 | LEU | CA-CB-CG | 7.24 | 131.96 | 115.30 |
| 1 | 2-A | 36 | LEU | CB-CG-CD2 | 7.24 | 123.31 | 111.00 |
| 1 | 67-A | 98 | ARG | NE-CZ-NH1 | 7.24 | 123.92 | 120.30 |
| 1 | 17-A | 128 | TYR | CB-CG-CD2 | 7.24 | 125.34 | 121.00 |
| 1 | 86-A | 128 | TYR | CB-CG-CD1 | 7.24 | 125.34 | 121.00 |
| 1 | 65-A | 12 | ARG | CG-CD-NE | 7.23 | 126.99 | 111.80 |
| 1 | 32-A | 98 | ARG | NE-CZ-NH1 | 7.23 | 123.92 | 120.30 |
| 1 | 51-A | 1 | MET | CG-SD-CE | 7.22 | 111.75 | 100.20 |
| 1 | 75-A | 62 | LEU | CB-CG-CD1 | 7.21 | 123.26 | 111.00 |
| 1 | 64-A | 154 | GLU | CG-CD-OE2 | 7.20 | 132.70 | 118.30 |
| 1 | 113-A | 21 | PRO | CA-C-N | 7.20 | 133.04 | 117.20 |
| 1 | 122-A | 98 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 1 | 14-A | 129 | GLU | N-CA-C | 7.20 | 130.43 | 111.00 |
| 1 | 108-A | 98 | ARG | CG-CD-NE | -7.19 | 96.70 | 111.80 |
| 1 | 125-A | 23 | ASN | N-CA-C | 7.19 | 130.41 | 111.00 |
| 1 | 46-A | 20 | MET | N-CA-CB | 7.19 | 123.53 | 110.60 |
| 1 | 13-A | 33 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 1 | 61-A | 159 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 1 | 55-A | 20 | MET | CG-SD-CE | 7.17 | 111.68 | 100.20 |
| 1 | 18-A | 88 | VAL | CB-CA-C | -7.17 | 97.77 | 111.40 |
| 1 | 15-A | 61 | ILE | CG1-CB-CG2 | -7.17 | 95.63 | 111.40 |
| 1 | 52-A | 129 | GLU | CB-CA-C | 7.17 | 124.74 | 110.40 |
| 1 | 97-A | 2 | ILE | CG1-CB-CG2 | 7.17 | 127.17 | 111.40 |
| 1 | 103-A | 33 | ARG | NE-CZ-NH2 | -7.17 | 116.72 | 120.30 |
| 1 | 74-A | 128 | TYR | CB-CG-CD2 | 7.16 | 125.30 | 121.00 |
| 1 | 112-A | 1 | MET | C-N-CA | 7.16 | 139.59 | 121.70 |
| 1 | 78-A | 149 | HIS | CB-CA-C | 7.15 | 124.70 | 110.40 |
| 1 | 110-A | 18 | ASN | N-CA-C | 7.13 | 130.26 | 111.00 |
| 1 | 116-A | 62 | LEU | CA-CB-CG | -7.13 | 98.89 | 115.30 |
| 1 | 110-A | 20 | MET | C-N-CD | -7.13 | 104.91 | 120.60 |
| 1 | 44-A | 12 | ARG | CB-CG-CD | 7.13 | 130.13 | 111.60 |
| 1 | 63-A | 33 | ARG | NE-CZ-NH1 | 7.13 | 123.86 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 70-A | 126 | PRO | CB-CA-C | -7.13 | 94.18 | 112.00 |
| 1 | 19-A | 128 | TYR | CB-CG-CD1 | 7.13 | 125.28 | 121.00 |
| 1 | 64-A | 12 | ARG | NH1-CZ-NH2 | -7.12 | 111.56 | 119.40 |
| 1 | 17-A | 11 | ASP | CB-CG-OD1 | -7.12 | 111.89 | 118.30 |
| 1 | 96-A | 52 | ARG | NE-CZ-NH1 | -7.12 | 116.74 | 120.30 |
| 1 | 80-A | 158 | ARG | CG-CD-NE | -7.11 | 96.86 | 111.80 |
| 1 | 124-A | 4 | LEU | CB-CG-CD2 | 7.11 | 123.09 | 111.00 |
| 1 | 6-A | 4 | LEU | CB-CG-CD2 | -7.11 | 98.91 | 111.00 |
| 1 | 4-A | 17 | GLU | CA-CB-CG | 7.11 | 129.04 | 113.40 |
| 1 | 67-A | 12 | ARG | NE-CZ-NH2 | 7.10 | 123.85 | 120.30 |
| 1 | 67-A | 101 | GLU | CG-CD-OE2 | 7.10 | 132.50 | 118.30 |
| 1 | 63-A | 101 | GLU | CA-CB-CG | 7.10 | 129.01 | 113.40 |
| 1 | 85-A | 1 | MET | C-N-CA | 7.09 | 139.43 | 121.70 |
| 1 | 32-A | 98 | ARG | NE-CZ-NH2 | -7.09 | 116.76 | 120.30 |
| 1 | 44-A | 79 | ASP | CB-CG-OD1 | -7.09 | 111.92 | 118.30 |
| 1 | 60-A | 128 | TYR | CB-CA-C | -7.07 | 96.27 | 110.40 |
| 1 | 70-A | 52 | ARG | NE-CZ-NH1 | -7.05 | 116.77 | 120.30 |
| 1 | 66-A | 52 | ARG | NE-CZ-NH2 | 7.05 | 123.82 | 120.30 |
| 1 | 82-A | 126 | PRO | C-N-CA | 7.04 | 139.31 | 121.70 |
| 1 | 19-A | 128 | TYR | CB-CG-CD2 | -7.04 | 116.78 | 121.00 |
| 1 | 35-A | 127 | ASP | CB-CA-C | 7.03 | 124.46 | 110.40 |
| 1 | 7-A | 154 | GLU | CG-CD-OE2 | 7.03 | 132.35 | 118.30 |
| 1 | 73-A | 4 | LEU | CB-CG-CD2 | 7.02 | 122.94 | 111.00 |
| 1 | 2-A | 98 | ARG | CG-CD-NE | 7.02 | 126.54 | 111.80 |
| 1 | 36-A | 12 | ARG | NE-CZ-NH2 | -7.01 | 116.79 | 120.30 |
| 1 | 80-A | 20 | MET | CB-CG-SD | 7.01 | 133.43 | 112.40 |
| 1 | 33-A | 127 | ASP | CB-CA-C | 7.00 | 124.40 | 110.40 |
| 1 | 44-A | 12 | ARG | CG-CD-NE | 7.00 | 126.50 | 111.80 |
| 1 | 103-A | 98 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 1 | 31-A | 129 | GLU | N-CA-C | 6.99 | 129.88 | 111.00 |
| 1 | 77-A | 127 | ASP | CB-CG-OD2 | 6.99 | 124.59 | 118.30 |
| 1 | 21-A | 20 | MET | CG-SD-CE | 6.99 | 111.38 | 100.20 |
| 1 | 33-A | 36 | LEU | CA-CB-CG | 6.98 | 131.36 | 115.30 |
| 1 | 43-A | 79 | ASP | CB-CG-OD2 | 6.98 | 124.58 | 118.30 |
| 1 | 56-A | 128 | TYR | CA-CB-CG | 6.98 | 126.66 | 113.40 |
| 1 | 40-A | 62 | LEU | CB-CG-CD1 | 6.98 | 122.86 | 111.00 |
| 1 | 44-A | 12 | ARG | NE-CZ-NH1 | 6.97 | 123.79 | 120.30 |
| 1 | 112-A | 87 | ASP | CB-CG-OD1 | 6.97 | 124.57 | 118.30 |
| 1 | 18-A | 128 | TYR | CA-CB-CG | 6.97 | 126.64 | 113.40 |
| 1 | 28-A | 12 | ARG | CD-NE-CZ | 6.97 | 133.36 | 123.60 |
| 1 | 92-A | 104 | LEU | CB-CG-CD2 | 6.97 | 122.84 | 111.00 |
| 1 | 8-A | 24 | LEU | N-CA-C | 6.96 | 129.78 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 98-A | 118 | GLU | CA-CB-CG | 6.95 | 128.69 | 113.40 |
| 1 | 100-A | 20 | MET | CG-SD-CE | 6.95 | 111.32 | 100.20 |
| 1 | 1-A | 144 | ASP | CB-CG-OD2 | -6.95 | 112.05 | 118.30 |
| 1 | 67-A | 159 | ARG | CA-CB-CG | 6.94 | 128.67 | 113.40 |
| 1 | 79-A | 156 | LEU | CA-CB-CG | 6.94 | 131.27 | 115.30 |
| 1 | 76-A | 52 | ARG | CG-CD-NE | 6.94 | 126.37 | 111.80 |
| 1 | 100-A | 132 | ASP | CB-CG-OD2 | -6.93 | 112.06 | 118.30 |
| 1 | 57-A | 128 | TYR | CB-CA-C | -6.93 | 96.54 | 110.40 |
| 1 | 6-A | 158 | ARG | NE-CZ-NH1 | 6.93 | 123.76 | 120.30 |
| 1 | 38-A | 12 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 1 | 83-A | 20 | MET | CB-CG-SD | 6.92 | 133.16 | 112.40 |
| 1 | 16-A | 62 | LEU | CB-CG-CD2 | -6.92 | 99.24 | 111.00 |
| 1 | 119-A | 20 | MET | CA-CB-CG | 6.92 | 125.06 | 113.30 |
| 1 | 39-A | 20 | MET | C-N-CD | -6.92 | 105.39 | 120.60 |
| 1 | 74-A | 128 | TYR | N-CA-C | 6.92 | 129.67 | 111.00 |
| 1 | 4-A | 11 | ASP | CB-CG-OD2 | 6.91 | 124.52 | 118.30 |
| 1 | 7-A | 36 | LEU | CA-CB-CG | 6.91 | 131.19 | 115.30 |
| 1 | 56-A | 98 | ARG | NE-CZ-NH1 | 6.91 | 123.75 | 120.30 |
| 1 | 111-A | 156 | LEU | CB-CG-CD2 | 6.90 | 122.73 | 111.00 |
| 1 | 92-A | 44 | ARG | NE-CZ-NH2 | -6.89 | 116.86 | 120.30 |
| 1 | 106-A | 44 | ARG | CG-CD-NE | 6.89 | 126.27 | 111.80 |
| 1 | 9-A | 79 | ASP | CB-CG-OD1 | -6.88 | 112.11 | 118.30 |
| 1 | 104-A | 98 | ARG | CB-CG-CD | 6.88 | 129.49 | 111.60 |
| 1 | 67-A | 16 | MET | CG-SD-CE | -6.88 | 89.20 | 100.20 |
| 1 | 85-A | 126 | PRO | N-CA-C | 6.88 | 129.98 | 112.10 |
| 1 | 85-A | 158 | ARG | CA-CB-CG | 6.88 | 128.53 | 113.40 |
| 1 | 91-A | 52 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | 11-A | 127 | ASP | CB-CG-OD1 | 6.87 | 124.49 | 118.30 |
| 1 | 31-A | 128 | TYR | CA-CB-CG | 6.87 | 126.45 | 113.40 |
| 1 | 34-A | 24 | LEU | CA-CB-CG | 6.87 | 131.09 | 115.30 |
| 1 | 35-A | 4 | LEU | CB-CG-CD2 | 6.87 | 122.67 | 111.00 |
| 1 | 13-A | 158 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 1 | 125-A | 18 | ASN | CA-C-N | 6.86 | 132.29 | 117.20 |
| 1 | 84-A | 126 | PRO | N-CA-C | 6.85 | 129.90 | 112.10 |
| 1 | 55-A | 92 | MET | CG-SD-CE | 6.85 | 111.15 | 100.20 |
| 1 | 125-A | 18 | ASN | N-CA-C | 6.84 | 129.48 | 111.00 |
| 1 | 39-A | 127 | ASP | CB-CG-OD2 | 6.84 | 124.45 | 118.30 |
| 1 | 6-A | 127 | ASP | N-CA-C | 6.84 | 129.46 | 111.00 |
| 1 | 115-A | 12 | ARG | NE-CZ-NH1 | 6.83 | 123.72 | 120.30 |
| 1 | 65-A | 130 | PRO | N-CA-C | 6.83 | 129.87 | 112.10 |
| 1 | 19-A | 52 | ARG | NE-CZ-NH2 | 6.83 | 123.72 | 120.30 |
| 1 | 116-A | 16 | MET | CG-SD-CE | -6.83 | 89.27 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 5-A | 158 | ARG | NE-CZ-NH1 | 6.83 | 123.72 | 120.30 |
| 1 | 123-A | 20 | MET | C-N-CD | -6.82 | 105.59 | 120.60 |
| 1 | 51-A | 20 | MET | CG-SD-CE | 6.82 | 111.11 | 100.20 |
| 1 | 90-A | 20 | MET | CG-SD-CE | -6.82 | 89.29 | 100.20 |
| 1 | 56-A | 98 | ARG | NE-CZ-NH2 | -6.81 | 116.89 | 120.30 |
| 1 | 106-A | 98 | ARG | NE-CZ-NH1 | 6.81 | 123.71 | 120.30 |
| 1 | 46-A | 132 | ASP | CB-CG-OD1 | 6.81 | 124.43 | 118.30 |
| 1 | 88-A | 159 | ARG | NE-CZ-NH2 | 6.81 | 123.70 | 120.30 |
| 1 | 91-A | 11 | ASP | CB-CG-OD2 | 6.81 | 124.43 | 118.30 |
| 1 | 12-A | 127 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | 3-A | 86 | GLY | N-CA-C | 6.80 | 130.10 | 113.10 |
| 1 | 100-A | 20 | MET | N-CA-C | 6.80 | 129.35 | 111.00 |
| 1 | 101-A | 87 | ASP | N-CA-CB | -6.79 | 98.39 | 110.60 |
| 1 | 124-A | 20 | MET | CB-CG-SD | 6.78 | 132.75 | 112.40 |
| 1 | 104-A | 132 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | 103-A | 21 | PRO | CB-CA-C | 6.78 | 128.95 | 112.00 |
| 1 | 55-A | 127 | ASP | N-CA-C | 6.78 | 129.30 | 111.00 |
| 1 | 124-A | 19 | ALA | N-CA-C | 6.78 | 129.29 | 111.00 |
| 1 | 20-A | 144 | ASP | CB-CG-OD1 | 6.77 | 124.39 | 118.30 |
| 1 | 11-A | 98 | ARG | CA-CB-CG | 6.77 | 128.28 | 113.40 |
| 1 | 68-A | 126 | PRO | N-CA-C | -6.76 | 94.52 | 112.10 |
| 1 | 99-A | 20 | MET | N-CA-C | 6.75 | 129.24 | 111.00 |
| 1 | 94-A | 18 | ASN | N-CA-C | 6.75 | 129.22 | 111.00 |
| 1 | 98-A | 98 | ARG | NE-CZ-NH2 | -6.75 | 116.93 | 120.30 |
| 1 | 61-A | 127 | ASP | CB-CG-OD2 | 6.74 | 124.37 | 118.30 |
| 1 | 120-A | 20 | MET | CA-CB-CG | 6.74 | 124.76 | 113.30 |
| 1 | 68-A | 127 | ASP | CB-CG-OD1 | -6.73 | 112.24 | 118.30 |
| 1 | 105-A | 20 | MET | CA-CB-CG | 6.73 | 124.75 | 113.30 |
| 1 | 17-A | 20 | MET | C-N-CD | -6.72 | 105.82 | 120.60 |
| 1 | 55-A | 24 | LEU | CA-CB-CG | 6.71 | 130.73 | 115.30 |
| 1 | 45-A | 156 | LEU | CB-CG-CD1 | -6.71 | 99.60 | 111.00 |
| 1 | 64-A | 1 | MET | CB-CG-SD | -6.70 | 92.31 | 112.40 |
| 1 | 10-A | 8 | LEU | CB-CG-CD1 | 6.69 | 122.38 | 111.00 |
| 1 | 114-A | 150 | SER | CA-CB-OG | -6.69 | 93.14 | 111.20 |
| 1 | 31-A | 20 | MET | CG-SD-CE | 6.69 | 110.90 | 100.20 |
| 1 | 79-A | 127 | ASP | CB-CG-OD1 | -6.69 | 112.28 | 118.30 |
| 1 | 39-A | 58 | LYS | CB-CA-C | 6.68 | 123.75 | 110.40 |
| 1 | 62-A | 159 | ARG | NE-CZ-NH2 | 6.68 | 123.64 | 120.30 |
| 1 | 112-A | 87 | ASP | CB-CG-OD2 | -6.67 | 112.29 | 118.30 |
| 1 | 105-A | 1 | MET | CB-CA-C | 6.67 | 123.75 | 110.40 |
| 1 | 111-A | 19 | ALA | N-CA-C | 6.66 | 128.99 | 111.00 |
| 1 | 17-A | 11 | ASP | CB-CG-OD2 | 6.65 | 124.28 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 42-A | 61 | ILE | CG1-CB-CG2 | -6.65 | 96.78 | 111.40 |
| 1 | 48-A | 4 | LEU | CA-CB-CG | 6.65 | 130.59 | 115.30 |
| 1 | 71-A | 128 | TYR | CB-CA-C | -6.65 | 97.11 | 110.40 |
| 1 | 18-A | 98 | ARG | NE-CZ-NH2 | -6.64 | 116.98 | 120.30 |
| 1 | 84-A | 44 | ARG | NE-CZ-NH1 | 6.64 | 123.62 | 120.30 |
| 1 | 8-A | 44 | ARG | NE-CZ-NH2 | -6.64 | 116.98 | 120.30 |
| 1 | 98-A | 12 | ARG | NH1-CZ-NH2 | 6.64 | 126.70 | 119.40 |
| 1 | 102-A | 20 | MET | CB-CG-SD | 6.64 | 132.31 | 112.40 |
| 1 | 24-A | 158 | ARG | NE-CZ-NH2 | 6.63 | 123.62 | 120.30 |
| 1 | 82-A | 101 | GLU | CA-CB-CG | 6.63 | 128.00 | 113.40 |
| 1 | 17-A | 79 | ASP | CB-CG-OD2 | -6.63 | 112.33 | 118.30 |
| 1 | 110-A | 1 | MET | CG-SD-CE | 6.63 | 110.81 | 100.20 |
| 1 | 22-A | 62 | LEU | CB-CG-CD2 | 6.63 | 122.27 | 111.00 |
| 1 | 117-A | 4 | LEU | CB-CG-CD2 | 6.63 | 122.27 | 111.00 |
| 1 | 9-A | 79 | ASP | CB-CG-OD2 | 6.62 | 124.26 | 118.30 |
| 1 | 96-A | 106 | LYS | CA-CB-CG | 6.62 | 127.96 | 113.40 |
| 1 | 21-A | 98 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | 40-A | 158 | ARG | NE-CZ-NH2 | -6.61 | 116.99 | 120.30 |
| 1 | 25-A | 36 | LEU | CB-CG-CD2 | 6.60 | 122.22 | 111.00 |
| 1 | 125-A | 12 | ARG | NE-CZ-NH2 | -6.60 | 117.00 | 120.30 |
| 1 | 50-A | 127 | ASP | CB-CG-OD2 | 6.60 | 124.24 | 118.30 |
| 1 | 38-A | 127 | ASP | CB-CG-OD1 | -6.59 | 112.37 | 118.30 |
| 1 | 47-A | 22 | TRP | CB-CG-CD1 | -6.59 | 118.43 | 127.00 |
| 1 | 12-A | 4 | LEU | CB-CG-CD2 | 6.59 | 122.20 | 111.00 |
| 1 | 40-A | 60 | ILE | CG1-CB-CG2 | -6.59 | 96.91 | 111.40 |
| 1 | 103-A | 21 | PRO | CA-CB-CG | -6.59 | 91.48 | 104.00 |
| 1 | 26-A | 62 | LEU | CB-CG-CD2 | 6.58 | 122.19 | 111.00 |
| 1 | 68-A | 130 | PRO | C-N-CA | 6.58 | 138.16 | 121.70 |
| 1 | 14-A | 98 | ARG | NE-CZ-NH2 | -6.58 | 117.01 | 120.30 |
| 1 | 90-A | 132 | ASP | CB-CG-OD2 | -6.57 | 112.39 | 118.30 |
| 1 | 116-A | 19 | ALA | N-CA-C | 6.57 | 128.73 | 111.00 |
| 1 | 89-A | 128 | TYR | CA-CB-CG | 6.56 | 125.87 | 113.40 |
| 1 | 124-A | 156 | LEU | CA-CB-CG | 6.56 | 130.38 | 115.30 |
| 1 | 89-A | 1 | MET | CG-SD-CE | -6.55 | 89.71 | 100.20 |
| 1 | 62-A | 44 | ARG | NE-CZ-NH1 | 6.55 | 123.58 | 120.30 |
| 1 | 73-A | 20 | MET | CG-SD-CE | 6.55 | 110.68 | 100.20 |
| 1 | 93-A | 128 | TYR | N-CA-CB | -6.55 | 98.81 | 110.60 |
| 1 | 84-A | 158 | ARG | NE-CZ-NH2 | -6.54 | 117.03 | 120.30 |
| 1 | 119-A | 127 | ASP | CB-CG-OD1 | 6.54 | 124.19 | 118.30 |
| 1 | 19-A | 127 | ASP | CB-CG-OD1 | 6.54 | 124.18 | 118.30 |
| 1 | 18-A | 16 | MET | CA-CB-CG | 6.53 | 124.41 | 113.30 |
| 1 | 88-A | 87 | ASP | CB-CG-OD2 | -6.53 | 112.42 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 1-A | 62 | LEU | CA-CB-CG | 6.52 | 130.30 | 115.30 |
| 1 | 89-A | 12 | ARG | CD-NE-CZ | 6.51 | 132.72 | 123.60 |
| 1 | 7-A | 1 | MET | CG-SD-CE | 6.51 | 110.62 | 100.20 |
| 1 | 10-A | 159 | ARG | NE-CZ-NH1 | 6.51 | 123.56 | 120.30 |
| 1 | 91-A | 130 | PRO | CA-C-O | -6.50 | 104.59 | 120.20 |
| 1 | 36-A | 120 | GLU | N-CA-C | 6.50 | 128.56 | 111.00 |
| 1 | 63-A | 33 | ARG | NE-CZ-NH2 | -6.50 | 117.05 | 120.30 |
| 1 | 14-A | 127 | ASP | N-CA-C | 6.50 | 128.55 | 111.00 |
| 1 | 2-A | 52 | ARG | NE-CZ-NH1 | 6.49 | 123.55 | 120.30 |
| 1 | 88-A | 119 | VAL | CB-CA-C | -6.49 | 99.08 | 111.40 |
| 1 | 91-A | 62 | LEU | CB-CG-CD1 | 6.49 | 122.03 | 111.00 |
| 1 | 94-A | 1 | MET | CA-CB-CG | -6.48 | 102.28 | 113.30 |
| 1 | 107-A | 132 | ASP | CB-CG-OD2 | 6.48 | 124.14 | 118.30 |
| 1 | 63-A | 16 | MET | CG-SD-CE | 6.48 | 110.56 | 100.20 |
| 1 | 83-A | 20 | MET | N-CA-CB | 6.47 | 122.25 | 110.60 |
| 1 | 41-A | 129 | GLU | N-CA-C | 6.47 | 128.47 | 111.00 |
| 1 | 29-A | 16 | MET | CG-SD-CE | -6.47 | 89.85 | 100.20 |
| 1 | 88-A | 33 | ARG | NE-CZ-NH1 | 6.47 | 123.53 | 120.30 |
| 1 | 83-A | 125 | PHE | C-N-CD | -6.47 | 106.37 | 120.60 |
| 1 | 109-A | 129 | GLU | OE1-CD-OE2 | -6.46 | 115.54 | 123.30 |
| 1 | 125-A | 12 | ARG | NE-CZ-NH1 | 6.46 | 123.53 | 120.30 |
| 1 | 76-A | 129 | GLU | N-CA-C | -6.46 | 93.56 | 111.00 |
| 1 | 82-A | 22 | TRP | CA-CB-CG | 6.46 | 125.97 | 113.70 |
| 1 | 29-A | 11 | ASP | CB-CG-OD1 | -6.45 | 112.49 | 118.30 |
| 1 | 64-A | 128 | TYR | N-CA-C | 6.44 | 128.40 | 111.00 |
| 1 | 91-A | 20 | MET | CB-CG-SD | 6.44 | 131.73 | 112.40 |
| 1 | 111-A | 12 | ARG | NE-CZ-NH2 | -6.44 | 117.08 | 120.30 |
| 1 | 64-A | 86 | GLY | N-CA-C | -6.43 | 97.03 | 113.10 |
| 1 | 79-A | 20 | MET | C-N-CD | -6.42 | 106.47 | 120.60 |
| 1 | 13-A | 125 | PHE | C-N-CD | -6.42 | 106.48 | 120.60 |
| 1 | 109-A | 106 | LYS | CB-CA-C | 6.42 | 123.24 | 110.40 |
| 1 | 72-A | 12 | ARG | NE-CZ-NH2 | -6.42 | 117.09 | 120.30 |
| 1 | 23-A | 98 | ARG | NE-CZ-NH2 | 6.42 | 123.51 | 120.30 |
| 1 | 91-A | 130 | PRO | CA-C-N | 6.42 | 131.31 | 117.20 |
| 1 | 11-A | 44 | ARG | NE-CZ-NH2 | -6.41 | 117.09 | 120.30 |
| 1 | 107-A | 20 | MET | CA-CB-CG | 6.41 | 124.19 | 113.30 |
| 1 | 88-A | 12 | ARG | CG-CD-NE | -6.40 | 98.36 | 111.80 |
| 1 | 113-A | 24 | LEU | CA-CB-CG | 6.40 | 130.03 | 115.30 |
| 1 | 24-A | 12 | ARG | NE-CZ-NH2 | -6.40 | 117.10 | 120.30 |
| 1 | 58-A | 128 | TYR | CB-CA-C | -6.40 | 97.60 | 110.40 |
| 1 | 61-A | 127 | ASP | N-CA-C | 6.39 | 128.26 | 111.00 |
| 1 | 13-A | 98 | ARG | NE-CZ-NH1 | 6.39 | 123.50 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 106-A | 79 | ASP | N-CA-CB | -6.38 | 99.11 | 110.60 |
| 1 | 125-A | 44 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 1 | 83-A | 135 | SER | CB-CA-C | -6.37 | 98.00 | 110.10 |
| 1 | 115-A | 12 | ARG | NE-CZ-NH2 | -6.37 | 117.11 | 120.30 |
| 1 | 104-A | 16 | MET | CG-SD-CE | 6.36 | 110.38 | 100.20 |
| 1 | 119-A | 21 | PRO | CA-C-N | -6.36 | 103.20 | 117.20 |
| 1 | 12-A | 127 | ASP | CB-CG-OD1 | 6.36 | 124.03 | 118.30 |
| 1 | 52-A | 1 | MET | CG-SD-CE | 6.36 | 110.37 | 100.20 |
| 1 | 51-A | 98 | ARG | CG-CD-NE | 6.36 | 125.15 | 111.80 |
| 1 | 91-A | 12 | ARG | NE-CZ-NH2 | -6.35 | 117.13 | 120.30 |
| 1 | 81-A | 12 | ARG | NE-CZ-NH2 | -6.34 | 117.13 | 120.30 |
| 1 | 26-A | 11 | ASP | CB-CG-OD1 | -6.34 | 112.59 | 118.30 |
| 1 | 64-A | 12 | ARG | CG-CD-NE | 6.34 | 125.11 | 111.80 |
| 1 | 56-A | 2 | ILE | CG1-CB-CG2 | -6.34 | 97.46 | 111.40 |
| 1 | 119-A | 11 | ASP | CB-CG-OD1 | -6.34 | 112.60 | 118.30 |
| 1 | 88-A | 79 | ASP | CB-CG-OD1 | 6.33 | 124.00 | 118.30 |
| 1 | 8-A | 87 | ASP | CB-CG-OD2 | 6.33 | 124.00 | 118.30 |
| 1 | 67-A | 125 | PHE | C-N-CA | -6.32 | 95.45 | 122.00 |
| 1 | 120-A | 21 | PRO | CA-C-N | -6.32 | 103.30 | 117.20 |
| 1 | 2-A | 108 | GLN | CA-CB-CG | 6.32 | 127.30 | 113.40 |
| 1 | 40-A | 129 | GLU | N-CA-C | 6.32 | 128.06 | 111.00 |
| 1 | 104-A | 19 | ALA | N-CA-CB | 6.32 | 118.94 | 110.10 |
| 1 | 35-A | 88 | VAL | CB-CA-C | -6.32 | 99.40 | 111.40 |
| 1 | 60-A | 101 | GLU | CA-CB-CG | -6.32 | 99.51 | 113.40 |
| 1 | 55-A | 128 | TYR | CB-CA-C | 6.31 | 123.03 | 110.40 |
| 1 | 54-A | 154 | GLU | CG-CD-OE2 | -6.31 | 105.67 | 118.30 |
| 1 | 55-A | 52 | ARG | NE-CZ-NH1 | -6.31 | 117.14 | 120.30 |
| 1 | 85-A | 21 | PRO | CA-N-CD | -6.31 | 102.66 | 111.50 |
| 1 | 82-A | 126 | PRO | N-CA-C | 6.31 | 128.50 | 112.10 |
| 1 | 119-A | 22 | TRP | CA-CB-CG | -6.31 | 101.71 | 113.70 |
| 1 | 31-A | 20 | MET | C-N-CD | -6.31 | 106.72 | 120.60 |
| 1 | 78-A | 8 | LEU | CB-CG-CD1 | 6.30 | 121.72 | 111.00 |
| 1 | 71-A | 128 | TYR | CB-CG-CD1 | -6.30 | 117.22 | 121.00 |
| 1 | 116-A | 8 | LEU | CB-CG-CD1 | -6.30 | 100.29 | 111.00 |
| 1 | 73-A | 16 | MET | CG-SD-CE | -6.30 | 90.12 | 100.20 |
| 1 | 3-A | 17 | GLU | CB-CA-C | 6.30 | 122.99 | 110.40 |
| 1 | 41-A | 158 | ARG | NE-CZ-NH2 | 6.29 | 123.45 | 120.30 |
| 1 | 1-A | 140 | PHE | CB-CG-CD2 | -6.29 | 116.39 | 120.80 |
| 1 | 101-A | 20 | MET | N-CA-CB | 6.29 | 121.93 | 110.60 |
| 1 | 115-A | 1 | MET | CB-CA-C | 6.29 | 122.98 | 110.40 |
| 1 | 109-A | 2 | ILE | N-CA-CB | 6.29 | 125.26 | 110.80 |
| 1 | 56-A | 131 | ASP | CB-CG-OD1 | -6.28 | 112.65 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 96-A | 22 | TRP | CB-CA-C | 6.27 | 122.95 | 110.40 |
| 1 | 97-A | 88 | VAL | CG1-CB-CG2 | -6.27 | 100.86 | 110.90 |
| 1 | 78-A | 44 | ARG | NE-CZ-NH1 | 6.27 | 123.44 | 120.30 |
| 1 | 97-A | 20 | MET | CG-SD-CE | 6.26 | 110.22 | 100.20 |
| 1 | 122-A | 17 | GLU | CB-CA-C | 6.26 | 122.92 | 110.40 |
| 1 | 2-A | 79 | ASP | CB-CG-OD1 | 6.26 | 123.93 | 118.30 |
| 1 | 76-A | 129 | GLU | C-N-CD | 6.25 | 141.54 | 128.40 |
| 1 | 111-A | 42 | MET | CG-SD-CE | 6.25 | 110.20 | 100.20 |
| 1 | 76-A | 22 | TRP | CB-CG-CD2 | 6.24 | 134.71 | 126.60 |
| 1 | 57-A | 12 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 1 | 84-A | 130 | PRO | C-N-CA | 6.24 | 137.29 | 121.70 |
| 1 | 42-A | 98 | ARG | CG-CD-NE | 6.23 | 124.89 | 111.80 |
| 1 | 81-A | 20 | MET | CB-CG-SD | 6.23 | 131.09 | 112.40 |
| 1 | 82-A | 1 | MET | CG-SD-CE | 6.23 | 110.17 | 100.20 |
| 1 | 28-A | 127 | ASP | CB-CA-C | 6.23 | 122.86 | 110.40 |
| 1 | 77-A | 127 | ASP | N-CA-C | 6.22 | 127.81 | 111.00 |
| 1 | 75-A | 158 | ARG | NE-CZ-NH2 | -6.22 | 117.19 | 120.30 |
| 1 | 60-A | 42 | MET | CG-SD-CE | 6.22 | 110.15 | 100.20 |
| 1 | 73-A | 127 | ASP | N-CA-C | 6.22 | 127.79 | 111.00 |
| 1 | 106-A | 22 | TRP | N-CA-CB | 6.22 | 121.80 | 110.60 |
| 1 | 67-A | 101 | GLU | CA-CB-CG | 6.22 | 127.08 | 113.40 |
| 1 | 6-A | 22 | TRP | N-CA-C | -6.21 | 94.22 | 111.00 |
| 1 | 32-A | 128 | TYR | N-CA-CB | 6.21 | 121.79 | 110.60 |
| 1 | 36-A | 12 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 1 | 85-A | 130 | PRO | CA-C-O | -6.21 | 105.29 | 120.20 |
| 1 | 69-A | 16 | MET | CG-SD-CE | -6.21 | 90.27 | 100.20 |
| 1 | 3-A | 17 | GLU | CA-C-N | -6.20 | 103.56 | 117.20 |
| 1 | 84-A | 129 | GLU | N-CA-C | -6.20 | 94.27 | 111.00 |
| 1 | 108-A | 20 | MET | CA-CB-CG | 6.20 | 123.83 | 113.30 |
| 1 | 73-A | 42 | MET | CG-SD-CE | 6.19 | 110.11 | 100.20 |
| 1 | 33-A | 54 | LEU | CB-CG-CD1 | 6.19 | 121.52 | 111.00 |
| 1 | 8-A | 154 | GLU | CA-CB-CG | 6.19 | 127.01 | 113.40 |
| 1 | 12-A | 128 | TYR | C-N-CA | -6.18 | 106.24 | 121.70 |
| 1 | 92-A | 129 | GLU | CB-CA-C | 6.18 | 122.77 | 110.40 |
| 1 | 82-A | 149 | HIS | CB-CA-C | 6.18 | 122.76 | 110.40 |
| 1 | 46-A | 19 | ALA | C-N-CA | -6.18 | 106.26 | 121.70 |
| 1 | 108-A | 33 | ARG | CA-CB-CG | 6.18 | 126.99 | 113.40 |
| 1 | 92-A | 62 | LEU | CB-CG-CD2 | 6.17 | 121.50 | 111.00 |
| 1 | 52-A | 98 | ARG | NE-CZ-NH1 | 6.17 | 123.39 | 120.30 |
| 1 | 115-A | 104 | LEU | CB-CG-CD1 | 6.17 | 121.49 | 111.00 |
| 1 | 6-A | 158 | ARG | NE-CZ-NH2 | -6.16 | 117.22 | 120.30 |
| 1 | 6-A | 44 | ARG | CG-CD-NE | 6.16 | 124.73 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 83-A | 106 | LYS | CD-CE-NZ | 6.16 | 125.86 | 111.70 |
| 1 | 97-A | 24 | LEU | CA-CB-CG | 6.15 | 129.45 | 115.30 |
| 1 | 68-A | 16 | MET | CA-CB-CG | 6.14 | 123.74 | 113.30 |
| 1 | 113-A | 21 | PRO | CA-C-O | -6.14 | 105.46 | 120.20 |
| 1 | 114-A | 21 | PRO | CA-C-O | -6.14 | 105.47 | 120.20 |
| 1 | 61-A | 102 | GLN | CA-CB-CG | 6.13 | 126.88 | 113.40 |
| 1 | 39-A | 16 | MET | CA-CB-CG | 6.12 | 123.71 | 113.30 |
| 1 | 11-A | 126 | PRO | CA-C-O | 6.12 | 134.89 | 120.20 |
| 1 | 90-A | 44 | ARG | CA-CB-CG | 6.12 | 126.87 | 113.40 |
| 1 | 4-A | 154 | GLU | CG-CD-OE1 | -6.12 | 106.06 | 118.30 |
| 1 | 88-A | 12 | ARG | NE-CZ-NH2 | -6.12 | 117.24 | 120.30 |
| 1 | 111-A | 12 | ARG | NE-CZ-NH1 | 6.11 | 123.36 | 120.30 |
| 1 | 7-A | 126 | PRO | CA-C-N | 6.10 | 130.62 | 117.20 |
| 1 | 38-A | 44 | ARG | NE-CZ-NH2 | -6.10 | 117.25 | 120.30 |
| 1 | 66-A | 52 | ARG | NE-CZ-NH1 | -6.10 | 117.25 | 120.30 |
| 1 | 32-A | 20 | MET | CG-SD-CE | 6.10 | 109.96 | 100.20 |
| 1 | 5-A | 154 | GLU | CG-CD-OE2 | 6.09 | 130.48 | 118.30 |
| 1 | 70-A | 129 | GLU | N-CA-C | -6.09 | 94.56 | 111.00 |
| 1 | 56-A | 20 | MET | C-N-CD | 6.09 | 141.18 | 128.40 |
| 1 | 9-A | 8 | LEU | CA-CB-CG | -6.08 | 101.33 | 115.30 |
| 1 | 21-A | 16 | MET | CA-CB-CG | 6.07 | 123.63 | 113.30 |
| 1 | 47-A | 52 | ARG | NE-CZ-NH2 | 6.07 | 123.34 | 120.30 |
| 1 | 72-A | 128 | TYR | N-CA-C | 6.07 | 127.40 | 111.00 |
| 1 | 85-A | 87 | ASP | CB-CG-OD1 | 6.07 | 123.77 | 118.30 |
| 1 | 114-A | 20 | MET | C-N-CA | -6.07 | 96.51 | 122.00 |
| 1 | 83-A | 1 | MET | CG-SD-CE | 6.07 | 109.91 | 100.20 |
| 1 | 109-A | 20 | MET | C-N-CD | 6.07 | 141.15 | 128.40 |
| 1 | 115-A | 156 | LEU | CB-CG-CD2 | 6.07 | 121.32 | 111.00 |
| 1 | 85-A | 130 | PRO | C-N-CA | 6.07 | 136.86 | 121.70 |
| 1 | 97-A | 24 | LEU | CB-CG-CD1 | -6.07 | 100.69 | 111.00 |
| 1 | 35-A | 127 | ASP | CB-CG-OD2 | 6.06 | 123.75 | 118.30 |
| 1 | 59-A | 1 | MET | CB-CG-SD | 6.05 | 130.56 | 112.40 |
| 1 | 96-A | 158 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 1 | 25-A | 16 | MET | CG-SD-CE | 6.04 | 109.87 | 100.20 |
| 1 | 3-A | 20 | MET | CG-SD-CE | 6.04 | 109.86 | 100.20 |
| 1 | 60-A | 128 | TYR | N-CA-C | 6.04 | 127.30 | 111.00 |
| 1 | 111-A | 30 | TRP | CD1-CG-CD2 | -6.04 | 101.47 | 106.30 |
| 1 | 67-A | 127 | ASP | CB-CG-OD2 | -6.03 | 112.87 | 118.30 |
| 1 | 91-A | 36 | LEU | CB-CG-CD2 | -6.03 | 100.75 | 111.00 |
| 1 | 9-A | 62 | LEU | CB-CG-CD1 | -6.03 | 100.75 | 111.00 |
| 1 | 120-A | 18 | ASN | N-CA-C | 6.03 | 127.28 | 111.00 |
| 1 | 66-A | 126 | PRO | N-CA-C | 6.02 | 127.76 | 112.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 59-A | 16 | MET | CB-CG-SD | -6.01 | 94.37 | 112.40 |
| 1 | 83-A | 52 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 1 | 109-A | 33 | ARG | CA-CB-CG | 6.00 | 126.60 | 113.40 |
| 1 | 2-A | 20 | MET | CA-CB-CG | 6.00 | 123.50 | 113.30 |
| 1 | 95-A | 12 | ARG | CB-CG-CD | 6.00 | 127.20 | 111.60 |
| 1 | 104-A | 127 | ASP | N-CA-CB | 6.00 | 121.40 | 110.60 |
| 1 | 10-A | 20 | MET | C-N-CD | 6.00 | 140.99 | 128.40 |
| 1 | 64-A | 16 | MET | CA-CB-CG | 6.00 | 123.49 | 113.30 |
| 1 | 26-A | 154 | GLU | OE1-CD-OE2 | -5.99 | 116.11 | 123.30 |
| 1 | 62-A | 101 | GLU | CA-CB-CG | 5.99 | 126.58 | 113.40 |
| 1 | 3-A | 17 | GLU | CA-C-O | 5.99 | 132.68 | 120.10 |
| 1 | 59-A | 58 | LYS | CA-CB-CG | -5.99 | 100.22 | 113.40 |
| 1 | 55-A | 44 | ARG | CG-CD-NE | -5.98 | 99.23 | 111.80 |
| 1 | 9-A | 62 | LEU | CB-CG-CD2 | 5.97 | 121.16 | 111.00 |
| 1 | 50-A | 106 | LYS | CD-CE-NZ | 5.97 | 125.44 | 111.70 |
| 1 | 54-A | 127 | ASP | N-CA-C | 5.97 | 127.13 | 111.00 |
| 1 | 96-A | 132 | ASP | CB-CG-OD1 | 5.97 | 123.68 | 118.30 |
| 1 | 29-A | 144 | ASP | CB-CA-C | 5.97 | 122.34 | 110.40 |
| 1 | 5-A | 28 | LEU | CA-CB-CG | 5.96 | 129.02 | 115.30 |
| 1 | 8-A | 20 | MET | CG-SD-CE | 5.96 | 109.73 | 100.20 |
| 1 | 28-A | 144 | ASP | N-CA-CB | -5.96 | 99.88 | 110.60 |
| 1 | 33-A | 92 | MET | CG-SD-CE | 5.95 | 109.73 | 100.20 |
| 1 | 14-A | 126 | PRO | CB-CA-C | -5.95 | 97.12 | 112.00 |
| 1 | 46-A | 12 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 1 | 121-A | 142 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | 11-A | 98 | ARG | CG-CD-NE | 5.95 | 124.28 | 111.80 |
| 1 | 45-A | 118 | GLU | CA-CB-CG | 5.95 | 126.48 | 113.40 |
| 1 | 96-A | 54 | LEU | CB-CG-CD1 | 5.94 | 121.10 | 111.00 |
| 1 | 33-A | 62 | LEU | CB-CG-CD1 | 5.94 | 121.09 | 111.00 |
| 1 | 112-A | 88 | VAL | N-CA-C | 5.94 | 127.03 | 111.00 |
| 1 | 18-A | 20 | MET | CG-SD-CE | 5.93 | 109.69 | 100.20 |
| 1 | 63-A | 33 | ARG | CG-CD-NE | -5.93 | 99.35 | 111.80 |
| 1 | 64-A | 16 | MET | CB-CG-SD | -5.93 | 94.62 | 112.40 |
| 1 | 75-A | 127 | ASP | N-CA-CB | -5.93 | 99.93 | 110.60 |
| 1 | 46-A | 20 | MET | CB-CA-C | 5.92 | 122.25 | 110.40 |
| 1 | 59-A | 128 | TYR | CB-CA-C | -5.92 | 98.56 | 110.40 |
| 1 | 9-A | 19 | ALA | N-CA-C | 5.92 | 126.98 | 111.00 |
| 1 | 22-A | 33 | ARG | CB-CA-C | -5.92 | 98.57 | 110.40 |
| 1 | 42-A | 62 | LEU | CB-CG-CD1 | 5.91 | 121.05 | 111.00 |
| 1 | 34-A | 1 | MET | CB-CG-SD | 5.91 | 130.14 | 112.40 |
| 1 | 24-A | 62 | LEU | CB-CG-CD2 | 5.91 | 121.05 | 111.00 |
| 1 | 96-A | 20 | MET | CG-SD-CE | -5.91 | 90.75 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 42-A | 12 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | 81-A | 87 | ASP | CB-CG-OD1 | 5.90 | 123.61 | 118.30 |
| 1 | 67-A | 98 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | 73-A | 16 | MET | CB-CG-SD | -5.90 | 94.71 | 112.40 |
| 1 | 94-A | 44 | ARG | CG-CD-NE | 5.90 | 124.18 | 111.80 |
| 1 | 7-A | 87 | ASP | N-CA-CB | 5.89 | 121.21 | 110.60 |
| 1 | 93-A | 20 | MET | CA-CB-CG | 5.89 | 123.31 | 113.30 |
| 1 | 55-A | 20 | MET | CB-CG-SD | -5.88 | 94.76 | 112.40 |
| 1 | 1-A | 98 | ARG | CG-CD-NE | 5.88 | 124.15 | 111.80 |
| 1 | 125-A | 19 | ALA | N-CA-C | 5.88 | 126.87 | 111.00 |
| 1 | 38-A | 44 | ARG | NE-CZ-NH1 | 5.87 | 123.24 | 120.30 |
| 1 | 45-A | 119 | VAL | CB-CA-C | 5.87 | 122.56 | 111.40 |
| 1 | 54-A | 20 | MET | CA-CB-CG | 5.87 | 123.28 | 113.30 |
| 1 | 122-A | 33 | ARG | NE-CZ-NH2 | -5.87 | 117.36 | 120.30 |
| 1 | 51-A | 154 | GLU | N-CA-CB | 5.87 | 121.16 | 110.60 |
| 1 | 103-A | 127 | ASP | CB-CA-C | -5.87 | 98.67 | 110.40 |
| 1 | 9-A | 8 | LEU | CB-CA-C | -5.86 | 99.06 | 110.20 |
| 1 | 51-A | 154 | GLU | OE1-CD-OE2 | 5.86 | 130.33 | 123.30 |
| 1 | 73-A | 79 | ASP | CB-CG-OD2 | 5.86 | 123.57 | 118.30 |
| 1 | 11-A | 12 | ARG | CD-NE-CZ | 5.86 | 131.80 | 123.60 |
| 1 | 9-A | 98 | ARG | NE-CZ-NH1 | -5.85 | 117.37 | 120.30 |
| 1 | 86-A | 127 | ASP | N-CA-C | 5.85 | 126.80 | 111.00 |
| 1 | 11-A | 158 | ARG | CG-CD-NE | 5.85 | 124.09 | 111.80 |
| 1 | 53-A | 20 | MET | C-N-CD | 5.85 | 140.68 | 128.40 |
| 1 | 29-A | 20 | MET | C-N-CD | 5.85 | 140.68 | 128.40 |
| 1 | 46-A | 54 | LEU | CB-CG-CD2 | 5.84 | 120.94 | 111.00 |
| 1 | 21-A | 4 | LEU | CA-CB-CG | 5.84 | 128.74 | 115.30 |
| 1 | 67-A | 20 | MET | N-CA-C | -5.84 | 95.24 | 111.00 |
| 1 | 98-A | 20 | MET | N-CA-C | 5.84 | 126.76 | 111.00 |
| 1 | 66-A | 130 | PRO | N-CA-C | 5.83 | 127.27 | 112.10 |
| 1 | 34-A | 128 | TYR | N-CA-C | 5.83 | 126.75 | 111.00 |
| 1 | 97-A | 159 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 1 | 98-A | 98 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 1 | 6-A | 24 | LEU | CB-CG-CD2 | -5.83 | 101.09 | 111.00 |
| 1 | 88-A | 44 | ARG | CG-CD-NE | 5.83 | 124.05 | 111.80 |
| 1 | 82-A | 33 | ARG | CG-CD-NE | 5.83 | 124.04 | 111.80 |
| 1 | 59-A | 16 | MET | N-CA-CB | -5.83 | 100.11 | 110.60 |
| 1 | 118-A | 98 | ARG | NE-CZ-NH2 | -5.83 | 117.39 | 120.30 |
| 1 | 33-A | 98 | ARG | NE-CZ-NH1 | -5.82 | 117.39 | 120.30 |
| 1 | 68-A | 129 | GLU | OE1-CD-OE2 | -5.82 | 116.31 | 123.30 |
| 1 | 70-A | 98 | ARG | CB-CG-CD | 5.82 | 126.74 | 111.60 |
| 1 | 23-A | 33 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 55-A | 129 | GLU | N-CA-C | -5.82 | 95.28 | 111.00 |
| 1 | 70-A | 98 | ARG | CD-NE-CZ | 5.82 | 131.75 | 123.60 |
| 1 | 97-A | 24 | LEU | CB-CA-C | -5.82 | 99.14 | 110.20 |
| 1 | 11-A | 104 | LEU | CB-CG-CD1 | 5.81 | 120.88 | 111.00 |
| 1 | 32-A | 157 | GLU | CA-CB-CG | -5.80 | 100.63 | 113.40 |
| 1 | 84-A | 142 | ASP | CB-CG-OD2 | 5.80 | 123.52 | 118.30 |
| 1 | 19-A | 36 | LEU | CA-CB-CG | 5.80 | 128.64 | 115.30 |
| 1 | 40-A | 138 | SER | N-CA-CB | 5.80 | 119.20 | 110.50 |
| 1 | 123-A | 24 | LEU | CB-CG-CD1 | 5.80 | 120.86 | 111.00 |
| 1 | 25-A | 104 | LEU | CB-CG-CD1 | 5.80 | 120.86 | 111.00 |
| 1 | 15-A | 58 | LYS | CD-CE-NZ | 5.80 | 125.03 | 111.70 |
| 1 | 22-A | 12 | ARG | CG-CD-NE | 5.80 | 123.97 | 111.80 |
| 1 | 20-A | 127 | ASP | N-CA-C | 5.79 | 126.65 | 111.00 |
| 1 | 80-A | 129 | GLU | N-CA-C | -5.79 | 95.36 | 111.00 |
| 1 | 7-A | 23 | ASN | N-CA-CB | -5.79 | 100.18 | 110.60 |
| 1 | 90-A | 108 | GLN | N-CA-CB | -5.79 | 100.18 | 110.60 |
| 1 | 93-A | 44 | ARG | NE-CZ-NH1 | 5.79 | 123.19 | 120.30 |
| 1 | 29-A | 12 | ARG | CB-CG-CD | 5.79 | 126.65 | 111.60 |
| 1 | 45-A | 20 | MET | CA-CB-CG | 5.79 | 123.14 | 113.30 |
| 1 | 74-A | 128 | TYR | CB-CA-C | -5.79 | 98.83 | 110.40 |
| 1 | 80-A | 98 | ARG | CD-NE-CZ | 5.79 | 131.70 | 123.60 |
| 1 | 92-A | 12 | ARG | CG-CD-NE | -5.79 | 99.65 | 111.80 |
| 1 | 13-A | 128 | TYR | N-CA-C | -5.78 | 95.39 | 111.00 |
| 1 | 112-A | 20 | MET | CG-SD-CE | -5.78 | 90.95 | 100.20 |
| 1 | 3-A | 4 | LEU | CB-CG-CD2 | 5.78 | 120.83 | 111.00 |
| 1 | 103-A | 21 | PRO | CA-N-CD | -5.78 | 103.41 | 111.50 |
| 1 | 114-A | 44 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 1 | 121-A | 142 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | 117-A | 30 | TRP | CA-CB-CG | 5.78 | 124.68 | 113.70 |
| 1 | 44-A | 44 | ARG | NE-CZ-NH1 | -5.78 | 117.41 | 120.30 |
| 1 | 52-A | 12 | ARG | NE-CZ-NH2 | 5.77 | 123.19 | 120.30 |
| 1 | 75-A | 28 | LEU | CA-CB-CG | -5.77 | 102.02 | 115.30 |
| 1 | 115-A | 20 | MET | N-CA-CB | 5.77 | 120.99 | 110.60 |
| 1 | 90-A | 79 | ASP | CB-CA-C | 5.77 | 121.95 | 110.40 |
| 1 | 95-A | 92 | MET | CG-SD-CE | 5.77 | 109.43 | 100.20 |
| 1 | 85-A | 130 | PRO | O-C-N | 5.76 | 131.92 | 122.70 |
| 1 | 1-A | 140 | PHE | CB-CG-CD1 | 5.76 | 124.83 | 120.80 |
| 1 | 7-A | 132 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | 111-A | 159 | ARG | CG-CD-NE | 5.76 | 123.89 | 111.80 |
| 1 | 21-A | 132 | ASP | CB-CG-OD1 | 5.76 | 123.48 | 118.30 |
| 1 | 41-A | 21 | PRO | N-CA-C | 5.76 | 127.06 | 112.10 |
| 1 | 59-A | 102 | GLN | CA-CB-CG | 5.76 | 126.06 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 87-A | 20 | MET | CA-CB-CG | 5.76 | 123.09 | 113.30 |
| 1 | 124-A | 52 | ARG | NE-CZ-NH1 | -5.76 | 117.42 | 120.30 |
| 1 | 56-A | 108 | GLN | N-CA-CB | -5.75 | 100.25 | 110.60 |
| 1 | 61-A | 11 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | 90-A | 21 | PRO | CA-C-O | -5.75 | 106.40 | 120.20 |
| 1 | 39-A | 16 | MET | N-CA-CB | 5.75 | 120.94 | 110.60 |
| 1 | 47-A | 127 | ASP | CB-CG-OD2 | 5.75 | 123.47 | 118.30 |
| 1 | 76-A | 16 | MET | CG-SD-CE | 5.75 | 109.39 | 100.20 |
| 1 | 11-A | 154 | GLU | OE1-CD-OE2 | 5.74 | 130.19 | 123.30 |
| 1 | 78-A | 157 | GLU | CA-CB-CG | 5.74 | 126.03 | 113.40 |
| 1 | 117-A | 20 | MET | CA-CB-CG | -5.74 | 103.54 | 113.30 |
| 1 | 70-A | 65 | GLN | CB-CA-C | 5.74 | 121.88 | 110.40 |
| 1 | 122-A | 52 | ARG | NE-CZ-NH2 | 5.74 | 123.17 | 120.30 |
| 1 | 99-A | 58 | LYS | CD-CE-NZ | 5.73 | 124.89 | 111.70 |
| 1 | 16-A | 156 | LEU | CB-CG-CD1 | -5.73 | 101.25 | 111.00 |
| 1 | 117-A | 20 | MET | C-N-CD | 5.73 | 140.44 | 128.40 |
| 1 | 4-A | 119 | VAL | CB-CA-C | -5.73 | 100.51 | 111.40 |
| 1 | 42-A | 20 | MET | C-N-CA | 5.73 | 146.07 | 122.00 |
| 1 | 57-A | 16 | MET | CG-SD-CE | -5.73 | 91.03 | 100.20 |
| 1 | 113-A | 127 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | 38-A | 16 | MET | CB-CG-SD | 5.73 | 129.58 | 112.40 |
| 1 | 86-A | 79 | ASP | CB-CG-OD2 | 5.73 | 123.45 | 118.30 |
| 1 | 124-A | 98 | ARG | CG-CD-NE | 5.73 | 123.83 | 111.80 |
| 1 | 124-A | 158 | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 1 | 49-A | 104 | LEU | CB-CG-CD1 | -5.72 | 101.27 | 111.00 |
| 1 | 20-A | 128 | TYR | CB-CG-CD2 | -5.72 | 117.57 | 121.00 |
| 1 | 28-A | 1 | MET | CB-CA-C | 5.72 | 121.84 | 110.40 |
| 1 | 33-A | 127 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | 45-A | 33 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | 28-A | 101 | GLU | CA-CB-CG | 5.71 | 125.95 | 113.40 |
| 1 | 46-A | 20 | MET | CG-SD-CE | 5.71 | 109.33 | 100.20 |
| 1 | 92-A | 32 | LYS | CA-CB-CG | 5.71 | 125.95 | 113.40 |
| 1 | 74-A | 127 | ASP | N-CA-C | 5.70 | 126.40 | 111.00 |
| 1 | 76-A | 22 | TRP | CB-CG-CD1 | -5.70 | 119.59 | 127.00 |
| 1 | 58-A | 128 | TYR | N-CA-C | 5.70 | 126.39 | 111.00 |
| 1 | 48-A | 129 | GLU | N-CA-CB | -5.70 | 100.35 | 110.60 |
| 1 | 17-A | 87 | ASP | CB-CG-OD2 | 5.69 | 123.42 | 118.30 |
| 1 | 124-A | 21 | PRO | CA-CB-CG | -5.69 | 93.18 | 104.00 |
| 1 | 121-A | 158 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 1 | 54-A | 11 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | 109-A | 2 | ILE | N-CA-C | -5.69 | 95.64 | 111.00 |
| 1 | 5-A | 111 | TYR | N-CA-C | 5.68 | 126.34 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 38-A | 98 | ARG | NE-CZ-NH1 | -5.68 | 117.46 | 120.30 |
| 1 | 125-A | 127 | ASP | CB-CG-OD1 | 5.68 | 123.41 | 118.30 |
| 1 | 4-A | 154 | GLU | CG-CD-OE2 | 5.68 | 129.66 | 118.30 |
| 1 | 11-A | 128 | TYR | CB-CG-CD2 | 5.68 | 124.41 | 121.00 |
| 1 | 45-A | 129 | GLU | N-CA-C | 5.68 | 126.33 | 111.00 |
| 1 | 49-A | 104 | LEU | CB-CG-CD2 | 5.68 | 120.65 | 111.00 |
| 1 | 58-A | 128 | TYR | CB-CG-CD1 | 5.68 | 124.41 | 121.00 |
| 1 | 106-A | 20 | MET | C-N-CD | -5.68 | 108.11 | 120.60 |
| 1 | 94-A | 19 | ALA | N-CA-C | 5.67 | 126.32 | 111.00 |
| 1 | 94-A | 20 | MET | CA-CB-CG | 5.67 | 122.95 | 113.30 |
| 1 | 8-A | 22 | TRP | CB-CA-C | 5.67 | 121.74 | 110.40 |
| 1 | 18-A | 52 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 |
| 1 | 73-A | 127 | ASP | CB-CG-OD1 | 5.67 | 123.40 | 118.30 |
| 1 | 105-A | 127 | ASP | CB-CG-OD1 | -5.67 | 113.20 | 118.30 |
| 1 | 26-A | 20 | MET | N-CA-CB | -5.67 | 100.40 | 110.60 |
| 1 | 103-A | 66 | PRO | N-CA-C | 5.67 | 126.84 | 112.10 |
| 1 | 34-A | 128 | TYR | CA-CB-CG | 5.66 | 124.15 | 113.40 |
| 1 | 100-A | 159 | ARG | NE-CZ-NH1 | 5.66 | 123.13 | 120.30 |
| 1 | 108-A | 129 | GLU | CB-CA-C | -5.65 | 99.10 | 110.40 |
| 1 | 110-A | 156 | LEU | CB-CG-CD2 | 5.65 | 120.61 | 111.00 |
| 1 | 61-A | 61 | ILE | CG1-CB-CG2 | -5.65 | 98.97 | 111.40 |
| 1 | 10-A | 87 | ASP | CB-CA-C | 5.64 | 121.69 | 110.40 |
| 1 | 120-A | 16 | MET | CA-CB-CG | 5.64 | 122.89 | 113.30 |
| 1 | 117-A | 12 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 1 | 63-A | 44 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | 84-A | 108 | GLN | CA-CB-CG | 5.63 | 125.79 | 113.40 |
| 1 | 42-A | 20 | MET | N-CA-C | 5.63 | 126.20 | 111.00 |
| 1 | 44-A | 33 | ARG | NE-CZ-NH1 | -5.63 | 117.48 | 120.30 |
| 1 | 24-A | 126 | PRO | CA-C-O | -5.63 | 106.69 | 120.20 |
| 1 | 32-A | 159 | ARG | NE-CZ-NH2 | -5.63 | 117.49 | 120.30 |
| 1 | 106-A | 4 | LEU | CB-CG-CD2 | 5.63 | 120.56 | 111.00 |
| 1 | 92-A | 88 | VAL | CA-CB-CG2 | 5.62 | 119.34 | 110.90 |
| 1 | 102-A | 52 | ARG | NE-CZ-NH2 | 5.62 | 123.11 | 120.30 |
| 1 | 10-A | 154 | GLU | CG-CD-OE2 | -5.62 | 107.06 | 118.30 |
| 1 | 35-A | 88 | VAL | C-N-CD | 5.62 | 140.21 | 128.40 |
| 1 | 36-A | 121 | GLY | N-CA-C | 5.62 | 127.15 | 113.10 |
| 1 | 101-A | 126 | PRO | CA-C-N | -5.62 | 104.83 | 117.20 |
| 1 | 103-A | 20 | MET | CB-CG-SD | -5.62 | 95.53 | 112.40 |
| 1 | 32-A | 98 | ARG | CG-CD-NE | 5.62 | 123.60 | 111.80 |
| 1 | 55-A | 127 | ASP | N-CA-CB | -5.62 | 100.49 | 110.60 |
| 1 | 114-A | 44 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 1 | 8-A | 12 | ARG | NE-CZ-NH1 | 5.62 | 123.11 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 111-A | 87 | ASP | CB-CG-OD2 | 5.62 | 123.36 | 118.30 |
| 1 | 50-A | 127 | ASP | N-CA-C | 5.62 | 126.16 | 111.00 |
| 1 | 29-A | 36 | LEU | CA-CB-CG | 5.61 | 128.21 | 115.30 |
| 1 | 33-A | 127 | ASP | N-CA-CB | -5.61 | 100.50 | 110.60 |
| 1 | 94-A | 28 | LEU | CB-CA-C | 5.61 | 120.87 | 110.20 |
| 1 | 118-A | 128 | TYR | CA-CB-CG | 5.61 | 124.07 | 113.40 |
| 1 | 4-A | 62 | LEU | CB-CG-CD2 | 5.61 | 120.54 | 111.00 |
| 1 | 72-A | 22 | TRP | CA-CB-CG | -5.61 | 103.04 | 113.70 |
| 1 | 111-A | 20 | MET | C-N-CD | 5.61 | 140.18 | 128.40 |
| 1 | 8-A | 154 | GLU | CG-CD-OE1 | 5.61 | 129.51 | 118.30 |
| 1 | 28-A | 127 | ASP | CB-CG-OD2 | 5.61 | 123.35 | 118.30 |
| 1 | 29-A | 154 | GLU | CB-CG-CD | 5.61 | 129.34 | 114.20 |
| 1 | 17-A | 98 | ARG | NE-CZ-NH2 | -5.60 | 117.50 | 120.30 |
| 1 | 79-A | 127 | ASP | N-CA-C | 5.60 | 126.13 | 111.00 |
| 1 | 92-A | 24 | LEU | CB-CG-CD2 | 5.60 | 120.52 | 111.00 |
| 1 | 86-A | 20 | MET | CA-CB-CG | 5.59 | 122.81 | 113.30 |
| 1 | 46-A | 12 | ARG | NE-CZ-NH2 | -5.59 | 117.50 | 120.30 |
| 1 | 6-A | 104 | LEU | CB-CG-CD1 | 5.59 | 120.50 | 111.00 |
| 1 | 6-A | 44 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | 93-A | 154 | GLU | OE1-CD-OE2 | 5.59 | 130.01 | 123.30 |
| 1 | 31-A | 127 | ASP | CA-C-O | 5.59 | 131.84 | 120.10 |
| 1 | 84-A | 127 | ASP | CB-CA-C | -5.59 | 99.23 | 110.40 |
| 1 | 57-A | 120 | GLU | CB-CG-CD | 5.58 | 129.27 | 114.20 |
| 1 | 114-A | 119 | VAL | N-CA-C | -5.58 | 95.92 | 111.00 |
| 1 | 36-A | 128 | TYR | CB-CG-CD1 | 5.58 | 124.35 | 121.00 |
| 1 | 108-A | 129 | GLU | N-CA-C | 5.58 | 126.06 | 111.00 |
| 1 | 33-A | 16 | MET | CG-SD-CE | 5.58 | 109.12 | 100.20 |
| 1 | 53-A | 1 | MET | CG-SD-CE | 5.57 | 109.12 | 100.20 |
| 1 | 57-A | 127 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 1 | 37-A | 128 | TYR | CB-CA-C | 5.57 | 121.53 | 110.40 |
| 1 | 53-A | 129 | GLU | N-CA-C | -5.57 | 95.97 | 111.00 |
| 1 | 84-A | 28 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 1 | 108-A | 8 | LEU | CB-CG-CD1 | 5.57 | 120.46 | 111.00 |
| 1 | 62-A | 126 | PRO | CA-C-O | -5.57 | 106.84 | 120.20 |
| 1 | 89-A | 158 | ARG | NE-CZ-NH2 | -5.57 | 117.52 | 120.30 |
| 1 | 34-A | 127 | ASP | CB-CG-OD1 | 5.56 | 123.31 | 118.30 |
| 1 | 64-A | 62 | LEU | CB-CG-CD2 | 5.56 | 120.46 | 111.00 |
| 1 | 116-A | 4 | LEU | CA-CB-CG | 5.56 | 128.09 | 115.30 |
| 1 | 19-A | 127 | ASP | N-CA-C | 5.56 | 126.01 | 111.00 |
| 1 | 17-A | 22 | TRP | CB-CA-C | -5.56 | 99.29 | 110.40 |
| 1 | 38-A | 52 | ARG | NE-CZ-NH1 | -5.56 | 117.52 | 120.30 |
| 1 | 84-A | 116 | ASP | CB-CG-OD2 | 5.55 | 123.30 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 90-A | 20 | MET | CB-CG-SD | 5.55 | 129.06 | 112.40 |
| 1 | 100-A | 44 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | 123-A | 20 | MET | CG-SD-CE | 5.55 | 109.08 | 100.20 |
| 1 | 48-A | 12 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | 26-A | 20 | MET | CB-CG-SD | -5.55 | 95.76 | 112.40 |
| 1 | 67-A | 127 | ASP | CB-CA-C | 5.55 | 121.49 | 110.40 |
| 1 | 104-A | 21 | PRO | N-CA-C | 5.55 | 126.52 | 112.10 |
| 1 | 110-A | 23 | ASN | N-CA-C | 5.54 | 125.97 | 111.00 |
| 1 | 57-A | 102 | GLN | CA-CB-CG | 5.54 | 125.59 | 113.40 |
| 1 | 83-A | 44 | ARG | CG-CD-NE | 5.54 | 123.44 | 111.80 |
| 1 | 101-A | 22 | TRP | CA-CB-CG | -5.54 | 103.18 | 113.70 |
| 1 | 100-A | 128 | TYR | CA-CB-CG | 5.54 | 123.92 | 113.40 |
| 1 | 63-A | 16 | MET | N-CA-CB | -5.53 | 100.64 | 110.60 |
| 1 | 12-A | 98 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 1 | 87-A | 42 | MET | CG-SD-CE | -5.53 | 91.36 | 100.20 |
| 1 | 122-A | 17 | GLU | N-CA-C | -5.53 | 96.08 | 111.00 |
| 1 | 13-A | 128 | TYR | N-CA-CB | 5.52 | 120.54 | 110.60 |
| 1 | 17-A | 98 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | 2-A | 1 | MET | CG-SD-CE | -5.52 | 91.38 | 100.20 |
| 1 | 6-A | 127 | ASP | N-CA-CB | -5.51 | 100.67 | 110.60 |
| 1 | 101-A | 20 | MET | CB-CG-SD | 5.51 | 128.94 | 112.40 |
| 1 | 117-A | 104 | LEU | CB-CG-CD2 | 5.51 | 120.37 | 111.00 |
| 1 | 6-A | 20 | MET | CG-SD-CE | -5.51 | 91.38 | 100.20 |
| 1 | 10-A | 98 | ARG | CG-CD-NE | 5.51 | 123.37 | 111.80 |
| 1 | 81-A | 22 | TRP | CA-CB-CG | 5.51 | 124.17 | 113.70 |
| 1 | 77-A | 20 | MET | CG-SD-CE | -5.50 | 91.39 | 100.20 |
| 1 | 123-A | 30 | TRP | CB-CG-CD2 | 5.50 | 133.76 | 126.60 |
| 1 | 35-A | 116 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | 78-A | 1 | MET | C-N-CA | 5.50 | 135.45 | 121.70 |
| 1 | 102-A | 20 | MET | C-N-CD | -5.49 | 108.51 | 120.60 |
| 1 | 34-A | 16 | MET | CB-CG-SD | 5.49 | 128.87 | 112.40 |
| 1 | 124-A | 1 | MET | CB-CG-SD | -5.49 | 95.93 | 112.40 |
| 1 | 12-A | 23 | ASN | O-C-N | 5.49 | 131.48 | 122.70 |
| 1 | 80-A | 1 | MET | C-N-CA | 5.48 | 135.41 | 121.70 |
| 1 | 58-A | 20 | MET | N-CA-C | -5.48 | 96.20 | 111.00 |
| 1 | 81-A | 24 | LEU | CA-CB-CG | 5.48 | 127.90 | 115.30 |
| 1 | 70-A | 159 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 1 | 41-A | 12 | ARG | CG-CD-NE | 5.47 | 123.30 | 111.80 |
| 1 | 79-A | 79 | ASP | CB-CA-C | 5.47 | 121.34 | 110.40 |
| 1 | 93-A | 116 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | 107-A | 154 | GLU | CG-CD-OE2 | 5.47 | 129.24 | 118.30 |
| 1 | 112-A | 10 | VAL | CB-CA-C | -5.46 | 101.02 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 10-A | 154 | GLU | CB-CG-CD | -5.46 | 99.45 | 114.20 |
| 1 | 66-A | 12 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | 92-A | 32 | LYS | CB-CG-CD | 5.46 | 125.80 | 111.60 |
| 1 | 4-A | 131 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | 52-A | 4 | LEU | CB-CG-CD2 | -5.46 | 101.72 | 111.00 |
| 1 | 54-A | 159 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | 64-A | 28 | LEU | CB-CA-C | 5.46 | 120.57 | 110.20 |
| 1 | 113-A | 20 | MET | CA-CB-CG | 5.46 | 122.58 | 113.30 |
| 1 | 84-A | 130 | PRO | CA-C-O | -5.46 | 107.11 | 120.20 |
| 1 | 48-A | 22 | TRP | N-CA-C | 5.45 | 125.72 | 111.00 |
| 1 | 48-A | 12 | ARG | NE-CZ-NH2 | -5.45 | 117.57 | 120.30 |
| 1 | 50-A | 52 | ARG | NE-CZ-NH2 | 5.45 | 123.03 | 120.30 |
| 1 | 70-A | 36 | LEU | CA-CB-CG | 5.45 | 127.84 | 115.30 |
| 1 | 87-A | 20 | MET | N-CA-CB | 5.45 | 120.41 | 110.60 |
| 1 | 55-A | 159 | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 1 | 115-A | 24 | LEU | C-N-CD | 5.45 | 139.84 | 128.40 |
| 1 | 41-A | 48 | GLU | CA-CB-CG | 5.45 | 125.38 | 113.40 |
| 1 | 98-A | 1 | MET | CA-CB-CG | 5.45 | 122.56 | 113.30 |
| 1 | 116-A | 131 | ASP | CB-CG-OD1 | 5.45 | 123.20 | 118.30 |
| 1 | 19-A | 12 | ARG | CG-CD-NE | 5.44 | 123.23 | 111.80 |
| 1 | 54-A | 23 | ASN | N-CA-C | 5.44 | 125.70 | 111.00 |
| 1 | 18-A | 22 | TRP | CB-CA-C | -5.44 | 99.52 | 110.40 |
| 1 | 19-A | 129 | GLU | N-CA-C | 5.43 | 125.67 | 111.00 |
| 1 | 32-A | 156 | LEU | CB-CG-CD1 | 5.43 | 120.24 | 111.00 |
| 1 | 110-A | 11 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | 125-A | 127 | ASP | CB-CG-OD2 | -5.43 | 113.41 | 118.30 |
| 1 | 26-A | 144 | ASP | CB-CA-C | -5.43 | 99.54 | 110.40 |
| 1 | 41-A | 23 | ASN | CB-CA-C | 5.43 | 121.26 | 110.40 |
| 1 | 98-A | 98 | ARG | CG-CD-NE | -5.43 | 100.39 | 111.80 |
| 1 | 9-A | 158 | ARG | NE-CZ-NH2 | -5.43 | 117.59 | 120.30 |
| 1 | 90-A | 44 | ARG | CG-CD-NE | 5.43 | 123.19 | 111.80 |
| 1 | 29-A | 156 | LEU | CA-CB-CG | 5.42 | 127.78 | 115.30 |
| 1 | 55-A | 16 | MET | CG-SD-CE | -5.42 | 91.52 | 100.20 |
| 1 | 44-A | 44 | ARG | NE-CZ-NH2 | 5.42 | 123.01 | 120.30 |
| 1 | 50-A | 44 | ARG | NE-CZ-NH1 | -5.42 | 117.59 | 120.30 |
| 1 | 34-A | 127 | ASP | N-CA-C | 5.42 | 125.63 | 111.00 |
| 1 | 81-A | 54 | LEU | CB-CG-CD1 | -5.42 | 101.79 | 111.00 |
| 1 | 35-A | 154 | GLU | CA-CB-CG | 5.41 | 125.31 | 113.40 |
| 1 | 43-A | 52 | ARG | NE-CZ-NH2 | 5.41 | 123.01 | 120.30 |
| 1 | 90-A | 44 | ARG | CB-CG-CD | 5.41 | 125.67 | 111.60 |
| 1 | 35-A | 16 | MET | CB-CG-SD | 5.41 | 128.63 | 112.40 |
| 1 | 57-A | 70 | ASP | CB-CG-OD1 | -5.41 | 113.43 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 118-A | 150 | SER | CA-CB-OG | -5.41 | 96.59 | 111.20 |
| 1 | 99-A | 128 | TYR | CA-CB-CG | 5.41 | 123.67 | 113.40 |
| 1 | 101-A | 126 | PRO | C-N-CA | 5.41 | 135.22 | 121.70 |
| 1 | 3-A | 112 | LEU | CA-CB-CG | 5.41 | 127.73 | 115.30 |
| 1 | 51-A | 70 | ASP | CB-CG-OD1 | -5.41 | 113.44 | 118.30 |
| 1 | 72-A | 120 | GLU | N-CA-C | 5.41 | 125.59 | 111.00 |
| 1 | 69-A | 98 | ARG | NE-CZ-NH1 | -5.40 | 117.60 | 120.30 |
| 1 | 114-A | 58 | LYS | CD-CE-NZ | 5.40 | 124.13 | 111.70 |
| 1 | 5-A | 36 | LEU | CB-CG-CD2 | 5.40 | 120.18 | 111.00 |
| 1 | 55-A | 54 | LEU | CB-CG-CD2 | -5.40 | 101.82 | 111.00 |
| 1 | 96-A | 23 | ASN | N-CA-C | 5.40 | 125.57 | 111.00 |
| 1 | 53-A | 127 | ASP | CB-CG-OD2 | 5.39 | 123.16 | 118.30 |
| 1 | 85-A | 44 | ARG | NE-CZ-NH2 | 5.39 | 123.00 | 120.30 |
| 1 | 102-A | 33 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 1 | 17-A | 16 | MET | CB-CG-SD | -5.39 | 96.23 | 112.40 |
| 1 | 88-A | 4 | LEU | CB-CG-CD1 | -5.39 | 101.84 | 111.00 |
| 1 | 15-A | 127 | ASP | N-CA-C | 5.39 | 125.55 | 111.00 |
| 1 | 43-A | 22 | TRP | CB-CG-CD2 | -5.39 | 119.60 | 126.60 |
| 1 | 64-A | 23 | ASN | N-CA-CB | 5.39 | 120.30 | 110.60 |
| 1 | 78-A | 158 | ARG | NE-CZ-NH1 | -5.39 | 117.61 | 120.30 |
| 1 | 105-A | 21 | PRO | CA-C-N | 5.38 | 129.04 | 117.20 |
| 1 | 104-A | 20 | MET | CA-CB-CG | 5.38 | 122.44 | 113.30 |
| 1 | 77-A | 22 | TRP | N-CA-C | 5.38 | 125.52 | 111.00 |
| 1 | 102-A | 21 | PRO | CA-N-CD | -5.38 | 103.97 | 111.50 |
| 1 | 108-A | 44 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | 11-A | 154 | GLU | CB-CG-CD | -5.38 | 99.68 | 114.20 |
| 1 | 38-A | 21 | PRO | N-CA-C | 5.38 | 126.08 | 112.10 |
| 1 | 40-A | 128 | TYR | CB-CG-CD2 | -5.38 | 117.77 | 121.00 |
| 1 | 67-A | 159 | ARG | N-CA-CB | -5.37 | 100.93 | 110.60 |
| 1 | 82-A | 127 | ASP | CB-CA-C | -5.37 | 99.65 | 110.40 |
| 1 | 120-A | 23 | ASN | N-CA-C | 5.37 | 125.51 | 111.00 |
| 1 | 4-A | 33 | ARG | NE-CZ-NH2 | -5.37 | 117.61 | 120.30 |
| 1 | 58-A | 132 | ASP | CB-CG-OD2 | -5.37 | 113.47 | 118.30 |
| 1 | 36-A | 129 | GLU | N-CA-CB | 5.37 | 120.27 | 110.60 |
| 1 | 23-A | 20 | MET | CG-SD-CE | 5.37 | 108.79 | 100.20 |
| 1 | 35-A | 128 | TYR | CA-CB-CG | 5.37 | 123.60 | 113.40 |
| 1 | 22-A | 98 | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 1 | 43-A | 127 | ASP | CB-CG-OD1 | -5.37 | 113.47 | 118.30 |
| 1 | 93-A | 104 | LEU | CB-CG-CD1 | -5.37 | 101.88 | 111.00 |
| 1 | 41-A | 158 | ARG | NE-CZ-NH1 | -5.36 | 117.62 | 120.30 |
| 1 | 60-A | 127 | ASP | N-CA-CB | -5.36 | 100.95 | 110.60 |
| 1 | 66-A | 127 | ASP | CB-CG-OD1 | -5.36 | 113.47 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 78-A | 129 | GLU | C-N-CD | 5.36 | 139.66 | 128.40 |
| 1 | 83-A | 20 | MET | N-CA-C | -5.36 | 96.53 | 111.00 |
| 1 | 11-A | 54 | LEU | CB-CG-CD1 | -5.36 | 101.89 | 111.00 |
| 1 | 35-A | 112 | LEU | CB-CG-CD1 | 5.36 | 120.11 | 111.00 |
| 1 | 2-A | 4 | LEU | CA-CB-CG | 5.36 | 127.62 | 115.30 |
| 1 | 45-A | 87 | ASP | CB-CA-C | 5.35 | 121.10 | 110.40 |
| 1 | 107-A | 87 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 1 | 53-A | 52 | ARG | NE-CZ-NH1 | -5.35 | 117.63 | 120.30 |
| 1 | 24-A | 127 | ASP | CB-CG-OD2 | -5.34 | 113.49 | 118.30 |
| 1 | 120-A | 42 | MET | CG-SD-CE | -5.34 | 91.66 | 100.20 |
| 1 | 71-A | 36 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 1 | 81-A | 130 | PRO | N-CA-C | 5.34 | 125.98 | 112.10 |
| 1 | 121-A | 20 | MET | N-CA-CB | 5.34 | 120.20 | 110.60 |
| 1 | 33-A | 20 | MET | CB-CG-SD | 5.33 | 128.41 | 112.40 |
| 1 | 35-A | 112 | LEU | CB-CG-CD2 | -5.33 | 101.93 | 111.00 |
| 1 | 75-A | 128 | TYR | N-CA-C | 5.33 | 125.40 | 111.00 |
| 1 | 69-A | 127 | ASP | CA-C-N | -5.33 | 105.47 | 117.20 |
| 1 | 89-A | 22 | TRP | CA-CB-CG | -5.33 | 103.57 | 113.70 |
| 1 | 68-A | 17 | GLU | OE1-CD-OE2 | -5.33 | 116.90 | 123.30 |
| 1 | 70-A | 36 | LEU | CB-CG-CD1 | 5.33 | 120.06 | 111.00 |
| 1 | 95-A | 20 | MET | CB-CG-SD | -5.33 | 96.41 | 112.40 |
| 1 | 108-A | 1 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 1 | 61-A | 42 | MET | CG-SD-CE | -5.33 | 91.68 | 100.20 |
| 1 | 18-A | 20 | MET | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | 41-A | 127 | ASP | O-C-N | 5.32 | 131.22 | 122.70 |
| 1 | 68-A | 67 | GLY | N-CA-C | 5.32 | 126.41 | 113.10 |
| 1 | 110-A | 30 | TRP | CB-CG-CD1 | 5.32 | 133.92 | 127.00 |
| 1 | 116-A | 158 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | 31-A | 127 | ASP | N-CA-C | 5.32 | 125.36 | 111.00 |
| 1 | 92-A | 70 | ASP | CB-CA-C | 5.32 | 121.04 | 110.40 |
| 1 | 17-A | 158 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 1 | 125-A | 20 | MET | N-CA-C | 5.32 | 125.35 | 111.00 |
| 1 | 29-A | 144 | ASP | N-CA-CB | -5.31 | 101.04 | 110.60 |
| 1 | 48-A | 104 | LEU | CB-CG-CD2 | 5.31 | 120.03 | 111.00 |
| 1 | 51-A | 127 | ASP | N-CA-C | 5.31 | 125.34 | 111.00 |
| 1 | 112-A | 20 | MET | CA-CB-CG | 5.31 | 122.33 | 113.30 |
| 1 | 41-A | 128 | TYR | O-C-N | -5.31 | 114.21 | 122.70 |
| 1 | 51-A | 129 | GLU | N-CA-C | 5.31 | 125.33 | 111.00 |
| 1 | 34-A | 20 | MET | CA-CB-CG | -5.30 | 104.29 | 113.30 |
| 1 | 99-A | 158 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | 74-A | 142 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | 12-A | 158 | ARG | NE-CZ-NH2 | 5.29 | 122.95 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 63-A | 58 | LYS | CA-CB-CG | 5.29 | 125.05 | 113.40 |
| 1 | 77-A | 12 | ARG | NE-CZ-NH2 | -5.29 | 117.65 | 120.30 |
| 1 | 56-A | 127 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | 99-A | 127 | ASP | CB-CG-OD1 | -5.29 | 113.54 | 118.30 |
| 1 | 66-A | 16 | MET | CB-CA-C | -5.29 | 99.83 | 110.40 |
| 1 | 66-A | 130 | PRO | CA-C-O | -5.29 | 107.52 | 120.20 |
| 1 | 2-A | 127 | ASP | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | 64-A | 68 | THR | CB-CA-C | -5.28 | 97.34 | 111.60 |
| 1 | 90-A | 44 | ARG | NE-CZ-NH2 | 5.28 | 122.94 | 120.30 |
| 1 | 52-A | 61 | ILE | CG1-CB-CG2 | -5.28 | 99.79 | 111.40 |
| 1 | 72-A | 24 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 1 | 120-A | 22 | TRP | N-CA-C | 5.28 | 125.24 | 111.00 |
| 1 | 94-A | 33 | ARG | NE-CZ-NH2 | -5.27 | 117.66 | 120.30 |
| 1 | 115-A | 88 | VAL | N-CA-C | -5.27 | 96.76 | 111.00 |
| 1 | 6-A | 86 | GLY | N-CA-C | 5.27 | 126.28 | 113.10 |
| 1 | 93-A | 52 | ARG | NE-CZ-NH1 | -5.27 | 117.66 | 120.30 |
| 1 | 32-A | 131 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |
| 1 | 60-A | 28 | LEU | CB-CG-CD2 | -5.27 | 102.04 | 111.00 |
| 1 | 21-A | 98 | ARG | CG-CD-NE | -5.27 | 100.74 | 111.80 |
| 1 | 125-A | 44 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 1 | 45-A | 85 | CYS | CB-CA-C | -5.26 | 99.87 | 110.40 |
| 1 | 121-A | 85 | CYS | CB-CA-C | -5.26 | 99.87 | 110.40 |
| 1 | 125-A | 22 | TRP | CA-CB-CG | 5.26 | 123.70 | 113.70 |
| 1 | 102-A | 33 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 1 | 83-A | 129 | GLU | C-N-CA | -5.26 | 99.91 | 122.00 |
| 1 | 72-A | 16 | MET | CB-CG-SD | -5.25 | 96.64 | 112.40 |
| 1 | 116-A | 136 | VAL | CG1-CB-CG2 | -5.25 | 102.49 | 110.90 |
| 1 | 51-A | 127 | ASP | CB-CG-OD1 | -5.25 | 113.57 | 118.30 |
| 1 | 10-A | 98 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | 22-A | 131 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |
| 1 | 43-A | 54 | LEU | CB-CG-CD1 | 5.25 | 119.92 | 111.00 |
| 1 | 122-A | 106 | LYS | CA-CB-CG | 5.25 | 124.94 | 113.40 |
| 1 | 34-A | 125 | PHE | CB-CG-CD2 | -5.24 | 117.13 | 120.80 |
| 1 | 78-A | 158 | ARG | NE-CZ-NH2 | 5.24 | 122.92 | 120.30 |
| 1 | 117-A | 42 | MET | CG-SD-CE | 5.24 | 108.59 | 100.20 |
| 1 | 55-A | 24 | LEU | C-N-CD | 5.24 | 139.40 | 128.40 |
| 1 | 81-A | 109 | LYS | CD-CE-NZ | 5.24 | 123.75 | 111.70 |
| 1 | 118-A | 24 | LEU | C-N-CD | 5.24 | 139.40 | 128.40 |
| 1 | 7-A | 127 | ASP | CB-CG-OD1 | 5.24 | 123.01 | 118.30 |
| 1 | 105-A | 22 | TRP | N-CA-CB | 5.24 | 120.02 | 110.60 |
| 1 | 62-A | 12 | ARG | CG-CD-NE | 5.23 | 122.78 | 111.80 |
| 1 | 33-A | 12 | ARG | NE-CZ-NH2 | -5.23 | 117.69 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 91-A | 11 | ASP | CB-CG-OD1 | -5.23 | 113.60 | 118.30 |
| 1 | 53-A | 12 | ARG | NE-CZ-NH1 | -5.22 | 117.69 | 120.30 |
| 1 | 3-A | 49 | SER | CB-CA-C | -5.22 | 100.18 | 110.10 |
| 1 | 13-A | 92 | MET | CG-SD-CE | -5.22 | 91.85 | 100.20 |
| 1 | 53-A | 12 | ARG | NE-CZ-NH2 | 5.22 | 122.91 | 120.30 |
| 1 | 64-A | 12 | ARG | NE-CZ-NH1 | -5.22 | 117.69 | 120.30 |
| 1 | 64-A | 87 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | 121-A | 23 | ASN | N-CA-C | 5.22 | 125.08 | 111.00 |
| 1 | 9-A | 84 | ALA | C-N-CA | -5.21 | 108.66 | 121.70 |
| 1 | 91-A | 129 | GLU | N-CA-C | -5.21 | 96.92 | 111.00 |
| 1 | 28-A | 104 | LEU | CB-CG-CD2 | -5.21 | 102.14 | 111.00 |
| 1 | 19-A | 79 | ASP | CB-CA-C | 5.21 | 120.82 | 110.40 |
| 1 | 62-A | 28 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 1 | 101-A | 108 | GLN | CA-CB-CG | 5.21 | 124.86 | 113.40 |
| 1 | 28-A | 12 | ARG | CB-CG-CD | 5.21 | 125.14 | 111.60 |
| 1 | 65-A | 20 | MET | CB-CG-SD | -5.21 | 96.78 | 112.40 |
| 1 | 107-A | 11 | ASP | CB-CG-OD1 | 5.21 | 122.98 | 118.30 |
| 1 | 102-A | 127 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | 102-A | 52 | ARG | NE-CZ-NH1 | -5.20 | 117.70 | 120.30 |
| 1 | 109-A | 1 | MET | N-CA-C | 5.20 | 125.04 | 111.00 |
| 1 | 6-A | 36 | LEU | CB-CG-CD2 | 5.20 | 119.84 | 111.00 |
| 1 | 15-A | 101 | GLU | CA-CB-CG | 5.20 | 124.84 | 113.40 |
| 1 | 27-A | 58 | LYS | CB-CG-CD | 5.20 | 125.11 | 111.60 |
| 1 | 44-A | 12 | ARG | NH1-CZ-NH2 | -5.20 | 113.68 | 119.40 |
| 1 | 121-A | 98 | ARG | CG-CD-NE | 5.20 | 122.72 | 111.80 |
| 1 | 77-A | 127 | ASP | CB-CA-C | -5.20 | 100.01 | 110.40 |
| 1 | 16-A | 79 | ASP | CB-CG-OD2 | -5.19 | 113.63 | 118.30 |
| 1 | 44-A | 11 | ASP | CB-CG-OD1 | 5.19 | 122.97 | 118.30 |
| 1 | 107-A | 132 | ASP | CB-CA-C | -5.19 | 100.02 | 110.40 |
| 1 | 18-A | 101 | GLU | CA-CB-CG | 5.19 | 124.82 | 113.40 |
| 1 | 18-A | 127 | ASP | CB-CA-C | -5.19 | 100.02 | 110.40 |
| 1 | 95-A | 98 | ARG | CG-CD-NE | 5.19 | 122.69 | 111.80 |
| 1 | 20-A | 92 | MET | CG-SD-CE | 5.19 | 108.50 | 100.20 |
| 1 | 63-A | 106 | LYS | CA-CB-CG | -5.19 | 101.99 | 113.40 |
| 1 | 84-A | 120 | GLU | C-N-CA | 5.19 | 133.19 | 122.30 |
| 1 | 29-A | 20 | MET | CG-SD-CE | 5.18 | 108.50 | 100.20 |
| 1 | 117-A | 30 | TRP | CB-CG-CD2 | 5.18 | 133.34 | 126.60 |
| 1 | 123-A | 127 | ASP | CB-CG-OD2 | 5.18 | 122.97 | 118.30 |
| 1 | 64-A | 24 | LEU | N-CA-C | -5.18 | 97.01 | 111.00 |
| 1 | 82-A | 20 | MET | CB-CG-SD | 5.18 | 127.94 | 112.40 |
| 1 | 114-A | 109 | LYS | CB-CA-C | -5.18 | 100.04 | 110.40 |
| 1 | 121-A | 18 | ASN | N-CA-C | 5.18 | 124.97 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 22-A | 127 | ASP | CB-CG-OD1 | -5.17 | 113.64 | 118.30 |
| 1 | 97-A | 88 | VAL | CB-CA-C | -5.17 | 101.58 | 111.40 |
| 1 | 70-A | 98 | ARG | NE-CZ-NH2 | -5.17 | 117.72 | 120.30 |
| 1 | 72-A | 44 | ARG | CA-CB-CG | -5.17 | 102.03 | 113.40 |
| 1 | 68-A | 37 | ASN | N-CA-CB | 5.17 | 119.90 | 110.60 |
| 1 | 39-A | 131 | ASP | CB-CG-OD1 | 5.16 | 122.94 | 118.30 |
| 1 | 85-A | 20 | MET | CG-SD-CE | 5.16 | 108.45 | 100.20 |
| 1 | 7-A | 126 | PRO | CA-C-O | -5.16 | 107.82 | 120.20 |
| 1 | 9-A | 125 | PHE | CB-CG-CD1 | -5.16 | 117.19 | 120.80 |
| 1 | 13-A | 36 | LEU | CB-CG-CD2 | 5.15 | 119.76 | 111.00 |
| 1 | 107-A | 1 | MET | CG-SD-CE | 5.15 | 108.45 | 100.20 |
| 1 | 37-A | 1 | MET | CB-CG-SD | 5.15 | 127.86 | 112.40 |
| 1 | 103-A | 21 | PRO | CA-C-O | -5.15 | 107.84 | 120.20 |
| 1 | 21-A | 36 | LEU | CA-CB-CG | -5.15 | 103.45 | 115.30 |
| 1 | 41-A | 1 | MET | CG-SD-CE | -5.15 | 91.96 | 100.20 |
| 1 | 87-A | 153 | PHE | CB-CG-CD2 | -5.15 | 117.19 | 120.80 |
| 1 | 61-A | 20 | MET | CG-SD-CE | -5.14 | 91.97 | 100.20 |
| 1 | 105-A | 21 | PRO | N-CA-CB | -5.14 | 96.94 | 102.60 |
| 1 | 27-A | 20 | MET | CB-CG-SD | 5.14 | 127.83 | 112.40 |
| 1 | 2-A | 12 | ARG | CB-CG-CD | 5.14 | 124.96 | 111.60 |
| 1 | 12-A | 72 | VAL | CG1-CB-CG2 | -5.14 | 102.68 | 110.90 |
| 1 | 26-A | 33 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 |
| 1 | 53-A | 127 | ASP | CA-C-N | -5.14 | 105.89 | 117.20 |
| 1 | 20-A | 120 | GLU | OE1-CD-OE2 | -5.14 | 117.14 | 123.30 |
| 1 | 73-A | 44 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 1 | 95-A | 1 | MET | CB-CA-C | 5.13 | 120.66 | 110.40 |
| 1 | 98-A | 23 | ASN | CB-CA-C | -5.13 | 100.14 | 110.40 |
| 1 | 46-A | 129 | GLU | C-N-CD | -5.13 | 109.32 | 120.60 |
| 1 | 2-A | 112 | LEU | CB-CG-CD1 | -5.12 | 102.30 | 111.00 |
| 1 | 77-A | 87 | ASP | CB-CG-OD2 | -5.12 | 113.69 | 118.30 |
| 1 | 56-A | 102 | GLN | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 1 | 64-A | 134 | GLU | N-CA-CB | 5.12 | 119.81 | 110.60 |
| 1 | 36-A | 1 | MET | CB-CG-SD | 5.11 | 127.74 | 112.40 |
| 1 | 48-A | 22 | TRP | CB-CG-CD1 | -5.11 | 120.35 | 127.00 |
| 1 | 99-A | 66 | PRO | N-CA-C | 5.11 | 125.39 | 112.10 |
| 1 | 108-A | 20 | MET | CB-CG-SD | -5.11 | 97.06 | 112.40 |
| 1 | 11-A | 4 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | 64-A | 12 | ARG | CD-NE-CZ | -5.11 | 116.44 | 123.60 |
| 1 | 32-A | 20 | MET | CB-CG-SD | -5.11 | 97.07 | 112.40 |
| 1 | 41-A | 33 | ARG | NE-CZ-NH1 | 5.11 | 122.85 | 120.30 |
| 1 | 72-A | 126 | PRO | C-N-CA | 5.11 | 134.47 | 121.70 |
| 1 | 41-A | 24 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 83-A | 2 | ILE | N-CA-CB | 5.11 | 122.55 | 110.80 |
| 1 | 61-A | 87 | ASP | N-CA-C | -5.10 | 97.22 | 111.00 |
| 1 | 109-A | 20 | MET | CB-CG-SD | -5.10 | 97.09 | 112.40 |
| 1 | 113-A | 127 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | 103-A | 21 | PRO | O-C-N | 5.10 | 130.86 | 122.70 |
| 1 | 5-A | 128 | TYR | N-CA-CB | -5.10 | 101.42 | 110.60 |
| 1 | 117-A | 23 | ASN | N-CA-CB | -5.10 | 101.42 | 110.60 |
| 1 | 80-A | 1 | MET | O-C-N | 5.10 | 130.86 | 122.70 |
| 1 | 102-A | 60 | ILE | CG1-CB-CG2 | 5.10 | 122.61 | 111.40 |
| 1 | 119-A | 30 | TRP | CA-CB-CG | -5.10 | 104.02 | 113.70 |
| 1 | 44-A | 24 | LEU | CB-CG-CD2 | 5.09 | 119.66 | 111.00 |
| 1 | 118-A | 128 | TYR | CB-CG-CD2 | 5.09 | 124.06 | 121.00 |
| 1 | 82-A | 127 | ASP | N-CA-C | 5.09 | 124.75 | 111.00 |
| 1 | 118-A | 120 | GLU | N-CA-CB | 5.09 | 119.77 | 110.60 |
| 1 | 47-A | 52 | ARG | NE-CZ-NH1 | -5.09 | 117.76 | 120.30 |
| 1 | 28-A | 48 | GLU | OE1-CD-OE2 | 5.09 | 129.41 | 123.30 |
| 1 | 61-A | 16 | MET | CG-SD-CE | -5.09 | 92.06 | 100.20 |
| 1 | 95-A | 98 | ARG | NE-CZ-NH2 | -5.09 | 117.76 | 120.30 |
| 1 | 96-A | 11 | ASP | CB-CG-OD1 | -5.09 | 113.72 | 118.30 |
| 1 | 50-A | 79 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 1 | 71-A | 127 | ASP | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | 3-A | 52 | ARG | NE-CZ-NH1 | -5.08 | 117.76 | 120.30 |
| 1 | 39-A | 24 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |
| 1 | 65-A | 42 | MET | CG-SD-CE | -5.08 | 92.07 | 100.20 |
| 1 | 97-A | 22 | TRP | CB-CA-C | 5.08 | 120.56 | 110.40 |
| 1 | 30-A | 11 | ASP | CB-CG-OD1 | -5.08 | 113.73 | 118.30 |
| 1 | 102-A | 153 | PHE | CB-CG-CD2 | -5.08 | 117.25 | 120.80 |
| 1 | 3-A | 49 | SER | N-CA-CB | -5.08 | 102.88 | 110.50 |
| 1 | 24-A | 132 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | 29-A | 104 | LEU | CB-CG-CD1 | 5.07 | 119.62 | 111.00 |
| 1 | 121-A | 28 | LEU | CB-CA-C | 5.07 | 119.84 | 110.20 |
| 1 | 21-A | 22 | TRP | CB-CG-CD2 | 5.07 | 133.19 | 126.60 |
| 1 | 5-A | 159 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 1 | 28-A | 134 | GLU | CA-CB-CG | 5.07 | 124.55 | 113.40 |
| 1 | 98-A | 24 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 1 | 5-A | 4 | LEU | CB-CG-CD2 | 5.07 | 119.61 | 111.00 |
| 1 | 65-A | 154 | GLU | OE1-CD-OE2 | -5.07 | 117.22 | 123.30 |
| 1 | 119-A | 127 | ASP | CB-CG-OD2 | -5.07 | 113.74 | 118.30 |
| 1 | 122-A | 18 | ASN | N-CA-CB | -5.07 | 101.48 | 110.60 |
| 1 | 93-A | 62 | LEU | CB-CG-CD2 | -5.06 | 102.40 | 111.00 |
| 1 | 10-A | 58 | LYS | CD-CE-NZ | 5.06 | 123.34 | 111.70 |
| 1 | 81-A | 20 | MET | N-CA-CB | 5.06 | 119.71 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 82-A | 127 | ASP | CB-CG-OD1 | -5.06 | 113.75 | 118.30 |
| 1 | 108-A | 30 | TRP | N-CA-CB | -5.06 | 101.49 | 110.60 |
| 1 | 24-A | 98 | ARG | CA-CB-CG | -5.06 | 102.27 | 113.40 |
| 1 | 68-A | 156 | LEU | CA-CB-CG | 5.06 | 126.93 | 115.30 |
| 1 | 68-A | 158 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 1 | 70-A | 70 | ASP | CB-CG-OD2 | 5.06 | 122.85 | 118.30 |
| 1 | 4-A | 129 | GLU | N-CA-C | -5.05 | 97.36 | 111.00 |
| 1 | 81-A | 128 | TYR | N-CA-C | 5.05 | 124.65 | 111.00 |
| 1 | 4-A | 17 | GLU | N-CA-CB | 5.05 | 119.69 | 110.60 |
| 1 | 108-A | 22 | TRP | CA-CB-CG | -5.05 | 104.10 | 113.70 |
| 1 | 96-A | 42 | MET | CG-SD-CE | 5.05 | 108.28 | 100.20 |
| 1 | 117-A | 54 | LEU | CB-CG-CD1 | -5.05 | 102.42 | 111.00 |
| 1 | 31-A | 79 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |
| 1 | 50-A | 106 | LYS | N-CA-CB | -5.05 | 101.52 | 110.60 |
| 1 | 108-A | 18 | ASN | N-CA-C | 5.04 | 124.62 | 111.00 |
| 1 | 99-A | 44 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | 119-A | 20 | MET | CB-CA-C | 5.04 | 120.49 | 110.40 |
| 1 | 65-A | 12 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 1 | 63-A | 154 | GLU | OE1-CD-OE2 | -5.04 | 117.25 | 123.30 |
| 1 | 104-A | 11 | ASP | CB-CG-OD1 | -5.04 | 113.76 | 118.30 |
| 1 | 72-A | 128 | TYR | CB-CG-CD1 | -5.04 | 117.98 | 121.00 |
| 1 | 70-A | 70 | ASP | CB-CG-OD1 | -5.04 | 113.77 | 118.30 |
| 1 | 10-A | 128 | TYR | CB-CA-C | 5.04 | 120.47 | 110.40 |
| 1 | 30-A | 20 | MET | CA-CB-CG | 5.04 | 121.86 | 113.30 |
| 1 | 59-A | 154 | GLU | CA-CB-CG | -5.04 | 102.32 | 113.40 |
| 1 | 76-A | 126 | PRO | O-C-N | 5.03 | 130.75 | 122.70 |
| 1 | 83-A | 79 | ASP | CB-CG-OD2 | -5.03 | 113.77 | 118.30 |
| 1 | 99-A | 126 | PRO | CB-CA-C | -5.03 | 99.42 | 112.00 |
| 1 | 37-A | 58 | LYS | CA-CB-CG | 5.03 | 124.47 | 113.40 |
| 1 | 121-A | 92 | MET | CG-SD-CE | 5.03 | 108.25 | 100.20 |
| 1 | 7-A | 116 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | 97-A | 4 | LEU | CB-CG-CD2 | 5.03 | 119.55 | 111.00 |
| 1 | 86-A | 158 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 1 | 50-A | 12 | ARG | CG-CD-NE | -5.02 | 101.25 | 111.80 |
| 1 | 69-A | 16 | MET | CA-CB-CG | 5.02 | 121.84 | 113.30 |
| 1 | 40-A | 52 | ARG | CA-CB-CG | 5.02 | 124.44 | 113.40 |
| 1 | 42-A | 1 | MET | CB-CG-SD | 5.02 | 127.45 | 112.40 |
| 1 | 85-A | 11 | ASP | CB-CG-OD1 | -5.02 | 113.78 | 118.30 |
| 1 | 115-A | 104 | LEU | CA-CB-CG | 5.02 | 126.84 | 115.30 |
| 1 | 7-A | 156 | LEU | CA-CB-CG | 5.01 | 126.84 | 115.30 |
| 1 | 24-A | 12 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 1 | 91-A | 36 | LEU | CA-CB-CG | -5.01 | 103.77 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 38-A | 52 | ARG | NE-CZ-NH2 | 5.01 | 122.81 | 120.30 |
| 1 | 92-A | 104 | LEU | C-N-CD | 5.01 | 138.93 | 128.40 |
| 1 | 80-A | 44 | ARG | CG-CD-NE | 5.01 | 122.33 | 111.80 |
| 1 | 124-A | 28 | LEU | CB-CG-CD2 | -5.01 | 102.48 | 111.00 |
| 1 | 30-A | 20 | MET | CB-CG-SD | 5.01 | 127.43 | 112.40 |
| 1 | 73-A | 36 | LEU | CB-CG-CD1 | 5.01 | 119.52 | 111.00 |
| 1 | 10-A | 127 | ASP | N-CA-C | 5.01 | 124.52 | 111.00 |
| 1 | 48-A | 128 | TYR | CB-CG-CD2 | 5.01 | 124.00 | 121.00 |
| 1 | 115-A | 88 | VAL | CB-CA-C | 5.01 | 120.91 | 111.40 |
| 1 | 4-A | 126 | PRO | C-N-CA | 5.00 | 134.21 | 121.70 |
| 1 | 37-A | 127 | ASP | N-CA-CB | 5.00 | 119.61 | 110.60 |
| 1 | 94-A | 21 | PRO | CA-C-N | 5.00 | 128.21 | 117.20 |
| 1 | 108-A | 18 | ASN | CB-CA-C | -5.00 | 100.39 | 110.40 |
| 1 | 11-A | 158 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |
| 1 | 24-A | 126 | PRO | CA-C-N | 5.00 | 128.21 | 117.20 |
| 1 | 123-A | 21 | PRO | CB-CA-C | 5.00 | 124.51 | 112.00 |
| 1 | 67-A | 126 | PRO | C-N-CA | -5.00 | 109.20 | 121.70 |
| 1 | 88-A | 128 | TYR | CA-CB-CG | 5.00 | 122.90 | 113.40 |

There are no chirality outliers.

All (267) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | 1-A | 128 | TYR | Peptide |
| 1 | 10-A | 126 | PRO | Peptide |
| 1 | 10-A | 127 | ASP | Peptide |
| 1 | 10-A | 128 | TYR | Peptide |
| 1 | 10-A | 21 | PRO | Peptide |
| 1 | 100-A | 21 | PRO | Peptide |
| 1 | 100-A | 23 | ASN | Peptide |
| 1 | 100-A | 67 | GLY | Peptide |
| 1 | 101-A | 127 | ASP | Peptide |
| 1 | 101-A | 21 | PRO | Peptide |
| 1 | 101-A | 67 | GLY | Peptide |
| 1 | 101-A | 86 | GLY | Peptide |
| 1 | 102-A | 126 | PRO | Mainchain,Peptide |
| 1 | 102-A | 127 | ASP | Peptide |
| 1 | 102-A | 21 | PRO | Peptide |
| 1 | 103-A | 22 | TRP | Peptide |
| 1 | 103-A | 23 | ASN | Peptide |
| 1 | 104-A | 127 | ASP | Peptide |
| 1 | 104-A | 17 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 105-A | 23 | ASN | Peptide |
| 1 | 106-A | 23 | ASN | Peptide |
| 1 | 107-A | 21 | PRO | Peptide |
| 1 | 108-A | 19 | ALA | Peptide |
| 1 | 108-A | 20 | MET | Peptide |
| 1 | 108-A | 21 | PRO | Peptide |
| 1 | 109-A | 19 | ALA | Peptide |
| 1 | 109-A | 20 | MET | Peptide |
| 1 | 109-A | 21 | PRO | Peptide |
| 1 | 11-A | 126 | PRO | Peptide |
| 1 | 11-A | 128 | TYR | Peptide |
| 1 | 11-A | 22 | TRP | Peptide |
| 1 | 110-A | 1 | MET | Peptide |
| 1 | 110-A | 19 | ALA | Peptide |
| 1 | 110-A | 21 | PRO | Peptide |
| 1 | 111-A | 18 | ASN | Peptide |
| 1 | 111-A | 21 | PRO | Peptide |
| 1 | 111-A | 22 | TRP | Peptide |
| 1 | 112-A | 18 | ASN | Peptide |
| 1 | 112-A | 50 | ILE | Peptide |
| 1 | 112-A | 87 | ASP | Peptide |
| 1 | 113-A | 1 | MET | Peptide |
| 1 | 114-A | 19 | ALA | Peptide |
| 1 | 114-A | 20 | MET | Peptide |
| 1 | 114-A | 21 | PRO | Peptide |
| 1 | 114-A | 22 | TRP | Peptide |
| 1 | 115-A | 126 | PRO | Peptide |
| 1 | 115-A | 20 | MET | Peptide |
| 1 | 115-A | 21 | PRO | Peptide |
| 1 | 116-A | 20 | MET | Peptide |
| 1 | 116-A | 21 | PRO | Peptide |
| 1 | 117-A | 19 | ALA | Peptide |
| 1 | 117-A | 20 | MET | Peptide |
| 1 | 118-A | 18 | ASN | Peptide |
| 1 | 118-A | 19 | ALA | Peptide |
| 1 | 118-A | 21 | PRO | Peptide |
| 1 | 119-A | 21 | PRO | Mainchain |
| 1 | 12-A | 126 | PRO | Peptide |
| 1 | 12-A | 127 | ASP | Peptide |
| 1 | 12-A | 128 | TYR | Peptide |
| 1 | 120-A | 118 | GLU | Peptide |
| 1 | 120-A | 21 | PRO | Mainchain |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 121-A | 17 | GLU | Mainchain |
| 1 | 121-A | 19 | ALA | Peptide |
| 1 | 121-A | 20 | MET | Peptide |
| 1 | 121-A | 21 | PRO | Peptide |
| 1 | 121-A | 85 | CYS | Mainchain |
| 1 | 122-A | 19 | ALA | Peptide |
| 1 | 123-A | 17 | GLU | Peptide |
| 1 | 123-A | 19 | ALA | Peptide |
| 1 | 124-A | 1 | MET | Peptide |
| 1 | 124-A | 23 | ASN | Peptide |
| 1 | 125-A | 1 | MET | Peptide |
| 1 | 125-A | 20 | MET | Peptide |
| 1 | 13-A | 127 | ASP | Peptide |
| 1 | 13-A | 128 | TYR | Peptide |
| 1 | 13-A | 22 | TRP | Peptide |
| 1 | 14-A | 126 | PRO | Peptide |
| 1 | 14-A | 127 | ASP | Peptide |
| 1 | 15-A | 126 | PRO | Mainchain |
| 1 | 15-A | 127 | ASP | Peptide |
| 1 | 15-A | 128 | TYR | Peptide |
| 1 | 16-A | 126 | PRO | Peptide |
| 1 | 16-A | 128 | TYR | Peptide |
| 1 | 16-A | 20 | MET | Peptide |
| 1 | 16-A | 22 | TRP | Peptide |
| 1 | 17-A | 118 | GLU | Peptide |
| 1 | 17-A | 126 | PRO | Peptide |
| 1 | 17-A | 128 | TYR | Peptide |
| 1 | 17-A | 22 | TRP | Peptide |
| 1 | 18-A | 126 | PRO | Peptide |
| 1 | 18-A | 22 | TRP | Peptide |
| 1 | 19-A | 126 | PRO | Peptide |
| 1 | 19-A | 20 | MET | Peptide |
| 1 | 2-A | 126 | PRO | Peptide |
| 1 | 2-A | 128 | TYR | Peptide |
| 1 | 2-A | 16 | MET | Peptide |
| 1 | 21-A | 128 | TYR | Peptide |
| 1 | 22-A | 126 | PRO | Peptide |
| 1 | 22-A | 127 | ASP | Peptide |
| 1 | 22-A | 128 | TYR | Peptide |
| 1 | 23-A | 126 | PRO | Peptide |
| 1 | 23-A | 127 | ASP | Peptide |
| 1 | 23-A | 21 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 24-A | 114 | HIS | Sidechain |
| 1 | 24-A | 126 | PRO | Peptide |
| 1 | 26-A | 128 | TYR | Peptide |
| 1 | 27-A | 19 | ALA | Peptide |
| 1 | 29-A | 128 | TYR | Peptide |
| 1 | 29-A | 64 | SER | Peptide |
| 1 | 3-A | 126 | PRO | Peptide |
| 1 | 3-A | 128 | TYR | Peptide |
| 1 | 3-A | 16 | MET | Peptide |
| 1 | 30-A | 128 | TYR | Peptide |
| 1 | 31-A | 1 | MET | Peptide |
| 1 | 31-A | 127 | ASP | Peptide |
| 1 | 32-A | 127 | ASP | Peptide |
| 1 | 32-A | 128 | TYR | Peptide |
| 1 | 33-A | 127 | ASP | Peptide |
| 1 | 36-A | 127 | ASP | Peptide |
| 1 | 36-A | 128 | TYR | Peptide |
| 1 | 38-A | 20 | MET | Peptide |
| 1 | 39-A | 126 | PRO | Peptide |
| 1 | 39-A | 127 | ASP | Peptide |
| 1 | 39-A | 20 | MET | Peptide |
| 1 | 4-A | 126 | PRO | Peptide |
| 1 | 4-A | 127 | ASP | Peptide |
| 1 | 4-A | 128 | TYR | Peptide |
| 1 | 40-A | 126 | PRO | Peptide |
| 1 | 40-A | 127 | ASP | Peptide |
| 1 | 41-A | 126 | PRO | Peptide |
| 1 | 41-A | 127 | ASP | Peptide |
| 1 | 41-A | 20 | MET | Peptide |
| 1 | 42-A | 127 | ASP | Peptide |
| 1 | 43-A | 126 | PRO | Peptide |
| 1 | 43-A | 127 | ASP | Peptide |
| 1 | 43-A | 128 | TYR | Peptide |
| 1 | 44-A | 126 | PRO | Peptide |
| 1 | 44-A | 20 | MET | Peptide |
| 1 | 45-A | 126 | PRO | Peptide |
| 1 | 46-A | 127 | ASP | Peptide |
| 1 | 46-A | 19 | ALA | Peptide |
| 1 | 47-A | 126 | PRO | Peptide |
| 1 | 47-A | 127 | ASP | Peptide |
| 1 | 48-A | 126 | PRO | Peptide |
| 1 | 49-A | 126 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 49-A | 128 | TYR | Peptide |
| 1 | 5-A | 110 | LEU | Peptide |
| 1 | 5-A | 126 | PRO | Peptide |
| 1 | 50-A | 126 | PRO | Peptide |
| 1 | 50-A | 127 | ASP | Peptide |
| 1 | 52-A | 126 | PRO | Peptide |
| 1 | 52-A | 21 | PRO | Peptide |
| 1 | 54-A | 126 | PRO | Peptide |
| 1 | 54-A | 127 | ASP | Peptide |
| 1 | 54-A | 22 | TRP | Peptide |
| 1 | 54-A | 23 | ASN | Peptide |
| 1 | 55-A | 126 | PRO | Peptide |
| 1 | 55-A | 127 | ASP | Peptide |
| 1 | 56-A | 126 | PRO | Peptide |
| 1 | 56-A | 128 | TYR | Peptide |
| 1 | 57-A | 126 | PRO | Peptide |
| 1 | 57-A | 128 | TYR | Peptide |
| 1 | 58-A | 126 | PRO | Peptide |
| 1 | 58-A | 128 | TYR | Peptide |
| 1 | 59-A | 128 | TYR | Peptide |
| 1 | 6-A | 126 | PRO | Peptide |
| 1 | 6-A | 127 | ASP | Peptide |
| 1 | 60-A | 128 | TYR | Peptide |
| 1 | 61-A | 128 | TYR | Peptide |
| 1 | 62-A | 129 | GLU | Peptide |
| 1 | 63-A | 1 | MET | Peptide |
| 1 | 63-A | 22 | TRP | Peptide |
| 1 | 63-A | 67 | GLY | Peptide |
| 1 | 64-A | 126 | PRO | Peptide |
| 1 | 64-A | 128 | TYR | Peptide |
| 1 | 64-A | 23 | ASN | Peptide |
| 1 | 65-A | 120 | GLU | Peptide |
| 1 | 65-A | 126 | PRO | Peptide |
| 1 | 66-A | 120 | GLU | Peptide |
| 1 | 66-A | 125 | PHE | Peptide |
| 1 | 66-A | 126 | PRO | Peptide |
| 1 | 66-A | 128 | TYR | Peptide |
| 1 | 66-A | 129 | GLU | Peptide |
| 1 | 66-A | 20 | MET | Peptide |
| 1 | 67-A | 125 | PHE | Peptide |
| 1 | 67-A | 127 | ASP | Peptide |
| 1 | 68-A | 125 | PHE | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 68-A | 127 | ASP | Peptide |
| 1 | 68-A | 128 | TYR | Peptide |
| 1 | 69-A | 1 | MET | Peptide |
| 1 | 69-A | 128 | TYR | Peptide |
| 1 | 69-A | 130 | PRO | Peptide |
| 1 | 7-A | 110 | LEU | Mainchain |
| 1 | 7-A | 126 | PRO | Peptide |
| 1 | 7-A | 127 | ASP | Peptide |
| 1 | 7-A | 128 | TYR | Peptide |
| 1 | 7-A | 22 | TRP | Peptide |
| 1 | 70-A | 128 | TYR | Peptide |
| 1 | 70-A | 68 | THR | Peptide |
| 1 | 71-A | 126 | PRO | Peptide |
| 1 | 71-A | 128 | TYR | Peptide |
| 1 | 72-A | 126 | PRO | Peptide |
| 1 | 73-A | 126 | PRO | Peptide |
| 1 | 73-A | 128 | TYR | Peptide |
| 1 | 73-A | 68 | THR | Peptide |
| 1 | 74-A | 128 | TYR | Peptide |
| 1 | 75-A | 126 | PRO | Peptide |
| 1 | 75-A | 127 | ASP | Peptide |
| 1 | 75-A | 128 | TYR | Peptide |
| 1 | 75-A | 19 | ALA | Peptide |
| 1 | 76-A | 126 | PRO | Peptide |
| 1 | 76-A | 127 | ASP | Peptide |
| 1 | 76-A | 128 | TYR | Peptide |
| 1 | 77-A | 126 | PRO | Peptide |
| 1 | 77-A | 128 | TYR | Peptide |
| 1 | 77-A | 22 | TRP | Peptide |
| 1 | 78-A | 20 | MET | Peptide |
| 1 | 78-A | 22 | TRP | Peptide |
| 1 | 79-A | 20 | MET | Peptide |
| 1 | 8-A | 126 | PRO | Peptide |
| 1 | 8-A | 21 | PRO | Peptide |
| 1 | 8-A | 23 | ASN | Peptide |
| 1 | 8-A | 85 | CYS | Peptide |
| 1 | 81-A | 128 | TYR | Peptide |
| 1 | 82-A | 128 | TYR | Peptide |
| 1 | 83-A | 124 | HIS | Peptide |
| 1 | 83-A | 22 | TRP | Peptide |
| 1 | 84-A | 21 | PRO | Peptide |
| 1 | 85-A | 1 | MET | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | 86-A | 129 | GLU | Peptide |
| 1 | 87-A | 128 | TYR | Peptide |
| 1 | 87-A | 129 | GLU | Peptide |
| 1 | 87-A | 87 | ASP | Peptide |
| 1 | 88-A | 119 | VAL | Peptide |
| 1 | 88-A | 129 | GLU | Peptide |
| 1 | 89-A | 129 | GLU | Peptide |
| 1 | 89-A | 21 | PRO | Peptide |
| 1 | 9-A | 114 | HIS | Sidechain |
| 1 | 9-A | 127 | ASP | Peptide |
| 1 | 9-A | 23 | ASN | Peptide |
| 1 | 9-A | 85 | CYS | Peptide |
| 1 | 90-A | 129 | GLU | Peptide |
| 1 | 90-A | 17 | GLU | Peptide |
| 1 | 90-A | 19 | ALA | Peptide |
| 1 | 91-A | 17 | GLU | Peptide |
| 1 | 91-A | 19 | ALA | Peptide |
| 1 | 91-A | 21 | PRO | Peptide |
| 1 | 92-A | 17 | GLU | Peptide |
| 1 | 92-A | 21 | PRO | Peptide |
| 1 | 93-A | 138 | SER | Peptide |
| 1 | 93-A | 19 | ALA | Peptide |
| 1 | 93-A | 20 | MET | Peptide |
| 1 | 93-A | 21 | PRO | Peptide |
| 1 | 94-A | 17 | GLU | Peptide |
| 1 | 94-A | 20 | MET | Peptide |
| 1 | 94-A | 86 | GLY | Peptide |
| 1 | 95-A | 17 | GLU | Peptide |
| 1 | 95-A | 20 | MET | Peptide |
| 1 | 96-A | 120 | GLU | Peptide |
| 1 | 96-A | 17 | GLU | Peptide |
| 1 | 96-A | 19 | ALA | Peptide |
| 1 | 96-A | 20 | MET | Peptide |
| 1 | 98-A | 126 | PRO | Peptide |
| 1 | 98-A | 23 | ASN | Peptide |
| 1 | 99-A | 20 | MET | Peptide |
| 1 | 99-A | 21 | PRO | Peptide |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 2-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 3-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 4-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 5-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 6-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 7-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 8-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 9-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 10-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 11-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 12-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 13-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 14-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 15-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 16-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 17-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 18-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 19-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 20-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 21-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 22-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 23-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 24-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 25-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 26-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 27-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 28-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 29-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 30-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 31-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 32-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 33-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 34-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 35-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 36-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 37-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 38-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 39-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 40-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 41-A | 1270 | 1221 | 1221 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 42-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 43-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 44-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 45-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 46-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 47-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 48-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 49-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 50-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 51-A | 1270 | 1221 | 1222 | 0 | 0 |
| 1 | 52-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 53-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 54-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 55-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 56-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 57-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 58-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 59-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 60-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 61-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 62-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 63-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 64-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 65-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 66-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 67-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 68-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 69-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 70-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 71-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 72-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 73-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 74-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 75-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 76-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 77-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 78-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 79-A | 1270 | 1221 | 1222 | 0 | 0 |
| 1 | 80-A | 1270 | 1221 | 1222 | 0 | 0 |
| 1 | 81-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 82-A | 1270 | 1221 | 1222 | 0 | 0 |
| 1 | 83-A | 1270 | 1221 | 1221 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 84-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 85-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 86-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 87-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 88-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 89-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 90-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 91-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 92-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 93-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 94-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 95-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 96-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 97-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 98-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 99-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 100-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 101-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 102-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 103-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 104-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 105-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 106-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 107-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 108-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 109-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 110-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 111-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 112-A | 1270 | 1221 | 1220 | 0 | 0 |
| 1 | 113-A | 1270 | 1221 | 1219 | 0 | 0 |
| 1 | 114-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 115-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 116-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 117-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 118-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 119-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 120-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 121-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 122-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 123-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 124-A | 1270 | 1221 | 1221 | 0 | 0 |
| 1 | 125-A | 1270 | 1221 | 1221 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 1-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 2-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 3-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 4-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 5-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 6-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 7-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 8-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 9-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 10-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 11-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 12-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 13-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 14-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 15-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 16-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 17-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 18-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 19-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 20-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 21-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 22-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 23-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 24-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 25-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 26-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 27-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 28-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 29-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 30-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 31-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 32-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 33-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 34-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 35-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 36-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 37-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 38-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 39-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 40-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 41-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 42-A | 32 | 17 | 17 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 43-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 44-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 45-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 46-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 47-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 48-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 49-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 50-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 51-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 52-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 53-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 54-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 55-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 56-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 57-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 58-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 59-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 60-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 61-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 62-A | 32 | 17 | 16 | 0 | 0 |
| 2 | 63-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 64-A | 32 | 17 | 16 | 0 | 0 |
| 2 | 65-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 66-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 67-A | 32 | 17 | 16 | 0 | 0 |
| 2 | 68-A | 32 | 17 | 16 | 0 | 0 |
| 2 | 69-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 70-A | 32 | 17 | 15 | 0 | 0 |
| 2 | 71-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 72-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 73-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 74-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 75-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 76-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 77-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 78-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 79-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 80-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 81-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 82-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 83-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 84-A | 32 | 17 | 17 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 85-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 86-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 87-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 88-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 89-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 90-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 91-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 92-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 93-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 94-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 95-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 96-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 97-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 98-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 99-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 100-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 101-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 102-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 103-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 104-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 105-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 106-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 107-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 108-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 109-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 110-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 111-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 112-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 113-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 114-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 115-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 116-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 117-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 118-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 119-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 120-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 121-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 122-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 123-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 124-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 125-A | 32 | 17 | 17 | 0 | 0 |
| 3 | 1-A | 48 | 25 | 25 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 2-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 3-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 4-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 5-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 6-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 7-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 8-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 9-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 10-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 11-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 12-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 13-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 14-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 15-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 16-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 17-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 18-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 19-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 20-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 21-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 22-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 23-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 24-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 25-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 26-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 27-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 28-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 29-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 30-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 31-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 32-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 33-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 34-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 35-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 36-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 37-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 38-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 39-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 40-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 41-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 42-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 43-A | 48 | 25 | 25 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 44-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 45-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 46-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 47-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 48-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 49-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 50-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 51-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 52-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 53-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 54-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 55-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 56-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 57-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 58-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 59-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 60-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 61-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 62-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 63-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 64-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 65-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 66-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 67-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 68-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 69-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 70-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 71-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 72-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 73-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 74-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 75-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 76-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 77-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 78-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 79-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 80-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 81-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 82-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 83-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 84-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 85-A | 48 | 25 | 25 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 86-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 87-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 88-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 89-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 90-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 91-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 92-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 93-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 94-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 95-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 96-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 97-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 98-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 99-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 100-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 101-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 102-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 103-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 104-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 105-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 106-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 107-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 108-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 109-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 110-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 111-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 112-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 113-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 114-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 115-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 116-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 117-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 118-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 119-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 120-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 121-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 122-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 123-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 124-A | 48 | 25 | 25 | 0 | 0 |
| 3 | 125-A | 48 | 25 | 25 | 0 | 0 |
| 4 | 1-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 2-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 3-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 4-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 5-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 6-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 7-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 8-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 9-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 10-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 11-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 12-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 13-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 14-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 15-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 16-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 17-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 18-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 19-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 20-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 21-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 22-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 23-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 24-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 25-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 26-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 27-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 28-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 29-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 30-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 31-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 32-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 33-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 34-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 35-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 36-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 37-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 38-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 39-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 40-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 41-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 42-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 43-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 44-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 45-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 46-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 47-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 48-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 49-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 50-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 51-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 52-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 53-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 54-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 55-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 56-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 57-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 58-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 59-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 60-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 61-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 62-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 63-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 64-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 65-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 66-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 67-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 68-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 69-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 70-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 71-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 72-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 73-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 74-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 75-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 76-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 77-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 78-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 79-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 80-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 81-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 82-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 83-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 84-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 85-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 86-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 87-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 88-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 89-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 90-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 91-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 92-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 93-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 94-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 95-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 96-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 97-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 98-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 99-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 100-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 101-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 102-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 103-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 104-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 105-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 106-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 107-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 108-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 109-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 110-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 111-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 112-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 113-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 114-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 115-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 116-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 117-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 118-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 119-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 120-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 121-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 122-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 123-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 124-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 125-A | 2 | 0 | 0 | 0 | 0 |
| 5 | 1-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 2-A | 91 | 0 | 0 | 0 | 0 |
| 5 | 3-A | 82 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | 4-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 5-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 6-A | 112 | 0 | 0 | 0 | 0 |
| 5 | 7-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 8-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 9-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 10-A | 90 | 0 | 0 | 0 | 0 |
| 5 | 11-A | 110 | 0 | 0 | 0 | 0 |
| 5 | 12-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 13-A | 117 | 0 | 0 | 0 | 0 |
| 5 | 14-A | 116 | 0 | 0 | 0 | 0 |
| 5 | 15-A | 113 | 0 | 0 | 0 | 0 |
| 5 | 16-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 17-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 18-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 19-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 20-A | 100 | 0 | 0 | 0 | 0 |
| 5 | 21-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 22-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 23-A | 110 | 0 | 0 | 0 | 0 |
| 5 | 24-A | 97 | 0 | 0 | 0 | 0 |
| 5 | 25-A | 106 | 0 | 0 | 0 | 0 |
| 5 | 26-A | 112 | 0 | 0 | 0 | 0 |
| 5 | 27-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 28-A | 100 | 0 | 0 | 0 | 0 |
| 5 | 29-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 30-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 31-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 32-A | 106 | 0 | 0 | 0 | 0 |
| 5 | 33-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 34-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 35-A | 100 | 0 | 0 | 0 | 0 |
| 5 | 36-A | 104 | 0 | 0 | 0 | 0 |
| 5 | 37-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 38-A | 119 | 0 | 0 | 0 | 0 |
| 5 | 39-A | 118 | 0 | 0 | 0 | 0 |
| 5 | 40-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 41-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 42-A | 97 | 0 | 0 | 0 | 0 |
| 5 | 43-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 44-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 45-A | 107 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | 46-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 47-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 48-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 49-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 50-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 51-A | 104 | 0 | 0 | 0 | 0 |
| 5 | 52-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 53-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 54-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 55-A | 106 | 0 | 0 | 0 | 0 |
| 5 | 56-A | 110 | 0 | 0 | 0 | 0 |
| 5 | 57-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 58-A | 116 | 0 | 0 | 0 | 0 |
| 5 | 59-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 60-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 61-A | 109 | 0 | 0 | 0 | 0 |
| 5 | 62-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 63-A | 110 | 0 | 0 | 0 | 0 |
| 5 | 64-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 65-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 66-A | 104 | 0 | 0 | 0 | 0 |
| 5 | 67-A | 99 | 0 | 0 | 0 | 0 |
| 5 | 68-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 69-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 70-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 71-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 72-A | 97 | 0 | 0 | 0 | 0 |
| 5 | 73-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 74-A | 111 | 0 | 0 | 0 | 0 |
| 5 | 75-A | 109 | 0 | 0 | 0 | 0 |
| 5 | 76-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 77-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 78-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 79-A | 115 | 0 | 0 | 0 | 0 |
| 5 | 80-A | 109 | 0 | 0 | 0 | 0 |
| 5 | 81-A | 106 | 0 | 0 | 0 | 0 |
| 5 | 82-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 83-A | 116 | 0 | 0 | 0 | 0 |
| 5 | 84-A | 111 | 0 | 0 | 0 | 0 |
| 5 | 85-A | 118 | 0 | 0 | 0 | 0 |
| 5 | 86-A | 109 | 0 | 0 | 0 | 0 |
| 5 | 87-A | 113 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 5 | 88-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 89-A | 109 | 0 | 0 | 0 | 0 |
| 5 | 90-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 91-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 92-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 93-A | 117 | 0 | 0 | 0 | 0 |
| 5 | 94-A | 121 | 0 | 0 | 0 | 0 |
| 5 | 95-A | 111 | 0 | 0 | 0 | 0 |
| 5 | 96-A | 104 | 0 | 0 | 0 | 0 |
| 5 | 97-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 98-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 99-A | 99 | 0 | 0 | 0 | 0 |
| 5 | 100-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 101-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 102-A | 100 | 0 | 0 | 0 | 0 |
| 5 | 103-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 104-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 105-A | 90 | 0 | 0 | 0 | 0 |
| 5 | 106-A | 91 | 0 | 0 | 0 | 0 |
| 5 | 107-A | 113 | 0 | 0 | 0 | 0 |
| 5 | 108-A | 108 | 0 | 0 | 0 | 0 |
| 5 | 109-A | 111 | 0 | 0 | 0 | 0 |
| 5 | 110-A | 113 | 0 | 0 | 0 | 0 |
| 5 | 111-A | 109 | 0 | 0 | 0 | 0 |
| 5 | 112-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 113-A | 101 | 0 | 0 | 0 | 0 |
| 5 | 114-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 115-A | 102 | 0 | 0 | 0 | 0 |
| 5 | 116-A | 101 | 0 | 0 | 0 | 0 |
| 5 | 117-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 118-A | 107 | 0 | 0 | 0 | 0 |
| 5 | 119-A | 106 | 0 | 0 | 0 | 0 |
| 5 | 120-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 121-A | 115 | 0 | 0 | 0 | 0 |
| 5 | 122-A | 97 | 0 | 0 | 0 | 0 |
| 5 | 123-A | 105 | 0 | 0 | 0 | 0 |
| 5 | 124-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 125-A | 102 | 0 | 0 | 0 | 0 |
| All | All | 181958 | 157875 | 157860 | 0 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1 | 1-A | 156/159 (98%) | 145 (93%) | 8 (5%) | 3 (2%) | 8 | 0 |
| 1 | 2-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 3-A | 156/159 (98%) | 147 (94%) | 4 (3%) | 5 (3%) | 4 | 0 |
| 1 | 4-A | 156/159 (98%) | 147 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |
| 1 | 5-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 6-A | 156/159 (98%) | 147 (94%) | 5 (3%) | 4 (3%) | 5 | 0 |
| 1 | 7-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 8-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 9-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 10-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 11-A | 156/159 (98%) | 144 (92%) | 11 (7%) | 1 (1%) | 25 | 5 |
| 1 | 12-A | 156/159 (98%) | 141 (90%) | 12 (8%) | 3 (2%) | 8 | 0 |
| 1 | 13-A | 156/159 (98%) | 147 (94%) | 3 (2%) | 6 (4%) | 3 | 0 |
| 1 | 14-A | 156/159 (98%) | 148 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 15-A | 156/159 (98%) | 144 (92%) | 10 (6%) | 2 (1%) | 12 | 1 |
| 1 | 16-A | 156/159 (98%) | 150 (96%) | 2 (1%) | 4 (3%) | 5 | 0 |
| 1 | 17-A | 156/159 (98%) | 149 (96%) | 4 (3%) | 3 (2%) | 8 | 0 |
| 1 | 18-A | 156/159 (98%) | 146 (94%) | 7 (4%) | 3 (2%) | 8 | 0 |
| 1 | 19-A | 156/159 (98%) | 149 (96%) | 2 (1%) | 5 (3%) | 4 | 0 |
| 1 | 20-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 21-A | 156/159 (98%) | 150 (96%) | 4 (3%) | 2 (1%) | 12 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1 | 22-A | 156/159 (98%) | 143 (92%) | 10 (6%) | 3 (2%) | 8 | 0 |
| 1 | 23-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 24-A | 156/159 (98%) | 145 (93%) | 9 (6%) | 2 (1%) | 12 | 1 |
| 1 | 25-A | 156/159 (98%) | 147 (94%) | 5 (3%) | 4 (3%) | 5 | 0 |
| 1 | 26-A | 156/159 (98%) | 148 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 27-A | 156/159 (98%) | 149 (96%) | 5 (3%) | 2 (1%) | 12 | 1 |
| 1 | 28-A | 156/159 (98%) | 145 (93%) | 10 (6%) | 1 (1%) | 25 | 5 |
| 1 | 29-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 30-A | 156/159 (98%) | 144 (92%) | 7 (4%) | 5 (3%) | 4 | 0 |
| 1 | 31-A | 156/159 (98%) | 148 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 32-A | 156/159 (98%) | 151 (97%) | 4 (3%) | 1 (1%) | 25 | 5 |
| 1 | 33-A | 156/159 (98%) | 149 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 34-A | 156/159 (98%) | 149 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 35-A | 156/159 (98%) | 144 (92%) | 9 (6%) | 3 (2%) | 8 | 0 |
| 1 | 36-A | 156/159 (98%) | 145 (93%) | 5 (3%) | 6 (4%) | 3 | 0 |
| 1 | 37-A | 156/159 (98%) | 145 (93%) | 8 (5%) | 3 (2%) | 8 | 0 |
| 1 | 38-A | 156/159 (98%) | 143 (92%) | 10 (6%) | 3 (2%) | 8 | 0 |
| 1 | 39-A | 156/159 (98%) | 146 (94%) | 7 (4%) | 3 (2%) | 8 | 0 |
| 1 | 40-A | 156/159 (98%) | 148 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 41-A | 156/159 (98%) | 142 (91%) | 9 (6%) | 5 (3%) | 4 | 0 |
| 1 | 42-A | 156/159 (98%) | 147 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |
| 1 | 43-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 44-A | 156/159 (98%) | 148 (95%) | 6 (4%) | 2 (1%) | 12 | 1 |
| 1 | 45-A | 156/159 (98%) | 144 (92%) | 11 (7%) | 1 (1%) | 25 | 5 |
| 1 | 46-A | 156/159 (98%) | 149 (96%) | 4 (3%) | 3 (2%) | 8 | 0 |
| 1 | 47-A | 156/159 (98%) | 150 (96%) | 4 (3%) | 2 (1%) | 12 | 1 |
| 1 | 48-A | 156/159 (98%) | 144 (92%) | 7 (4%) | 5 (3%) | 4 | 0 |
| 1 | 49-A | 156/159 (98%) | 149 (96%) | 2 (1%) | 5 (3%) | 4 | 0 |
| 1 | 50-A | 156/159 (98%) | 151 (97%) | 3 (2%) | 2 (1%) | 12 | 1 |
| 1 | 51-A | 156/159 (98%) | 148 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 52-A | 156/159 (98%) | 149 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1 | 53-A | 156/159 (98%) | 148 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 54-A | 156/159 (98%) | 146 (94%) | 8 (5%) | 2 (1%) | 12 | 1 |
| 1 | 55-A | 156/159 (98%) | 146 (94%) | 8 (5%) | 2 (1%) | 12 | 1 |
| 1 | 56-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 57-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 58-A | 156/159 (98%) | 148 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 59-A | 156/159 (98%) | 149 (96%) | 4 (3%) | 3 (2%) | 8 | 0 |
| 1 | 60-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 61-A | 156/159 (98%) | 149 (96%) | 3 (2%) | 4 (3%) | 5 | 0 |
| 1 | 62-A | 156/159 (98%) | 148 (95%) | 3 (2%) | 5 (3%) | 4 | 0 |
| 1 | 63-A | 156/159 (98%) | 144 (92%) | 5 (3%) | 7 (4%) | 2 | 0 |
| 1 | 64-A | 156/159 (98%) | 136 (87%) | 7 (4%) | 13 (8%) | 1 | 0 |
| 1 | 65-A | 156/159 (98%) | 140 (90%) | 10 (6%) | 6 (4%) | 3 | 0 |
| 1 | 66-A | 156/159 (98%) | 146 (94%) | 2 (1%) | 8 (5%) | 2 | 0 |
| 1 | 67-A | 156/159 (98%) | 143 (92%) | 8 (5%) | 5 (3%) | 4 | 0 |
| 1 | 68-A | 156/159 (98%) | 146 (94%) | 6 (4%) | 4 (3%) | 5 | 0 |
| 1 | 69-A | 156/159 (98%) | 147 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |
| 1 | 70-A | 156/159 (98%) | 149 (96%) | 5 (3%) | 2 (1%) | 12 | 1 |
| 1 | 71-A | 156/159 (98%) | 145 (93%) | 9 (6%) | 2 (1%) | 12 | 1 |
| 1 | 72-A | 156/159 (98%) | 147 (94%) | 5 (3%) | 4 (3%) | 5 | 0 |
| 1 | 73-A | 156/159 (98%) | 148 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 74-A | 156/159 (98%) | 147 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |
| 1 | 75-A | 156/159 (98%) | 151 (97%) | 3 (2%) | 2 (1%) | 12 | 1 |
| 1 | 76-A | 156/159 (98%) | 143 (92%) | 8 (5%) | 5 (3%) | 4 | 0 |
| 1 | 77-A | 156/159 (98%) | 149 (96%) | 3 (2%) | 4 (3%) | 5 | 0 |
| 1 | 78-A | 156/159 (98%) | 148 (95%) | 6 (4%) | 2 (1%) | 12 | 1 |
| 1 | 79-A | 156/159 (98%) | 143 (92%) | 6 (4%) | 7 (4%) | 2 | 0 |
| 1 | 80-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 81-A | 156/159 (98%) | 146 (94%) | 6 (4%) | 4 (3%) | 5 | 0 |
| 1 | 82-A | 156/159 (98%) | 141 (90%) | 8 (5%) | 7 (4%) | 2 | 0 |
| 1 | 83-A | 156/159 (98%) | 147 (94%) | 4 (3%) | 5 (3%) | 4 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1 | 84-A | 156/159 (98%) | 144 (92%) | 6 (4%) | 6 (4%) | 3 | 0 |
| 1 | 85-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 86-A | 156/159 (98%) | 147 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |
| 1 | 87-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 88-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 89-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 90-A | 156/159 (98%) | 144 (92%) | 6 (4%) | 6 (4%) | 3 | 0 |
| 1 | 91-A | 156/159 (98%) | 145 (93%) | 5 (3%) | 6 (4%) | 3 | 0 |
| 1 | 92-A | 156/159 (98%) | 145 (93%) | 5 (3%) | 6 (4%) | 3 | 0 |
| 1 | 93-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 94-A | 156/159 (98%) | 147 (94%) | 2 (1%) | 7 (4%) | 2 | 0 |
| 1 | 95-A | 156/159 (98%) | 148 (95%) | 3 (2%) | 5 (3%) | 4 | 0 |
| 1 | 96-A | 156/159 (98%) | 142 (91%) | 10 (6%) | 4 (3%) | 5 | 0 |
| 1 | 97-A | 156/159 (98%) | 140 (90%) | 10 (6%) | 6 (4%) | 3 | 0 |
| 1 | 98-A | 156/159 (98%) | 145 (93%) | 6 (4%) | 5 (3%) | 4 | 0 |
| 1 | 99-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 100-A | 156/159 (98%) | 145 (93%) | 5 (3%) | 6 (4%) | 3 | 0 |
| 1 | 101-A | 156/159 (98%) | 146 (94%) | 4 (3%) | 6 (4%) | 3 | 0 |
| 1 | 102-A | 156/159 (98%) | 148 (95%) | 4 (3%) | 4 (3%) | 5 | 0 |
| 1 | 103-A | 156/159 (98%) | 147 (94%) | 3 (2%) | 6 (4%) | 3 | 0 |
| 1 | 104-A | 156/159 (98%) | 144 (92%) | 6 (4%) | 6 (4%) | 3 | 0 |
| 1 | 105-A | 156/159 (98%) | 141 (90%) | 12 (8%) | 3 (2%) | 8 | 0 |
| 1 | 106-A | 156/159 (98%) | 144 (92%) | 5 (3%) | 7 (4%) | 2 | 0 |
| 1 | 107-A | 156/159 (98%) | 146 (94%) | 6 (4%) | 4 (3%) | 5 | 0 |
| 1 | 108-A | 156/159 (98%) | 145 (93%) | 7 (4%) | 4 (3%) | 5 | 0 |
| 1 | 109-A | 156/159 (98%) | 145 (93%) | 8 (5%) | 3 (2%) | 8 | 0 |
| 1 | 110-A | 156/159 (98%) | 143 (92%) | 10 (6%) | 3 (2%) | 8 | 0 |
| 1 | 111-A | 156/159 (98%) | 147 (94%) | 5 (3%) | 4 (3%) | 5 | 0 |
| 1 | 112-A | 156/159 (98%) | 143 (92%) | 9 (6%) | 4 (3%) | 5 | 0 |
| 1 | 113-A | 156/159 (98%) | 146 (94%) | 7 (4%) | 3 (2%) | 8 | 0 |
| 1 | 114-A | 156/159 (98%) | 145 (93%) | 6 (4%) | 5 (3%) | 4 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|---|
| 1 | 115-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 116-A | 156/159 (98%) | 147 (94%) | 5 (3%) | 4 (3%) | 5 | 0 |
| 1 | 117-A | 156/159 (98%) | 143 (92%) | 7 (4%) | 6 (4%) | 3 | 0 |
| 1 | 118-A | 156/159 (98%) | 143 (92%) | 8 (5%) | 5 (3%) | 4 | 0 |
| 1 | 119-A | 156/159 (98%) | 143 (92%) | 8 (5%) | 5 (3%) | 4 | 0 |
| 1 | 120-A | 156/159 (98%) | 144 (92%) | 6 (4%) | 6 (4%) | 3 | 0 |
| 1 | 121-A | 156/159 (98%) | 140 (90%) | 10 (6%) | 6 (4%) | 3 | 0 |
| 1 | 122-A | 156/159 (98%) | 143 (92%) | 5 (3%) | 8 (5%) | 2 | 0 |
| 1 | 123-A | 156/159 (98%) | 146 (94%) | 5 (3%) | 5 (3%) | 4 | 0 |
| 1 | 124-A | 156/159 (98%) | 145 (93%) | 6 (4%) | 5 (3%) | 4 | 0 |
| 1 | 125-A | 156/159 (98%) | 142 (91%) | 9 (6%) | 5 (3%) | 4 | 0 |
| All | All | 19500/19875 (98%) | 18238 (94%) | 756 (4%) | 506 (3%) | 5 | 0 |

All (506) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1-A | 17 | GLU |
| 1 | 1-A | 127 | ASP |
| 1 | 2-A | 17 | GLU |
| 1 | 2-A | 18 | ASN |
| 1 | 3-A | 17 | GLU |
| 1 | 3-A | 87 | ASP |
| 1 | 3-A | 128 | TYR |
| 1 | 4-A | 87 | ASP |
| 1 | 4-A | 127 | ASP |
| 1 | 6-A | 22 | TRP |
| 1 | 6-A | 127 | ASP |
| 1 | 6-A | 128 | TYR |
| 1 | 7-A | 23 | ASN |
| 1 | 7-A | 87 | ASP |
| 1 | 7-A | 127 | ASP |
| 1 | 8-A | 127 | ASP |
| 1 | 9-A | 87 | ASP |
| 1 | 9-A | 128 | TYR |
| 1 | 10-A | 127 | ASP |
| 1 | 10-A | 128 | TYR |
| 1 | 11-A | 127 | ASP |
| 1 | 12-A | 125 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 12-A | 126 | PRO |
| 1 | 13-A | 127 | ASP |
| 1 | 13-A | 129 | GLU |
| 1 | 17-A | 21 | PRO |
| 1 | 17-A | 127 | ASP |
| 1 | 19-A | 127 | ASP |
| 1 | 19-A | 128 | TYR |
| 1 | 20-A | 87 | ASP |
| 1 | 20-A | 127 | ASP |
| 1 | 20-A | 128 | TYR |
| 1 | 21-A | 127 | ASP |
| 1 | 21-A | 128 | TYR |
| 1 | 22-A | 128 | TYR |
| 1 | 24-A | 127 | ASP |
| 1 | 25-A | 22 | TRP |
| 1 | 25-A | 127 | ASP |
| 1 | 27-A | 128 | TYR |
| 1 | 29-A | 21 | PRO |
| 1 | 29-A | 66 | PRO |
| 1 | 29-A | 128 | TYR |
| 1 | 31-A | 127 | ASP |
| 1 | 32-A | 127 | ASP |
| 1 | 35-A | 126 | PRO |
| 1 | 35-A | 127 | ASP |
| 1 | 36-A | 21 | PRO |
| 1 | 36-A | 121 | GLY |
| 1 | 36-A | 127 | ASP |
| 1 | 37-A | 21 | PRO |
| 1 | 37-A | 126 | PRO |
| 1 | 38-A | 22 | TRP |
| 1 | 39-A | 20 | MET |
| 1 | 39-A | 21 | PRO |
| 1 | 39-A | 22 | TRP |
| 1 | 40-A | 21 | PRO |
| 1 | 40-A | 127 | ASP |
| 1 | 41-A | 21 | PRO |
| 1 | 41-A | 127 | ASP |
| 1 | 42-A | 21 | PRO |
| 1 | 42-A | 23 | ASN |
| 1 | 42-A | 129 | GLU |
| 1 | 43-A | 21 | PRO |
| 1 | 43-A | 127 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 43-A | 129 | GLU |
| 1 | 44-A | 21 | PRO |
| 1 | 44-A | 127 | ASP |
| 1 | 45-A | 127 | ASP |
| 1 | 47-A | 22 | TRP |
| 1 | 48-A | 21 | PRO |
| 1 | 48-A | 22 | TRP |
| 1 | 48-A | 127 | ASP |
| 1 | 49-A | 22 | TRP |
| 1 | 49-A | 127 | ASP |
| 1 | 49-A | 129 | GLU |
| 1 | 50-A | 127 | ASP |
| 1 | 53-A | 128 | TYR |
| 1 | 55-A | 128 | TYR |
| 1 | 56-A | 68 | THR |
| 1 | 56-A | 127 | ASP |
| 1 | 56-A | 128 | TYR |
| 1 | 57-A | 127 | ASP |
| 1 | 57-A | 128 | TYR |
| 1 | 58-A | 128 | TYR |
| 1 | 59-A | 128 | TYR |
| 1 | 60-A | 127 | ASP |
| 1 | 61-A | 21 | PRO |
| 1 | 61-A | 127 | ASP |
| 1 | 61-A | 128 | TYR |
| 1 | 61-A | 129 | GLU |
| 1 | 62-A | 21 | PRO |
| 1 | 62-A | 127 | ASP |
| 1 | 62-A | 128 | TYR |
| 1 | 62-A | 131 | ASP |
| 1 | 63-A | 131 | ASP |
| 1 | 64-A | 23 | ASN |
| 1 | 64-A | 24 | LEU |
| 1 | 64-A | 67 | GLY |
| 1 | 64-A | 127 | ASP |
| 1 | 64-A | 129 | GLU |
| 1 | 64-A | 130 | PRO |
| 1 | 65-A | 23 | ASN |
| 1 | 65-A | 67 | GLY |
| 1 | 65-A | 68 | THR |
| 1 | 65-A | 129 | GLU |
| 1 | 65-A | 130 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 66-A | 22 | TRP |
| 1 | 66-A | 68 | THR |
| 1 | 66-A | 126 | PRO |
| 1 | 66-A | 129 | GLU |
| 1 | 67-A | 67 | GLY |
| 1 | 67-A | 68 | THR |
| 1 | 67-A | 126 | PRO |
| 1 | 68-A | 68 | THR |
| 1 | 68-A | 129 | GLU |
| 1 | 68-A | 131 | ASP |
| 1 | 69-A | 68 | THR |
| 1 | 69-A | 126 | PRO |
| 1 | 70-A | 68 | THR |
| 1 | 71-A | 127 | ASP |
| 1 | 72-A | 127 | ASP |
| 1 | 73-A | 68 | THR |
| 1 | 73-A | 120 | GLU |
| 1 | 73-A | 127 | ASP |
| 1 | 74-A | 127 | ASP |
| 1 | 76-A | 2 | ILE |
| 1 | 76-A | 21 | PRO |
| 1 | 76-A | 127 | ASP |
| 1 | 77-A | 2 | ILE |
| 1 | 77-A | 21 | PRO |
| 1 | 77-A | 127 | ASP |
| 1 | 78-A | 2 | ILE |
| 1 | 78-A | 21 | PRO |
| 1 | 79-A | 2 | ILE |
| 1 | 79-A | 21 | PRO |
| 1 | 79-A | 24 | LEU |
| 1 | 79-A | 87 | ASP |
| 1 | 79-A | 127 | ASP |
| 1 | 80-A | 127 | ASP |
| 1 | 80-A | 130 | PRO |
| 1 | 81-A | 2 | ILE |
| 1 | 82-A | 21 | PRO |
| 1 | 82-A | 127 | ASP |
| 1 | 82-A | 131 | ASP |
| 1 | 83-A | 23 | ASN |
| 1 | 83-A | 127 | ASP |
| 1 | 83-A | 131 | ASP |
| 1 | 84-A | 130 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 84-A | 131 | ASP |
| 1 | 85-A | 21 | PRO |
| 1 | 85-A | 131 | ASP |
| 1 | 86-A | 21 | PRO |
| 1 | 86-A | 127 | ASP |
| 1 | 86-A | 130 | PRO |
| 1 | 87-A | 130 | PRO |
| 1 | 88-A | 130 | PRO |
| 1 | 89-A | 23 | ASN |
| 1 | 89-A | 130 | PRO |
| 1 | 90-A | 17 | GLU |
| 1 | 90-A | 18 | ASN |
| 1 | 90-A | 23 | ASN |
| 1 | 91-A | 17 | GLU |
| 1 | 91-A | 18 | ASN |
| 1 | 91-A | 21 | PRO |
| 1 | 91-A | 130 | PRO |
| 1 | 92-A | 19 | ALA |
| 1 | 92-A | 21 | PRO |
| 1 | 92-A | 127 | ASP |
| 1 | 92-A | 130 | PRO |
| 1 | 93-A | 20 | MET |
| 1 | 93-A | 21 | PRO |
| 1 | 93-A | 23 | ASN |
| 1 | 94-A | 17 | GLU |
| 1 | 94-A | 19 | ALA |
| 1 | 94-A | 20 | MET |
| 1 | 94-A | 128 | TYR |
| 1 | 95-A | 18 | ASN |
| 1 | 95-A | 20 | MET |
| 1 | 95-A | 21 | PRO |
| 1 | 96-A | 18 | ASN |
| 1 | 96-A | 23 | ASN |
| 1 | 97-A | 18 | ASN |
| 1 | 97-A | 19 | ALA |
| 1 | 97-A | 23 | ASN |
| 1 | 97-A | 24 | LEU |
| 1 | 98-A | 22 | TRP |
| 1 | 98-A | 23 | ASN |
| 1 | 98-A | 67 | GLY |
| 1 | 99-A | 23 | ASN |
| 1 | 99-A | 24 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 99-A | 127 | ASP |
| 1 | 100-A | 23 | ASN |
| 1 | 100-A | 24 | LEU |
| 1 | 101-A | 22 | TRP |
| 1 | 101-A | 87 | ASP |
| 1 | 102-A | 127 | ASP |
| 1 | 103-A | 21 | PRO |
| 1 | 103-A | 22 | TRP |
| 1 | 103-A | 23 | ASN |
| 1 | 103-A | 128 | TYR |
| 1 | 104-A | 20 | MET |
| 1 | 104-A | 21 | PRO |
| 1 | 104-A | 22 | TRP |
| 1 | 104-A | 23 | ASN |
| 1 | 104-A | 128 | TYR |
| 1 | 105-A | 21 | PRO |
| 1 | 105-A | 22 | TRP |
| 1 | 106-A | 18 | ASN |
| 1 | 106-A | 21 | PRO |
| 1 | 106-A | 22 | TRP |
| 1 | 106-A | 66 | PRO |
| 1 | 106-A | 67 | GLY |
| 1 | 107-A | 17 | GLU |
| 1 | 107-A | 18 | ASN |
| 1 | 107-A | 20 | MET |
| 1 | 110-A | 19 | ALA |
| 1 | 110-A | 21 | PRO |
| 1 | 111-A | 20 | MET |
| 1 | 112-A | 2 | ILE |
| 1 | 112-A | 23 | ASN |
| 1 | 113-A | 19 | ALA |
| 1 | 113-A | 21 | PRO |
| 1 | 113-A | 23 | ASN |
| 1 | 114-A | 20 | MET |
| 1 | 115-A | 17 | GLU |
| 1 | 115-A | 22 | TRP |
| 1 | 116-A | 17 | GLU |
| 1 | 116-A | 19 | ALA |
| 1 | 116-A | 22 | TRP |
| 1 | 117-A | 17 | GLU |
| 1 | 118-A | 17 | GLU |
| 1 | 118-A | 18 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 118-A | 20 | MET |
| 1 | 118-A | 137 | PHE |
| 1 | 119-A | 23 | ASN |
| 1 | 120-A | 19 | ALA |
| 1 | 120-A | 21 | PRO |
| 1 | 120-A | 66 | PRO |
| 1 | 121-A | 17 | GLU |
| 1 | 121-A | 20 | MET |
| 1 | 121-A | 21 | PRO |
| 1 | 121-A | 22 | TRP |
| 1 | 122-A | 20 | MET |
| 1 | 122-A | 21 | PRO |
| 1 | 122-A | 22 | TRP |
| 1 | 122-A | 23 | ASN |
| 1 | 122-A | 24 | LEU |
| 1 | 123-A | 21 | PRO |
| 1 | 123-A | 23 | ASN |
| 1 | 123-A | 24 | LEU |
| 1 | 124-A | 17 | GLU |
| 1 | 124-A | 18 | ASN |
| 1 | 124-A | 21 | PRO |
| 1 | 124-A | 24 | LEU |
| 1 | 125-A | 18 | ASN |
| 1 | 125-A | 22 | TRP |
| 1 | 125-A | 24 | LEU |
| 1 | 5-A | 87 | ASP |
| 1 | 6-A | 87 | ASP |
| 1 | 8-A | 87 | ASP |
| 1 | 8-A | 128 | TYR |
| 1 | 9-A | 22 | TRP |
| 1 | 12-A | 127 | ASP |
| 1 | 15-A | 87 | ASP |
| 1 | 16-A | 128 | TYR |
| 1 | 17-A | 119 | VAL |
| 1 | 22-A | 127 | ASP |
| 1 | 23-A | 121 | GLY |
| 1 | 23-A | 130 | PRO |
| 1 | 25-A | 18 | ASN |
| 1 | 30-A | 87 | ASP |
| 1 | 36-A | 86 | GLY |
| 1 | 36-A | 120 | GLU |
| 1 | 37-A | 127 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 38-A | 21 | PRO |
| 1 | 38-A | 126 | PRO |
| 1 | 46-A | 129 | GLU |
| 1 | 46-A | 130 | PRO |
| 1 | 47-A | 127 | ASP |
| 1 | 60-A | 23 | ASN |
| 1 | 60-A | 128 | TYR |
| 1 | 63-A | 18 | ASN |
| 1 | 63-A | 67 | GLY |
| 1 | 63-A | 68 | THR |
| 1 | 63-A | 130 | PRO |
| 1 | 64-A | 68 | THR |
| 1 | 64-A | 90 | GLU |
| 1 | 65-A | 126 | PRO |
| 1 | 66-A | 23 | ASN |
| 1 | 66-A | 67 | GLY |
| 1 | 67-A | 131 | ASP |
| 1 | 68-A | 127 | ASP |
| 1 | 70-A | 126 | PRO |
| 1 | 72-A | 67 | GLY |
| 1 | 72-A | 121 | GLY |
| 1 | 75-A | 23 | ASN |
| 1 | 76-A | 23 | ASN |
| 1 | 80-A | 2 | ILE |
| 1 | 81-A | 137 | PHE |
| 1 | 82-A | 2 | ILE |
| 1 | 82-A | 90 | GLU |
| 1 | 82-A | 130 | PRO |
| 1 | 83-A | 130 | PRO |
| 1 | 84-A | 2 | ILE |
| 1 | 85-A | 127 | ASP |
| 1 | 89-A | 18 | ASN |
| 1 | 89-A | 128 | TYR |
| 1 | 90-A | 19 | ALA |
| 1 | 90-A | 130 | PRO |
| 1 | 92-A | 17 | GLU |
| 1 | 93-A | 17 | GLU |
| 1 | 94-A | 23 | ASN |
| 1 | 95-A | 17 | GLU |
| 1 | 99-A | 128 | TYR |
| 1 | 101-A | 23 | ASN |
| 1 | 102-A | 87 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 108-A | 18 | ASN |
| 1 | 109-A | 17 | GLU |
| 1 | 111-A | 2 | ILE |
| 1 | 111-A | 22 | TRP |
| 1 | 114-A | 17 | GLU |
| 1 | 114-A | 19 | ALA |
| 1 | 114-A | 22 | TRP |
| 1 | 115-A | 86 | GLY |
| 1 | 116-A | 37 | ASN |
| 1 | 117-A | 23 | ASN |
| 1 | 117-A | 137 | PHE |
| 1 | 120-A | 20 | MET |
| 1 | 120-A | 23 | ASN |
| 1 | 121-A | 19 | ALA |
| 1 | 121-A | 24 | LEU |
| 1 | 122-A | 17 | GLU |
| 1 | 122-A | 67 | GLY |
| 1 | 123-A | 17 | GLU |
| 1 | 125-A | 21 | PRO |
| 1 | 2-A | 126 | PRO |
| 1 | 3-A | 69 | ASP |
| 1 | 3-A | 126 | PRO |
| 1 | 5-A | 21 | PRO |
| 1 | 5-A | 128 | TYR |
| 1 | 7-A | 128 | TYR |
| 1 | 13-A | 128 | TYR |
| 1 | 14-A | 128 | TYR |
| 1 | 15-A | 126 | PRO |
| 1 | 18-A | 69 | ASP |
| 1 | 19-A | 22 | TRP |
| 1 | 23-A | 127 | ASP |
| 1 | 29-A | 127 | ASP |
| 1 | 30-A | 128 | TYR |
| 1 | 34-A | 21 | PRO |
| 1 | 35-A | 69 | ASP |
| 1 | 43-A | 23 | ASN |
| 1 | 49-A | 128 | TYR |
| 1 | 55-A | 127 | ASP |
| 1 | 58-A | 127 | ASP |
| 1 | 59-A | 129 | GLU |
| 1 | 64-A | 21 | PRO |
| 1 | 64-A | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 64-A | 137 | PHE |
| 1 | 66-A | 130 | PRO |
| 1 | 66-A | 131 | ASP |
| 1 | 67-A | 128 | TYR |
| 1 | 72-A | 68 | THR |
| 1 | 75-A | 126 | PRO |
| 1 | 77-A | 20 | MET |
| 1 | 79-A | 130 | PRO |
| 1 | 81-A | 127 | ASP |
| 1 | 81-A | 130 | PRO |
| 1 | 82-A | 23 | ASN |
| 1 | 84-A | 126 | PRO |
| 1 | 87-A | 21 | PRO |
| 1 | 87-A | 127 | ASP |
| 1 | 87-A | 143 | ALA |
| 1 | 92-A | 90 | GLU |
| 1 | 95-A | 19 | ALA |
| 1 | 97-A | 22 | TRP |
| 1 | 100-A | 22 | TRP |
| 1 | 100-A | 90 | GLU |
| 1 | 101-A | 67 | GLY |
| 1 | 101-A | 127 | ASP |
| 1 | 104-A | 18 | ASN |
| 1 | 107-A | 21 | PRO |
| 1 | 108-A | 128 | TYR |
| 1 | 109-A | 19 | ALA |
| 1 | 111-A | 21 | PRO |
| 1 | 112-A | 19 | ALA |
| 1 | 115-A | 19 | ALA |
| 1 | 115-A | 37 | ASN |
| 1 | 119-A | 137 | PHE |
| 1 | 120-A | 22 | TRP |
| 1 | 122-A | 128 | TYR |
| 1 | 124-A | 90 | GLU |
| 1 | 9-A | 130 | PRO |
| 1 | 10-A | 22 | TRP |
| 1 | 13-A | 87 | ASP |
| 1 | 13-A | 126 | PRO |
| 1 | 14-A | 127 | ASP |
| 1 | 16-A | 20 | MET |
| 1 | 16-A | 86 | GLY |
| 1 | 18-A | 89 | PRO |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 19-A | 21 | PRO |
| 1 | 20-A | 129 | GLU |
| 1 | 22-A | 143 | ALA |
| 1 | 24-A | 22 | TRP |
| 1 | 26-A | 128 | TYR |
| 1 | 28-A | 128 | TYR |
| 1 | 30-A | 19 | ALA |
| 1 | 30-A | 90 | GLU |
| 1 | 33-A | 128 | TYR |
| 1 | 40-A | 23 | ASN |
| 1 | 41-A | 129 | GLU |
| 1 | 46-A | 21 | PRO |
| 1 | 49-A | 69 | ASP |
| 1 | 51-A | 143 | ALA |
| 1 | 54-A | 127 | ASP |
| 1 | 54-A | 129 | GLU |
| 1 | 57-A | 21 | PRO |
| 1 | 62-A | 129 | GLU |
| 1 | 63-A | 128 | TYR |
| 1 | 84-A | 22 | TRP |
| 1 | 88-A | 21 | PRO |
| 1 | 90-A | 143 | ALA |
| 1 | 94-A | 21 | PRO |
| 1 | 98-A | 24 | LEU |
| 1 | 100-A | 86 | GLY |
| 1 | 101-A | 126 | PRO |
| 1 | 106-A | 17 | GLU |
| 1 | 108-A | 17 | GLU |
| 1 | 108-A | 21 | PRO |
| 1 | 112-A | 21 | PRO |
| 1 | 117-A | 21 | PRO |
| 1 | 118-A | 19 | ALA |
| 1 | 119-A | 21 | PRO |
| 1 | 1-A | 128 | TYR |
| 1 | 2-A | 127 | ASP |
| 1 | 5-A | 111 | TYR |
| 1 | 8-A | 22 | TRP |
| 1 | 8-A | 129 | GLU |
| 1 | 9-A | 129 | GLU |
| 1 | 10-A | 24 | LEU |
| 1 | 14-A | 129 | GLU |
| 1 | 18-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 23-A | 129 | GLU |
| 1 | 41-A | 23 | ASN |
| 1 | 41-A | 66 | PRO |
| 1 | 52-A | 21 | PRO |
| 1 | 53-A | 24 | LEU |
| 1 | 53-A | 127 | ASP |
| 1 | 60-A | 129 | GLU |
| 1 | 64-A | 131 | ASP |
| 1 | 80-A | 24 | LEU |
| 1 | 80-A | 129 | GLU |
| 1 | 83-A | 22 | TRP |
| 1 | 85-A | 130 | PRO |
| 1 | 91-A | 23 | ASN |
| 1 | 91-A | 67 | GLY |
| 1 | 94-A | 18 | ASN |
| 1 | 96-A | 21 | PRO |
| 1 | 100-A | 126 | PRO |
| 1 | 102-A | 23 | ASN |
| 1 | 105-A | 127 | ASP |
| 1 | 106-A | 65 | GLN |
| 1 | 109-A | 20 | MET |
| 1 | 110-A | 143 | ALA |
| 1 | 114-A | 23 | ASN |
| 1 | 119-A | 17 | GLU |
| 1 | 119-A | 22 | TRP |
| 1 | 123-A | 18 | ASN |
| 1 | 4-A | 21 | PRO |
| 1 | 16-A | 21 | PRO |
| 1 | 19-A | 129 | GLU |
| 1 | 36-A | 126 | PRO |
| 1 | 48-A | 66 | PRO |
| 1 | 50-A | 129 | GLU |
| 1 | 56-A | 129 | GLU |
| 1 | 57-A | 129 | GLU |
| 1 | 58-A | 129 | GLU |
| 1 | 76-A | 126 | PRO |
| 1 | 84-A | 129 | GLU |
| 1 | 88-A | 22 | TRP |
| 1 | 88-A | 120 | GLU |
| 1 | 96-A | 20 | MET |
| 1 | 98-A | 69 | ASP |
| 1 | 102-A | 18 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 103-A | 88 | VAL |
| 1 | 117-A | 19 | ALA |
| 1 | 117-A | 20 | MET |
| 1 | 125-A | 20 | MET |
| 1 | 13-A | 24 | LEU |
| 1 | 25-A | 21 | PRO |
| 1 | 30-A | 86 | GLY |
| 1 | 69-A | 130 | PRO |
| 1 | 59-A | 126 | PRO |
| 1 | 63-A | 21 | PRO |
| 1 | 74-A | 126 | PRO |
| 1 | 23-A | 21 | PRO |
| 1 | 27-A | 21 | PRO |
| 1 | 48-A | 89 | PRO |
| 1 | 71-A | 21 | PRO |
| 1 | 79-A | 20 | MET |
| 1 | 97-A | 21 | PRO |
| 1 | 103-A | 129 | GLU |
| 1 | 2-A | 21 | PRO |
| 1 | 20-A | 130 | PRO |
| 1 | 64-A | 126 | PRO |
| 1 | 74-A | 21 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 1-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 2-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 3-A | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 | 0 |
| 1 | 4-A | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 | 0 |
| 1 | 5-A | 135/135 (100%) | 120 (89%) | 15 (11%) | 6 | 0 |
| 1 | 6-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 7-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 8-A | 135/135 (100%) | 115 (85%) | 20 (15%) | 3 | 0 |
| 1 | 9-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 10-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 11-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 12-A | 135/135 (100%) | 115 (85%) | 20 (15%) | 3 | 0 |
| 1 | 13-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 14-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 15-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 16-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 17-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 18-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 19-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 20-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 21-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 22-A | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 | 0 |
| 1 | 23-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 24-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 25-A | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 | 0 |
| 1 | 26-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 27-A | 135/135 (100%) | 120 (89%) | 15 (11%) | 6 | 0 |
| 1 | 28-A | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 | 0 |
| 1 | 29-A | 135/135 (100%) | 111 (82%) | 24 (18%) | 2 | 0 |
| 1 | 30-A | 135/135 (100%) | 120 (89%) | 15 (11%) | 6 | 0 |
| 1 | 31-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 32-A | 135/135 (100%) | 111 (82%) | 24 (18%) | 2 | 0 |
| 1 | 33-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 34-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 35-A | 135/135 (100%) | 115 (85%) | 20 (15%) | 3 | 0 |
| 1 | 36-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 37-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 38-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 39-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 40-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 41-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 42-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 43-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 44-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 45-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 46-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 47-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 48-A | 135/135 (100%) | 115 (85%) | 20 (15%) | 3 | 0 |
| 1 | 49-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 50-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 51-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 52-A | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 | 0 |
| 1 | 53-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 54-A | 135/135 (100%) | 120 (89%) | 15 (11%) | 6 | 0 |
| 1 | 55-A | 135/135 (100%) | 120 (89%) | 15 (11%) | 6 | 0 |
| 1 | 56-A | 135/135 (100%) | 111 (82%) | 24 (18%) | 2 | 0 |
| 1 | 57-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 58-A | 135/135 (100%) | 121 (90%) | 14 (10%) | 7 | 0 |
| 1 | 59-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 60-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 61-A | 135/135 (100%) | 121 (90%) | 14 (10%) | 7 | 0 |
| 1 | 62-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 63-A | 135/135 (100%) | 121 (90%) | 14 (10%) | 7 | 0 |
| 1 | 64-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 65-A | 135/135 (100%) | 115 (85%) | 20 (15%) | 3 | 0 |
| 1 | 66-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 67-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 68-A | 135/135 (100%) | 113 (84%) | 22 (16%) | 2 | 0 |
| 1 | 69-A | 135/135 (100%) | 113 (84%) | 22 (16%) | 2 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 70-A | 135/135 (100%) | 113 (84%) | 22 (16%) | 2 | 0 |
| 1 | 71-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 72-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 73-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 74-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 75-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 76-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 77-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 78-A | 135/135 (100%) | 124 (92%) | 11 (8%) | 11 | 0 |
| 1 | 79-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 80-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 81-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 82-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 83-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 84-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 85-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 86-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 87-A | 135/135 (100%) | 112 (83%) | 23 (17%) | 2 | 0 |
| 1 | 88-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 89-A | 135/135 (100%) | 113 (84%) | 22 (16%) | 2 | 0 |
| 1 | 90-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 91-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 92-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 93-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 94-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| 1 | 95-A | 135/135 (100%) | 120 (89%) | 15 (11%) | 6 | 0 |
| 1 | 96-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 97-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 98-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 99-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 100-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|------------|-------------|---|
| 1 | 101-A | 135/135 (100%) | 115 (85%) | 20 (15%) | 3 | 0 |
| 1 | 102-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 103-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 104-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 105-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 106-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 107-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 108-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 109-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 110-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 111-A | 135/135 (100%) | 114 (84%) | 21 (16%) | 2 | 0 |
| 1 | 112-A | 135/135 (100%) | 127 (94%) | 8 (6%) | 19 | 2 |
| 1 | 113-A | 135/135 (100%) | 124 (92%) | 11 (8%) | 11 | 0 |
| 1 | 114-A | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 | 0 |
| 1 | 115-A | 135/135 (100%) | 111 (82%) | 24 (18%) | 2 | 0 |
| 1 | 116-A | 135/135 (100%) | 116 (86%) | 19 (14%) | 3 | 0 |
| 1 | 117-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 118-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 119-A | 135/135 (100%) | 124 (92%) | 11 (8%) | 11 | 0 |
| 1 | 120-A | 135/135 (100%) | 121 (90%) | 14 (10%) | 7 | 0 |
| 1 | 121-A | 135/135 (100%) | 117 (87%) | 18 (13%) | 4 | 0 |
| 1 | 122-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 123-A | 135/135 (100%) | 125 (93%) | 10 (7%) | 13 | 1 |
| 1 | 124-A | 135/135 (100%) | 119 (88%) | 16 (12%) | 5 | 0 |
| 1 | 125-A | 135/135 (100%) | 118 (87%) | 17 (13%) | 4 | 0 |
| All | All | 16875/16875 (100%) | 14694 (87%) | 2181 (13%) | 4 | 0 |

All (2181) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1-A | 1 | MET |
| 1 | 1-A | 12 | ARG |
| 1 | 1-A | 17 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1-A | 20 | MET |
| 1 | 1-A | 23 | ASN |
| 1 | 1-A | 36 | LEU |
| 1 | 1-A | 37 | ASN |
| 1 | 1-A | 44 | ARG |
| 1 | 1-A | 52 | ARG |
| 1 | 1-A | 59 | ASN |
| 1 | 1-A | 70 | ASP |
| 1 | 1-A | 76 | LYS |
| 1 | 1-A | 79 | ASP |
| 1 | 1-A | 87 | ASP |
| 1 | 1-A | 106 | LYS |
| 1 | 1-A | 108 | GLN |
| 1 | 1-A | 114 | HIS |
| 1 | 1-A | 119 | VAL |
| 1 | 1-A | 128 | TYR |
| 1 | 1-A | 134 | GLU |
| 1 | 1-A | 140 | PHE |
| 1 | 1-A | 144 | ASP |
| 1 | 1-A | 154 | GLU |
| 1 | 2-A | 1 | MET |
| 1 | 2-A | 4 | LEU |
| 1 | 2-A | 12 | ARG |
| 1 | 2-A | 17 | GLU |
| 1 | 2-A | 33 | ARG |
| 1 | 2-A | 49 | SER |
| 1 | 2-A | 52 | ARG |
| 1 | 2-A | 59 | ASN |
| 1 | 2-A | 62 | LEU |
| 1 | 2-A | 65 | GLN |
| 1 | 2-A | 76 | LYS |
| 1 | 2-A | 87 | ASP |
| 1 | 2-A | 106 | LYS |
| 1 | 2-A | 108 | GLN |
| 1 | 2-A | 127 | ASP |
| 1 | 2-A | 128 | TYR |
| 1 | 2-A | 146 | GLN |
| 1 | 2-A | 154 | GLU |
| 1 | 3-A | 1 | MET |
| 1 | 3-A | 17 | GLU |
| 1 | 3-A | 20 | MET |
| 1 | 3-A | 23 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 3-A | 52 | ARG |
| 1 | 3-A | 59 | ASN |
| 1 | 3-A | 65 | GLN |
| 1 | 3-A | 76 | LYS |
| 1 | 3-A | 106 | LYS |
| 1 | 3-A | 114 | HIS |
| 1 | 3-A | 128 | TYR |
| 1 | 3-A | 154 | GLU |
| 1 | 3-A | 155 | ILE |
| 1 | 4-A | 1 | MET |
| 1 | 4-A | 8 | LEU |
| 1 | 4-A | 20 | MET |
| 1 | 4-A | 24 | LEU |
| 1 | 4-A | 36 | LEU |
| 1 | 4-A | 52 | ARG |
| 1 | 4-A | 61 | ILE |
| 1 | 4-A | 62 | LEU |
| 1 | 4-A | 76 | LYS |
| 1 | 4-A | 106 | LYS |
| 1 | 4-A | 108 | GLN |
| 1 | 4-A | 128 | TYR |
| 1 | 4-A | 154 | GLU |
| 1 | 5-A | 12 | ARG |
| 1 | 5-A | 20 | MET |
| 1 | 5-A | 24 | LEU |
| 1 | 5-A | 44 | ARG |
| 1 | 5-A | 49 | SER |
| 1 | 5-A | 52 | ARG |
| 1 | 5-A | 62 | LEU |
| 1 | 5-A | 76 | LYS |
| 1 | 5-A | 101 | GLU |
| 1 | 5-A | 108 | GLN |
| 1 | 5-A | 114 | HIS |
| 1 | 5-A | 118 | GLU |
| 1 | 5-A | 127 | ASP |
| 1 | 5-A | 137 | PHE |
| 1 | 5-A | 154 | GLU |
| 1 | 6-A | 1 | MET |
| 1 | 6-A | 20 | MET |
| 1 | 6-A | 23 | ASN |
| 1 | 6-A | 30 | TRP |
| 1 | 6-A | 36 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 6-A | 44 | ARG |
| 1 | 6-A | 52 | ARG |
| 1 | 6-A | 62 | LEU |
| 1 | 6-A | 65 | GLN |
| 1 | 6-A | 76 | LYS |
| 1 | 6-A | 98 | ARG |
| 1 | 6-A | 106 | LYS |
| 1 | 6-A | 114 | HIS |
| 1 | 6-A | 115 | ILE |
| 1 | 6-A | 132 | ASP |
| 1 | 6-A | 148 | SER |
| 1 | 6-A | 154 | GLU |
| 1 | 6-A | 156 | LEU |
| 1 | 7-A | 1 | MET |
| 1 | 7-A | 18 | ASN |
| 1 | 7-A | 20 | MET |
| 1 | 7-A | 22 | TRP |
| 1 | 7-A | 23 | ASN |
| 1 | 7-A | 24 | LEU |
| 1 | 7-A | 36 | LEU |
| 1 | 7-A | 49 | SER |
| 1 | 7-A | 52 | ARG |
| 1 | 7-A | 59 | ASN |
| 1 | 7-A | 65 | GLN |
| 1 | 7-A | 76 | LYS |
| 1 | 7-A | 101 | GLU |
| 1 | 7-A | 106 | LYS |
| 1 | 7-A | 116 | ASP |
| 1 | 7-A | 127 | ASP |
| 1 | 7-A | 138 | SER |
| 1 | 7-A | 148 | SER |
| 1 | 7-A | 154 | GLU |
| 1 | 8-A | 1 | MET |
| 1 | 8-A | 8 | LEU |
| 1 | 8-A | 20 | MET |
| 1 | 8-A | 22 | TRP |
| 1 | 8-A | 24 | LEU |
| 1 | 8-A | 36 | LEU |
| 1 | 8-A | 45 | HIS |
| 1 | 8-A | 52 | ARG |
| 1 | 8-A | 59 | ASN |
| 1 | 8-A | 61 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 8-A | 62 | LEU |
| 1 | 8-A | 76 | LYS |
| 1 | 8-A | 79 | ASP |
| 1 | 8-A | 85 | CYS |
| 1 | 8-A | 106 | LYS |
| 1 | 8-A | 114 | HIS |
| 1 | 8-A | 128 | TYR |
| 1 | 8-A | 132 | ASP |
| 1 | 8-A | 141 | HIS |
| 1 | 8-A | 154 | GLU |
| 1 | 9-A | 8 | LEU |
| 1 | 9-A | 11 | ASP |
| 1 | 9-A | 17 | GLU |
| 1 | 9-A | 20 | MET |
| 1 | 9-A | 22 | TRP |
| 1 | 9-A | 23 | ASN |
| 1 | 9-A | 33 | ARG |
| 1 | 9-A | 36 | LEU |
| 1 | 9-A | 52 | ARG |
| 1 | 9-A | 61 | ILE |
| 1 | 9-A | 62 | LEU |
| 1 | 9-A | 65 | GLN |
| 1 | 9-A | 76 | LYS |
| 1 | 9-A | 85 | CYS |
| 1 | 9-A | 101 | GLU |
| 1 | 9-A | 106 | LYS |
| 1 | 9-A | 119 | VAL |
| 1 | 9-A | 128 | TYR |
| 1 | 9-A | 129 | GLU |
| 1 | 9-A | 154 | GLU |
| 1 | 9-A | 158 | ARG |
| 1 | 10-A | 2 | ILE |
| 1 | 10-A | 11 | ASP |
| 1 | 10-A | 12 | ARG |
| 1 | 10-A | 20 | MET |
| 1 | 10-A | 23 | ASN |
| 1 | 10-A | 24 | LEU |
| 1 | 10-A | 49 | SER |
| 1 | 10-A | 52 | ARG |
| 1 | 10-A | 59 | ASN |
| 1 | 10-A | 62 | LEU |
| 1 | 10-A | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 10-A | 76 | LYS |
| 1 | 10-A | 79 | ASP |
| 1 | 10-A | 87 | ASP |
| 1 | 10-A | 88 | VAL |
| 1 | 10-A | 101 | GLU |
| 1 | 10-A | 106 | LYS |
| 1 | 10-A | 119 | VAL |
| 1 | 10-A | 128 | TYR |
| 1 | 10-A | 148 | SER |
| 1 | 10-A | 154 | GLU |
| 1 | 11-A | 1 | MET |
| 1 | 11-A | 4 | LEU |
| 1 | 11-A | 11 | ASP |
| 1 | 11-A | 12 | ARG |
| 1 | 11-A | 16 | MET |
| 1 | 11-A | 20 | MET |
| 1 | 11-A | 33 | ARG |
| 1 | 11-A | 52 | ARG |
| 1 | 11-A | 59 | ASN |
| 1 | 11-A | 87 | ASP |
| 1 | 11-A | 98 | ARG |
| 1 | 11-A | 106 | LYS |
| 1 | 11-A | 108 | GLN |
| 1 | 11-A | 129 | GLU |
| 1 | 11-A | 154 | GLU |
| 1 | 11-A | 158 | ARG |
| 1 | 12-A | 11 | ASP |
| 1 | 12-A | 12 | ARG |
| 1 | 12-A | 18 | ASN |
| 1 | 12-A | 20 | MET |
| 1 | 12-A | 21 | PRO |
| 1 | 12-A | 23 | ASN |
| 1 | 12-A | 33 | ARG |
| 1 | 12-A | 37 | ASN |
| 1 | 12-A | 49 | SER |
| 1 | 12-A | 52 | ARG |
| 1 | 12-A | 59 | ASN |
| 1 | 12-A | 87 | ASP |
| 1 | 12-A | 108 | GLN |
| 1 | 12-A | 109 | LYS |
| 1 | 12-A | 118 | GLU |
| 1 | 12-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 12-A | 134 | GLU |
| 1 | 12-A | 135 | SER |
| 1 | 12-A | 139 | GLU |
| 1 | 12-A | 154 | GLU |
| 1 | 13-A | 17 | GLU |
| 1 | 13-A | 20 | MET |
| 1 | 13-A | 23 | ASN |
| 1 | 13-A | 33 | ARG |
| 1 | 13-A | 36 | LEU |
| 1 | 13-A | 37 | ASN |
| 1 | 13-A | 52 | ARG |
| 1 | 13-A | 61 | ILE |
| 1 | 13-A | 62 | LEU |
| 1 | 13-A | 65 | GLN |
| 1 | 13-A | 98 | ARG |
| 1 | 13-A | 108 | GLN |
| 1 | 13-A | 120 | GLU |
| 1 | 13-A | 127 | ASP |
| 1 | 13-A | 156 | LEU |
| 1 | 13-A | 158 | ARG |
| 1 | 13-A | 159 | ARG |
| 1 | 14-A | 1 | MET |
| 1 | 14-A | 11 | ASP |
| 1 | 14-A | 12 | ARG |
| 1 | 14-A | 17 | GLU |
| 1 | 14-A | 18 | ASN |
| 1 | 14-A | 20 | MET |
| 1 | 14-A | 33 | ARG |
| 1 | 14-A | 36 | LEU |
| 1 | 14-A | 44 | ARG |
| 1 | 14-A | 52 | ARG |
| 1 | 14-A | 59 | ASN |
| 1 | 14-A | 77 | SER |
| 1 | 14-A | 98 | ARG |
| 1 | 14-A | 106 | LYS |
| 1 | 14-A | 108 | GLN |
| 1 | 14-A | 109 | LYS |
| 1 | 14-A | 142 | ASP |
| 1 | 14-A | 159 | ARG |
| 1 | 15-A | 1 | MET |
| 1 | 15-A | 11 | ASP |
| 1 | 15-A | 16 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 15-A | 17 | GLU |
| 1 | 15-A | 18 | ASN |
| 1 | 15-A | 20 | MET |
| 1 | 15-A | 33 | ARG |
| 1 | 15-A | 52 | ARG |
| 1 | 15-A | 54 | LEU |
| 1 | 15-A | 58 | LYS |
| 1 | 15-A | 62 | LEU |
| 1 | 15-A | 76 | LYS |
| 1 | 15-A | 79 | ASP |
| 1 | 15-A | 98 | ARG |
| 1 | 15-A | 108 | GLN |
| 1 | 15-A | 127 | ASP |
| 1 | 15-A | 136 | VAL |
| 1 | 15-A | 142 | ASP |
| 1 | 15-A | 154 | GLU |
| 1 | 16-A | 1 | MET |
| 1 | 16-A | 16 | MET |
| 1 | 16-A | 17 | GLU |
| 1 | 16-A | 20 | MET |
| 1 | 16-A | 22 | TRP |
| 1 | 16-A | 33 | ARG |
| 1 | 16-A | 36 | LEU |
| 1 | 16-A | 45 | HIS |
| 1 | 16-A | 59 | ASN |
| 1 | 16-A | 62 | LEU |
| 1 | 16-A | 106 | LYS |
| 1 | 16-A | 108 | GLN |
| 1 | 16-A | 118 | GLU |
| 1 | 16-A | 128 | TYR |
| 1 | 16-A | 138 | SER |
| 1 | 16-A | 142 | ASP |
| 1 | 17-A | 1 | MET |
| 1 | 17-A | 12 | ARG |
| 1 | 17-A | 18 | ASN |
| 1 | 17-A | 20 | MET |
| 1 | 17-A | 22 | TRP |
| 1 | 17-A | 28 | LEU |
| 1 | 17-A | 33 | ARG |
| 1 | 17-A | 48 | GLU |
| 1 | 17-A | 49 | SER |
| 1 | 17-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 17-A | 58 | LYS |
| 1 | 17-A | 59 | ASN |
| 1 | 17-A | 60 | ILE |
| 1 | 17-A | 62 | LEU |
| 1 | 17-A | 65 | GLN |
| 1 | 17-A | 68 | THR |
| 1 | 17-A | 87 | ASP |
| 1 | 17-A | 119 | VAL |
| 1 | 17-A | 127 | ASP |
| 1 | 17-A | 138 | SER |
| 1 | 17-A | 142 | ASP |
| 1 | 17-A | 148 | SER |
| 1 | 17-A | 156 | LEU |
| 1 | 18-A | 1 | MET |
| 1 | 18-A | 10 | VAL |
| 1 | 18-A | 12 | ARG |
| 1 | 18-A | 16 | MET |
| 1 | 18-A | 18 | ASN |
| 1 | 18-A | 20 | MET |
| 1 | 18-A | 22 | TRP |
| 1 | 18-A | 44 | ARG |
| 1 | 18-A | 49 | SER |
| 1 | 18-A | 52 | ARG |
| 1 | 18-A | 58 | LYS |
| 1 | 18-A | 62 | LEU |
| 1 | 18-A | 65 | GLN |
| 1 | 18-A | 98 | ARG |
| 1 | 18-A | 106 | LYS |
| 1 | 18-A | 128 | TYR |
| 1 | 18-A | 129 | GLU |
| 1 | 18-A | 142 | ASP |
| 1 | 18-A | 156 | LEU |
| 1 | 19-A | 1 | MET |
| 1 | 19-A | 12 | ARG |
| 1 | 19-A | 16 | MET |
| 1 | 19-A | 18 | ASN |
| 1 | 19-A | 20 | MET |
| 1 | 19-A | 22 | TRP |
| 1 | 19-A | 23 | ASN |
| 1 | 19-A | 33 | ARG |
| 1 | 19-A | 36 | LEU |
| 1 | 19-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 19-A | 58 | LYS |
| 1 | 19-A | 59 | ASN |
| 1 | 19-A | 62 | LEU |
| 1 | 19-A | 70 | ASP |
| 1 | 19-A | 79 | ASP |
| 1 | 19-A | 87 | ASP |
| 1 | 19-A | 101 | GLU |
| 1 | 19-A | 106 | LYS |
| 1 | 19-A | 118 | GLU |
| 1 | 19-A | 128 | TYR |
| 1 | 19-A | 154 | GLU |
| 1 | 19-A | 155 | ILE |
| 1 | 19-A | 159 | ARG |
| 1 | 20-A | 1 | MET |
| 1 | 20-A | 2 | ILE |
| 1 | 20-A | 12 | ARG |
| 1 | 20-A | 18 | ASN |
| 1 | 20-A | 23 | ASN |
| 1 | 20-A | 52 | ARG |
| 1 | 20-A | 64 | SER |
| 1 | 20-A | 65 | GLN |
| 1 | 20-A | 87 | ASP |
| 1 | 20-A | 106 | LYS |
| 1 | 20-A | 116 | ASP |
| 1 | 20-A | 120 | GLU |
| 1 | 20-A | 127 | ASP |
| 1 | 20-A | 128 | TYR |
| 1 | 20-A | 150 | SER |
| 1 | 20-A | 154 | GLU |
| 1 | 20-A | 158 | ARG |
| 1 | 21-A | 1 | MET |
| 1 | 21-A | 4 | LEU |
| 1 | 21-A | 8 | LEU |
| 1 | 21-A | 12 | ARG |
| 1 | 21-A | 18 | ASN |
| 1 | 21-A | 20 | MET |
| 1 | 21-A | 52 | ARG |
| 1 | 21-A | 59 | ASN |
| 1 | 21-A | 87 | ASP |
| 1 | 21-A | 98 | ARG |
| 1 | 21-A | 104 | LEU |
| 1 | 21-A | 106 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 21-A | 120 | GLU |
| 1 | 21-A | 127 | ASP |
| 1 | 21-A | 128 | TYR |
| 1 | 21-A | 134 | GLU |
| 1 | 21-A | 144 | ASP |
| 1 | 21-A | 158 | ARG |
| 1 | 22-A | 8 | LEU |
| 1 | 22-A | 12 | ARG |
| 1 | 22-A | 20 | MET |
| 1 | 22-A | 33 | ARG |
| 1 | 22-A | 52 | ARG |
| 1 | 22-A | 58 | LYS |
| 1 | 22-A | 64 | SER |
| 1 | 22-A | 76 | LYS |
| 1 | 22-A | 114 | HIS |
| 1 | 22-A | 120 | GLU |
| 1 | 22-A | 128 | TYR |
| 1 | 22-A | 158 | ARG |
| 1 | 22-A | 159 | ARG |
| 1 | 23-A | 1 | MET |
| 1 | 23-A | 18 | ASN |
| 1 | 23-A | 23 | ASN |
| 1 | 23-A | 33 | ARG |
| 1 | 23-A | 48 | GLU |
| 1 | 23-A | 54 | LEU |
| 1 | 23-A | 61 | ILE |
| 1 | 23-A | 62 | LEU |
| 1 | 23-A | 76 | LYS |
| 1 | 23-A | 98 | ARG |
| 1 | 23-A | 118 | GLU |
| 1 | 23-A | 119 | VAL |
| 1 | 23-A | 120 | GLU |
| 1 | 23-A | 127 | ASP |
| 1 | 23-A | 128 | TYR |
| 1 | 23-A | 138 | SER |
| 1 | 23-A | 148 | SER |
| 1 | 24-A | 1 | MET |
| 1 | 24-A | 12 | ARG |
| 1 | 24-A | 16 | MET |
| 1 | 24-A | 18 | ASN |
| 1 | 24-A | 33 | ARG |
| 1 | 24-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 24-A | 76 | LYS |
| 1 | 24-A | 89 | PRO |
| 1 | 24-A | 109 | LYS |
| 1 | 24-A | 118 | GLU |
| 1 | 24-A | 119 | VAL |
| 1 | 24-A | 120 | GLU |
| 1 | 24-A | 128 | TYR |
| 1 | 24-A | 134 | GLU |
| 1 | 24-A | 138 | SER |
| 1 | 24-A | 148 | SER |
| 1 | 24-A | 158 | ARG |
| 1 | 25-A | 12 | ARG |
| 1 | 25-A | 18 | ASN |
| 1 | 25-A | 23 | ASN |
| 1 | 25-A | 33 | ARG |
| 1 | 25-A | 36 | LEU |
| 1 | 25-A | 44 | ARG |
| 1 | 25-A | 48 | GLU |
| 1 | 25-A | 52 | ARG |
| 1 | 25-A | 62 | LEU |
| 1 | 25-A | 106 | LYS |
| 1 | 25-A | 127 | ASP |
| 1 | 25-A | 128 | TYR |
| 1 | 25-A | 129 | GLU |
| 1 | 26-A | 12 | ARG |
| 1 | 26-A | 16 | MET |
| 1 | 26-A | 18 | ASN |
| 1 | 26-A | 20 | MET |
| 1 | 26-A | 33 | ARG |
| 1 | 26-A | 52 | ARG |
| 1 | 26-A | 54 | LEU |
| 1 | 26-A | 59 | ASN |
| 1 | 26-A | 62 | LEU |
| 1 | 26-A | 64 | SER |
| 1 | 26-A | 106 | LYS |
| 1 | 26-A | 114 | HIS |
| 1 | 26-A | 119 | VAL |
| 1 | 26-A | 128 | TYR |
| 1 | 26-A | 148 | SER |
| 1 | 26-A | 154 | GLU |
| 1 | 27-A | 4 | LEU |
| 1 | 27-A | 16 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 27-A | 17 | GLU |
| 1 | 27-A | 20 | MET |
| 1 | 27-A | 33 | ARG |
| 1 | 27-A | 36 | LEU |
| 1 | 27-A | 44 | ARG |
| 1 | 27-A | 54 | LEU |
| 1 | 27-A | 62 | LEU |
| 1 | 27-A | 79 | ASP |
| 1 | 27-A | 114 | HIS |
| 1 | 27-A | 127 | ASP |
| 1 | 27-A | 128 | TYR |
| 1 | 27-A | 136 | VAL |
| 1 | 27-A | 148 | SER |
| 1 | 28-A | 1 | MET |
| 1 | 28-A | 8 | LEU |
| 1 | 28-A | 16 | MET |
| 1 | 28-A | 33 | ARG |
| 1 | 28-A | 54 | LEU |
| 1 | 28-A | 58 | LYS |
| 1 | 28-A | 65 | GLN |
| 1 | 28-A | 79 | ASP |
| 1 | 28-A | 106 | LYS |
| 1 | 28-A | 127 | ASP |
| 1 | 28-A | 138 | SER |
| 1 | 28-A | 146 | GLN |
| 1 | 28-A | 156 | LEU |
| 1 | 29-A | 8 | LEU |
| 1 | 29-A | 12 | ARG |
| 1 | 29-A | 16 | MET |
| 1 | 29-A | 20 | MET |
| 1 | 29-A | 23 | ASN |
| 1 | 29-A | 33 | ARG |
| 1 | 29-A | 36 | LEU |
| 1 | 29-A | 52 | ARG |
| 1 | 29-A | 54 | LEU |
| 1 | 29-A | 59 | ASN |
| 1 | 29-A | 62 | LEU |
| 1 | 29-A | 64 | SER |
| 1 | 29-A | 65 | GLN |
| 1 | 29-A | 79 | ASP |
| 1 | 29-A | 87 | ASP |
| 1 | 29-A | 88 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 29-A | 104 | LEU |
| 1 | 29-A | 114 | HIS |
| 1 | 29-A | 118 | GLU |
| 1 | 29-A | 129 | GLU |
| 1 | 29-A | 140 | PHE |
| 1 | 29-A | 144 | ASP |
| 1 | 29-A | 154 | GLU |
| 1 | 29-A | 157 | GLU |
| 1 | 30-A | 16 | MET |
| 1 | 30-A | 20 | MET |
| 1 | 30-A | 33 | ARG |
| 1 | 30-A | 59 | ASN |
| 1 | 30-A | 62 | LEU |
| 1 | 30-A | 87 | ASP |
| 1 | 30-A | 101 | GLU |
| 1 | 30-A | 114 | HIS |
| 1 | 30-A | 119 | VAL |
| 1 | 30-A | 127 | ASP |
| 1 | 30-A | 134 | GLU |
| 1 | 30-A | 137 | PHE |
| 1 | 30-A | 144 | ASP |
| 1 | 30-A | 156 | LEU |
| 1 | 30-A | 157 | GLU |
| 1 | 31-A | 16 | MET |
| 1 | 31-A | 18 | ASN |
| 1 | 31-A | 23 | ASN |
| 1 | 31-A | 33 | ARG |
| 1 | 31-A | 49 | SER |
| 1 | 31-A | 58 | LYS |
| 1 | 31-A | 64 | SER |
| 1 | 31-A | 65 | GLN |
| 1 | 31-A | 108 | GLN |
| 1 | 31-A | 114 | HIS |
| 1 | 31-A | 119 | VAL |
| 1 | 31-A | 128 | TYR |
| 1 | 31-A | 129 | GLU |
| 1 | 31-A | 134 | GLU |
| 1 | 31-A | 144 | ASP |
| 1 | 31-A | 154 | GLU |
| 1 | 31-A | 159 | ARG |
| 1 | 32-A | 1 | MET |
| 1 | 32-A | 12 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 32-A | 16 | MET |
| 1 | 32-A | 18 | ASN |
| 1 | 32-A | 20 | MET |
| 1 | 32-A | 23 | ASN |
| 1 | 32-A | 24 | LEU |
| 1 | 32-A | 33 | ARG |
| 1 | 32-A | 36 | LEU |
| 1 | 32-A | 52 | ARG |
| 1 | 32-A | 59 | ASN |
| 1 | 32-A | 62 | LEU |
| 1 | 32-A | 65 | GLN |
| 1 | 32-A | 87 | ASP |
| 1 | 32-A | 98 | ARG |
| 1 | 32-A | 114 | HIS |
| 1 | 32-A | 118 | GLU |
| 1 | 32-A | 119 | VAL |
| 1 | 32-A | 128 | TYR |
| 1 | 32-A | 129 | GLU |
| 1 | 32-A | 134 | GLU |
| 1 | 32-A | 148 | SER |
| 1 | 32-A | 156 | LEU |
| 1 | 32-A | 159 | ARG |
| 1 | 33-A | 1 | MET |
| 1 | 33-A | 12 | ARG |
| 1 | 33-A | 16 | MET |
| 1 | 33-A | 23 | ASN |
| 1 | 33-A | 33 | ARG |
| 1 | 33-A | 36 | LEU |
| 1 | 33-A | 44 | ARG |
| 1 | 33-A | 58 | LYS |
| 1 | 33-A | 59 | ASN |
| 1 | 33-A | 62 | LEU |
| 1 | 33-A | 65 | GLN |
| 1 | 33-A | 76 | LYS |
| 1 | 33-A | 79 | ASP |
| 1 | 33-A | 98 | ARG |
| 1 | 33-A | 108 | GLN |
| 1 | 33-A | 114 | HIS |
| 1 | 33-A | 118 | GLU |
| 1 | 33-A | 119 | VAL |
| 1 | 33-A | 128 | TYR |
| 1 | 33-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 33-A | 132 | ASP |
| 1 | 33-A | 134 | GLU |
| 1 | 33-A | 154 | GLU |
| 1 | 34-A | 1 | MET |
| 1 | 34-A | 2 | ILE |
| 1 | 34-A | 12 | ARG |
| 1 | 34-A | 20 | MET |
| 1 | 34-A | 24 | LEU |
| 1 | 34-A | 28 | LEU |
| 1 | 34-A | 33 | ARG |
| 1 | 34-A | 58 | LYS |
| 1 | 34-A | 59 | ASN |
| 1 | 34-A | 65 | GLN |
| 1 | 34-A | 76 | LYS |
| 1 | 34-A | 114 | HIS |
| 1 | 34-A | 127 | ASP |
| 1 | 34-A | 128 | TYR |
| 1 | 34-A | 134 | GLU |
| 1 | 34-A | 138 | SER |
| 1 | 34-A | 154 | GLU |
| 1 | 35-A | 1 | MET |
| 1 | 35-A | 12 | ARG |
| 1 | 35-A | 16 | MET |
| 1 | 35-A | 20 | MET |
| 1 | 35-A | 24 | LEU |
| 1 | 35-A | 28 | LEU |
| 1 | 35-A | 33 | ARG |
| 1 | 35-A | 58 | LYS |
| 1 | 35-A | 59 | ASN |
| 1 | 35-A | 65 | GLN |
| 1 | 35-A | 76 | LYS |
| 1 | 35-A | 79 | ASP |
| 1 | 35-A | 88 | VAL |
| 1 | 35-A | 108 | GLN |
| 1 | 35-A | 119 | VAL |
| 1 | 35-A | 127 | ASP |
| 1 | 35-A | 128 | TYR |
| 1 | 35-A | 132 | ASP |
| 1 | 35-A | 154 | GLU |
| 1 | 35-A | 159 | ARG |
| 1 | 36-A | 11 | ASP |
| 1 | 36-A | 12 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 36-A | 20 | MET |
| 1 | 36-A | 28 | LEU |
| 1 | 36-A | 37 | ASN |
| 1 | 36-A | 58 | LYS |
| 1 | 36-A | 65 | GLN |
| 1 | 36-A | 76 | LYS |
| 1 | 36-A | 108 | GLN |
| 1 | 36-A | 118 | GLU |
| 1 | 36-A | 119 | VAL |
| 1 | 36-A | 127 | ASP |
| 1 | 36-A | 128 | TYR |
| 1 | 36-A | 129 | GLU |
| 1 | 36-A | 134 | GLU |
| 1 | 36-A | 139 | GLU |
| 1 | 36-A | 146 | GLN |
| 1 | 37-A | 1 | MET |
| 1 | 37-A | 20 | MET |
| 1 | 37-A | 21 | PRO |
| 1 | 37-A | 37 | ASN |
| 1 | 37-A | 54 | LEU |
| 1 | 37-A | 58 | LYS |
| 1 | 37-A | 59 | ASN |
| 1 | 37-A | 62 | LEU |
| 1 | 37-A | 87 | ASP |
| 1 | 37-A | 105 | PRO |
| 1 | 37-A | 106 | LYS |
| 1 | 37-A | 114 | HIS |
| 1 | 37-A | 127 | ASP |
| 1 | 37-A | 129 | GLU |
| 1 | 37-A | 146 | GLN |
| 1 | 37-A | 150 | SER |
| 1 | 37-A | 158 | ARG |
| 1 | 38-A | 1 | MET |
| 1 | 38-A | 2 | ILE |
| 1 | 38-A | 8 | LEU |
| 1 | 38-A | 12 | ARG |
| 1 | 38-A | 16 | MET |
| 1 | 38-A | 20 | MET |
| 1 | 38-A | 21 | PRO |
| 1 | 38-A | 22 | TRP |
| 1 | 38-A | 37 | ASN |
| 1 | 38-A | 54 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 38-A | 58 | LYS |
| 1 | 38-A | 59 | ASN |
| 1 | 38-A | 101 | GLU |
| 1 | 38-A | 106 | LYS |
| 1 | 38-A | 114 | HIS |
| 1 | 38-A | 138 | SER |
| 1 | 38-A | 150 | SER |
| 1 | 39-A | 1 | MET |
| 1 | 39-A | 11 | ASP |
| 1 | 39-A | 12 | ARG |
| 1 | 39-A | 20 | MET |
| 1 | 39-A | 21 | PRO |
| 1 | 39-A | 22 | TRP |
| 1 | 39-A | 24 | LEU |
| 1 | 39-A | 37 | ASN |
| 1 | 39-A | 44 | ARG |
| 1 | 39-A | 58 | LYS |
| 1 | 39-A | 60 | ILE |
| 1 | 39-A | 62 | LEU |
| 1 | 39-A | 102 | GLN |
| 1 | 39-A | 106 | LYS |
| 1 | 39-A | 108 | GLN |
| 1 | 39-A | 114 | HIS |
| 1 | 39-A | 127 | ASP |
| 1 | 39-A | 128 | TYR |
| 1 | 39-A | 129 | GLU |
| 1 | 39-A | 134 | GLU |
| 1 | 39-A | 148 | SER |
| 1 | 40-A | 1 | MET |
| 1 | 40-A | 11 | ASP |
| 1 | 40-A | 20 | MET |
| 1 | 40-A | 21 | PRO |
| 1 | 40-A | 22 | TRP |
| 1 | 40-A | 37 | ASN |
| 1 | 40-A | 54 | LEU |
| 1 | 40-A | 58 | LYS |
| 1 | 40-A | 60 | ILE |
| 1 | 40-A | 87 | ASP |
| 1 | 40-A | 101 | GLU |
| 1 | 40-A | 106 | LYS |
| 1 | 40-A | 108 | GLN |
| 1 | 40-A | 118 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 40-A | 128 | TYR |
| 1 | 40-A | 129 | GLU |
| 1 | 40-A | 148 | SER |
| 1 | 41-A | 1 | MET |
| 1 | 41-A | 11 | ASP |
| 1 | 41-A | 21 | PRO |
| 1 | 41-A | 33 | ARG |
| 1 | 41-A | 48 | GLU |
| 1 | 41-A | 58 | LYS |
| 1 | 41-A | 66 | PRO |
| 1 | 41-A | 79 | ASP |
| 1 | 41-A | 98 | ARG |
| 1 | 41-A | 101 | GLU |
| 1 | 41-A | 104 | LEU |
| 1 | 41-A | 106 | LYS |
| 1 | 41-A | 108 | GLN |
| 1 | 41-A | 128 | TYR |
| 1 | 41-A | 129 | GLU |
| 1 | 41-A | 148 | SER |
| 1 | 41-A | 156 | LEU |
| 1 | 42-A | 12 | ARG |
| 1 | 42-A | 18 | ASN |
| 1 | 42-A | 20 | MET |
| 1 | 42-A | 24 | LEU |
| 1 | 42-A | 33 | ARG |
| 1 | 42-A | 37 | ASN |
| 1 | 42-A | 48 | GLU |
| 1 | 42-A | 58 | LYS |
| 1 | 42-A | 65 | GLN |
| 1 | 42-A | 70 | ASP |
| 1 | 42-A | 87 | ASP |
| 1 | 42-A | 101 | GLU |
| 1 | 42-A | 104 | LEU |
| 1 | 42-A | 127 | ASP |
| 1 | 42-A | 128 | TYR |
| 1 | 42-A | 129 | GLU |
| 1 | 42-A | 139 | GLU |
| 1 | 43-A | 12 | ARG |
| 1 | 43-A | 16 | MET |
| 1 | 43-A | 18 | ASN |
| 1 | 43-A | 21 | PRO |
| 1 | 43-A | 24 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 43-A | 33 | ARG |
| 1 | 43-A | 44 | ARG |
| 1 | 43-A | 54 | LEU |
| 1 | 43-A | 58 | LYS |
| 1 | 43-A | 65 | GLN |
| 1 | 43-A | 98 | ARG |
| 1 | 43-A | 101 | GLU |
| 1 | 43-A | 102 | GLN |
| 1 | 43-A | 106 | LYS |
| 1 | 43-A | 119 | VAL |
| 1 | 43-A | 120 | GLU |
| 1 | 43-A | 127 | ASP |
| 1 | 43-A | 128 | TYR |
| 1 | 43-A | 129 | GLU |
| 1 | 43-A | 138 | SER |
| 1 | 43-A | 148 | SER |
| 1 | 43-A | 154 | GLU |
| 1 | 43-A | 159 | ARG |
| 1 | 44-A | 12 | ARG |
| 1 | 44-A | 20 | MET |
| 1 | 44-A | 22 | TRP |
| 1 | 44-A | 23 | ASN |
| 1 | 44-A | 24 | LEU |
| 1 | 44-A | 33 | ARG |
| 1 | 44-A | 44 | ARG |
| 1 | 44-A | 50 | ILE |
| 1 | 44-A | 52 | ARG |
| 1 | 44-A | 54 | LEU |
| 1 | 44-A | 65 | GLN |
| 1 | 44-A | 76 | LYS |
| 1 | 44-A | 79 | ASP |
| 1 | 44-A | 98 | ARG |
| 1 | 44-A | 101 | GLU |
| 1 | 44-A | 104 | LEU |
| 1 | 44-A | 106 | LYS |
| 1 | 44-A | 127 | ASP |
| 1 | 44-A | 128 | TYR |
| 1 | 44-A | 129 | GLU |
| 1 | 44-A | 132 | ASP |
| 1 | 45-A | 1 | MET |
| 1 | 45-A | 11 | ASP |
| 1 | 45-A | 12 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 45-A | 16 | MET |
| 1 | 45-A | 18 | ASN |
| 1 | 45-A | 20 | MET |
| 1 | 45-A | 22 | TRP |
| 1 | 45-A | 24 | LEU |
| 1 | 45-A | 33 | ARG |
| 1 | 45-A | 44 | ARG |
| 1 | 45-A | 58 | LYS |
| 1 | 45-A | 98 | ARG |
| 1 | 45-A | 102 | GLN |
| 1 | 45-A | 104 | LEU |
| 1 | 45-A | 106 | LYS |
| 1 | 45-A | 108 | GLN |
| 1 | 45-A | 118 | GLU |
| 1 | 45-A | 126 | PRO |
| 1 | 45-A | 128 | TYR |
| 1 | 45-A | 134 | GLU |
| 1 | 45-A | 154 | GLU |
| 1 | 45-A | 156 | LEU |
| 1 | 45-A | 159 | ARG |
| 1 | 46-A | 1 | MET |
| 1 | 46-A | 11 | ASP |
| 1 | 46-A | 12 | ARG |
| 1 | 46-A | 20 | MET |
| 1 | 46-A | 22 | TRP |
| 1 | 46-A | 44 | ARG |
| 1 | 46-A | 54 | LEU |
| 1 | 46-A | 58 | LYS |
| 1 | 46-A | 87 | ASP |
| 1 | 46-A | 98 | ARG |
| 1 | 46-A | 104 | LEU |
| 1 | 46-A | 106 | LYS |
| 1 | 46-A | 127 | ASP |
| 1 | 46-A | 128 | TYR |
| 1 | 46-A | 129 | GLU |
| 1 | 46-A | 132 | ASP |
| 1 | 46-A | 135 | SER |
| 1 | 46-A | 154 | GLU |
| 1 | 47-A | 4 | LEU |
| 1 | 47-A | 11 | ASP |
| 1 | 47-A | 12 | ARG |
| 1 | 47-A | 18 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 47-A | 22 | TRP |
| 1 | 47-A | 33 | ARG |
| 1 | 47-A | 48 | GLU |
| 1 | 47-A | 54 | LEU |
| 1 | 47-A | 58 | LYS |
| 1 | 47-A | 87 | ASP |
| 1 | 47-A | 98 | ARG |
| 1 | 47-A | 104 | LEU |
| 1 | 47-A | 106 | LYS |
| 1 | 47-A | 119 | VAL |
| 1 | 47-A | 127 | ASP |
| 1 | 47-A | 128 | TYR |
| 1 | 47-A | 154 | GLU |
| 1 | 48-A | 1 | MET |
| 1 | 48-A | 4 | LEU |
| 1 | 48-A | 12 | ARG |
| 1 | 48-A | 18 | ASN |
| 1 | 48-A | 22 | TRP |
| 1 | 48-A | 24 | LEU |
| 1 | 48-A | 33 | ARG |
| 1 | 48-A | 44 | ARG |
| 1 | 48-A | 48 | GLU |
| 1 | 48-A | 52 | ARG |
| 1 | 48-A | 60 | ILE |
| 1 | 48-A | 66 | PRO |
| 1 | 48-A | 76 | LYS |
| 1 | 48-A | 98 | ARG |
| 1 | 48-A | 106 | LYS |
| 1 | 48-A | 109 | LYS |
| 1 | 48-A | 119 | VAL |
| 1 | 48-A | 127 | ASP |
| 1 | 48-A | 142 | ASP |
| 1 | 48-A | 154 | GLU |
| 1 | 49-A | 1 | MET |
| 1 | 49-A | 12 | ARG |
| 1 | 49-A | 16 | MET |
| 1 | 49-A | 22 | TRP |
| 1 | 49-A | 23 | ASN |
| 1 | 49-A | 24 | LEU |
| 1 | 49-A | 33 | ARG |
| 1 | 49-A | 44 | ARG |
| 1 | 49-A | 48 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 49-A | 52 | ARG |
| 1 | 49-A | 54 | LEU |
| 1 | 49-A | 58 | LYS |
| 1 | 49-A | 76 | LYS |
| 1 | 49-A | 98 | ARG |
| 1 | 49-A | 109 | LYS |
| 1 | 49-A | 116 | ASP |
| 1 | 49-A | 120 | GLU |
| 1 | 49-A | 127 | ASP |
| 1 | 49-A | 136 | VAL |
| 1 | 49-A | 154 | GLU |
| 1 | 49-A | 155 | ILE |
| 1 | 50-A | 1 | MET |
| 1 | 50-A | 18 | ASN |
| 1 | 50-A | 22 | TRP |
| 1 | 50-A | 44 | ARG |
| 1 | 50-A | 58 | LYS |
| 1 | 50-A | 60 | ILE |
| 1 | 50-A | 65 | GLN |
| 1 | 50-A | 76 | LYS |
| 1 | 50-A | 87 | ASP |
| 1 | 50-A | 98 | ARG |
| 1 | 50-A | 109 | LYS |
| 1 | 50-A | 116 | ASP |
| 1 | 50-A | 120 | GLU |
| 1 | 50-A | 128 | TYR |
| 1 | 50-A | 148 | SER |
| 1 | 50-A | 154 | GLU |
| 1 | 51-A | 1 | MET |
| 1 | 51-A | 12 | ARG |
| 1 | 51-A | 18 | ASN |
| 1 | 51-A | 20 | MET |
| 1 | 51-A | 22 | TRP |
| 1 | 51-A | 44 | ARG |
| 1 | 51-A | 54 | LEU |
| 1 | 51-A | 70 | ASP |
| 1 | 51-A | 98 | ARG |
| 1 | 51-A | 118 | GLU |
| 1 | 51-A | 119 | VAL |
| 1 | 51-A | 120 | GLU |
| 1 | 51-A | 127 | ASP |
| 1 | 51-A | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 51-A | 134 | GLU |
| 1 | 51-A | 135 | SER |
| 1 | 51-A | 138 | SER |
| 1 | 52-A | 1 | MET |
| 1 | 52-A | 22 | TRP |
| 1 | 52-A | 23 | ASN |
| 1 | 52-A | 44 | ARG |
| 1 | 52-A | 49 | SER |
| 1 | 52-A | 52 | ARG |
| 1 | 52-A | 65 | GLN |
| 1 | 52-A | 79 | ASP |
| 1 | 52-A | 98 | ARG |
| 1 | 52-A | 118 | GLU |
| 1 | 52-A | 127 | ASP |
| 1 | 52-A | 128 | TYR |
| 1 | 52-A | 129 | GLU |
| 1 | 53-A | 17 | GLU |
| 1 | 53-A | 18 | ASN |
| 1 | 53-A | 22 | TRP |
| 1 | 53-A | 23 | ASN |
| 1 | 53-A | 44 | ARG |
| 1 | 53-A | 52 | ARG |
| 1 | 53-A | 54 | LEU |
| 1 | 53-A | 61 | ILE |
| 1 | 53-A | 65 | GLN |
| 1 | 53-A | 78 | VAL |
| 1 | 53-A | 79 | ASP |
| 1 | 53-A | 120 | GLU |
| 1 | 53-A | 127 | ASP |
| 1 | 53-A | 128 | TYR |
| 1 | 53-A | 135 | SER |
| 1 | 53-A | 148 | SER |
| 1 | 54-A | 1 | MET |
| 1 | 54-A | 16 | MET |
| 1 | 54-A | 18 | ASN |
| 1 | 54-A | 21 | PRO |
| 1 | 54-A | 24 | LEU |
| 1 | 54-A | 44 | ARG |
| 1 | 54-A | 65 | GLN |
| 1 | 54-A | 78 | VAL |
| 1 | 54-A | 79 | ASP |
| 1 | 54-A | 106 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 54-A | 108 | GLN |
| 1 | 54-A | 128 | TYR |
| 1 | 54-A | 132 | ASP |
| 1 | 54-A | 146 | GLN |
| 1 | 54-A | 154 | GLU |
| 1 | 55-A | 1 | MET |
| 1 | 55-A | 2 | ILE |
| 1 | 55-A | 12 | ARG |
| 1 | 55-A | 16 | MET |
| 1 | 55-A | 24 | LEU |
| 1 | 55-A | 33 | ARG |
| 1 | 55-A | 44 | ARG |
| 1 | 55-A | 52 | ARG |
| 1 | 55-A | 78 | VAL |
| 1 | 55-A | 106 | LYS |
| 1 | 55-A | 109 | LYS |
| 1 | 55-A | 114 | HIS |
| 1 | 55-A | 128 | TYR |
| 1 | 55-A | 131 | ASP |
| 1 | 55-A | 146 | GLN |
| 1 | 56-A | 1 | MET |
| 1 | 56-A | 2 | ILE |
| 1 | 56-A | 8 | LEU |
| 1 | 56-A | 12 | ARG |
| 1 | 56-A | 16 | MET |
| 1 | 56-A | 18 | ASN |
| 1 | 56-A | 24 | LEU |
| 1 | 56-A | 28 | LEU |
| 1 | 56-A | 33 | ARG |
| 1 | 56-A | 48 | GLU |
| 1 | 56-A | 52 | ARG |
| 1 | 56-A | 65 | GLN |
| 1 | 56-A | 70 | ASP |
| 1 | 56-A | 78 | VAL |
| 1 | 56-A | 98 | ARG |
| 1 | 56-A | 102 | GLN |
| 1 | 56-A | 106 | LYS |
| 1 | 56-A | 109 | LYS |
| 1 | 56-A | 120 | GLU |
| 1 | 56-A | 127 | ASP |
| 1 | 56-A | 128 | TYR |
| 1 | 56-A | 131 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 56-A | 138 | SER |
| 1 | 56-A | 146 | GLN |
| 1 | 57-A | 11 | ASP |
| 1 | 57-A | 12 | ARG |
| 1 | 57-A | 24 | LEU |
| 1 | 57-A | 48 | GLU |
| 1 | 57-A | 58 | LYS |
| 1 | 57-A | 68 | THR |
| 1 | 57-A | 70 | ASP |
| 1 | 57-A | 98 | ARG |
| 1 | 57-A | 106 | LYS |
| 1 | 57-A | 108 | GLN |
| 1 | 57-A | 119 | VAL |
| 1 | 57-A | 127 | ASP |
| 1 | 57-A | 128 | TYR |
| 1 | 57-A | 134 | GLU |
| 1 | 57-A | 135 | SER |
| 1 | 57-A | 148 | SER |
| 1 | 57-A | 154 | GLU |
| 1 | 58-A | 1 | MET |
| 1 | 58-A | 16 | MET |
| 1 | 58-A | 23 | ASN |
| 1 | 58-A | 33 | ARG |
| 1 | 58-A | 48 | GLU |
| 1 | 58-A | 49 | SER |
| 1 | 58-A | 70 | ASP |
| 1 | 58-A | 87 | ASP |
| 1 | 58-A | 98 | ARG |
| 1 | 58-A | 108 | GLN |
| 1 | 58-A | 128 | TYR |
| 1 | 58-A | 139 | GLU |
| 1 | 58-A | 146 | GLN |
| 1 | 58-A | 154 | GLU |
| 1 | 59-A | 1 | MET |
| 1 | 59-A | 11 | ASP |
| 1 | 59-A | 16 | MET |
| 1 | 59-A | 20 | MET |
| 1 | 59-A | 23 | ASN |
| 1 | 59-A | 24 | LEU |
| 1 | 59-A | 33 | ARG |
| 1 | 59-A | 68 | THR |
| 1 | 59-A | 78 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 59-A | 98 | ARG |
| 1 | 59-A | 101 | GLU |
| 1 | 59-A | 106 | LYS |
| 1 | 59-A | 108 | GLN |
| 1 | 59-A | 118 | GLU |
| 1 | 59-A | 119 | VAL |
| 1 | 59-A | 120 | GLU |
| 1 | 59-A | 127 | ASP |
| 1 | 59-A | 128 | TYR |
| 1 | 59-A | 138 | SER |
| 1 | 59-A | 139 | GLU |
| 1 | 59-A | 159 | ARG |
| 1 | 60-A | 1 | MET |
| 1 | 60-A | 2 | ILE |
| 1 | 60-A | 12 | ARG |
| 1 | 60-A | 16 | MET |
| 1 | 60-A | 18 | ASN |
| 1 | 60-A | 20 | MET |
| 1 | 60-A | 23 | ASN |
| 1 | 60-A | 24 | LEU |
| 1 | 60-A | 52 | ARG |
| 1 | 60-A | 58 | LYS |
| 1 | 60-A | 62 | LEU |
| 1 | 60-A | 79 | ASP |
| 1 | 60-A | 118 | GLU |
| 1 | 60-A | 119 | VAL |
| 1 | 60-A | 128 | TYR |
| 1 | 60-A | 157 | GLU |
| 1 | 61-A | 1 | MET |
| 1 | 61-A | 8 | LEU |
| 1 | 61-A | 16 | MET |
| 1 | 61-A | 28 | LEU |
| 1 | 61-A | 30 | TRP |
| 1 | 61-A | 37 | ASN |
| 1 | 61-A | 52 | ARG |
| 1 | 61-A | 102 | GLN |
| 1 | 61-A | 120 | GLU |
| 1 | 61-A | 128 | TYR |
| 1 | 61-A | 132 | ASP |
| 1 | 61-A | 138 | SER |
| 1 | 61-A | 156 | LEU |
| 1 | 61-A | 159 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 62-A | 1 | MET |
| 1 | 62-A | 11 | ASP |
| 1 | 62-A | 12 | ARG |
| 1 | 62-A | 16 | MET |
| 1 | 62-A | 23 | ASN |
| 1 | 62-A | 24 | LEU |
| 1 | 62-A | 28 | LEU |
| 1 | 62-A | 33 | ARG |
| 1 | 62-A | 36 | LEU |
| 1 | 62-A | 61 | ILE |
| 1 | 62-A | 78 | VAL |
| 1 | 62-A | 102 | GLN |
| 1 | 62-A | 120 | GLU |
| 1 | 62-A | 128 | TYR |
| 1 | 62-A | 132 | ASP |
| 1 | 62-A | 146 | GLN |
| 1 | 63-A | 1 | MET |
| 1 | 63-A | 16 | MET |
| 1 | 63-A | 24 | LEU |
| 1 | 63-A | 33 | ARG |
| 1 | 63-A | 49 | SER |
| 1 | 63-A | 52 | ARG |
| 1 | 63-A | 58 | LYS |
| 1 | 63-A | 76 | LYS |
| 1 | 63-A | 78 | VAL |
| 1 | 63-A | 98 | ARG |
| 1 | 63-A | 119 | VAL |
| 1 | 63-A | 120 | GLU |
| 1 | 63-A | 128 | TYR |
| 1 | 63-A | 148 | SER |
| 1 | 64-A | 1 | MET |
| 1 | 64-A | 11 | ASP |
| 1 | 64-A | 16 | MET |
| 1 | 64-A | 24 | LEU |
| 1 | 64-A | 28 | LEU |
| 1 | 64-A | 33 | ARG |
| 1 | 64-A | 44 | ARG |
| 1 | 64-A | 52 | ARG |
| 1 | 64-A | 68 | THR |
| 1 | 64-A | 70 | ASP |
| 1 | 64-A | 79 | ASP |
| 1 | 64-A | 87 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 64-A | 98 | ARG |
| 1 | 64-A | 119 | VAL |
| 1 | 64-A | 126 | PRO |
| 1 | 64-A | 128 | TYR |
| 1 | 64-A | 137 | PHE |
| 1 | 64-A | 159 | ARG |
| 1 | 65-A | 1 | MET |
| 1 | 65-A | 4 | LEU |
| 1 | 65-A | 11 | ASP |
| 1 | 65-A | 12 | ARG |
| 1 | 65-A | 16 | MET |
| 1 | 65-A | 18 | ASN |
| 1 | 65-A | 24 | LEU |
| 1 | 65-A | 49 | SER |
| 1 | 65-A | 58 | LYS |
| 1 | 65-A | 79 | ASP |
| 1 | 65-A | 106 | LYS |
| 1 | 65-A | 118 | GLU |
| 1 | 65-A | 126 | PRO |
| 1 | 65-A | 127 | ASP |
| 1 | 65-A | 128 | TYR |
| 1 | 65-A | 129 | GLU |
| 1 | 65-A | 138 | SER |
| 1 | 65-A | 140 | PHE |
| 1 | 65-A | 148 | SER |
| 1 | 65-A | 159 | ARG |
| 1 | 66-A | 12 | ARG |
| 1 | 66-A | 18 | ASN |
| 1 | 66-A | 24 | LEU |
| 1 | 66-A | 25 | PRO |
| 1 | 66-A | 33 | ARG |
| 1 | 66-A | 52 | ARG |
| 1 | 66-A | 106 | LYS |
| 1 | 66-A | 118 | GLU |
| 1 | 66-A | 119 | VAL |
| 1 | 66-A | 127 | ASP |
| 1 | 66-A | 129 | GLU |
| 1 | 66-A | 139 | GLU |
| 1 | 67-A | 12 | ARG |
| 1 | 67-A | 16 | MET |
| 1 | 67-A | 18 | ASN |
| 1 | 67-A | 24 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 67-A | 33 | ARG |
| 1 | 67-A | 49 | SER |
| 1 | 67-A | 52 | ARG |
| 1 | 67-A | 65 | GLN |
| 1 | 67-A | 77 | SER |
| 1 | 67-A | 79 | ASP |
| 1 | 67-A | 106 | LYS |
| 1 | 67-A | 118 | GLU |
| 1 | 67-A | 119 | VAL |
| 1 | 67-A | 120 | GLU |
| 1 | 67-A | 128 | TYR |
| 1 | 67-A | 129 | GLU |
| 1 | 67-A | 139 | GLU |
| 1 | 67-A | 159 | ARG |
| 1 | 68-A | 1 | MET |
| 1 | 68-A | 16 | MET |
| 1 | 68-A | 18 | ASN |
| 1 | 68-A | 23 | ASN |
| 1 | 68-A | 24 | LEU |
| 1 | 68-A | 33 | ARG |
| 1 | 68-A | 36 | LEU |
| 1 | 68-A | 52 | ARG |
| 1 | 68-A | 58 | LYS |
| 1 | 68-A | 65 | GLN |
| 1 | 68-A | 79 | ASP |
| 1 | 68-A | 89 | PRO |
| 1 | 68-A | 106 | LYS |
| 1 | 68-A | 116 | ASP |
| 1 | 68-A | 118 | GLU |
| 1 | 68-A | 120 | GLU |
| 1 | 68-A | 128 | TYR |
| 1 | 68-A | 129 | GLU |
| 1 | 68-A | 134 | GLU |
| 1 | 68-A | 135 | SER |
| 1 | 68-A | 146 | GLN |
| 1 | 68-A | 159 | ARG |
| 1 | 69-A | 1 | MET |
| 1 | 69-A | 16 | MET |
| 1 | 69-A | 17 | GLU |
| 1 | 69-A | 18 | ASN |
| 1 | 69-A | 20 | MET |
| 1 | 69-A | 32 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 69-A | 33 | ARG |
| 1 | 69-A | 37 | ASN |
| 1 | 69-A | 45 | HIS |
| 1 | 69-A | 52 | ARG |
| 1 | 69-A | 61 | ILE |
| 1 | 69-A | 79 | ASP |
| 1 | 69-A | 98 | ARG |
| 1 | 69-A | 106 | LYS |
| 1 | 69-A | 108 | GLN |
| 1 | 69-A | 116 | ASP |
| 1 | 69-A | 127 | ASP |
| 1 | 69-A | 129 | GLU |
| 1 | 69-A | 146 | GLN |
| 1 | 69-A | 155 | ILE |
| 1 | 69-A | 156 | LEU |
| 1 | 69-A | 159 | ARG |
| 1 | 70-A | 1 | MET |
| 1 | 70-A | 16 | MET |
| 1 | 70-A | 17 | GLU |
| 1 | 70-A | 20 | MET |
| 1 | 70-A | 22 | TRP |
| 1 | 70-A | 23 | ASN |
| 1 | 70-A | 32 | LYS |
| 1 | 70-A | 37 | ASN |
| 1 | 70-A | 44 | ARG |
| 1 | 70-A | 52 | ARG |
| 1 | 70-A | 61 | ILE |
| 1 | 70-A | 76 | LYS |
| 1 | 70-A | 79 | ASP |
| 1 | 70-A | 88 | VAL |
| 1 | 70-A | 101 | GLU |
| 1 | 70-A | 102 | GLN |
| 1 | 70-A | 106 | LYS |
| 1 | 70-A | 116 | ASP |
| 1 | 70-A | 118 | GLU |
| 1 | 70-A | 129 | GLU |
| 1 | 70-A | 146 | GLN |
| 1 | 70-A | 148 | SER |
| 1 | 71-A | 1 | MET |
| 1 | 71-A | 16 | MET |
| 1 | 71-A | 18 | ASN |
| 1 | 71-A | 23 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 71-A | 32 | LYS |
| 1 | 71-A | 36 | LEU |
| 1 | 71-A | 37 | ASN |
| 1 | 71-A | 44 | ARG |
| 1 | 71-A | 52 | ARG |
| 1 | 71-A | 61 | ILE |
| 1 | 71-A | 65 | GLN |
| 1 | 71-A | 68 | THR |
| 1 | 71-A | 76 | LYS |
| 1 | 71-A | 79 | ASP |
| 1 | 71-A | 106 | LYS |
| 1 | 71-A | 116 | ASP |
| 1 | 71-A | 118 | GLU |
| 1 | 71-A | 120 | GLU |
| 1 | 71-A | 127 | ASP |
| 1 | 71-A | 129 | GLU |
| 1 | 71-A | 135 | SER |
| 1 | 72-A | 1 | MET |
| 1 | 72-A | 16 | MET |
| 1 | 72-A | 22 | TRP |
| 1 | 72-A | 23 | ASN |
| 1 | 72-A | 33 | ARG |
| 1 | 72-A | 36 | LEU |
| 1 | 72-A | 37 | ASN |
| 1 | 72-A | 44 | ARG |
| 1 | 72-A | 49 | SER |
| 1 | 72-A | 52 | ARG |
| 1 | 72-A | 58 | LYS |
| 1 | 72-A | 62 | LEU |
| 1 | 72-A | 76 | LYS |
| 1 | 72-A | 106 | LYS |
| 1 | 72-A | 118 | GLU |
| 1 | 72-A | 120 | GLU |
| 1 | 72-A | 135 | SER |
| 1 | 73-A | 1 | MET |
| 1 | 73-A | 18 | ASN |
| 1 | 73-A | 20 | MET |
| 1 | 73-A | 36 | LEU |
| 1 | 73-A | 37 | ASN |
| 1 | 73-A | 52 | ARG |
| 1 | 73-A | 58 | LYS |
| 1 | 73-A | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 73-A | 76 | LYS |
| 1 | 73-A | 108 | GLN |
| 1 | 73-A | 118 | GLU |
| 1 | 73-A | 119 | VAL |
| 1 | 73-A | 128 | TYR |
| 1 | 73-A | 138 | SER |
| 1 | 73-A | 144 | ASP |
| 1 | 73-A | 154 | GLU |
| 1 | 74-A | 1 | MET |
| 1 | 74-A | 8 | LEU |
| 1 | 74-A | 16 | MET |
| 1 | 74-A | 18 | ASN |
| 1 | 74-A | 22 | TRP |
| 1 | 74-A | 23 | ASN |
| 1 | 74-A | 24 | LEU |
| 1 | 74-A | 28 | LEU |
| 1 | 74-A | 36 | LEU |
| 1 | 74-A | 44 | ARG |
| 1 | 74-A | 52 | ARG |
| 1 | 74-A | 58 | LYS |
| 1 | 74-A | 68 | THR |
| 1 | 74-A | 106 | LYS |
| 1 | 74-A | 108 | GLN |
| 1 | 74-A | 119 | VAL |
| 1 | 74-A | 129 | GLU |
| 1 | 74-A | 144 | ASP |
| 1 | 74-A | 156 | LEU |
| 1 | 75-A | 1 | MET |
| 1 | 75-A | 8 | LEU |
| 1 | 75-A | 20 | MET |
| 1 | 75-A | 22 | TRP |
| 1 | 75-A | 23 | ASN |
| 1 | 75-A | 30 | TRP |
| 1 | 75-A | 32 | LYS |
| 1 | 75-A | 33 | ARG |
| 1 | 75-A | 44 | ARG |
| 1 | 75-A | 48 | GLU |
| 1 | 75-A | 62 | LEU |
| 1 | 75-A | 65 | GLN |
| 1 | 75-A | 79 | ASP |
| 1 | 75-A | 87 | ASP |
| 1 | 75-A | 106 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 75-A | 128 | TYR |
| 1 | 75-A | 129 | GLU |
| 1 | 75-A | 148 | SER |
| 1 | 75-A | 158 | ARG |
| 1 | 76-A | 1 | MET |
| 1 | 76-A | 2 | ILE |
| 1 | 76-A | 8 | LEU |
| 1 | 76-A | 22 | TRP |
| 1 | 76-A | 24 | LEU |
| 1 | 76-A | 44 | ARG |
| 1 | 76-A | 62 | LEU |
| 1 | 76-A | 70 | ASP |
| 1 | 76-A | 76 | LYS |
| 1 | 76-A | 87 | ASP |
| 1 | 76-A | 104 | LEU |
| 1 | 76-A | 108 | GLN |
| 1 | 76-A | 129 | GLU |
| 1 | 76-A | 138 | SER |
| 1 | 76-A | 154 | GLU |
| 1 | 76-A | 158 | ARG |
| 1 | 77-A | 1 | MET |
| 1 | 77-A | 8 | LEU |
| 1 | 77-A | 18 | ASN |
| 1 | 77-A | 20 | MET |
| 1 | 77-A | 23 | ASN |
| 1 | 77-A | 58 | LYS |
| 1 | 77-A | 62 | LEU |
| 1 | 77-A | 127 | ASP |
| 1 | 77-A | 128 | TYR |
| 1 | 77-A | 129 | GLU |
| 1 | 77-A | 156 | LEU |
| 1 | 77-A | 158 | ARG |
| 1 | 78-A | 1 | MET |
| 1 | 78-A | 8 | LEU |
| 1 | 78-A | 18 | ASN |
| 1 | 78-A | 23 | ASN |
| 1 | 78-A | 44 | ARG |
| 1 | 78-A | 68 | THR |
| 1 | 78-A | 118 | GLU |
| 1 | 78-A | 127 | ASP |
| 1 | 78-A | 128 | TYR |
| 1 | 78-A | 132 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 78-A | 148 | SER |
| 1 | 79-A | 1 | MET |
| 1 | 79-A | 2 | ILE |
| 1 | 79-A | 4 | LEU |
| 1 | 79-A | 18 | ASN |
| 1 | 79-A | 21 | PRO |
| 1 | 79-A | 22 | TRP |
| 1 | 79-A | 23 | ASN |
| 1 | 79-A | 36 | LEU |
| 1 | 79-A | 44 | ARG |
| 1 | 79-A | 52 | ARG |
| 1 | 79-A | 70 | ASP |
| 1 | 79-A | 106 | LYS |
| 1 | 79-A | 119 | VAL |
| 1 | 79-A | 127 | ASP |
| 1 | 79-A | 128 | TYR |
| 1 | 79-A | 134 | GLU |
| 1 | 79-A | 135 | SER |
| 1 | 79-A | 148 | SER |
| 1 | 79-A | 156 | LEU |
| 1 | 79-A | 158 | ARG |
| 1 | 79-A | 159 | ARG |
| 1 | 80-A | 1 | MET |
| 1 | 80-A | 16 | MET |
| 1 | 80-A | 17 | GLU |
| 1 | 80-A | 22 | TRP |
| 1 | 80-A | 28 | LEU |
| 1 | 80-A | 58 | LYS |
| 1 | 80-A | 68 | THR |
| 1 | 80-A | 87 | ASP |
| 1 | 80-A | 101 | GLU |
| 1 | 80-A | 108 | GLN |
| 1 | 80-A | 119 | VAL |
| 1 | 80-A | 127 | ASP |
| 1 | 80-A | 129 | GLU |
| 1 | 80-A | 137 | PHE |
| 1 | 80-A | 138 | SER |
| 1 | 80-A | 156 | LEU |
| 1 | 80-A | 158 | ARG |
| 1 | 80-A | 159 | ARG |
| 1 | 81-A | 1 | MET |
| 1 | 81-A | 17 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 81-A | 20 | MET |
| 1 | 81-A | 22 | TRP |
| 1 | 81-A | 33 | ARG |
| 1 | 81-A | 52 | ARG |
| 1 | 81-A | 54 | LEU |
| 1 | 81-A | 58 | LYS |
| 1 | 81-A | 87 | ASP |
| 1 | 81-A | 98 | ARG |
| 1 | 81-A | 119 | VAL |
| 1 | 81-A | 127 | ASP |
| 1 | 81-A | 129 | GLU |
| 1 | 81-A | 130 | PRO |
| 1 | 81-A | 137 | PHE |
| 1 | 81-A | 156 | LEU |
| 1 | 81-A | 158 | ARG |
| 1 | 81-A | 159 | ARG |
| 1 | 82-A | 2 | ILE |
| 1 | 82-A | 17 | GLU |
| 1 | 82-A | 18 | ASN |
| 1 | 82-A | 20 | MET |
| 1 | 82-A | 23 | ASN |
| 1 | 82-A | 24 | LEU |
| 1 | 82-A | 33 | ARG |
| 1 | 82-A | 54 | LEU |
| 1 | 82-A | 58 | LYS |
| 1 | 82-A | 98 | ARG |
| 1 | 82-A | 101 | GLU |
| 1 | 82-A | 119 | VAL |
| 1 | 82-A | 120 | GLU |
| 1 | 82-A | 127 | ASP |
| 1 | 82-A | 129 | GLU |
| 1 | 82-A | 134 | GLU |
| 1 | 82-A | 158 | ARG |
| 1 | 83-A | 1 | MET |
| 1 | 83-A | 2 | ILE |
| 1 | 83-A | 10 | VAL |
| 1 | 83-A | 20 | MET |
| 1 | 83-A | 33 | ARG |
| 1 | 83-A | 58 | LYS |
| 1 | 83-A | 98 | ARG |
| 1 | 83-A | 108 | GLN |
| 1 | 83-A | 119 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 83-A | 120 | GLU |
| 1 | 83-A | 126 | PRO |
| 1 | 83-A | 127 | ASP |
| 1 | 83-A | 129 | GLU |
| 1 | 83-A | 138 | SER |
| 1 | 83-A | 148 | SER |
| 1 | 83-A | 158 | ARG |
| 1 | 84-A | 1 | MET |
| 1 | 84-A | 10 | VAL |
| 1 | 84-A | 18 | ASN |
| 1 | 84-A | 22 | TRP |
| 1 | 84-A | 44 | ARG |
| 1 | 84-A | 49 | SER |
| 1 | 84-A | 52 | ARG |
| 1 | 84-A | 58 | LYS |
| 1 | 84-A | 60 | ILE |
| 1 | 84-A | 76 | LYS |
| 1 | 84-A | 106 | LYS |
| 1 | 84-A | 108 | GLN |
| 1 | 84-A | 120 | GLU |
| 1 | 84-A | 126 | PRO |
| 1 | 84-A | 128 | TYR |
| 1 | 84-A | 129 | GLU |
| 1 | 84-A | 142 | ASP |
| 1 | 84-A | 154 | GLU |
| 1 | 85-A | 12 | ARG |
| 1 | 85-A | 20 | MET |
| 1 | 85-A | 22 | TRP |
| 1 | 85-A | 32 | LYS |
| 1 | 85-A | 33 | ARG |
| 1 | 85-A | 52 | ARG |
| 1 | 85-A | 54 | LEU |
| 1 | 85-A | 65 | GLN |
| 1 | 85-A | 104 | LEU |
| 1 | 85-A | 106 | LYS |
| 1 | 85-A | 108 | GLN |
| 1 | 85-A | 114 | HIS |
| 1 | 85-A | 118 | GLU |
| 1 | 85-A | 119 | VAL |
| 1 | 85-A | 126 | PRO |
| 1 | 85-A | 127 | ASP |
| 1 | 85-A | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 85-A | 138 | SER |
| 1 | 85-A | 148 | SER |
| 1 | 86-A | 12 | ARG |
| 1 | 86-A | 17 | GLU |
| 1 | 86-A | 20 | MET |
| 1 | 86-A | 32 | LYS |
| 1 | 86-A | 52 | ARG |
| 1 | 86-A | 54 | LEU |
| 1 | 86-A | 104 | LEU |
| 1 | 86-A | 108 | GLN |
| 1 | 86-A | 114 | HIS |
| 1 | 86-A | 119 | VAL |
| 1 | 86-A | 127 | ASP |
| 1 | 86-A | 128 | TYR |
| 1 | 86-A | 129 | GLU |
| 1 | 86-A | 130 | PRO |
| 1 | 86-A | 135 | SER |
| 1 | 86-A | 139 | GLU |
| 1 | 86-A | 158 | ARG |
| 1 | 87-A | 12 | ARG |
| 1 | 87-A | 17 | GLU |
| 1 | 87-A | 18 | ASN |
| 1 | 87-A | 20 | MET |
| 1 | 87-A | 21 | PRO |
| 1 | 87-A | 24 | LEU |
| 1 | 87-A | 33 | ARG |
| 1 | 87-A | 48 | GLU |
| 1 | 87-A | 52 | ARG |
| 1 | 87-A | 58 | LYS |
| 1 | 87-A | 70 | ASP |
| 1 | 87-A | 76 | LYS |
| 1 | 87-A | 79 | ASP |
| 1 | 87-A | 87 | ASP |
| 1 | 87-A | 88 | VAL |
| 1 | 87-A | 98 | ARG |
| 1 | 87-A | 104 | LEU |
| 1 | 87-A | 106 | LYS |
| 1 | 87-A | 108 | GLN |
| 1 | 87-A | 118 | GLU |
| 1 | 87-A | 119 | VAL |
| 1 | 87-A | 128 | TYR |
| 1 | 87-A | 139 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 88-A | 1 | MET |
| 1 | 88-A | 12 | ARG |
| 1 | 88-A | 16 | MET |
| 1 | 88-A | 17 | GLU |
| 1 | 88-A | 20 | MET |
| 1 | 88-A | 23 | ASN |
| 1 | 88-A | 44 | ARG |
| 1 | 88-A | 58 | LYS |
| 1 | 88-A | 65 | GLN |
| 1 | 88-A | 79 | ASP |
| 1 | 88-A | 104 | LEU |
| 1 | 88-A | 106 | LYS |
| 1 | 88-A | 108 | GLN |
| 1 | 88-A | 109 | LYS |
| 1 | 88-A | 119 | VAL |
| 1 | 88-A | 129 | GLU |
| 1 | 88-A | 132 | ASP |
| 1 | 88-A | 135 | SER |
| 1 | 88-A | 138 | SER |
| 1 | 89-A | 1 | MET |
| 1 | 89-A | 12 | ARG |
| 1 | 89-A | 17 | GLU |
| 1 | 89-A | 18 | ASN |
| 1 | 89-A | 20 | MET |
| 1 | 89-A | 21 | PRO |
| 1 | 89-A | 32 | LYS |
| 1 | 89-A | 33 | ARG |
| 1 | 89-A | 44 | ARG |
| 1 | 89-A | 52 | ARG |
| 1 | 89-A | 58 | LYS |
| 1 | 89-A | 61 | ILE |
| 1 | 89-A | 65 | GLN |
| 1 | 89-A | 76 | LYS |
| 1 | 89-A | 87 | ASP |
| 1 | 89-A | 104 | LEU |
| 1 | 89-A | 108 | GLN |
| 1 | 89-A | 109 | LYS |
| 1 | 89-A | 119 | VAL |
| 1 | 89-A | 128 | TYR |
| 1 | 89-A | 129 | GLU |
| 1 | 89-A | 132 | ASP |
| 1 | 90-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 90-A | 12 | ARG |
| 1 | 90-A | 20 | MET |
| 1 | 90-A | 22 | TRP |
| 1 | 90-A | 32 | LYS |
| 1 | 90-A | 44 | ARG |
| 1 | 90-A | 49 | SER |
| 1 | 90-A | 52 | ARG |
| 1 | 90-A | 70 | ASP |
| 1 | 90-A | 108 | GLN |
| 1 | 90-A | 109 | LYS |
| 1 | 90-A | 118 | GLU |
| 1 | 90-A | 119 | VAL |
| 1 | 90-A | 126 | PRO |
| 1 | 90-A | 127 | ASP |
| 1 | 90-A | 128 | TYR |
| 1 | 90-A | 132 | ASP |
| 1 | 90-A | 134 | GLU |
| 1 | 90-A | 148 | SER |
| 1 | 91-A | 8 | LEU |
| 1 | 91-A | 12 | ARG |
| 1 | 91-A | 20 | MET |
| 1 | 91-A | 21 | PRO |
| 1 | 91-A | 22 | TRP |
| 1 | 91-A | 32 | LYS |
| 1 | 91-A | 44 | ARG |
| 1 | 91-A | 48 | GLU |
| 1 | 91-A | 52 | ARG |
| 1 | 91-A | 62 | LEU |
| 1 | 91-A | 65 | GLN |
| 1 | 91-A | 70 | ASP |
| 1 | 91-A | 88 | VAL |
| 1 | 91-A | 108 | GLN |
| 1 | 91-A | 109 | LYS |
| 1 | 91-A | 127 | ASP |
| 1 | 91-A | 128 | TYR |
| 1 | 91-A | 154 | GLU |
| 1 | 91-A | 156 | LEU |
| 1 | 92-A | 4 | LEU |
| 1 | 92-A | 12 | ARG |
| 1 | 92-A | 20 | MET |
| 1 | 92-A | 21 | PRO |
| 1 | 92-A | 22 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 92-A | 32 | LYS |
| 1 | 92-A | 36 | LEU |
| 1 | 92-A | 44 | ARG |
| 1 | 92-A | 58 | LYS |
| 1 | 92-A | 61 | ILE |
| 1 | 92-A | 70 | ASP |
| 1 | 92-A | 104 | LEU |
| 1 | 92-A | 108 | GLN |
| 1 | 92-A | 118 | GLU |
| 1 | 92-A | 119 | VAL |
| 1 | 92-A | 128 | TYR |
| 1 | 92-A | 130 | PRO |
| 1 | 92-A | 134 | GLU |
| 1 | 92-A | 135 | SER |
| 1 | 92-A | 141 | HIS |
| 1 | 92-A | 154 | GLU |
| 1 | 93-A | 1 | MET |
| 1 | 93-A | 12 | ARG |
| 1 | 93-A | 20 | MET |
| 1 | 93-A | 22 | TRP |
| 1 | 93-A | 28 | LEU |
| 1 | 93-A | 32 | LYS |
| 1 | 93-A | 44 | ARG |
| 1 | 93-A | 58 | LYS |
| 1 | 93-A | 61 | ILE |
| 1 | 93-A | 70 | ASP |
| 1 | 93-A | 87 | ASP |
| 1 | 93-A | 108 | GLN |
| 1 | 93-A | 109 | LYS |
| 1 | 93-A | 110 | LEU |
| 1 | 93-A | 128 | TYR |
| 1 | 93-A | 134 | GLU |
| 1 | 93-A | 141 | HIS |
| 1 | 94-A | 1 | MET |
| 1 | 94-A | 12 | ARG |
| 1 | 94-A | 16 | MET |
| 1 | 94-A | 23 | ASN |
| 1 | 94-A | 28 | LEU |
| 1 | 94-A | 32 | LYS |
| 1 | 94-A | 87 | ASP |
| 1 | 94-A | 108 | GLN |
| 1 | 94-A | 109 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 94-A | 118 | GLU |
| 1 | 94-A | 127 | ASP |
| 1 | 94-A | 128 | TYR |
| 1 | 94-A | 138 | SER |
| 1 | 94-A | 139 | GLU |
| 1 | 94-A | 141 | HIS |
| 1 | 94-A | 154 | GLU |
| 1 | 94-A | 159 | ARG |
| 1 | 95-A | 1 | MET |
| 1 | 95-A | 12 | ARG |
| 1 | 95-A | 22 | TRP |
| 1 | 95-A | 23 | ASN |
| 1 | 95-A | 32 | LYS |
| 1 | 95-A | 49 | SER |
| 1 | 95-A | 54 | LEU |
| 1 | 95-A | 79 | ASP |
| 1 | 95-A | 87 | ASP |
| 1 | 95-A | 106 | LYS |
| 1 | 95-A | 108 | GLN |
| 1 | 95-A | 128 | TYR |
| 1 | 95-A | 134 | GLU |
| 1 | 95-A | 139 | GLU |
| 1 | 95-A | 154 | GLU |
| 1 | 96-A | 1 | MET |
| 1 | 96-A | 12 | ARG |
| 1 | 96-A | 16 | MET |
| 1 | 96-A | 18 | ASN |
| 1 | 96-A | 22 | TRP |
| 1 | 96-A | 24 | LEU |
| 1 | 96-A | 32 | LYS |
| 1 | 96-A | 33 | ARG |
| 1 | 96-A | 52 | ARG |
| 1 | 96-A | 54 | LEU |
| 1 | 96-A | 87 | ASP |
| 1 | 96-A | 88 | VAL |
| 1 | 96-A | 118 | GLU |
| 1 | 96-A | 119 | VAL |
| 1 | 96-A | 127 | ASP |
| 1 | 96-A | 128 | TYR |
| 1 | 96-A | 134 | GLU |
| 1 | 96-A | 139 | GLU |
| 1 | 96-A | 154 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 97-A | 1 | MET |
| 1 | 97-A | 2 | ILE |
| 1 | 97-A | 20 | MET |
| 1 | 97-A | 22 | TRP |
| 1 | 97-A | 32 | LYS |
| 1 | 97-A | 52 | ARG |
| 1 | 97-A | 88 | VAL |
| 1 | 97-A | 108 | GLN |
| 1 | 97-A | 119 | VAL |
| 1 | 97-A | 127 | ASP |
| 1 | 97-A | 134 | GLU |
| 1 | 97-A | 139 | GLU |
| 1 | 98-A | 18 | ASN |
| 1 | 98-A | 22 | TRP |
| 1 | 98-A | 49 | SER |
| 1 | 98-A | 52 | ARG |
| 1 | 98-A | 65 | GLN |
| 1 | 98-A | 87 | ASP |
| 1 | 98-A | 98 | ARG |
| 1 | 98-A | 108 | GLN |
| 1 | 98-A | 118 | GLU |
| 1 | 98-A | 127 | ASP |
| 1 | 98-A | 134 | GLU |
| 1 | 98-A | 135 | SER |
| 1 | 99-A | 8 | LEU |
| 1 | 99-A | 20 | MET |
| 1 | 99-A | 30 | TRP |
| 1 | 99-A | 52 | ARG |
| 1 | 99-A | 65 | GLN |
| 1 | 99-A | 98 | ARG |
| 1 | 99-A | 106 | LYS |
| 1 | 99-A | 108 | GLN |
| 1 | 99-A | 118 | GLU |
| 1 | 99-A | 127 | ASP |
| 1 | 99-A | 128 | TYR |
| 1 | 99-A | 129 | GLU |
| 1 | 100-A | 1 | MET |
| 1 | 100-A | 20 | MET |
| 1 | 100-A | 33 | ARG |
| 1 | 100-A | 49 | SER |
| 1 | 100-A | 52 | ARG |
| 1 | 100-A | 60 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 100-A | 65 | GLN |
| 1 | 100-A | 70 | ASP |
| 1 | 100-A | 79 | ASP |
| 1 | 100-A | 98 | ARG |
| 1 | 100-A | 108 | GLN |
| 1 | 100-A | 128 | TYR |
| 1 | 100-A | 129 | GLU |
| 1 | 100-A | 132 | ASP |
| 1 | 100-A | 146 | GLN |
| 1 | 100-A | 150 | SER |
| 1 | 101-A | 1 | MET |
| 1 | 101-A | 18 | ASN |
| 1 | 101-A | 20 | MET |
| 1 | 101-A | 23 | ASN |
| 1 | 101-A | 24 | LEU |
| 1 | 101-A | 52 | ARG |
| 1 | 101-A | 60 | ILE |
| 1 | 101-A | 65 | GLN |
| 1 | 101-A | 66 | PRO |
| 1 | 101-A | 68 | THR |
| 1 | 101-A | 79 | ASP |
| 1 | 101-A | 87 | ASP |
| 1 | 101-A | 108 | GLN |
| 1 | 101-A | 109 | LYS |
| 1 | 101-A | 119 | VAL |
| 1 | 101-A | 127 | ASP |
| 1 | 101-A | 129 | GLU |
| 1 | 101-A | 132 | ASP |
| 1 | 101-A | 146 | GLN |
| 1 | 101-A | 154 | GLU |
| 1 | 102-A | 20 | MET |
| 1 | 102-A | 52 | ARG |
| 1 | 102-A | 60 | ILE |
| 1 | 102-A | 65 | GLN |
| 1 | 102-A | 68 | THR |
| 1 | 102-A | 87 | ASP |
| 1 | 102-A | 98 | ARG |
| 1 | 102-A | 108 | GLN |
| 1 | 102-A | 129 | GLU |
| 1 | 102-A | 146 | GLN |
| 1 | 102-A | 148 | SER |
| 1 | 102-A | 154 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 103-A | 1 | MET |
| 1 | 103-A | 18 | ASN |
| 1 | 103-A | 20 | MET |
| 1 | 103-A | 21 | PRO |
| 1 | 103-A | 22 | TRP |
| 1 | 103-A | 23 | ASN |
| 1 | 103-A | 24 | LEU |
| 1 | 103-A | 33 | ARG |
| 1 | 103-A | 52 | ARG |
| 1 | 103-A | 60 | ILE |
| 1 | 103-A | 65 | GLN |
| 1 | 103-A | 79 | ASP |
| 1 | 103-A | 87 | ASP |
| 1 | 103-A | 89 | PRO |
| 1 | 103-A | 98 | ARG |
| 1 | 103-A | 108 | GLN |
| 1 | 103-A | 119 | VAL |
| 1 | 103-A | 128 | TYR |
| 1 | 103-A | 129 | GLU |
| 1 | 103-A | 146 | GLN |
| 1 | 103-A | 156 | LEU |
| 1 | 104-A | 1 | MET |
| 1 | 104-A | 11 | ASP |
| 1 | 104-A | 16 | MET |
| 1 | 104-A | 22 | TRP |
| 1 | 104-A | 23 | ASN |
| 1 | 104-A | 30 | TRP |
| 1 | 104-A | 33 | ARG |
| 1 | 104-A | 52 | ARG |
| 1 | 104-A | 60 | ILE |
| 1 | 104-A | 66 | PRO |
| 1 | 104-A | 98 | ARG |
| 1 | 104-A | 104 | LEU |
| 1 | 104-A | 108 | GLN |
| 1 | 104-A | 127 | ASP |
| 1 | 104-A | 129 | GLU |
| 1 | 104-A | 138 | SER |
| 1 | 104-A | 146 | GLN |
| 1 | 104-A | 148 | SER |
| 1 | 104-A | 150 | SER |
| 1 | 105-A | 1 | MET |
| 1 | 105-A | 18 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 105-A | 21 | PRO |
| 1 | 105-A | 23 | ASN |
| 1 | 105-A | 28 | LEU |
| 1 | 105-A | 34 | ASN |
| 1 | 105-A | 52 | ARG |
| 1 | 105-A | 60 | ILE |
| 1 | 105-A | 65 | GLN |
| 1 | 105-A | 88 | VAL |
| 1 | 105-A | 98 | ARG |
| 1 | 105-A | 101 | GLU |
| 1 | 105-A | 106 | LYS |
| 1 | 105-A | 108 | GLN |
| 1 | 105-A | 119 | VAL |
| 1 | 105-A | 127 | ASP |
| 1 | 105-A | 138 | SER |
| 1 | 105-A | 148 | SER |
| 1 | 105-A | 150 | SER |
| 1 | 106-A | 18 | ASN |
| 1 | 106-A | 22 | TRP |
| 1 | 106-A | 23 | ASN |
| 1 | 106-A | 33 | ARG |
| 1 | 106-A | 52 | ARG |
| 1 | 106-A | 98 | ARG |
| 1 | 106-A | 101 | GLU |
| 1 | 106-A | 106 | LYS |
| 1 | 106-A | 108 | GLN |
| 1 | 106-A | 127 | ASP |
| 1 | 106-A | 132 | ASP |
| 1 | 106-A | 150 | SER |
| 1 | 107-A | 33 | ARG |
| 1 | 107-A | 52 | ARG |
| 1 | 107-A | 65 | GLN |
| 1 | 107-A | 76 | LYS |
| 1 | 107-A | 79 | ASP |
| 1 | 107-A | 87 | ASP |
| 1 | 107-A | 106 | LYS |
| 1 | 107-A | 108 | GLN |
| 1 | 107-A | 129 | GLU |
| 1 | 107-A | 139 | GLU |
| 1 | 107-A | 142 | ASP |
| 1 | 107-A | 154 | GLU |
| 1 | 108-A | 1 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 108-A | 8 | LEU |
| 1 | 108-A | 18 | ASN |
| 1 | 108-A | 20 | MET |
| 1 | 108-A | 23 | ASN |
| 1 | 108-A | 33 | ARG |
| 1 | 108-A | 52 | ARG |
| 1 | 108-A | 65 | GLN |
| 1 | 108-A | 79 | ASP |
| 1 | 108-A | 87 | ASP |
| 1 | 108-A | 98 | ARG |
| 1 | 108-A | 106 | LYS |
| 1 | 108-A | 108 | GLN |
| 1 | 108-A | 115 | ILE |
| 1 | 108-A | 127 | ASP |
| 1 | 108-A | 128 | TYR |
| 1 | 108-A | 129 | GLU |
| 1 | 108-A | 142 | ASP |
| 1 | 108-A | 154 | GLU |
| 1 | 109-A | 1 | MET |
| 1 | 109-A | 20 | MET |
| 1 | 109-A | 23 | ASN |
| 1 | 109-A | 24 | LEU |
| 1 | 109-A | 52 | ARG |
| 1 | 109-A | 61 | ILE |
| 1 | 109-A | 65 | GLN |
| 1 | 109-A | 76 | LYS |
| 1 | 109-A | 79 | ASP |
| 1 | 109-A | 87 | ASP |
| 1 | 109-A | 101 | GLU |
| 1 | 109-A | 108 | GLN |
| 1 | 109-A | 120 | GLU |
| 1 | 109-A | 127 | ASP |
| 1 | 109-A | 128 | TYR |
| 1 | 109-A | 129 | GLU |
| 1 | 109-A | 132 | ASP |
| 1 | 109-A | 154 | GLU |
| 1 | 110-A | 1 | MET |
| 1 | 110-A | 20 | MET |
| 1 | 110-A | 22 | TRP |
| 1 | 110-A | 23 | ASN |
| 1 | 110-A | 28 | LEU |
| 1 | 110-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 110-A | 61 | ILE |
| 1 | 110-A | 65 | GLN |
| 1 | 110-A | 87 | ASP |
| 1 | 110-A | 88 | VAL |
| 1 | 110-A | 106 | LYS |
| 1 | 110-A | 108 | GLN |
| 1 | 110-A | 115 | ILE |
| 1 | 110-A | 127 | ASP |
| 1 | 110-A | 129 | GLU |
| 1 | 110-A | 132 | ASP |
| 1 | 110-A | 142 | ASP |
| 1 | 110-A | 144 | ASP |
| 1 | 110-A | 154 | GLU |
| 1 | 111-A | 20 | MET |
| 1 | 111-A | 22 | TRP |
| 1 | 111-A | 23 | ASN |
| 1 | 111-A | 24 | LEU |
| 1 | 111-A | 36 | LEU |
| 1 | 111-A | 49 | SER |
| 1 | 111-A | 52 | ARG |
| 1 | 111-A | 60 | ILE |
| 1 | 111-A | 61 | ILE |
| 1 | 111-A | 65 | GLN |
| 1 | 111-A | 76 | LYS |
| 1 | 111-A | 106 | LYS |
| 1 | 111-A | 127 | ASP |
| 1 | 111-A | 132 | ASP |
| 1 | 111-A | 134 | GLU |
| 1 | 111-A | 136 | VAL |
| 1 | 111-A | 148 | SER |
| 1 | 111-A | 150 | SER |
| 1 | 111-A | 154 | GLU |
| 1 | 111-A | 156 | LEU |
| 1 | 111-A | 159 | ARG |
| 1 | 112-A | 10 | VAL |
| 1 | 112-A | 24 | LEU |
| 1 | 112-A | 33 | ARG |
| 1 | 112-A | 52 | ARG |
| 1 | 112-A | 58 | LYS |
| 1 | 112-A | 61 | ILE |
| 1 | 112-A | 114 | HIS |
| 1 | 112-A | 154 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 113-A | 18 | ASN |
| 1 | 113-A | 20 | MET |
| 1 | 113-A | 22 | TRP |
| 1 | 113-A | 24 | LEU |
| 1 | 113-A | 60 | ILE |
| 1 | 113-A | 87 | ASP |
| 1 | 113-A | 98 | ARG |
| 1 | 113-A | 104 | LEU |
| 1 | 113-A | 118 | GLU |
| 1 | 113-A | 129 | GLU |
| 1 | 113-A | 150 | SER |
| 1 | 114-A | 24 | LEU |
| 1 | 114-A | 49 | SER |
| 1 | 114-A | 68 | THR |
| 1 | 114-A | 76 | LYS |
| 1 | 114-A | 109 | LYS |
| 1 | 114-A | 114 | HIS |
| 1 | 114-A | 126 | PRO |
| 1 | 114-A | 127 | ASP |
| 1 | 114-A | 128 | TYR |
| 1 | 114-A | 136 | VAL |
| 1 | 114-A | 148 | SER |
| 1 | 114-A | 157 | GLU |
| 1 | 115-A | 2 | ILE |
| 1 | 115-A | 16 | MET |
| 1 | 115-A | 18 | ASN |
| 1 | 115-A | 20 | MET |
| 1 | 115-A | 21 | PRO |
| 1 | 115-A | 22 | TRP |
| 1 | 115-A | 23 | ASN |
| 1 | 115-A | 32 | LYS |
| 1 | 115-A | 37 | ASN |
| 1 | 115-A | 52 | ARG |
| 1 | 115-A | 65 | GLN |
| 1 | 115-A | 79 | ASP |
| 1 | 115-A | 87 | ASP |
| 1 | 115-A | 88 | VAL |
| 1 | 115-A | 98 | ARG |
| 1 | 115-A | 104 | LEU |
| 1 | 115-A | 114 | HIS |
| 1 | 115-A | 120 | GLU |
| 1 | 115-A | 127 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 115-A | 136 | VAL |
| 1 | 115-A | 138 | SER |
| 1 | 115-A | 150 | SER |
| 1 | 115-A | 156 | LEU |
| 1 | 115-A | 159 | ARG |
| 1 | 116-A | 1 | MET |
| 1 | 116-A | 4 | LEU |
| 1 | 116-A | 11 | ASP |
| 1 | 116-A | 16 | MET |
| 1 | 116-A | 20 | MET |
| 1 | 116-A | 21 | PRO |
| 1 | 116-A | 22 | TRP |
| 1 | 116-A | 23 | ASN |
| 1 | 116-A | 24 | LEU |
| 1 | 116-A | 37 | ASN |
| 1 | 116-A | 52 | ARG |
| 1 | 116-A | 62 | LEU |
| 1 | 116-A | 68 | THR |
| 1 | 116-A | 79 | ASP |
| 1 | 116-A | 98 | ARG |
| 1 | 116-A | 118 | GLU |
| 1 | 116-A | 119 | VAL |
| 1 | 116-A | 136 | VAL |
| 1 | 116-A | 139 | GLU |
| 1 | 117-A | 1 | MET |
| 1 | 117-A | 11 | ASP |
| 1 | 117-A | 16 | MET |
| 1 | 117-A | 22 | TRP |
| 1 | 117-A | 23 | ASN |
| 1 | 117-A | 24 | LEU |
| 1 | 117-A | 37 | ASN |
| 1 | 117-A | 52 | ARG |
| 1 | 117-A | 65 | GLN |
| 1 | 117-A | 98 | ARG |
| 1 | 117-A | 104 | LEU |
| 1 | 117-A | 106 | LYS |
| 1 | 117-A | 119 | VAL |
| 1 | 117-A | 120 | GLU |
| 1 | 117-A | 128 | TYR |
| 1 | 117-A | 132 | ASP |
| 1 | 117-A | 138 | SER |
| 1 | 117-A | 139 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 118-A | 12 | ARG |
| 1 | 118-A | 16 | MET |
| 1 | 118-A | 20 | MET |
| 1 | 118-A | 22 | TRP |
| 1 | 118-A | 24 | LEU |
| 1 | 118-A | 30 | TRP |
| 1 | 118-A | 36 | LEU |
| 1 | 118-A | 37 | ASN |
| 1 | 118-A | 52 | ARG |
| 1 | 118-A | 98 | ARG |
| 1 | 118-A | 104 | LEU |
| 1 | 118-A | 109 | LYS |
| 1 | 118-A | 119 | VAL |
| 1 | 118-A | 128 | TYR |
| 1 | 118-A | 129 | GLU |
| 1 | 118-A | 132 | ASP |
| 1 | 118-A | 138 | SER |
| 1 | 118-A | 150 | SER |
| 1 | 119-A | 1 | MET |
| 1 | 119-A | 20 | MET |
| 1 | 119-A | 25 | PRO |
| 1 | 119-A | 30 | TRP |
| 1 | 119-A | 52 | ARG |
| 1 | 119-A | 58 | LYS |
| 1 | 119-A | 88 | VAL |
| 1 | 119-A | 98 | ARG |
| 1 | 119-A | 104 | LEU |
| 1 | 119-A | 132 | ASP |
| 1 | 119-A | 146 | GLN |
| 1 | 120-A | 1 | MET |
| 1 | 120-A | 8 | LEU |
| 1 | 120-A | 16 | MET |
| 1 | 120-A | 20 | MET |
| 1 | 120-A | 45 | HIS |
| 1 | 120-A | 48 | GLU |
| 1 | 120-A | 52 | ARG |
| 1 | 120-A | 58 | LYS |
| 1 | 120-A | 87 | ASP |
| 1 | 120-A | 98 | ARG |
| 1 | 120-A | 104 | LEU |
| 1 | 120-A | 139 | GLU |
| 1 | 120-A | 146 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 120-A | 150 | SER |
| 1 | 121-A | 10 | VAL |
| 1 | 121-A | 12 | ARG |
| 1 | 121-A | 20 | MET |
| 1 | 121-A | 24 | LEU |
| 1 | 121-A | 30 | TRP |
| 1 | 121-A | 52 | ARG |
| 1 | 121-A | 58 | LYS |
| 1 | 121-A | 70 | ASP |
| 1 | 121-A | 88 | VAL |
| 1 | 121-A | 98 | ARG |
| 1 | 121-A | 106 | LYS |
| 1 | 121-A | 119 | VAL |
| 1 | 121-A | 120 | GLU |
| 1 | 121-A | 129 | GLU |
| 1 | 121-A | 137 | PHE |
| 1 | 121-A | 142 | ASP |
| 1 | 121-A | 146 | GLN |
| 1 | 121-A | 154 | GLU |
| 1 | 122-A | 1 | MET |
| 1 | 122-A | 4 | LEU |
| 1 | 122-A | 20 | MET |
| 1 | 122-A | 23 | ASN |
| 1 | 122-A | 28 | LEU |
| 1 | 122-A | 30 | TRP |
| 1 | 122-A | 52 | ARG |
| 1 | 122-A | 70 | ASP |
| 1 | 122-A | 87 | ASP |
| 1 | 122-A | 98 | ARG |
| 1 | 122-A | 104 | LEU |
| 1 | 122-A | 106 | LYS |
| 1 | 122-A | 109 | LYS |
| 1 | 122-A | 129 | GLU |
| 1 | 122-A | 148 | SER |
| 1 | 122-A | 150 | SER |
| 1 | 123-A | 4 | LEU |
| 1 | 123-A | 20 | MET |
| 1 | 123-A | 22 | TRP |
| 1 | 123-A | 23 | ASN |
| 1 | 123-A | 24 | LEU |
| 1 | 123-A | 30 | TRP |
| 1 | 123-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 123-A | 58 | LYS |
| 1 | 123-A | 87 | ASP |
| 1 | 123-A | 98 | ARG |
| 1 | 124-A | 1 | MET |
| 1 | 124-A | 8 | LEU |
| 1 | 124-A | 21 | PRO |
| 1 | 124-A | 22 | TRP |
| 1 | 124-A | 23 | ASN |
| 1 | 124-A | 30 | TRP |
| 1 | 124-A | 48 | GLU |
| 1 | 124-A | 52 | ARG |
| 1 | 124-A | 77 | SER |
| 1 | 124-A | 98 | ARG |
| 1 | 124-A | 108 | GLN |
| 1 | 124-A | 118 | GLU |
| 1 | 124-A | 120 | GLU |
| 1 | 124-A | 139 | GLU |
| 1 | 124-A | 146 | GLN |
| 1 | 124-A | 157 | GLU |
| 1 | 125-A | 1 | MET |
| 1 | 125-A | 20 | MET |
| 1 | 125-A | 23 | ASN |
| 1 | 125-A | 24 | LEU |
| 1 | 125-A | 28 | LEU |
| 1 | 125-A | 30 | TRP |
| 1 | 125-A | 32 | LYS |
| 1 | 125-A | 52 | ARG |
| 1 | 125-A | 61 | ILE |
| 1 | 125-A | 65 | GLN |
| 1 | 125-A | 79 | ASP |
| 1 | 125-A | 108 | GLN |
| 1 | 125-A | 128 | TYR |
| 1 | 125-A | 129 | GLU |
| 1 | 125-A | 139 | GLU |
| 1 | 125-A | 155 | ILE |
| 1 | 125-A | 159 | ARG |

Some 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 ⓘ

125 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 | CSD | 52-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 48-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 70-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 58-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 63-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 121-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 85-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 37-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 8-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 19-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 65-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 5-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 107-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 30-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 88-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 40-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 2-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 103-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 16-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 38-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 41-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 114-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | CSD | 105-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 50-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 28-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 125-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 106-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 75-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 6-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 35-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 20-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 92-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 49-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 97-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 64-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 31-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 89-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 76-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 24-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 51-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 33-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 110-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 60-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 56-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 15-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 4-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 124-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 10-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 109-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 11-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 42-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 72-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 120-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 45-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 18-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 68-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 53-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | CSD | 117-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 101-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 104-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 111-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 57-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 14-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 98-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 93-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 29-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 71-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 26-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 55-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 115-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 86-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 47-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 91-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 73-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 44-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 1-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 119-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 3-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 67-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 123-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 116-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 80-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 78-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 87-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 66-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 13-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 46-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 77-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 32-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 108-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 82-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 7-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | CSD | 69-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 27-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 25-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 34-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 22-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 9-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 100-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 43-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 94-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 62-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 102-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 59-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 81-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 90-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 84-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 12-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 17-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 112-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 21-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 74-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 61-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 96-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 36-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 113-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 39-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 99-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 118-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 95-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 54-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 122-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 83-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 23-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |
| 1 | CSD | 79-A | 152 | 1 | 3,7,8 | 1.15 | 0 | 1,8,10 | 4.88 | 1 (100%) |

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 | CSD | 52-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 48-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 70-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 58-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 63-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 121-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 85-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 37-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 8-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 19-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 65-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 5-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 107-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 30-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 88-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 40-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 2-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 103-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 16-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 38-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 41-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 114-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 105-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 50-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 28-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 125-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 106-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 75-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 6-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 35-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 20-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 92-A | 152 | 1 | - | 2/2/6/8 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | CSD | 49-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 97-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 64-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 31-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 89-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 76-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 24-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 51-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 33-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 110-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 60-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 56-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 15-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 4-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 124-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 10-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 109-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 11-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 42-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 72-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 120-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 45-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 18-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 68-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 53-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 117-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 101-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 104-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 111-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 57-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 14-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 98-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 93-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 29-A | 152 | 1 | - | 2/2/6/8 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | CSD | 71-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 26-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 55-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 115-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 86-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 47-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 91-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 73-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 44-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 1-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 119-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 3-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 67-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 123-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 116-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 80-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 78-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 87-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 66-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 13-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 46-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 77-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 32-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 108-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 82-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 7-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 69-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 27-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 25-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 34-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 22-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 9-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 100-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 43-A | 152 | 1 | - | 2/2/6/8 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | CSD | 94-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 62-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 102-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 59-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 81-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 90-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 84-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 12-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 17-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 112-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 21-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 74-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 61-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 96-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 36-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 113-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 39-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 99-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 118-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 95-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 54-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 122-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 83-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 23-A | 152 | 1 | - | 2/2/6/8 | - |
| 1 | CSD | 79-A | 152 | 1 | - | 2/2/6/8 | - |

There are no bond length outliers.

All (125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | 52-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 48-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 70-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 58-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 63-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 121-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | 85-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 37-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 8-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 19-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 65-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 5-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 107-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 30-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 88-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 40-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 2-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 103-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 16-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 38-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 41-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 114-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 105-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 50-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 28-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 125-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 106-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 75-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 6-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 35-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 20-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 92-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 49-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 97-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 64-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 31-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 89-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 76-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 24-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 51-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 33-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 110-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 60-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 56-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 15-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 4-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 124-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 10-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | 109-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 11-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 42-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 72-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 120-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 45-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 18-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 68-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 53-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 117-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 101-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 104-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 111-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 57-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 14-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 98-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 93-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 29-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 71-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 26-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 55-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 115-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 86-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 47-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 91-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 73-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 44-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 1-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 119-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 3-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 67-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 123-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 116-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 80-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 78-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 87-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 66-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 13-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 46-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 77-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 32-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 108-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | 82-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 7-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 69-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 27-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 25-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 34-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 22-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 9-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 100-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 43-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 94-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 62-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 102-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 59-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 81-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 90-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 84-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 12-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 17-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 112-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 21-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 74-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 61-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 96-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 36-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 113-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 39-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 99-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 118-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 95-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 54-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 122-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 83-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 23-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |
| 1 | 79-A | 152 | CSD | OD1-SG-CB | 4.88 | 114.83 | 105.54 |

There are no chirality outliers.

All (250) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 52-A | 152 | CSD | N-CA-CB-SG |
| 1 | 52-A | 152 | CSD | CA-CB-SG-OD1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 48-A | 152 | CSD | N-CA-CB-SG |
| 1 | 48-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 70-A | 152 | CSD | N-CA-CB-SG |
| 1 | 70-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 58-A | 152 | CSD | N-CA-CB-SG |
| 1 | 58-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 63-A | 152 | CSD | N-CA-CB-SG |
| 1 | 63-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 121-A | 152 | CSD | N-CA-CB-SG |
| 1 | 121-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 85-A | 152 | CSD | N-CA-CB-SG |
| 1 | 85-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 37-A | 152 | CSD | N-CA-CB-SG |
| 1 | 37-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 8-A | 152 | CSD | N-CA-CB-SG |
| 1 | 8-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 19-A | 152 | CSD | N-CA-CB-SG |
| 1 | 19-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 65-A | 152 | CSD | N-CA-CB-SG |
| 1 | 65-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 5-A | 152 | CSD | N-CA-CB-SG |
| 1 | 5-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 107-A | 152 | CSD | N-CA-CB-SG |
| 1 | 107-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 30-A | 152 | CSD | N-CA-CB-SG |
| 1 | 30-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 88-A | 152 | CSD | N-CA-CB-SG |
| 1 | 88-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 40-A | 152 | CSD | N-CA-CB-SG |
| 1 | 40-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 2-A | 152 | CSD | N-CA-CB-SG |
| 1 | 2-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 103-A | 152 | CSD | N-CA-CB-SG |
| 1 | 103-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 16-A | 152 | CSD | N-CA-CB-SG |
| 1 | 16-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 38-A | 152 | CSD | N-CA-CB-SG |
| 1 | 38-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 41-A | 152 | CSD | N-CA-CB-SG |
| 1 | 41-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 114-A | 152 | CSD | N-CA-CB-SG |
| 1 | 114-A | 152 | CSD | CA-CB-SG-OD1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 105-A | 152 | CSD | N-CA-CB-SG |
| 1 | 105-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 50-A | 152 | CSD | N-CA-CB-SG |
| 1 | 50-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 28-A | 152 | CSD | N-CA-CB-SG |
| 1 | 28-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 125-A | 152 | CSD | N-CA-CB-SG |
| 1 | 125-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 106-A | 152 | CSD | N-CA-CB-SG |
| 1 | 106-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 75-A | 152 | CSD | N-CA-CB-SG |
| 1 | 75-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 6-A | 152 | CSD | N-CA-CB-SG |
| 1 | 6-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 35-A | 152 | CSD | N-CA-CB-SG |
| 1 | 35-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 20-A | 152 | CSD | N-CA-CB-SG |
| 1 | 20-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 92-A | 152 | CSD | N-CA-CB-SG |
| 1 | 92-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 49-A | 152 | CSD | N-CA-CB-SG |
| 1 | 49-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 97-A | 152 | CSD | N-CA-CB-SG |
| 1 | 97-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 64-A | 152 | CSD | N-CA-CB-SG |
| 1 | 64-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 31-A | 152 | CSD | N-CA-CB-SG |
| 1 | 31-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 89-A | 152 | CSD | N-CA-CB-SG |
| 1 | 89-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 76-A | 152 | CSD | N-CA-CB-SG |
| 1 | 76-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 24-A | 152 | CSD | N-CA-CB-SG |
| 1 | 24-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 51-A | 152 | CSD | N-CA-CB-SG |
| 1 | 51-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 33-A | 152 | CSD | N-CA-CB-SG |
| 1 | 33-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 110-A | 152 | CSD | N-CA-CB-SG |
| 1 | 110-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 60-A | 152 | CSD | N-CA-CB-SG |
| 1 | 60-A | 152 | CSD | CA-CB-SG-OD1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 56-A | 152 | CSD | N-CA-CB-SG |
| 1 | 56-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 15-A | 152 | CSD | N-CA-CB-SG |
| 1 | 15-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 4-A | 152 | CSD | N-CA-CB-SG |
| 1 | 4-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 124-A | 152 | CSD | N-CA-CB-SG |
| 1 | 124-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 10-A | 152 | CSD | N-CA-CB-SG |
| 1 | 10-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 109-A | 152 | CSD | N-CA-CB-SG |
| 1 | 109-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 11-A | 152 | CSD | N-CA-CB-SG |
| 1 | 11-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 42-A | 152 | CSD | N-CA-CB-SG |
| 1 | 42-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 72-A | 152 | CSD | N-CA-CB-SG |
| 1 | 72-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 120-A | 152 | CSD | N-CA-CB-SG |
| 1 | 120-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 45-A | 152 | CSD | N-CA-CB-SG |
| 1 | 45-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 18-A | 152 | CSD | N-CA-CB-SG |
| 1 | 18-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 68-A | 152 | CSD | N-CA-CB-SG |
| 1 | 68-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 53-A | 152 | CSD | N-CA-CB-SG |
| 1 | 53-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 117-A | 152 | CSD | N-CA-CB-SG |
| 1 | 117-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 101-A | 152 | CSD | N-CA-CB-SG |
| 1 | 101-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 104-A | 152 | CSD | N-CA-CB-SG |
| 1 | 104-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 111-A | 152 | CSD | N-CA-CB-SG |
| 1 | 111-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 57-A | 152 | CSD | N-CA-CB-SG |
| 1 | 57-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 14-A | 152 | CSD | N-CA-CB-SG |
| 1 | 14-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 98-A | 152 | CSD | N-CA-CB-SG |
| 1 | 98-A | 152 | CSD | CA-CB-SG-OD1 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 93-A | 152 | CSD | N-CA-CB-SG |
| 1 | 93-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 29-A | 152 | CSD | N-CA-CB-SG |
| 1 | 29-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 71-A | 152 | CSD | N-CA-CB-SG |
| 1 | 71-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 26-A | 152 | CSD | N-CA-CB-SG |
| 1 | 26-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 55-A | 152 | CSD | N-CA-CB-SG |
| 1 | 55-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 115-A | 152 | CSD | N-CA-CB-SG |
| 1 | 115-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 86-A | 152 | CSD | N-CA-CB-SG |
| 1 | 86-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 47-A | 152 | CSD | N-CA-CB-SG |
| 1 | 47-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 91-A | 152 | CSD | N-CA-CB-SG |
| 1 | 91-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 73-A | 152 | CSD | N-CA-CB-SG |
| 1 | 73-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 44-A | 152 | CSD | N-CA-CB-SG |
| 1 | 44-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 1-A | 152 | CSD | N-CA-CB-SG |
| 1 | 1-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 119-A | 152 | CSD | N-CA-CB-SG |
| 1 | 119-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 3-A | 152 | CSD | N-CA-CB-SG |
| 1 | 3-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 67-A | 152 | CSD | N-CA-CB-SG |
| 1 | 67-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 123-A | 152 | CSD | N-CA-CB-SG |
| 1 | 123-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 116-A | 152 | CSD | N-CA-CB-SG |
| 1 | 116-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 80-A | 152 | CSD | N-CA-CB-SG |
| 1 | 80-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 78-A | 152 | CSD | N-CA-CB-SG |
| 1 | 78-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 87-A | 152 | CSD | N-CA-CB-SG |
| 1 | 87-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 66-A | 152 | CSD | N-CA-CB-SG |
| 1 | 66-A | 152 | CSD | CA-CB-SG-OD1 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 13-A | 152 | CSD | N-CA-CB-SG |
| 1 | 13-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 46-A | 152 | CSD | N-CA-CB-SG |
| 1 | 46-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 77-A | 152 | CSD | N-CA-CB-SG |
| 1 | 77-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 32-A | 152 | CSD | N-CA-CB-SG |
| 1 | 32-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 108-A | 152 | CSD | N-CA-CB-SG |
| 1 | 108-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 82-A | 152 | CSD | N-CA-CB-SG |
| 1 | 82-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 7-A | 152 | CSD | N-CA-CB-SG |
| 1 | 7-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 69-A | 152 | CSD | N-CA-CB-SG |
| 1 | 69-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 27-A | 152 | CSD | N-CA-CB-SG |
| 1 | 27-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 25-A | 152 | CSD | N-CA-CB-SG |
| 1 | 25-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 34-A | 152 | CSD | N-CA-CB-SG |
| 1 | 34-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 22-A | 152 | CSD | N-CA-CB-SG |
| 1 | 22-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 9-A | 152 | CSD | N-CA-CB-SG |
| 1 | 9-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 100-A | 152 | CSD | N-CA-CB-SG |
| 1 | 100-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 43-A | 152 | CSD | N-CA-CB-SG |
| 1 | 43-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 94-A | 152 | CSD | N-CA-CB-SG |
| 1 | 94-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 62-A | 152 | CSD | N-CA-CB-SG |
| 1 | 62-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 102-A | 152 | CSD | N-CA-CB-SG |
| 1 | 102-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 59-A | 152 | CSD | N-CA-CB-SG |
| 1 | 59-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 81-A | 152 | CSD | N-CA-CB-SG |
| 1 | 81-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 90-A | 152 | CSD | N-CA-CB-SG |
| 1 | 90-A | 152 | CSD | CA-CB-SG-OD1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 84-A | 152 | CSD | N-CA-CB-SG |
| 1 | 84-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 12-A | 152 | CSD | N-CA-CB-SG |
| 1 | 12-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 17-A | 152 | CSD | N-CA-CB-SG |
| 1 | 17-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 112-A | 152 | CSD | N-CA-CB-SG |
| 1 | 112-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 21-A | 152 | CSD | N-CA-CB-SG |
| 1 | 21-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 74-A | 152 | CSD | N-CA-CB-SG |
| 1 | 74-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 61-A | 152 | CSD | N-CA-CB-SG |
| 1 | 61-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 96-A | 152 | CSD | N-CA-CB-SG |
| 1 | 96-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 36-A | 152 | CSD | N-CA-CB-SG |
| 1 | 36-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 113-A | 152 | CSD | N-CA-CB-SG |
| 1 | 113-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 39-A | 152 | CSD | N-CA-CB-SG |
| 1 | 39-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 99-A | 152 | CSD | N-CA-CB-SG |
| 1 | 99-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 118-A | 152 | CSD | N-CA-CB-SG |
| 1 | 118-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 95-A | 152 | CSD | N-CA-CB-SG |
| 1 | 95-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 54-A | 152 | CSD | N-CA-CB-SG |
| 1 | 54-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 122-A | 152 | CSD | N-CA-CB-SG |
| 1 | 122-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 83-A | 152 | CSD | N-CA-CB-SG |
| 1 | 83-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 23-A | 152 | CSD | N-CA-CB-SG |
| 1 | 23-A | 152 | CSD | CA-CB-SG-OD1 |
| 1 | 79-A | 152 | CSD | N-CA-CB-SG |
| 1 | 79-A | 152 | CSD | CA-CB-SG-OD1 |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 500 ligands modelled in this entry, 250 are monoatomic - leaving 250 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 31-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 34-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 124-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 54-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 26-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 14-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 36-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 124-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 20-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 7-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 99-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 72-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 51-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 97-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 79-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 82-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 80-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 66-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 11-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 3-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 67-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 40-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 74-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 55-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 25-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 78-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 45-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 99-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 16-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 83-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 76-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 125-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 85-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 87-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 44-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 64-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 24-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 3-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 68-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 52-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 111-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 18-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 94-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 60-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 110-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 28-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 84-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 91-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 100-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 15-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 5-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 67-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 70-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 35-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 35-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 31-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 80-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 22-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 41-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 103-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 23-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 78-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 57-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 52-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 73-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 22-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 88-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 32-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 119-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 39-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 2-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 50-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 7-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 1-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 13-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 79-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 97-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 55-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 98-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 10-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 43-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 85-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 62-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 112-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 116-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 40-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 93-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 96-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 17-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 77-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 6-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 69-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 98-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 12-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 111-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 89-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 75-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 106-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 95-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 25-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 34-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 29-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 64-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 59-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 32-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 115-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 8-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 42-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 46-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 102-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 93-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 114-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 81-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 71-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 58-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 108-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 74-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 21-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 53-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 63-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 117-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 56-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 66-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 39-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 49-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 61-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 90-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 48-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 6-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 62-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 18-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 65-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 58-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 102-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 47-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 81-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 120-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 51-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 104-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 33-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 76-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 20-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 101-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 29-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 30-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 70-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 88-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 63-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 117-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 109-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 19-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 44-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 100-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 105-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 71-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 120-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 86-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 16-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 38-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 38-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 41-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 69-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 17-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 122-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 47-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 95-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 106-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 43-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 8-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 92-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 13-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 84-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 61-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 59-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 50-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 45-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 24-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 122-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 123-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 89-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 42-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 5-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 30-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 113-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 115-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 49-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 4-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 118-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 27-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 114-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 110-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 105-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 94-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 103-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 11-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 86-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 10-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 91-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 119-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 73-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 87-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 77-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 125-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 37-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 37-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 104-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 19-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 68-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 121-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 92-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 113-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 56-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 4-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 123-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 33-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 118-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 48-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 26-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 12-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 121-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 72-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 9-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 83-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 23-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 108-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 2-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 21-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 82-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 90-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 15-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 107-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 101-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 116-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 28-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 36-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 112-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 14-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 2 | FOL | 75-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 109-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 53-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 3 | NAP | 9-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 46-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 57-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 54-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 60-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 1-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 65-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 27-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |
| 3 | NAP | 96-A | 202 | - | 45,52,52 | 2.96 | 9 (20%) | 56,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 107-A | 201 | - | 28,34,34 | 1.17 | 2 (7%) | 36,47,47 | 2.29 | 10 (27%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FOL | 31-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 34-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 124-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 54-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 26-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 14-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 36-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 124-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 20-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 7-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 99-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FOL | 72-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 51-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 97-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 79-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 82-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 80-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 66-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 11-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 3-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 67-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 40-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 74-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 55-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 25-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 78-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 45-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 99-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 16-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 83-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 76-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 125-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 85-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 87-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 44-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 64-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 24-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 3-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 68-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 52-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 111-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 18-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 94-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 60-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 110-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FOL | 28-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 84-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 91-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 100-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 15-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 5-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 67-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 70-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 35-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 35-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 31-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 80-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 22-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 41-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 103-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 23-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 78-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 57-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 52-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 73-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 22-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 88-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 32-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 119-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 39-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 2-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 50-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 7-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 1-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 13-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 79-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 97-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 55-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 98-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAP | 10-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 43-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 85-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 62-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 112-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 116-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 40-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 93-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 96-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 17-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 77-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 6-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 69-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 98-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 12-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 111-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 89-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 75-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 106-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 95-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 25-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 34-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 29-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 64-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 59-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 32-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 115-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 8-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 42-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 46-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 102-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 93-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 114-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 81-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAP | 71-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 58-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 108-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 74-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 21-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 53-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 63-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 117-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 56-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 66-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 39-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 49-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 61-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 90-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 48-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 6-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 62-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 18-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 65-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 58-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 102-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 47-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 81-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 120-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 51-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 104-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 33-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 76-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 20-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 101-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 29-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 30-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 70-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 88-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAP | 63-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 117-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 109-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 19-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 44-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 100-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 105-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 71-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 120-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 86-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 16-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 38-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 38-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 41-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 69-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 17-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 122-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 47-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 95-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 106-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 43-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 8-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 92-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 13-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 84-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 61-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 59-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 50-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 45-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 24-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 122-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 123-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 89-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 42-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAP | 5-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 30-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 113-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 115-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 49-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 4-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 118-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 27-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 114-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 110-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 105-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 94-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 103-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 11-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 86-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 10-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 91-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 119-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 73-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 87-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 77-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 125-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 37-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 37-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 104-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 19-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 68-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 121-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 92-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 113-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 56-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 4-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 123-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 33-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FOL | 118-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 48-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 26-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 12-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 121-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 72-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 9-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 83-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 23-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 108-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 2-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 21-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 82-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 90-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 15-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 107-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 101-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 116-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 28-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 36-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 112-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 14-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 2 | FOL | 75-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 109-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 53-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 3 | NAP | 9-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 46-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 57-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 54-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 60-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 1-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 65-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |
| 2 | FOL | 27-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |
| 3 | NAP | 96-A | 202 | - | - | 3/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FOL | 107-A | 201 | - | - | 5/16/22/22 | 0/3/3/3 |

All (1375) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3 | 80-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 66-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 24-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 94-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 35-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 103-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 55-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 116-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 77-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 69-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 64-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 81-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 71-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 74-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 3-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 56-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 62-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 70-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 63-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 44-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 120-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 115-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 91-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 41-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 37-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 104-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 121-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 72-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 82-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 36-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 112-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 53-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 96-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 40-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 45-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 16-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 85-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3 | 15-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 67-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 10-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 88-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 43-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 17-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 107-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 6-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 4-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 76-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 101-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 29-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 119-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 61-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 59-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 30-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 1-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 11-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 118-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 7-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 109-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 48-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 65-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 54-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 39-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 97-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 99-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 83-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 125-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 68-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 52-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 111-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 84-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 100-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 31-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 32-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 86-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 98-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 89-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 34-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 114-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 110-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3 | 90-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 51-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 38-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 47-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 123-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 105-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 12-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 108-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 21-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 57-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 23-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 14-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 124-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 25-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 26-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 22-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 78-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 117-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 13-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 79-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 75-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 106-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 8-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 46-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 93-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 18-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 58-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 102-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 33-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 20-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 122-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 95-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 42-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 50-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 5-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 49-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 27-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 73-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 87-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 19-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 92-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 113-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3 | 2-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 28-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 9-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 60-A | 202 | NAP | C2D-C1D | -11.57 | 1.36 | 1.53 |
| 3 | 80-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 66-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 24-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 94-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 35-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 103-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 55-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 116-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 77-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 69-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 64-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 81-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 71-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 74-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 3-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 56-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 62-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 70-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 63-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 44-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 120-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 115-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 91-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 41-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 37-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 104-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 121-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 72-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 82-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 36-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 112-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 53-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 96-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 40-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 45-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 16-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 85-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 15-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 67-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 10-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 88-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 43-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 17-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 107-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 6-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 4-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 76-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 101-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 29-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 119-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 61-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 59-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 30-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 1-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 11-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 118-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 7-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 109-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 48-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 65-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 54-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 39-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 97-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 99-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 83-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 125-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 68-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 52-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 111-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 84-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 100-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 31-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 32-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 86-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 98-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 89-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 34-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 114-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 110-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 90-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 51-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 38-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 47-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 123-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 105-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 12-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 108-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 21-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 57-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 23-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 14-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 124-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 25-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 26-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 22-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 78-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 117-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 13-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 79-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 75-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 106-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 8-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 46-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 93-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 18-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 58-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 102-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 33-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 20-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 122-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 95-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 42-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 50-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 5-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 49-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 27-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 73-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 87-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 19-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 92-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 113-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 2-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 28-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 9-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 60-A | 202 | NAP | O4B-C1B | 10.24 | 1.55 | 1.41 |
| 3 | 80-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 66-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 24-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 94-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 35-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 103-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 55-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 116-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 77-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 69-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 64-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 81-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 71-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 74-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 3-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 56-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 62-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 70-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 63-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 44-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 120-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 115-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 91-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 41-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 37-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 104-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 121-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 72-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 82-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 36-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 112-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 53-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 96-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 40-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 45-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 16-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 85-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 15-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 67-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 10-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 88-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 43-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 17-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 107-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 6-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 4-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 76-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 101-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 29-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 119-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 61-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 59-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 30-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 1-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 11-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 118-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 7-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 109-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 48-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 65-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 54-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 39-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 97-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 99-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 83-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 125-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 68-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 52-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 111-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 84-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 100-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 31-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 32-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 86-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 98-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 89-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 34-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 114-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 110-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 90-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 51-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 38-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 47-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 123-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 105-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 12-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 108-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 21-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 57-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 23-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 14-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 124-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 25-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 26-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 22-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 78-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 117-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 13-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 79-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 75-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 106-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 8-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 46-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 93-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 18-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 58-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 102-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 33-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 20-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 122-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 95-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 42-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 50-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 5-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 49-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 27-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 73-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 87-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 19-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 92-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 113-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 2-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 28-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 9-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 60-A | 202 | NAP | O4D-C1D | 8.99 | 1.53 | 1.41 |
| 3 | 80-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 66-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 24-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 94-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 35-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 103-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 55-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 116-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 77-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 69-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 64-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 81-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 71-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 74-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 3-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 56-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 62-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 70-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 63-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 44-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 120-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 115-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 91-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 41-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 37-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 104-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 121-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 72-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 82-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 36-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 112-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 53-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 96-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 40-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 45-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 16-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 85-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 15-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 67-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 10-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 88-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 43-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 17-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 107-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 6-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 4-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 76-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 101-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 29-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 119-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 61-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 59-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 30-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 1-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 11-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 118-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 7-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 109-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 48-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 65-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 54-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 39-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 97-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 99-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 83-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 125-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 68-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 52-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 111-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 84-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 100-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 31-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 32-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 86-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 98-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 89-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 34-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 114-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 110-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 90-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 51-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 38-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 47-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 123-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 105-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 12-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 108-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 21-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 57-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 23-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 14-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 124-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 25-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 26-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 22-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 78-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 117-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 13-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 79-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 75-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 106-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 8-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 46-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 93-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 18-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 58-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 102-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 33-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 20-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 122-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 95-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 42-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 50-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 5-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 49-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 27-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 73-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 87-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 19-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 92-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 113-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 2-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 28-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 9-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 60-A | 202 | NAP | O4B-C4B | -3.49 | 1.37 | 1.45 |
| 3 | 80-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 66-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 24-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 94-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 35-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 103-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 55-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 116-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 77-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 69-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 64-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 81-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 71-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 74-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 3-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 56-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 62-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 70-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 63-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 44-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 120-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 115-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 91-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 41-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 37-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 104-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 121-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 72-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 82-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 36-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 112-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 53-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 96-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 40-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 45-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 16-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 85-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 15-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 67-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 10-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 88-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 43-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 17-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 107-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 6-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 4-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 76-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 101-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 29-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 119-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 61-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 59-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 30-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 1-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 11-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 118-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 7-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 109-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 48-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 65-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 54-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 39-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 97-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 99-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 83-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 125-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 68-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 52-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 111-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 84-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 100-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 31-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 32-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 86-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 98-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 89-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 34-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 114-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 110-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 90-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 51-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 38-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 47-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 123-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 105-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 12-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 108-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 21-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 57-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 23-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 14-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 124-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 25-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 26-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 22-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 78-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 117-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 13-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 79-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 75-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 106-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 8-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 46-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 93-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 18-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 58-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 102-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 33-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 20-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 122-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 95-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 42-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 50-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 5-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 49-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 27-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 73-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 87-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 19-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 92-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 113-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 2-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 28-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 9-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 3 | 60-A | 202 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 80-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 66-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 24-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 94-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 35-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 103-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 55-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 116-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 77-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 69-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 64-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 81-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 71-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 74-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 3-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 56-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 62-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 70-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 63-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 44-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 120-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 115-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 91-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 41-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 37-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 104-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 121-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 72-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 82-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 36-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 112-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 53-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 96-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 40-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 45-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 16-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 85-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 15-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 67-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 10-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 88-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 43-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 17-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 107-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 6-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 4-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 76-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 101-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 29-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 119-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 61-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 59-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 30-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 1-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 11-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 118-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 7-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 109-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 48-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 65-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 54-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 39-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 97-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 99-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 83-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 125-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 68-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 52-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 111-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 84-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 100-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 31-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 32-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 86-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 98-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 89-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 34-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 114-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 110-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 90-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 51-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 38-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 47-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 123-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 105-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 12-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 108-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 21-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 57-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 23-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 14-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 124-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 25-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 26-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 22-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 78-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 117-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 13-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 79-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 75-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 106-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 8-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 46-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 93-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 18-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 58-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 102-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 33-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 20-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 122-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 95-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 42-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 50-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 5-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 49-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 27-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 73-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 87-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 19-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 92-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 113-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 2-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 28-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 9-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 3 | 60-A | 202 | NAP | O4D-C4D | -3.11 | 1.38 | 1.45 |
| 2 | 31-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 99-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 51-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 82-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 21-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 55-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 76-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 18-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 60-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 80-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 23-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 57-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 62-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 111-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 39-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 61-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 48-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 120-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 104-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 30-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 117-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 41-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 54-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 45-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 116-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 113-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 103-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 77-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 123-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 26-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 46-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 36-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 20-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 72-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 79-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 67-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 87-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 64-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 110-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 91-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 5-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 81-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 50-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 112-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 93-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 98-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 6-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 95-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 25-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 29-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 13-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 19-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 100-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 16-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 38-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 69-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 43-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 92-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 84-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 85-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 119-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 10-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 125-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 121-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 9-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 14-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 75-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 107-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 124-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 40-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 7-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 74-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 78-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 35-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 73-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 2-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 97-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 12-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 59-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 32-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 115-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 102-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 58-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 53-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 63-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 49-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 42-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 88-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 17-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 106-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 24-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 122-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 89-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 4-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 114-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 94-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 56-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 33-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 101-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 65-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 27-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 34-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 11-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 118-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 44-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 3-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 28-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 70-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 52-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 22-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 83-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 96-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 8-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 108-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 66-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 90-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 47-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 109-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 105-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 71-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 86-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 37-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 68-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 15-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 2 | 1-A | 201 | FOL | C4-C4A | 3.02 | 1.46 | 1.41 |
| 3 | 80-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 66-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 24-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 94-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 35-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 103-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 55-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 116-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 77-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 69-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 64-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 81-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 71-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 74-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 3-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 56-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 62-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 70-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 63-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 44-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 120-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 115-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 91-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 41-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 37-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 104-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 121-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 72-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 82-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 36-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 112-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 53-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 96-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 40-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 45-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 16-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 85-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 15-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 67-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 10-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 88-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 43-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 17-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 107-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 6-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 4-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 76-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 101-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 29-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 119-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 61-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 59-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 30-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 1-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 11-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 118-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 7-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 109-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 48-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 65-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 54-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 39-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 97-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 99-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 83-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 125-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 68-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 52-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 111-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 84-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 100-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 31-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 32-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 86-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 98-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 89-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 34-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 114-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 110-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 90-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 51-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 38-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 47-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 123-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 105-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 12-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 108-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 21-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 57-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 23-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 14-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 124-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 25-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 26-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 22-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 78-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 117-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 13-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 79-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 75-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 106-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 8-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 46-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 93-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 18-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 58-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 102-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 33-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 20-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 122-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 95-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 42-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 50-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 5-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 49-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 27-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 73-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 87-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 19-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 92-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 113-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 2-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 28-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 9-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 3 | 60-A | 202 | NAP | C2A-N3A | 2.89 | 1.36 | 1.32 |
| 2 | 31-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 99-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 51-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 82-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 21-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 55-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 76-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 18-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 60-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 80-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 23-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 57-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 62-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 111-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 39-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 61-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 48-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 120-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 104-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 30-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 117-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 41-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 54-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 45-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 116-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 113-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 103-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 77-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 123-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 26-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 46-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 36-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 20-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 72-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 79-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 67-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 87-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 64-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 110-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 91-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 5-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 81-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 50-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 112-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 93-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 98-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 6-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 95-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 25-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 29-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 13-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 19-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 100-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 16-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 38-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 69-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 43-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 92-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 84-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 85-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 119-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 10-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 125-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 121-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 9-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 14-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 75-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 107-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 124-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 40-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 7-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 74-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 78-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 35-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 73-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 2-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 97-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 12-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 59-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 32-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 115-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 102-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 58-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 53-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 63-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 49-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 42-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 88-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 17-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 106-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 24-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 122-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 89-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 4-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 114-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 94-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 56-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 33-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 101-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 65-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 27-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 34-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 11-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 118-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 44-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 3-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 28-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 70-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 52-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 22-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 83-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 96-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 8-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 108-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 66-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 90-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 47-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 109-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 105-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 71-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 86-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 37-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 68-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 15-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 2 | 1-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 3 | 80-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 66-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 24-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 94-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 35-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 103-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 55-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 116-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 77-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 69-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 64-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 81-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 71-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 74-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 3-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 56-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 62-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 70-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 63-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 44-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 120-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 115-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 91-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 41-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 37-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 104-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 121-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 72-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 82-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 36-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 112-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 53-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 96-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 40-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 45-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 16-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 85-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 15-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 67-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 10-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 88-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 43-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 17-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 107-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 6-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 4-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 76-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 101-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 29-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 119-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 61-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 59-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 30-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 1-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 11-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 118-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 7-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 109-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 48-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 65-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 54-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 39-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 97-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 99-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 83-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 125-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 68-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 52-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 111-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 84-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 100-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 31-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 32-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 86-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 98-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 89-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 34-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 114-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 110-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 90-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 51-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 38-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 47-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 123-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 105-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 12-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 108-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 21-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 57-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 23-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 14-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 124-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 25-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 26-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 22-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 78-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 117-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 13-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 79-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 75-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 106-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 8-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 46-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 93-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 18-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 58-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 102-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 33-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 20-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 122-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 95-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 42-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 50-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 5-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 49-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 27-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 73-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 87-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 19-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 92-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 113-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 2-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 28-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 9-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 60-A | 202 | NAP | C2N-N1N | 2.20 | 1.37 | 1.35 |
| 3 | 80-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 66-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 24-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 94-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 35-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 103-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 55-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 116-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 77-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 69-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 64-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 81-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 71-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 74-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 3-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 56-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 62-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 70-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 63-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 44-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 120-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 115-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 91-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 41-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 37-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 104-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 121-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 72-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 82-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 36-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 112-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 53-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 96-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 40-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 45-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 16-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 85-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 15-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 67-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 10-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 88-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 43-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 17-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 107-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 6-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 4-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 76-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 101-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 29-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 119-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 61-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 59-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 30-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 1-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 11-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 118-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 7-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 109-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 48-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 65-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 54-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 39-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 97-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 99-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 83-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 125-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 68-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 52-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 111-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 84-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 100-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 31-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 32-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 86-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 98-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 89-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 34-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 114-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 110-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 90-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 51-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 38-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 47-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 123-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 105-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 12-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 108-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 21-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 57-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 23-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 14-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 124-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 25-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 26-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 22-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 78-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 117-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 13-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 79-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 75-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 106-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 8-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 46-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 93-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 18-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 58-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 102-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 33-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 20-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 122-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 95-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 42-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 50-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 5-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 49-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 27-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 73-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 87-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 19-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 92-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 113-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 2-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 28-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 9-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |
| 3 | 60-A | 202 | NAP | C6A-N6A | 2.05 | 1.41 | 1.34 |

All (2250) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 31-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 99-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 51-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 82-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 21-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 55-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 76-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 18-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 60-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 80-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 23-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 57-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 62-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 111-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 39-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 61-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 48-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 120-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 104-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 30-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 117-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 41-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 54-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 45-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 116-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 113-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 103-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 77-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 123-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 26-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 46-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 36-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 20-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 72-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 79-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 67-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 87-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 64-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 110-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 91-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 5-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 81-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 50-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 112-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 93-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 98-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 6-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 95-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 25-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 29-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 13-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 19-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 100-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 16-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 38-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 69-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 43-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 92-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 84-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 85-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 119-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 10-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 125-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 121-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 9-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 14-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 75-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 107-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 124-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 40-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 7-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 74-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 78-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 35-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 73-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 2-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 97-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 12-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 59-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 32-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 115-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 102-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 58-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 53-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 63-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 49-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 42-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 88-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 17-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 106-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 24-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 122-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 89-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 4-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 114-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 94-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 56-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 33-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 101-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 65-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 27-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 34-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 11-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 118-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 44-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 3-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 28-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 70-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 52-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 22-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 83-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 96-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 8-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 108-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 66-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 90-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 47-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 109-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 105-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 71-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 86-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 37-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 68-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 15-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 1-A | 201 | FOL | N8-C8A-N1 | 6.92 | 123.72 | 115.82 |
| 2 | 31-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 99-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 51-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 82-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 21-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 55-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 76-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 18-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 60-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 80-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 23-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 57-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 62-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 111-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 39-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 61-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 48-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 120-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 104-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 30-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 117-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 41-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 54-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 45-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 116-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 113-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 103-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 77-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 123-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 26-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 46-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 36-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 20-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 72-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 79-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 67-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 87-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 64-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 110-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 91-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 5-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 81-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 50-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 112-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 93-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 98-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 6-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 95-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 25-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 29-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 13-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 19-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 100-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 16-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 38-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 69-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 43-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 92-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 84-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 85-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 119-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 10-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 125-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 121-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 9-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 14-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 75-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 107-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 124-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 40-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 7-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 74-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 78-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 35-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 73-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 2-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 97-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 12-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 59-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 32-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 115-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 102-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 58-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 53-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 63-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 49-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 42-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 88-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 17-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 106-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 24-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 122-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 89-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 4-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 114-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 94-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 56-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 33-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 101-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 65-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 27-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 34-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 11-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 118-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 44-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 3-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 28-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 70-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 52-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 22-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 83-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 96-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 8-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 108-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 66-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 90-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 47-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 109-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 105-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 71-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 86-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 37-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 68-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 15-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 2 | 1-A | 201 | FOL | C4A-C4-N3 | -5.06 | 116.50 | 123.43 |
| 3 | 80-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 66-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 24-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 94-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 35-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 103-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 55-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 116-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 77-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 69-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 64-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 81-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 71-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 74-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 3-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 56-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 62-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 70-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 63-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 44-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 120-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 115-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 91-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 41-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 37-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 104-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 121-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 72-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 82-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 36-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 112-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 53-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 96-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 40-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 45-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 16-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 85-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 15-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 67-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 10-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 88-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 43-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 17-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 107-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 6-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 4-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 76-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 101-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 29-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 119-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 61-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 59-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 30-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 1-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 11-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 118-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 7-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 109-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 48-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 65-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 54-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 39-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 97-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 99-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 83-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 125-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 68-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 52-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 111-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 84-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 100-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 31-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 32-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 86-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 98-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 89-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 34-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 114-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 110-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 90-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 51-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 38-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 47-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 123-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 105-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 12-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 108-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 21-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 57-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 23-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 14-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 124-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 25-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 26-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 22-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 78-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 117-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 13-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 79-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 75-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 106-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 8-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 46-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 93-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 18-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 58-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 102-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 33-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 20-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 122-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 95-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 42-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 50-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 5-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 49-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 27-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 73-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 87-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 19-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 92-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 113-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 2-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 28-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 9-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 3 | 60-A | 202 | NAP | C5A-C6A-N6A | 4.68 | 127.46 | 120.35 |
| 2 | 31-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 99-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 51-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 82-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 21-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 55-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 76-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 18-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 60-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 80-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 23-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 57-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 62-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 111-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 39-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 61-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 48-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 120-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 104-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 30-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 117-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 41-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 54-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 45-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 116-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 113-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 103-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 77-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 123-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 26-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 46-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 36-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 20-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 72-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 79-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 67-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 87-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 64-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 110-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 91-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 5-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 81-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 50-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 112-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 93-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 98-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 6-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 95-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 25-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 29-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 13-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 19-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 100-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 16-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 38-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 69-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 43-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 92-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 84-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 85-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 119-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 10-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 125-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 121-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 9-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 14-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 75-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 107-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 124-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 40-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 7-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 74-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 78-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 35-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 73-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 2-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 97-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 12-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 59-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 32-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 115-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 102-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 58-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 53-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 63-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 49-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 42-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 88-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 17-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 106-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 24-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 122-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 89-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 4-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 114-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 94-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 56-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 33-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 101-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 65-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 27-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 34-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 11-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 118-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 44-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 3-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 28-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 70-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 52-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 22-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 83-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 96-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 8-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 108-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 66-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 90-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 47-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 109-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 105-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 71-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 86-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 37-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 68-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 15-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 1-A | 201 | FOL | C4-N3-C2 | 4.49 | 123.06 | 115.93 |
| 2 | 31-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 99-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 51-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 82-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 21-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 55-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 76-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 18-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 60-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 80-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 23-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 57-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 62-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 111-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 39-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 61-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 48-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 120-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 104-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 30-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 117-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 41-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 54-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 45-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 116-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 113-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 103-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 77-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 123-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 26-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 46-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 36-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 20-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 72-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 79-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 67-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 87-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 64-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 110-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 91-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 5-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 81-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 50-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 112-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 93-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 98-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 6-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 95-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 25-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 29-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 13-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 19-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 100-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 16-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 38-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 69-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 43-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 92-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 84-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 85-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 119-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 10-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 125-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 121-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 9-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 14-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 75-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 107-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 124-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 40-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 7-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 74-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 78-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 35-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 73-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 2-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 97-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 12-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 59-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 32-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 115-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 102-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 58-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 53-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 63-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 49-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 42-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 88-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 17-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 106-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 24-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 122-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 89-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 4-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 114-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 94-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 56-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 33-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 101-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 65-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 27-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 34-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 11-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 118-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 44-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 3-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 28-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 70-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 52-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 22-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 83-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 96-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 8-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 108-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 66-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 90-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 47-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 109-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 105-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 71-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 86-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 37-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 68-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 15-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 1-A | 201 | FOL | C4-C4A-C8A | -4.46 | 117.00 | 119.95 |
| 2 | 31-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 99-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 51-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 82-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 21-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 55-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 76-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 18-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 60-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 80-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 23-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 57-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 62-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 111-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 39-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 61-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 48-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 120-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 104-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 30-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 117-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 41-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 54-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 45-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 116-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 113-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 103-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 77-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 123-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 26-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 46-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 36-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 20-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 72-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 79-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 67-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 87-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 64-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 110-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 91-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 5-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 81-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 50-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 112-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 93-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 98-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 6-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 95-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 25-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 29-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 13-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 19-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 100-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 16-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 38-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 69-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 43-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 92-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 84-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 85-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 119-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 10-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 125-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 121-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 9-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 14-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 75-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 107-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 124-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 40-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 7-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 74-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 78-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 35-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 73-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 2-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 97-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 12-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 59-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 32-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 115-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 102-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 58-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 53-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 63-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 49-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 42-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 88-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 17-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 106-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 24-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 122-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 89-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 4-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 114-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 94-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 56-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 33-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 101-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 65-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 27-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 34-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 11-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 118-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 44-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 3-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 28-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 70-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 52-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 22-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 83-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 96-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 8-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 108-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 66-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 90-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 47-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 109-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 105-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 71-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 86-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 37-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 68-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 15-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 1-A | 201 | FOL | C2-N1-C8A | 3.66 | 119.53 | 115.36 |
| 2 | 31-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 99-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 51-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 82-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 21-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 55-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 76-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 18-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 60-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 80-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 23-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 57-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 62-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 111-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 39-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 61-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 48-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 120-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 104-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 30-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 117-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 41-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 54-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 45-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 116-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 113-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 103-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 77-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 123-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 26-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 46-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 36-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 20-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 72-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 79-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 67-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 87-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 64-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 110-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 91-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 5-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 81-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 50-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 112-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 93-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 98-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 6-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 95-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 25-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 29-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 13-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 19-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 100-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 16-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 38-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 69-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 43-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 92-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 84-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 85-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 119-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 10-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 125-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 121-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 9-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 14-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 75-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 107-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 124-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 40-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 7-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 74-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 78-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 35-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 73-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 2-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 97-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 12-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 59-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 32-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 115-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 102-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 58-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 53-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 63-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 49-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 42-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 88-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 17-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 106-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 24-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 122-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 89-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 4-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 114-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 94-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 56-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 33-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 101-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 65-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 27-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 34-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 11-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 118-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 44-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 3-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 28-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 70-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 52-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 22-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 83-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 96-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 8-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 108-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 66-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 90-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 47-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 109-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 105-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 71-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 86-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 37-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 68-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 15-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 1-A | 201 | FOL | C7-N8-C8A | 3.23 | 119.94 | 116.69 |
| 2 | 31-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 99-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 51-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 82-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 21-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 55-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 76-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 18-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 60-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 80-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 23-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 57-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 62-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 111-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 39-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 61-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 48-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 120-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 104-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 30-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 117-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 41-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 54-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 45-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 116-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 113-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 103-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 77-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 123-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 26-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 46-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 36-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 20-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 72-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 79-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 67-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 87-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 64-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 110-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 91-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 5-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 81-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 50-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 112-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 93-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 98-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 6-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 95-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 25-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 29-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 13-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 19-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 100-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 16-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 38-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 69-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 43-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 92-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 84-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 85-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 119-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 10-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 125-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 121-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 9-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 14-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 75-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 107-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 124-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 40-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 7-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 74-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 78-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 35-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 73-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 2-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 97-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 12-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 59-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 32-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 115-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 102-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 58-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 53-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 63-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 49-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 42-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 88-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 17-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 106-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 24-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 122-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 89-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 4-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 114-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 94-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 56-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 33-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 101-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 65-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 27-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 34-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 11-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 118-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 44-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 3-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 28-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 70-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 52-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 22-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 83-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 96-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 8-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 108-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 66-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 90-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 47-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 109-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 105-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 71-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 86-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 37-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 68-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 15-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 1-A | 201 | FOL | N1-C2-N3 | -3.12 | 123.06 | 127.22 |
| 2 | 31-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 99-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 51-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 82-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 21-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 55-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 76-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 18-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 60-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 80-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 23-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 57-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 62-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 111-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 39-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 61-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 48-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 120-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 104-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 30-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 117-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 41-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 54-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 45-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 116-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 113-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 103-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 77-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 123-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 26-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 46-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 36-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 20-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 72-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 79-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 67-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 87-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 64-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 110-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 91-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 5-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 81-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 50-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 112-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 93-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 98-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 6-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 95-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 25-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 29-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 13-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 19-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 100-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 16-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 38-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 69-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 43-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 92-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 84-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 85-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 119-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 10-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 125-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 121-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 9-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 14-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 75-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 107-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 124-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 40-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 7-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 74-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 78-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 35-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 73-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 2-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 97-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 12-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 59-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 32-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 115-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 102-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 58-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 53-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 63-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 49-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 42-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 88-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 17-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 106-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 24-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 122-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 89-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 4-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 114-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 94-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 56-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 33-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 101-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 65-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 27-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 34-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 11-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 118-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 44-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 3-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 28-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 70-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 52-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 22-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 83-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 96-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 8-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 108-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 66-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 90-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 47-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 109-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 105-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 71-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 86-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 37-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 68-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 15-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 1-A | 201 | FOL | C7-C6-N5 | -3.11 | 118.81 | 120.85 |
| 2 | 31-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 99-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 51-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 82-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 21-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 55-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 76-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 18-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 60-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 80-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 23-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 57-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 62-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 111-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 39-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 61-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 48-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 120-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 104-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 30-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 117-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 41-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 54-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 45-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 116-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 113-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 103-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 77-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 123-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 26-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 46-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 36-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 20-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 72-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 79-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 67-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 87-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 64-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 110-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 91-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 5-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 81-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 50-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 112-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 93-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 98-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 6-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 95-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 25-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 29-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 13-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 19-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 100-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 16-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 38-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 69-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 43-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 92-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 84-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 85-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 119-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 10-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 125-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 121-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 9-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 14-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 75-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 107-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 124-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 40-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 7-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 74-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 78-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 35-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 73-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 2-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 97-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 12-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 59-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 32-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 115-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 102-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 58-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 53-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 63-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 49-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 42-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 88-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 17-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 106-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 24-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 122-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 89-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 4-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 114-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 94-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 56-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 33-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 101-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 65-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 27-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 34-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 11-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 118-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 44-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 3-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 28-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 70-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 52-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 22-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 83-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 96-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 8-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 108-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 66-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 90-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 47-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 109-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 105-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 71-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 86-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 37-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 68-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 15-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 2 | 1-A | 201 | FOL | C11-C-N | -3.01 | 111.29 | 117.06 |
| 3 | 80-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 66-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 24-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 94-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 35-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 103-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 55-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 116-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 77-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 69-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 64-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 81-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 71-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 74-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 3-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 56-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 62-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 70-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 63-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 44-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 120-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 115-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 91-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 41-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 37-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 104-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 121-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 72-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 82-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 36-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 112-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 53-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 96-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 40-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 45-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 16-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 85-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 15-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 67-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 10-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 88-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 43-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 17-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 107-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 6-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 4-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 76-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 101-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 29-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 119-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 61-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 59-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 30-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 1-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 11-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 118-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 7-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 109-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 48-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 65-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 54-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 39-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 97-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 99-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 83-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 125-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 68-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 52-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 111-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 84-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 100-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 31-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 32-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 86-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 98-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 89-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 34-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 114-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 110-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 90-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 51-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 38-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 47-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 123-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 105-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 12-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 108-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 21-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 57-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 23-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 14-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 124-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 25-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 26-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 22-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 78-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 117-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 13-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 79-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 75-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 106-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 8-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 46-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 93-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 18-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 58-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 102-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 33-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 20-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 122-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 95-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 42-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 50-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 5-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 49-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 27-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 73-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 87-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 19-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 92-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 113-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 2-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 28-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 9-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 60-A | 202 | NAP | C2N-C3N-C4N | 2.61 | 121.22 | 118.26 |
| 3 | 80-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 66-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 24-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 94-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 35-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 103-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 55-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 116-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 77-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 69-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 64-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 81-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 71-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 74-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 3-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 56-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 62-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 70-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 63-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 44-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 120-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 115-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 91-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 41-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 37-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 104-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 121-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 72-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 82-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 36-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 112-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 53-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 96-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 40-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 45-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 16-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 85-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 15-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 67-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 10-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 88-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 43-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 17-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 107-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 6-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 4-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 76-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 101-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 29-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 119-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 61-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 59-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 30-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 1-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 11-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 118-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 7-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 109-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 48-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 65-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 54-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 39-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 97-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 99-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 83-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 125-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 68-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 52-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 111-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 84-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 100-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 31-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 32-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 86-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 98-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 89-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 34-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 114-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 110-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 90-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 51-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 38-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 47-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 123-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 105-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 12-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 108-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 21-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 57-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 23-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 14-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 124-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 25-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 26-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 22-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 78-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 117-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 13-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 79-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 75-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 106-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 8-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 46-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 93-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 18-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 58-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 102-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 33-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 20-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 122-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 95-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 42-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 50-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 5-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 49-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 27-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 73-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 87-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 19-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 92-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 113-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 2-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 28-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 9-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 3 | 60-A | 202 | NAP | C1B-N9A-C4A | -2.59 | 122.09 | 126.64 |
| 2 | 31-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 99-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 51-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 82-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 21-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 55-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 76-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 18-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 60-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 80-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 23-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 57-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 62-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 111-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 39-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 61-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 48-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 120-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 104-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 30-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 117-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 41-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 54-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 45-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 116-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 113-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 103-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 77-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 123-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 26-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 46-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 36-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 20-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 72-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 79-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 67-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 87-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 64-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 110-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 91-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 5-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 81-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 50-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 112-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 93-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 98-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 6-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 95-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 25-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 29-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 13-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 19-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 100-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 16-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 38-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 69-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 43-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 92-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 84-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 85-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 119-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 10-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 125-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 121-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 9-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 14-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 75-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 107-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 124-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 40-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 7-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 74-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 78-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 35-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 73-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 2-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 97-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 12-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 59-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 32-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 115-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 102-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 58-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 53-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 63-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 49-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 42-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 88-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 17-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 106-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 24-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 122-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 89-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 4-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 114-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 94-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 56-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 33-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 101-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 65-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 27-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 34-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 11-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 118-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 44-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 3-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 28-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 70-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 52-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 22-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 83-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 96-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 8-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 108-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 66-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 90-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 47-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 109-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 105-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 71-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 86-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 37-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 68-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 15-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 2 | 1-A | 201 | FOL | O-C-N | 2.55 | 127.14 | 122.45 |
| 3 | 80-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 66-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 24-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 94-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 35-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 103-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 55-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 116-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 77-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 69-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 64-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 81-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 71-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 74-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 3-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 56-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 62-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 70-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 63-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 44-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 120-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 115-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 91-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 41-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 37-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 104-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 121-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 72-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 82-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 36-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 112-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 53-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 96-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 40-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 45-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 16-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 85-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 15-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 67-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 10-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 88-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 43-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 17-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 107-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 6-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 4-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 76-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 101-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 29-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 119-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 61-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 59-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 30-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 1-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 11-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 118-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 7-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 109-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 48-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 65-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 54-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 39-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 97-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 99-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 83-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 125-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 68-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 52-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 111-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 84-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 100-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 31-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 32-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 86-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 98-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 89-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 34-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 114-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 110-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 90-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 51-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 38-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 47-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 123-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 105-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 12-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 108-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 21-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 57-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 23-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 14-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 124-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 25-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 26-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 22-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 78-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 117-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 13-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 79-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 75-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 106-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 8-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 46-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 93-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 18-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 58-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 102-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 33-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 20-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 122-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 95-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 42-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 50-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 5-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 49-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 27-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 73-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 87-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 19-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 92-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 113-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 2-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 28-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 9-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 60-A | 202 | NAP | N3A-C2A-N1A | -2.40 | 124.93 | 128.68 |
| 3 | 80-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 66-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 24-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 94-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 35-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 103-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 55-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 116-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 77-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 69-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 64-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 81-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 71-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 74-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 3-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 56-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 62-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 70-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 63-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 44-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 120-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 115-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 91-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 41-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 37-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 104-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 121-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 72-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 82-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 36-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 112-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 53-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 96-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 40-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 45-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 16-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 85-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 15-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 67-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 10-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 88-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 43-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 17-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 107-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 6-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 4-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 76-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 101-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 29-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 119-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 61-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 59-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 30-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 1-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 11-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 118-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 7-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 109-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 48-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 65-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 54-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 39-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 97-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 99-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 83-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 125-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 68-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 52-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 111-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 84-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 100-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 31-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 32-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 86-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 98-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 89-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 34-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 114-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 110-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 90-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 51-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 38-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 47-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 123-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 105-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 12-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 108-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 21-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 57-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 23-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 14-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 124-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 25-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 26-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 22-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 78-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 117-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 13-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 79-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 75-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 106-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 8-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 46-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 93-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 18-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 58-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 102-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 33-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 20-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 122-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 95-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 42-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 50-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 5-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 49-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 27-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 73-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 87-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 19-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 92-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 113-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 2-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 28-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 9-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 60-A | 202 | NAP | N6A-C6A-N1A | -2.25 | 113.91 | 118.57 |
| 3 | 80-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 66-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 24-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 94-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 35-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 103-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 55-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 116-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 77-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 69-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 64-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 81-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 71-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 74-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 3-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 56-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 62-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 70-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 63-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 44-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 120-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 115-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 91-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 41-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 37-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 104-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 121-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 72-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 82-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 36-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 112-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 53-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 96-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 40-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 45-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 16-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 85-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 15-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 67-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 10-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 88-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 43-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 17-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 107-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 6-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 4-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 76-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 101-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 29-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 119-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 61-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 59-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 30-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 1-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 11-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 118-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 7-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 109-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 48-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 65-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 54-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 39-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 97-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 99-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 83-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 125-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 68-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 52-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 111-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 84-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 100-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 31-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 32-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 86-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 98-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 89-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 34-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 114-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 110-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 90-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 51-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 38-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 47-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 123-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 105-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 12-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 108-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 21-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 57-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 23-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 14-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 124-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 25-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 26-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 22-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 78-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 117-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 13-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 79-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 75-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 106-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 8-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 46-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 93-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 18-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 58-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 102-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 33-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 20-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 122-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 95-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 42-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 50-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 5-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 49-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 27-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 73-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 87-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 19-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 92-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 113-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 2-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 28-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 9-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 60-A | 202 | NAP | O4D-C1D-C2D | -2.09 | 103.87 | 106.93 |
| 3 | 80-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 66-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 24-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 94-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 35-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 103-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 55-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 116-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 77-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 69-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 64-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 81-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 71-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 74-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 3-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 56-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 62-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 70-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 63-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 44-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 120-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 115-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 91-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 41-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 37-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 104-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 121-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 72-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 82-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 36-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 112-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 53-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 96-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 40-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 45-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 16-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 85-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 15-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 67-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 10-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 88-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 43-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 17-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 107-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 6-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 4-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 76-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 101-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 29-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 119-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 61-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 59-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 30-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 1-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 11-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 118-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 7-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 109-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 48-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 65-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 54-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 39-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 97-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 99-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 83-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 125-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 68-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 52-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 111-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 84-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 100-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 31-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 32-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 86-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 98-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 89-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 34-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 114-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 110-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 90-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 51-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 38-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 47-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 123-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 105-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 12-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 108-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 21-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 57-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 23-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 14-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 124-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 25-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 26-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 22-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 78-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 117-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 13-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 79-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 75-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 106-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 8-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 46-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 93-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 18-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 58-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 102-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 33-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 20-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 122-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 95-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 42-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 50-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 5-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 49-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 27-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 73-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 87-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 19-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 92-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 113-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 2-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 28-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 9-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 60-A | 202 | NAP | C6N-N1N-C2N | -2.07 | 120.09 | 121.97 |
| 3 | 80-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 66-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 24-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 94-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 35-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 103-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 55-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 116-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 77-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 69-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 64-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 81-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 71-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 74-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 3-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 56-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 62-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 70-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 63-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 44-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 120-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 115-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 91-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 41-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 37-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 104-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 121-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 72-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 82-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 36-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 112-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 53-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 96-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 40-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 45-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 16-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 85-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 15-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 67-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 10-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 88-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 43-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 17-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 107-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 6-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 4-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 76-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 101-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 29-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 119-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 61-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 59-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 30-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 1-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 11-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 118-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 7-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 109-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 48-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 65-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 54-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 39-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 97-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 99-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 83-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 125-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 68-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 52-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 111-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 84-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 100-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 31-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 32-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 86-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 98-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 89-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 34-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 114-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 110-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 90-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 51-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 38-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 47-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 123-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 105-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 12-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 108-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 21-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 57-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 23-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 14-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 124-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 25-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 26-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 22-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 78-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 117-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 13-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 79-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 75-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 106-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 8-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 46-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 93-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 18-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 58-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 102-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 33-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 20-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 122-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 95-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 42-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 50-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 5-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 49-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 27-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 73-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 87-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 19-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 92-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 113-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 2-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 28-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 9-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |
| 3 | 60-A | 202 | NAP | O3B-C3B-C2B | 2.02 | 116.91 | 111.17 |

There are no chirality outliers.

All (1000) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 80-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 66-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 24-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 94-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 35-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 103-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 55-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 116-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 77-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 69-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 64-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 81-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 71-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 74-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 3-A | 202 | NAP | O4D-C1D-N1N-C6N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 56-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 62-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 70-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 63-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 44-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 120-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 115-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 91-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 41-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 37-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 104-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 121-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 72-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 82-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 36-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 112-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 53-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 96-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 40-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 45-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 16-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 85-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 15-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 67-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 10-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 88-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 43-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 17-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 107-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 6-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 4-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 76-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 101-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 29-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 119-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 61-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 59-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 30-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 1-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 11-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 118-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 7-A | 202 | NAP | O4D-C1D-N1N-C6N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 109-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 48-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 65-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 54-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 39-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 97-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 99-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 83-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 125-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 68-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 52-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 111-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 84-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 100-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 31-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 32-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 86-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 98-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 89-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 34-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 114-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 110-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 90-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 51-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 38-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 47-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 123-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 105-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 12-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 108-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 21-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 57-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 23-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 14-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 124-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 25-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 26-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 22-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 78-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 117-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 13-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 79-A | 202 | NAP | O4D-C1D-N1N-C6N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 75-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 106-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 8-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 46-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 93-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 18-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 58-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 102-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 33-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 20-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 122-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 95-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 42-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 50-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 5-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 49-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 27-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 73-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 87-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 19-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 92-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 113-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 2-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 28-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 9-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 60-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 31-A | 201 | FOL | O-C-C11-C12 |
| 2 | 99-A | 201 | FOL | O-C-C11-C12 |
| 2 | 51-A | 201 | FOL | O-C-C11-C12 |
| 2 | 82-A | 201 | FOL | O-C-C11-C12 |
| 2 | 21-A | 201 | FOL | O-C-C11-C12 |
| 2 | 55-A | 201 | FOL | O-C-C11-C12 |
| 2 | 76-A | 201 | FOL | O-C-C11-C12 |
| 2 | 18-A | 201 | FOL | O-C-C11-C12 |
| 2 | 60-A | 201 | FOL | O-C-C11-C12 |
| 2 | 80-A | 201 | FOL | O-C-C11-C12 |
| 2 | 23-A | 201 | FOL | O-C-C11-C12 |
| 2 | 57-A | 201 | FOL | O-C-C11-C12 |
| 2 | 62-A | 201 | FOL | O-C-C11-C12 |
| 2 | 111-A | 201 | FOL | O-C-C11-C12 |
| 2 | 39-A | 201 | FOL | O-C-C11-C12 |
| 2 | 61-A | 201 | FOL | O-C-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 48-A | 201 | FOL | O-C-C11-C12 |
| 2 | 120-A | 201 | FOL | O-C-C11-C12 |
| 2 | 104-A | 201 | FOL | O-C-C11-C12 |
| 2 | 30-A | 201 | FOL | O-C-C11-C12 |
| 2 | 117-A | 201 | FOL | O-C-C11-C12 |
| 2 | 41-A | 201 | FOL | O-C-C11-C12 |
| 2 | 54-A | 201 | FOL | O-C-C11-C12 |
| 2 | 45-A | 201 | FOL | O-C-C11-C12 |
| 2 | 116-A | 201 | FOL | O-C-C11-C12 |
| 2 | 113-A | 201 | FOL | O-C-C11-C12 |
| 2 | 103-A | 201 | FOL | O-C-C11-C12 |
| 2 | 77-A | 201 | FOL | O-C-C11-C12 |
| 2 | 123-A | 201 | FOL | O-C-C11-C12 |
| 2 | 26-A | 201 | FOL | O-C-C11-C12 |
| 2 | 46-A | 201 | FOL | O-C-C11-C12 |
| 2 | 36-A | 201 | FOL | O-C-C11-C12 |
| 2 | 20-A | 201 | FOL | O-C-C11-C12 |
| 2 | 72-A | 201 | FOL | O-C-C11-C12 |
| 2 | 79-A | 201 | FOL | O-C-C11-C12 |
| 2 | 67-A | 201 | FOL | O-C-C11-C12 |
| 2 | 87-A | 201 | FOL | O-C-C11-C12 |
| 2 | 64-A | 201 | FOL | O-C-C11-C12 |
| 2 | 110-A | 201 | FOL | O-C-C11-C12 |
| 2 | 91-A | 201 | FOL | O-C-C11-C12 |
| 2 | 5-A | 201 | FOL | O-C-C11-C12 |
| 2 | 81-A | 201 | FOL | O-C-C11-C12 |
| 2 | 50-A | 201 | FOL | O-C-C11-C12 |
| 2 | 112-A | 201 | FOL | O-C-C11-C12 |
| 2 | 93-A | 201 | FOL | O-C-C11-C12 |
| 2 | 98-A | 201 | FOL | O-C-C11-C12 |
| 2 | 6-A | 201 | FOL | O-C-C11-C12 |
| 2 | 95-A | 201 | FOL | O-C-C11-C12 |
| 2 | 25-A | 201 | FOL | O-C-C11-C12 |
| 2 | 29-A | 201 | FOL | O-C-C11-C12 |
| 2 | 13-A | 201 | FOL | O-C-C11-C12 |
| 2 | 19-A | 201 | FOL | O-C-C11-C12 |
| 2 | 100-A | 201 | FOL | O-C-C11-C12 |
| 2 | 16-A | 201 | FOL | O-C-C11-C12 |
| 2 | 38-A | 201 | FOL | O-C-C11-C12 |
| 2 | 69-A | 201 | FOL | O-C-C11-C12 |
| 2 | 43-A | 201 | FOL | O-C-C11-C12 |
| 2 | 92-A | 201 | FOL | O-C-C11-C12 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 84-A | 201 | FOL | O-C-C11-C12 |
| 2 | 85-A | 201 | FOL | O-C-C11-C12 |
| 2 | 119-A | 201 | FOL | O-C-C11-C12 |
| 2 | 10-A | 201 | FOL | O-C-C11-C12 |
| 2 | 125-A | 201 | FOL | O-C-C11-C12 |
| 2 | 121-A | 201 | FOL | O-C-C11-C12 |
| 2 | 9-A | 201 | FOL | O-C-C11-C12 |
| 2 | 14-A | 201 | FOL | O-C-C11-C12 |
| 2 | 75-A | 201 | FOL | O-C-C11-C12 |
| 2 | 107-A | 201 | FOL | O-C-C11-C12 |
| 2 | 124-A | 201 | FOL | O-C-C11-C12 |
| 2 | 40-A | 201 | FOL | O-C-C11-C12 |
| 2 | 7-A | 201 | FOL | O-C-C11-C12 |
| 2 | 74-A | 201 | FOL | O-C-C11-C12 |
| 2 | 78-A | 201 | FOL | O-C-C11-C12 |
| 2 | 35-A | 201 | FOL | O-C-C11-C12 |
| 2 | 73-A | 201 | FOL | O-C-C11-C12 |
| 2 | 2-A | 201 | FOL | O-C-C11-C12 |
| 2 | 97-A | 201 | FOL | O-C-C11-C12 |
| 2 | 12-A | 201 | FOL | O-C-C11-C12 |
| 2 | 59-A | 201 | FOL | O-C-C11-C12 |
| 2 | 32-A | 201 | FOL | O-C-C11-C12 |
| 2 | 115-A | 201 | FOL | O-C-C11-C12 |
| 2 | 102-A | 201 | FOL | O-C-C11-C12 |
| 2 | 58-A | 201 | FOL | O-C-C11-C12 |
| 2 | 53-A | 201 | FOL | O-C-C11-C12 |
| 2 | 63-A | 201 | FOL | O-C-C11-C12 |
| 2 | 49-A | 201 | FOL | O-C-C11-C12 |
| 2 | 42-A | 201 | FOL | O-C-C11-C12 |
| 2 | 88-A | 201 | FOL | O-C-C11-C12 |
| 2 | 17-A | 201 | FOL | O-C-C11-C12 |
| 2 | 106-A | 201 | FOL | O-C-C11-C12 |
| 2 | 24-A | 201 | FOL | O-C-C11-C12 |
| 2 | 122-A | 201 | FOL | O-C-C11-C12 |
| 2 | 89-A | 201 | FOL | O-C-C11-C12 |
| 2 | 4-A | 201 | FOL | O-C-C11-C12 |
| 2 | 114-A | 201 | FOL | O-C-C11-C12 |
| 2 | 94-A | 201 | FOL | O-C-C11-C12 |
| 2 | 56-A | 201 | FOL | O-C-C11-C12 |
| 2 | 33-A | 201 | FOL | O-C-C11-C12 |
| 2 | 101-A | 201 | FOL | O-C-C11-C12 |
| 2 | 65-A | 201 | FOL | O-C-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 27-A | 201 | FOL | O-C-C11-C12 |
| 2 | 34-A | 201 | FOL | O-C-C11-C12 |
| 2 | 11-A | 201 | FOL | O-C-C11-C12 |
| 2 | 118-A | 201 | FOL | O-C-C11-C12 |
| 2 | 44-A | 201 | FOL | O-C-C11-C12 |
| 2 | 3-A | 201 | FOL | O-C-C11-C12 |
| 2 | 28-A | 201 | FOL | O-C-C11-C12 |
| 2 | 70-A | 201 | FOL | O-C-C11-C12 |
| 2 | 52-A | 201 | FOL | O-C-C11-C12 |
| 2 | 22-A | 201 | FOL | O-C-C11-C12 |
| 2 | 83-A | 201 | FOL | O-C-C11-C12 |
| 2 | 96-A | 201 | FOL | O-C-C11-C12 |
| 2 | 8-A | 201 | FOL | O-C-C11-C12 |
| 2 | 108-A | 201 | FOL | O-C-C11-C12 |
| 2 | 66-A | 201 | FOL | O-C-C11-C12 |
| 2 | 90-A | 201 | FOL | O-C-C11-C12 |
| 2 | 47-A | 201 | FOL | O-C-C11-C12 |
| 2 | 109-A | 201 | FOL | O-C-C11-C12 |
| 2 | 105-A | 201 | FOL | O-C-C11-C12 |
| 2 | 71-A | 201 | FOL | O-C-C11-C12 |
| 2 | 86-A | 201 | FOL | O-C-C11-C12 |
| 2 | 37-A | 201 | FOL | O-C-C11-C12 |
| 2 | 68-A | 201 | FOL | O-C-C11-C12 |
| 2 | 15-A | 201 | FOL | O-C-C11-C12 |
| 2 | 1-A | 201 | FOL | O-C-C11-C12 |
| 2 | 31-A | 201 | FOL | N-C-C11-C12 |
| 2 | 99-A | 201 | FOL | N-C-C11-C12 |
| 2 | 51-A | 201 | FOL | N-C-C11-C12 |
| 2 | 82-A | 201 | FOL | N-C-C11-C12 |
| 2 | 21-A | 201 | FOL | N-C-C11-C12 |
| 2 | 55-A | 201 | FOL | N-C-C11-C12 |
| 2 | 76-A | 201 | FOL | N-C-C11-C12 |
| 2 | 18-A | 201 | FOL | N-C-C11-C12 |
| 2 | 60-A | 201 | FOL | N-C-C11-C12 |
| 2 | 80-A | 201 | FOL | N-C-C11-C12 |
| 2 | 23-A | 201 | FOL | N-C-C11-C12 |
| 2 | 57-A | 201 | FOL | N-C-C11-C12 |
| 2 | 62-A | 201 | FOL | N-C-C11-C12 |
| 2 | 111-A | 201 | FOL | N-C-C11-C12 |
| 2 | 39-A | 201 | FOL | N-C-C11-C12 |
| 2 | 61-A | 201 | FOL | N-C-C11-C12 |
| 2 | 48-A | 201 | FOL | N-C-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 120-A | 201 | FOL | N-C-C11-C12 |
| 2 | 104-A | 201 | FOL | N-C-C11-C12 |
| 2 | 30-A | 201 | FOL | N-C-C11-C12 |
| 2 | 117-A | 201 | FOL | N-C-C11-C12 |
| 2 | 41-A | 201 | FOL | N-C-C11-C12 |
| 2 | 54-A | 201 | FOL | N-C-C11-C12 |
| 2 | 45-A | 201 | FOL | N-C-C11-C12 |
| 2 | 116-A | 201 | FOL | N-C-C11-C12 |
| 2 | 113-A | 201 | FOL | N-C-C11-C12 |
| 2 | 103-A | 201 | FOL | N-C-C11-C12 |
| 2 | 77-A | 201 | FOL | N-C-C11-C12 |
| 2 | 123-A | 201 | FOL | N-C-C11-C12 |
| 2 | 26-A | 201 | FOL | N-C-C11-C12 |
| 2 | 46-A | 201 | FOL | N-C-C11-C12 |
| 2 | 36-A | 201 | FOL | N-C-C11-C12 |
| 2 | 20-A | 201 | FOL | N-C-C11-C12 |
| 2 | 72-A | 201 | FOL | N-C-C11-C12 |
| 2 | 79-A | 201 | FOL | N-C-C11-C12 |
| 2 | 67-A | 201 | FOL | N-C-C11-C12 |
| 2 | 87-A | 201 | FOL | N-C-C11-C12 |
| 2 | 64-A | 201 | FOL | N-C-C11-C12 |
| 2 | 110-A | 201 | FOL | N-C-C11-C12 |
| 2 | 91-A | 201 | FOL | N-C-C11-C12 |
| 2 | 5-A | 201 | FOL | N-C-C11-C12 |
| 2 | 81-A | 201 | FOL | N-C-C11-C12 |
| 2 | 50-A | 201 | FOL | N-C-C11-C12 |
| 2 | 112-A | 201 | FOL | N-C-C11-C12 |
| 2 | 93-A | 201 | FOL | N-C-C11-C12 |
| 2 | 98-A | 201 | FOL | N-C-C11-C12 |
| 2 | 6-A | 201 | FOL | N-C-C11-C12 |
| 2 | 95-A | 201 | FOL | N-C-C11-C12 |
| 2 | 25-A | 201 | FOL | N-C-C11-C12 |
| 2 | 29-A | 201 | FOL | N-C-C11-C12 |
| 2 | 13-A | 201 | FOL | N-C-C11-C12 |
| 2 | 19-A | 201 | FOL | N-C-C11-C12 |
| 2 | 100-A | 201 | FOL | N-C-C11-C12 |
| 2 | 16-A | 201 | FOL | N-C-C11-C12 |
| 2 | 38-A | 201 | FOL | N-C-C11-C12 |
| 2 | 69-A | 201 | FOL | N-C-C11-C12 |
| 2 | 43-A | 201 | FOL | N-C-C11-C12 |
| 2 | 92-A | 201 | FOL | N-C-C11-C12 |
| 2 | 84-A | 201 | FOL | N-C-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 85-A | 201 | FOL | N-C-C11-C12 |
| 2 | 119-A | 201 | FOL | N-C-C11-C12 |
| 2 | 10-A | 201 | FOL | N-C-C11-C12 |
| 2 | 125-A | 201 | FOL | N-C-C11-C12 |
| 2 | 121-A | 201 | FOL | N-C-C11-C12 |
| 2 | 9-A | 201 | FOL | N-C-C11-C12 |
| 2 | 14-A | 201 | FOL | N-C-C11-C12 |
| 2 | 75-A | 201 | FOL | N-C-C11-C12 |
| 2 | 107-A | 201 | FOL | N-C-C11-C12 |
| 2 | 124-A | 201 | FOL | N-C-C11-C12 |
| 2 | 40-A | 201 | FOL | N-C-C11-C12 |
| 2 | 7-A | 201 | FOL | N-C-C11-C12 |
| 2 | 74-A | 201 | FOL | N-C-C11-C12 |
| 2 | 78-A | 201 | FOL | N-C-C11-C12 |
| 2 | 35-A | 201 | FOL | N-C-C11-C12 |
| 2 | 73-A | 201 | FOL | N-C-C11-C12 |
| 2 | 2-A | 201 | FOL | N-C-C11-C12 |
| 2 | 97-A | 201 | FOL | N-C-C11-C12 |
| 2 | 12-A | 201 | FOL | N-C-C11-C12 |
| 2 | 59-A | 201 | FOL | N-C-C11-C12 |
| 2 | 32-A | 201 | FOL | N-C-C11-C12 |
| 2 | 115-A | 201 | FOL | N-C-C11-C12 |
| 2 | 102-A | 201 | FOL | N-C-C11-C12 |
| 2 | 58-A | 201 | FOL | N-C-C11-C12 |
| 2 | 53-A | 201 | FOL | N-C-C11-C12 |
| 2 | 63-A | 201 | FOL | N-C-C11-C12 |
| 2 | 49-A | 201 | FOL | N-C-C11-C12 |
| 2 | 42-A | 201 | FOL | N-C-C11-C12 |
| 2 | 88-A | 201 | FOL | N-C-C11-C12 |
| 2 | 17-A | 201 | FOL | N-C-C11-C12 |
| 2 | 106-A | 201 | FOL | N-C-C11-C12 |
| 2 | 24-A | 201 | FOL | N-C-C11-C12 |
| 2 | 122-A | 201 | FOL | N-C-C11-C12 |
| 2 | 89-A | 201 | FOL | N-C-C11-C12 |
| 2 | 4-A | 201 | FOL | N-C-C11-C12 |
| 2 | 114-A | 201 | FOL | N-C-C11-C12 |
| 2 | 94-A | 201 | FOL | N-C-C11-C12 |
| 2 | 56-A | 201 | FOL | N-C-C11-C12 |
| 2 | 33-A | 201 | FOL | N-C-C11-C12 |
| 2 | 101-A | 201 | FOL | N-C-C11-C12 |
| 2 | 65-A | 201 | FOL | N-C-C11-C12 |
| 2 | 27-A | 201 | FOL | N-C-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 34-A | 201 | FOL | N-C-C11-C12 |
| 2 | 11-A | 201 | FOL | N-C-C11-C12 |
| 2 | 118-A | 201 | FOL | N-C-C11-C12 |
| 2 | 44-A | 201 | FOL | N-C-C11-C12 |
| 2 | 3-A | 201 | FOL | N-C-C11-C12 |
| 2 | 28-A | 201 | FOL | N-C-C11-C12 |
| 2 | 70-A | 201 | FOL | N-C-C11-C12 |
| 2 | 52-A | 201 | FOL | N-C-C11-C12 |
| 2 | 22-A | 201 | FOL | N-C-C11-C12 |
| 2 | 83-A | 201 | FOL | N-C-C11-C12 |
| 2 | 96-A | 201 | FOL | N-C-C11-C12 |
| 2 | 8-A | 201 | FOL | N-C-C11-C12 |
| 2 | 108-A | 201 | FOL | N-C-C11-C12 |
| 2 | 66-A | 201 | FOL | N-C-C11-C12 |
| 2 | 90-A | 201 | FOL | N-C-C11-C12 |
| 2 | 47-A | 201 | FOL | N-C-C11-C12 |
| 2 | 109-A | 201 | FOL | N-C-C11-C12 |
| 2 | 105-A | 201 | FOL | N-C-C11-C12 |
| 2 | 71-A | 201 | FOL | N-C-C11-C12 |
| 2 | 86-A | 201 | FOL | N-C-C11-C12 |
| 2 | 37-A | 201 | FOL | N-C-C11-C12 |
| 2 | 68-A | 201 | FOL | N-C-C11-C12 |
| 2 | 15-A | 201 | FOL | N-C-C11-C12 |
| 2 | 1-A | 201 | FOL | N-C-C11-C12 |
| 2 | 31-A | 201 | FOL | O-C-C11-C16 |
| 2 | 31-A | 201 | FOL | N-C-C11-C16 |
| 2 | 99-A | 201 | FOL | O-C-C11-C16 |
| 2 | 99-A | 201 | FOL | N-C-C11-C16 |
| 2 | 51-A | 201 | FOL | O-C-C11-C16 |
| 2 | 51-A | 201 | FOL | N-C-C11-C16 |
| 2 | 82-A | 201 | FOL | O-C-C11-C16 |
| 2 | 82-A | 201 | FOL | N-C-C11-C16 |
| 2 | 21-A | 201 | FOL | O-C-C11-C16 |
| 2 | 21-A | 201 | FOL | N-C-C11-C16 |
| 2 | 55-A | 201 | FOL | O-C-C11-C16 |
| 2 | 55-A | 201 | FOL | N-C-C11-C16 |
| 2 | 76-A | 201 | FOL | O-C-C11-C16 |
| 2 | 76-A | 201 | FOL | N-C-C11-C16 |
| 2 | 18-A | 201 | FOL | O-C-C11-C16 |
| 2 | 18-A | 201 | FOL | N-C-C11-C16 |
| 2 | 60-A | 201 | FOL | O-C-C11-C16 |
| 2 | 60-A | 201 | FOL | N-C-C11-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 80-A | 201 | FOL | O-C-C11-C16 |
| 2 | 80-A | 201 | FOL | N-C-C11-C16 |
| 2 | 23-A | 201 | FOL | O-C-C11-C16 |
| 2 | 23-A | 201 | FOL | N-C-C11-C16 |
| 2 | 57-A | 201 | FOL | O-C-C11-C16 |
| 2 | 57-A | 201 | FOL | N-C-C11-C16 |
| 2 | 62-A | 201 | FOL | O-C-C11-C16 |
| 2 | 62-A | 201 | FOL | N-C-C11-C16 |
| 2 | 111-A | 201 | FOL | O-C-C11-C16 |
| 2 | 111-A | 201 | FOL | N-C-C11-C16 |
| 2 | 39-A | 201 | FOL | O-C-C11-C16 |
| 2 | 39-A | 201 | FOL | N-C-C11-C16 |
| 2 | 61-A | 201 | FOL | O-C-C11-C16 |
| 2 | 61-A | 201 | FOL | N-C-C11-C16 |
| 2 | 48-A | 201 | FOL | O-C-C11-C16 |
| 2 | 48-A | 201 | FOL | N-C-C11-C16 |
| 2 | 120-A | 201 | FOL | O-C-C11-C16 |
| 2 | 120-A | 201 | FOL | N-C-C11-C16 |
| 2 | 104-A | 201 | FOL | O-C-C11-C16 |
| 2 | 104-A | 201 | FOL | N-C-C11-C16 |
| 2 | 30-A | 201 | FOL | O-C-C11-C16 |
| 2 | 30-A | 201 | FOL | N-C-C11-C16 |
| 2 | 117-A | 201 | FOL | O-C-C11-C16 |
| 2 | 117-A | 201 | FOL | N-C-C11-C16 |
| 2 | 41-A | 201 | FOL | O-C-C11-C16 |
| 2 | 41-A | 201 | FOL | N-C-C11-C16 |
| 2 | 54-A | 201 | FOL | O-C-C11-C16 |
| 2 | 54-A | 201 | FOL | N-C-C11-C16 |
| 2 | 45-A | 201 | FOL | O-C-C11-C16 |
| 2 | 45-A | 201 | FOL | N-C-C11-C16 |
| 2 | 116-A | 201 | FOL | O-C-C11-C16 |
| 2 | 116-A | 201 | FOL | N-C-C11-C16 |
| 2 | 113-A | 201 | FOL | O-C-C11-C16 |
| 2 | 113-A | 201 | FOL | N-C-C11-C16 |
| 2 | 103-A | 201 | FOL | O-C-C11-C16 |
| 2 | 103-A | 201 | FOL | N-C-C11-C16 |
| 2 | 77-A | 201 | FOL | O-C-C11-C16 |
| 2 | 77-A | 201 | FOL | N-C-C11-C16 |
| 2 | 123-A | 201 | FOL | O-C-C11-C16 |
| 2 | 123-A | 201 | FOL | N-C-C11-C16 |
| 2 | 26-A | 201 | FOL | O-C-C11-C16 |
| 2 | 26-A | 201 | FOL | N-C-C11-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 46-A | 201 | FOL | O-C-C11-C16 |
| 2 | 46-A | 201 | FOL | N-C-C11-C16 |
| 2 | 36-A | 201 | FOL | O-C-C11-C16 |
| 2 | 36-A | 201 | FOL | N-C-C11-C16 |
| 2 | 20-A | 201 | FOL | O-C-C11-C16 |
| 2 | 20-A | 201 | FOL | N-C-C11-C16 |
| 2 | 72-A | 201 | FOL | O-C-C11-C16 |
| 2 | 72-A | 201 | FOL | N-C-C11-C16 |
| 2 | 79-A | 201 | FOL | O-C-C11-C16 |
| 2 | 79-A | 201 | FOL | N-C-C11-C16 |
| 2 | 67-A | 201 | FOL | O-C-C11-C16 |
| 2 | 67-A | 201 | FOL | N-C-C11-C16 |
| 2 | 87-A | 201 | FOL | O-C-C11-C16 |
| 2 | 87-A | 201 | FOL | N-C-C11-C16 |
| 2 | 64-A | 201 | FOL | O-C-C11-C16 |
| 2 | 64-A | 201 | FOL | N-C-C11-C16 |
| 2 | 110-A | 201 | FOL | O-C-C11-C16 |
| 2 | 110-A | 201 | FOL | N-C-C11-C16 |
| 2 | 91-A | 201 | FOL | O-C-C11-C16 |
| 2 | 91-A | 201 | FOL | N-C-C11-C16 |
| 2 | 5-A | 201 | FOL | O-C-C11-C16 |
| 2 | 5-A | 201 | FOL | N-C-C11-C16 |
| 2 | 81-A | 201 | FOL | O-C-C11-C16 |
| 2 | 81-A | 201 | FOL | N-C-C11-C16 |
| 2 | 50-A | 201 | FOL | O-C-C11-C16 |
| 2 | 50-A | 201 | FOL | N-C-C11-C16 |
| 2 | 112-A | 201 | FOL | O-C-C11-C16 |
| 2 | 112-A | 201 | FOL | N-C-C11-C16 |
| 2 | 93-A | 201 | FOL | O-C-C11-C16 |
| 2 | 93-A | 201 | FOL | N-C-C11-C16 |
| 2 | 98-A | 201 | FOL | O-C-C11-C16 |
| 2 | 98-A | 201 | FOL | N-C-C11-C16 |
| 2 | 6-A | 201 | FOL | O-C-C11-C16 |
| 2 | 6-A | 201 | FOL | N-C-C11-C16 |
| 2 | 95-A | 201 | FOL | O-C-C11-C16 |
| 2 | 95-A | 201 | FOL | N-C-C11-C16 |
| 2 | 25-A | 201 | FOL | O-C-C11-C16 |
| 2 | 25-A | 201 | FOL | N-C-C11-C16 |
| 2 | 29-A | 201 | FOL | O-C-C11-C16 |
| 2 | 29-A | 201 | FOL | N-C-C11-C16 |
| 2 | 13-A | 201 | FOL | O-C-C11-C16 |
| 2 | 13-A | 201 | FOL | N-C-C11-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 19-A | 201 | FOL | O-C-C11-C16 |
| 2 | 19-A | 201 | FOL | N-C-C11-C16 |
| 2 | 100-A | 201 | FOL | O-C-C11-C16 |
| 2 | 100-A | 201 | FOL | N-C-C11-C16 |
| 2 | 16-A | 201 | FOL | O-C-C11-C16 |
| 2 | 16-A | 201 | FOL | N-C-C11-C16 |
| 2 | 38-A | 201 | FOL | O-C-C11-C16 |
| 2 | 38-A | 201 | FOL | N-C-C11-C16 |
| 2 | 69-A | 201 | FOL | O-C-C11-C16 |
| 2 | 69-A | 201 | FOL | N-C-C11-C16 |
| 2 | 43-A | 201 | FOL | O-C-C11-C16 |
| 2 | 43-A | 201 | FOL | N-C-C11-C16 |
| 2 | 92-A | 201 | FOL | O-C-C11-C16 |
| 2 | 92-A | 201 | FOL | N-C-C11-C16 |
| 2 | 84-A | 201 | FOL | O-C-C11-C16 |
| 2 | 84-A | 201 | FOL | N-C-C11-C16 |
| 2 | 85-A | 201 | FOL | O-C-C11-C16 |
| 2 | 85-A | 201 | FOL | N-C-C11-C16 |
| 2 | 119-A | 201 | FOL | O-C-C11-C16 |
| 2 | 119-A | 201 | FOL | N-C-C11-C16 |
| 2 | 10-A | 201 | FOL | O-C-C11-C16 |
| 2 | 10-A | 201 | FOL | N-C-C11-C16 |
| 2 | 125-A | 201 | FOL | O-C-C11-C16 |
| 2 | 125-A | 201 | FOL | N-C-C11-C16 |
| 2 | 121-A | 201 | FOL | O-C-C11-C16 |
| 2 | 121-A | 201 | FOL | N-C-C11-C16 |
| 2 | 9-A | 201 | FOL | O-C-C11-C16 |
| 2 | 9-A | 201 | FOL | N-C-C11-C16 |
| 2 | 14-A | 201 | FOL | O-C-C11-C16 |
| 2 | 14-A | 201 | FOL | N-C-C11-C16 |
| 2 | 75-A | 201 | FOL | O-C-C11-C16 |
| 2 | 75-A | 201 | FOL | N-C-C11-C16 |
| 2 | 107-A | 201 | FOL | O-C-C11-C16 |
| 2 | 107-A | 201 | FOL | N-C-C11-C16 |
| 2 | 124-A | 201 | FOL | O-C-C11-C16 |
| 2 | 124-A | 201 | FOL | N-C-C11-C16 |
| 2 | 40-A | 201 | FOL | O-C-C11-C16 |
| 2 | 40-A | 201 | FOL | N-C-C11-C16 |
| 2 | 7-A | 201 | FOL | O-C-C11-C16 |
| 2 | 7-A | 201 | FOL | N-C-C11-C16 |
| 2 | 74-A | 201 | FOL | O-C-C11-C16 |
| 2 | 74-A | 201 | FOL | N-C-C11-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 78-A | 201 | FOL | O-C-C11-C16 |
| 2 | 78-A | 201 | FOL | N-C-C11-C16 |
| 2 | 35-A | 201 | FOL | O-C-C11-C16 |
| 2 | 35-A | 201 | FOL | N-C-C11-C16 |
| 2 | 73-A | 201 | FOL | O-C-C11-C16 |
| 2 | 73-A | 201 | FOL | N-C-C11-C16 |
| 2 | 2-A | 201 | FOL | O-C-C11-C16 |
| 2 | 2-A | 201 | FOL | N-C-C11-C16 |
| 2 | 97-A | 201 | FOL | O-C-C11-C16 |
| 2 | 97-A | 201 | FOL | N-C-C11-C16 |
| 2 | 12-A | 201 | FOL | O-C-C11-C16 |
| 2 | 12-A | 201 | FOL | N-C-C11-C16 |
| 2 | 59-A | 201 | FOL | O-C-C11-C16 |
| 2 | 59-A | 201 | FOL | N-C-C11-C16 |
| 2 | 32-A | 201 | FOL | O-C-C11-C16 |
| 2 | 32-A | 201 | FOL | N-C-C11-C16 |
| 2 | 115-A | 201 | FOL | O-C-C11-C16 |
| 2 | 115-A | 201 | FOL | N-C-C11-C16 |
| 2 | 102-A | 201 | FOL | O-C-C11-C16 |
| 2 | 102-A | 201 | FOL | N-C-C11-C16 |
| 2 | 58-A | 201 | FOL | O-C-C11-C16 |
| 2 | 58-A | 201 | FOL | N-C-C11-C16 |
| 2 | 53-A | 201 | FOL | O-C-C11-C16 |
| 2 | 53-A | 201 | FOL | N-C-C11-C16 |
| 2 | 63-A | 201 | FOL | O-C-C11-C16 |
| 2 | 63-A | 201 | FOL | N-C-C11-C16 |
| 2 | 49-A | 201 | FOL | O-C-C11-C16 |
| 2 | 49-A | 201 | FOL | N-C-C11-C16 |
| 2 | 42-A | 201 | FOL | O-C-C11-C16 |
| 2 | 42-A | 201 | FOL | N-C-C11-C16 |
| 2 | 88-A | 201 | FOL | O-C-C11-C16 |
| 2 | 88-A | 201 | FOL | N-C-C11-C16 |
| 2 | 17-A | 201 | FOL | O-C-C11-C16 |
| 2 | 17-A | 201 | FOL | N-C-C11-C16 |
| 2 | 106-A | 201 | FOL | O-C-C11-C16 |
| 2 | 106-A | 201 | FOL | N-C-C11-C16 |
| 2 | 24-A | 201 | FOL | O-C-C11-C16 |
| 2 | 24-A | 201 | FOL | N-C-C11-C16 |
| 2 | 122-A | 201 | FOL | O-C-C11-C16 |
| 2 | 122-A | 201 | FOL | N-C-C11-C16 |
| 2 | 89-A | 201 | FOL | O-C-C11-C16 |
| 2 | 89-A | 201 | FOL | N-C-C11-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | 4-A | 201 | FOL | O-C-C11-C16 |
| 2 | 4-A | 201 | FOL | N-C-C11-C16 |
| 2 | 114-A | 201 | FOL | O-C-C11-C16 |
| 2 | 114-A | 201 | FOL | N-C-C11-C16 |
| 2 | 94-A | 201 | FOL | O-C-C11-C16 |
| 2 | 94-A | 201 | FOL | N-C-C11-C16 |
| 2 | 56-A | 201 | FOL | O-C-C11-C16 |
| 2 | 56-A | 201 | FOL | N-C-C11-C16 |
| 2 | 33-A | 201 | FOL | O-C-C11-C16 |
| 2 | 33-A | 201 | FOL | N-C-C11-C16 |
| 2 | 101-A | 201 | FOL | O-C-C11-C16 |
| 2 | 101-A | 201 | FOL | N-C-C11-C16 |
| 2 | 65-A | 201 | FOL | O-C-C11-C16 |
| 2 | 65-A | 201 | FOL | N-C-C11-C16 |
| 2 | 27-A | 201 | FOL | O-C-C11-C16 |
| 2 | 27-A | 201 | FOL | N-C-C11-C16 |
| 2 | 34-A | 201 | FOL | O-C-C11-C16 |
| 2 | 34-A | 201 | FOL | N-C-C11-C16 |
| 2 | 11-A | 201 | FOL | O-C-C11-C16 |
| 2 | 11-A | 201 | FOL | N-C-C11-C16 |
| 2 | 118-A | 201 | FOL | O-C-C11-C16 |
| 2 | 118-A | 201 | FOL | N-C-C11-C16 |
| 2 | 44-A | 201 | FOL | O-C-C11-C16 |
| 2 | 44-A | 201 | FOL | N-C-C11-C16 |
| 2 | 3-A | 201 | FOL | O-C-C11-C16 |
| 2 | 3-A | 201 | FOL | N-C-C11-C16 |
| 2 | 28-A | 201 | FOL | O-C-C11-C16 |
| 2 | 28-A | 201 | FOL | N-C-C11-C16 |
| 2 | 70-A | 201 | FOL | O-C-C11-C16 |
| 2 | 70-A | 201 | FOL | N-C-C11-C16 |
| 2 | 52-A | 201 | FOL | O-C-C11-C16 |
| 2 | 52-A | 201 | FOL | N-C-C11-C16 |
| 2 | 22-A | 201 | FOL | O-C-C11-C16 |
| 2 | 22-A | 201 | FOL | N-C-C11-C16 |
| 2 | 83-A | 201 | FOL | O-C-C11-C16 |
| 2 | 83-A | 201 | FOL | N-C-C11-C16 |
| 2 | 96-A | 201 | FOL | O-C-C11-C16 |
| 2 | 96-A | 201 | FOL | N-C-C11-C16 |
| 2 | 8-A | 201 | FOL | O-C-C11-C16 |
| 2 | 8-A | 201 | FOL | N-C-C11-C16 |
| 2 | 108-A | 201 | FOL | O-C-C11-C16 |
| 2 | 108-A | 201 | FOL | N-C-C11-C16 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 2 | 66-A | 201 | FOL | O-C-C11-C16 |
| 2 | 66-A | 201 | FOL | N-C-C11-C16 |
| 2 | 90-A | 201 | FOL | O-C-C11-C16 |
| 2 | 90-A | 201 | FOL | N-C-C11-C16 |
| 2 | 47-A | 201 | FOL | O-C-C11-C16 |
| 2 | 47-A | 201 | FOL | N-C-C11-C16 |
| 2 | 109-A | 201 | FOL | O-C-C11-C16 |
| 2 | 109-A | 201 | FOL | N-C-C11-C16 |
| 2 | 105-A | 201 | FOL | O-C-C11-C16 |
| 2 | 105-A | 201 | FOL | N-C-C11-C16 |
| 2 | 71-A | 201 | FOL | O-C-C11-C16 |
| 2 | 71-A | 201 | FOL | N-C-C11-C16 |
| 2 | 86-A | 201 | FOL | O-C-C11-C16 |
| 2 | 86-A | 201 | FOL | N-C-C11-C16 |
| 2 | 37-A | 201 | FOL | O-C-C11-C16 |
| 2 | 37-A | 201 | FOL | N-C-C11-C16 |
| 2 | 68-A | 201 | FOL | O-C-C11-C16 |
| 2 | 68-A | 201 | FOL | N-C-C11-C16 |
| 2 | 15-A | 201 | FOL | O-C-C11-C16 |
| 2 | 15-A | 201 | FOL | N-C-C11-C16 |
| 2 | 1-A | 201 | FOL | O-C-C11-C16 |
| 2 | 1-A | 201 | FOL | N-C-C11-C16 |
| 3 | 80-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 66-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 24-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 94-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 35-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 103-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 55-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 116-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 77-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 69-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 64-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 81-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 71-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 74-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 3-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 56-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 62-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 70-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 63-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 44-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 120-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 115-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 91-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 41-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 37-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 104-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 121-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 72-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 82-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 36-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 112-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 53-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 96-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 40-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 45-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 16-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 85-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 15-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 67-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 10-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 88-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 43-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 17-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 107-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 6-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 4-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 76-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 101-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 29-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 119-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 61-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 59-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 30-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 1-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 11-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 118-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 7-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 109-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 48-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 65-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 54-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 39-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 97-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 99-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 83-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 125-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 68-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 52-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 111-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 84-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 100-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 31-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 32-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 86-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 98-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 89-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 34-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 114-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 110-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 90-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 51-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 38-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 47-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 123-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 105-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 12-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 108-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 21-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 57-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 23-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 14-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 124-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 25-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 26-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 22-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 78-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 117-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 13-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 79-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 75-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 106-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 8-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 46-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 93-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 18-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 58-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 102-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 33-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 20-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 122-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 95-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 42-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 50-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 5-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 49-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 27-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 73-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 87-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 19-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 92-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 113-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 2-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 28-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 9-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 60-A | 202 | NAP | PA-O3-PN-O5D |
| 2 | 31-A | 201 | FOL | N-CA-CB-CG |
| 2 | 99-A | 201 | FOL | N-CA-CB-CG |
| 2 | 51-A | 201 | FOL | N-CA-CB-CG |
| 2 | 82-A | 201 | FOL | N-CA-CB-CG |
| 2 | 21-A | 201 | FOL | N-CA-CB-CG |
| 2 | 55-A | 201 | FOL | N-CA-CB-CG |
| 2 | 76-A | 201 | FOL | N-CA-CB-CG |
| 2 | 18-A | 201 | FOL | N-CA-CB-CG |
| 2 | 60-A | 201 | FOL | N-CA-CB-CG |
| 2 | 80-A | 201 | FOL | N-CA-CB-CG |
| 2 | 23-A | 201 | FOL | N-CA-CB-CG |
| 2 | 57-A | 201 | FOL | N-CA-CB-CG |
| 2 | 62-A | 201 | FOL | N-CA-CB-CG |
| 2 | 111-A | 201 | FOL | N-CA-CB-CG |
| 2 | 39-A | 201 | FOL | N-CA-CB-CG |
| 2 | 61-A | 201 | FOL | N-CA-CB-CG |
| 2 | 48-A | 201 | FOL | N-CA-CB-CG |
| 2 | 120-A | 201 | FOL | N-CA-CB-CG |
| 2 | 104-A | 201 | FOL | N-CA-CB-CG |
| 2 | 30-A | 201 | FOL | N-CA-CB-CG |
| 2 | 117-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 2 | 41-A | 201 | FOL | N-CA-CB-CG |
| 2 | 54-A | 201 | FOL | N-CA-CB-CG |
| 2 | 45-A | 201 | FOL | N-CA-CB-CG |
| 2 | 116-A | 201 | FOL | N-CA-CB-CG |
| 2 | 113-A | 201 | FOL | N-CA-CB-CG |
| 2 | 103-A | 201 | FOL | N-CA-CB-CG |
| 2 | 77-A | 201 | FOL | N-CA-CB-CG |
| 2 | 123-A | 201 | FOL | N-CA-CB-CG |
| 2 | 26-A | 201 | FOL | N-CA-CB-CG |
| 2 | 46-A | 201 | FOL | N-CA-CB-CG |
| 2 | 36-A | 201 | FOL | N-CA-CB-CG |
| 2 | 20-A | 201 | FOL | N-CA-CB-CG |
| 2 | 72-A | 201 | FOL | N-CA-CB-CG |
| 2 | 79-A | 201 | FOL | N-CA-CB-CG |
| 2 | 67-A | 201 | FOL | N-CA-CB-CG |
| 2 | 87-A | 201 | FOL | N-CA-CB-CG |
| 2 | 64-A | 201 | FOL | N-CA-CB-CG |
| 2 | 110-A | 201 | FOL | N-CA-CB-CG |
| 2 | 91-A | 201 | FOL | N-CA-CB-CG |
| 2 | 5-A | 201 | FOL | N-CA-CB-CG |
| 2 | 81-A | 201 | FOL | N-CA-CB-CG |
| 2 | 50-A | 201 | FOL | N-CA-CB-CG |
| 2 | 112-A | 201 | FOL | N-CA-CB-CG |
| 2 | 93-A | 201 | FOL | N-CA-CB-CG |
| 2 | 98-A | 201 | FOL | N-CA-CB-CG |
| 2 | 6-A | 201 | FOL | N-CA-CB-CG |
| 2 | 95-A | 201 | FOL | N-CA-CB-CG |
| 2 | 25-A | 201 | FOL | N-CA-CB-CG |
| 2 | 29-A | 201 | FOL | N-CA-CB-CG |
| 2 | 13-A | 201 | FOL | N-CA-CB-CG |
| 2 | 19-A | 201 | FOL | N-CA-CB-CG |
| 2 | 100-A | 201 | FOL | N-CA-CB-CG |
| 2 | 16-A | 201 | FOL | N-CA-CB-CG |
| 2 | 38-A | 201 | FOL | N-CA-CB-CG |
| 2 | 69-A | 201 | FOL | N-CA-CB-CG |
| 2 | 43-A | 201 | FOL | N-CA-CB-CG |
| 2 | 92-A | 201 | FOL | N-CA-CB-CG |
| 2 | 84-A | 201 | FOL | N-CA-CB-CG |
| 2 | 85-A | 201 | FOL | N-CA-CB-CG |
| 2 | 119-A | 201 | FOL | N-CA-CB-CG |
| 2 | 10-A | 201 | FOL | N-CA-CB-CG |
| 2 | 125-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|--------------|
| 2 | 121-A | 201 | FOL | N-CA-CB-CG |
| 2 | 9-A | 201 | FOL | N-CA-CB-CG |
| 2 | 14-A | 201 | FOL | N-CA-CB-CG |
| 2 | 75-A | 201 | FOL | N-CA-CB-CG |
| 2 | 107-A | 201 | FOL | N-CA-CB-CG |
| 2 | 124-A | 201 | FOL | N-CA-CB-CG |
| 2 | 40-A | 201 | FOL | N-CA-CB-CG |
| 2 | 7-A | 201 | FOL | N-CA-CB-CG |
| 2 | 74-A | 201 | FOL | N-CA-CB-CG |
| 2 | 78-A | 201 | FOL | N-CA-CB-CG |
| 2 | 35-A | 201 | FOL | N-CA-CB-CG |
| 2 | 73-A | 201 | FOL | N-CA-CB-CG |
| 2 | 2-A | 201 | FOL | N-CA-CB-CG |
| 2 | 97-A | 201 | FOL | N-CA-CB-CG |
| 2 | 12-A | 201 | FOL | N-CA-CB-CG |
| 2 | 59-A | 201 | FOL | N-CA-CB-CG |
| 2 | 32-A | 201 | FOL | N-CA-CB-CG |
| 2 | 115-A | 201 | FOL | N-CA-CB-CG |
| 2 | 102-A | 201 | FOL | N-CA-CB-CG |
| 2 | 58-A | 201 | FOL | N-CA-CB-CG |
| 2 | 53-A | 201 | FOL | N-CA-CB-CG |
| 2 | 63-A | 201 | FOL | N-CA-CB-CG |
| 2 | 49-A | 201 | FOL | N-CA-CB-CG |
| 2 | 42-A | 201 | FOL | N-CA-CB-CG |
| 2 | 88-A | 201 | FOL | N-CA-CB-CG |
| 2 | 17-A | 201 | FOL | N-CA-CB-CG |
| 2 | 106-A | 201 | FOL | N-CA-CB-CG |
| 2 | 24-A | 201 | FOL | N-CA-CB-CG |
| 2 | 122-A | 201 | FOL | N-CA-CB-CG |
| 2 | 89-A | 201 | FOL | N-CA-CB-CG |
| 2 | 4-A | 201 | FOL | N-CA-CB-CG |
| 2 | 114-A | 201 | FOL | N-CA-CB-CG |
| 2 | 94-A | 201 | FOL | N-CA-CB-CG |
| 2 | 56-A | 201 | FOL | N-CA-CB-CG |
| 2 | 33-A | 201 | FOL | N-CA-CB-CG |
| 2 | 101-A | 201 | FOL | N-CA-CB-CG |
| 2 | 65-A | 201 | FOL | N-CA-CB-CG |
| 2 | 27-A | 201 | FOL | N-CA-CB-CG |
| 2 | 34-A | 201 | FOL | N-CA-CB-CG |
| 2 | 11-A | 201 | FOL | N-CA-CB-CG |
| 2 | 118-A | 201 | FOL | N-CA-CB-CG |
| 2 | 44-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 3-A | 201 | FOL | N-CA-CB-CG |
| 2 | 28-A | 201 | FOL | N-CA-CB-CG |
| 2 | 70-A | 201 | FOL | N-CA-CB-CG |
| 2 | 52-A | 201 | FOL | N-CA-CB-CG |
| 2 | 22-A | 201 | FOL | N-CA-CB-CG |
| 2 | 83-A | 201 | FOL | N-CA-CB-CG |
| 2 | 96-A | 201 | FOL | N-CA-CB-CG |
| 2 | 8-A | 201 | FOL | N-CA-CB-CG |
| 2 | 108-A | 201 | FOL | N-CA-CB-CG |
| 2 | 66-A | 201 | FOL | N-CA-CB-CG |
| 2 | 90-A | 201 | FOL | N-CA-CB-CG |
| 2 | 47-A | 201 | FOL | N-CA-CB-CG |
| 2 | 109-A | 201 | FOL | N-CA-CB-CG |
| 2 | 105-A | 201 | FOL | N-CA-CB-CG |
| 2 | 71-A | 201 | FOL | N-CA-CB-CG |
| 2 | 86-A | 201 | FOL | N-CA-CB-CG |
| 2 | 37-A | 201 | FOL | N-CA-CB-CG |
| 2 | 68-A | 201 | FOL | N-CA-CB-CG |
| 2 | 15-A | 201 | FOL | N-CA-CB-CG |
| 2 | 1-A | 201 | FOL | N-CA-CB-CG |
| 3 | 80-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 66-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 24-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 94-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 35-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 103-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 55-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 116-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 77-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 69-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 64-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 81-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 71-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 74-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 3-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 56-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 62-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 70-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 63-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 44-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 120-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 115-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 91-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 41-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 37-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 104-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 121-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 72-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 82-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 36-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 112-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 53-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 96-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 40-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 45-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 16-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 85-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 15-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 67-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 10-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 88-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 43-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 17-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 107-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 6-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 4-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 76-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 101-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 29-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 119-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 61-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 59-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 30-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 1-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 11-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 118-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 7-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 109-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 48-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 65-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 54-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 39-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 97-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 99-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 83-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 125-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 68-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 52-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 111-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 84-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 100-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 31-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 32-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 86-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 98-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 89-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 34-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 114-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 110-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 90-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 51-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 38-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 47-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 123-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 105-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 12-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 108-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 21-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 57-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 23-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 14-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 124-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 25-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 26-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 22-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 78-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 117-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 13-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 79-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 75-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 106-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 8-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 46-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 93-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 18-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 58-A | 202 | NAP | C2B-O2B-P2B-O3X |

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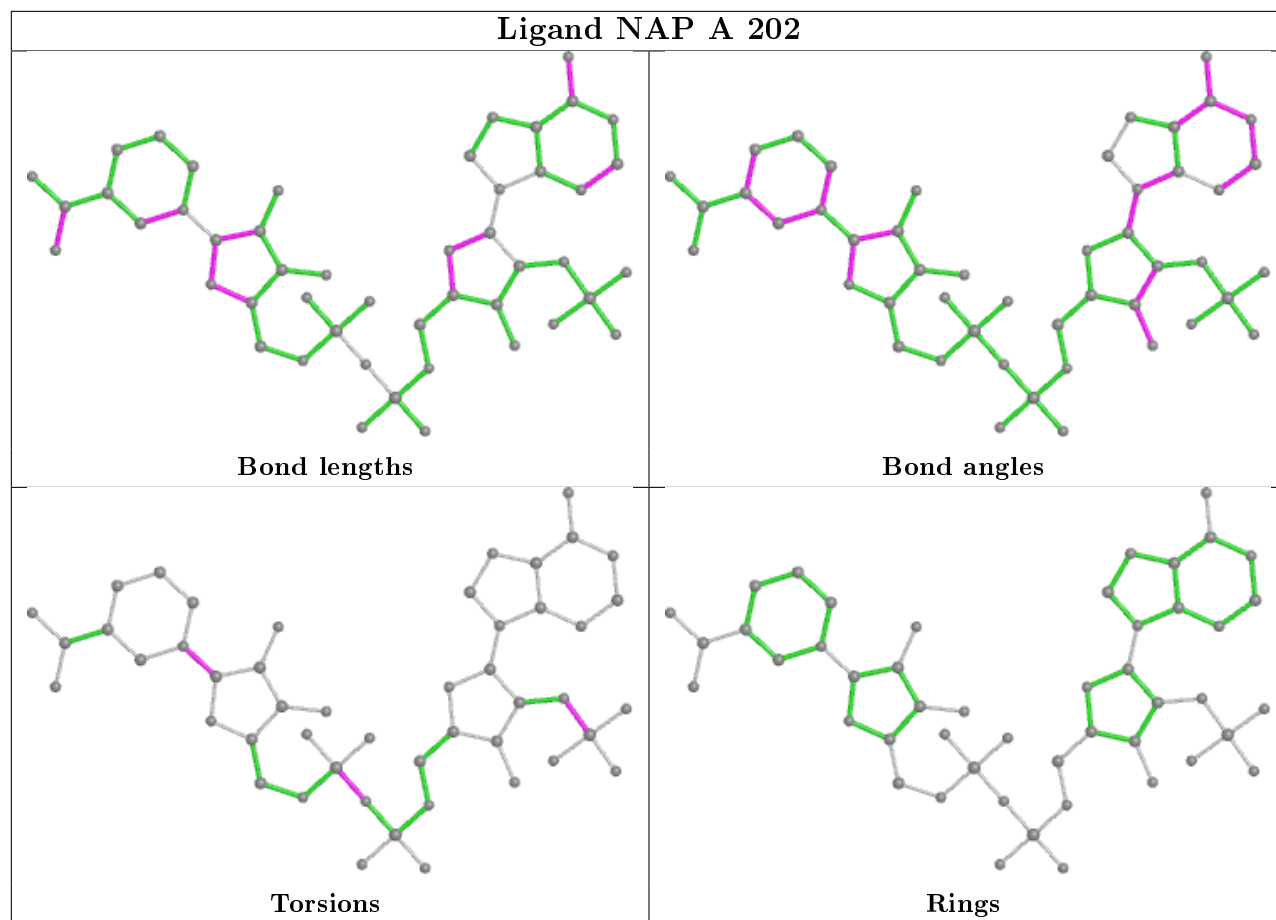
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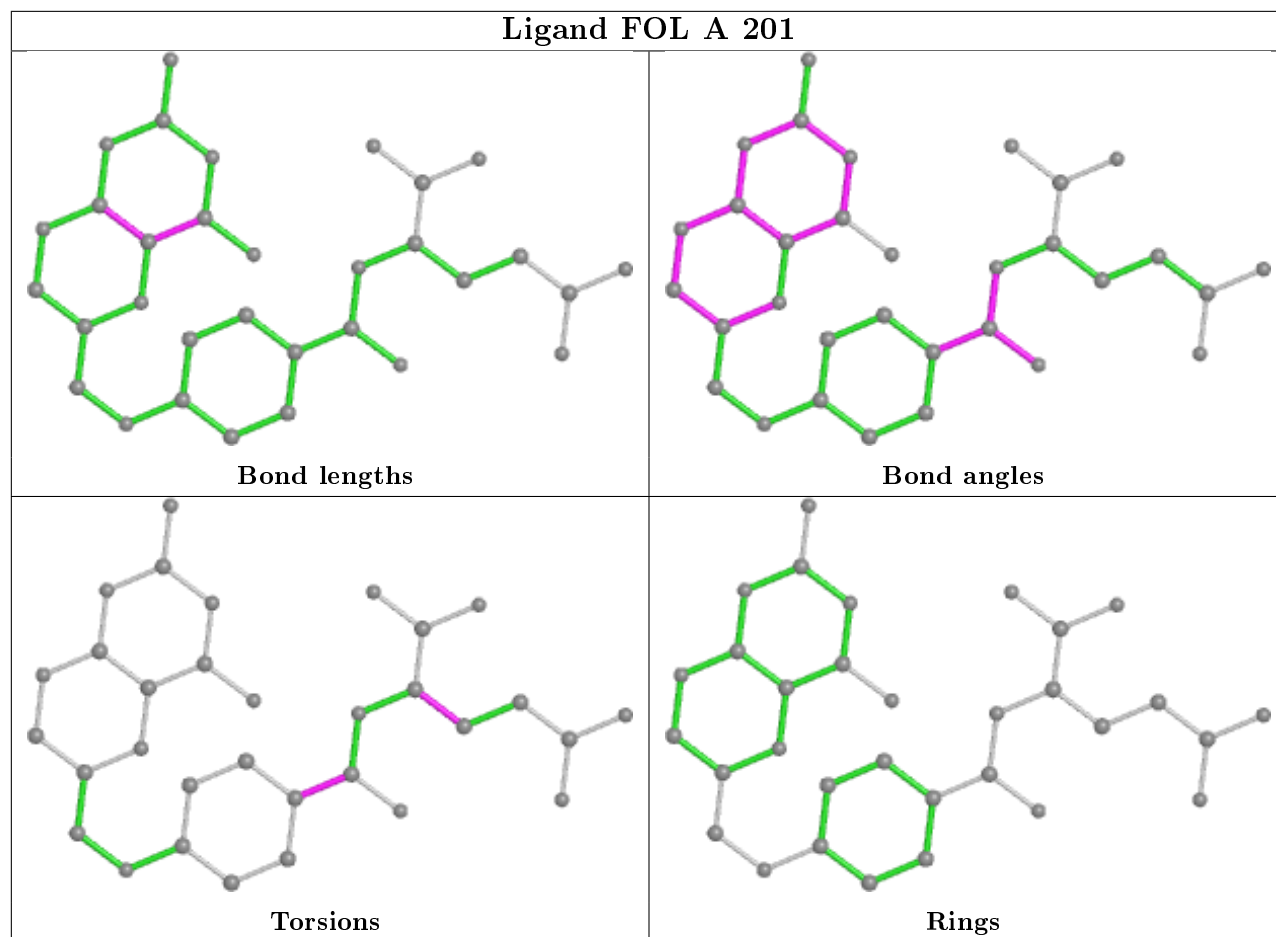
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 102-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 33-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 20-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 122-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 95-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 42-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 50-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 5-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 49-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 27-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 73-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 87-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 19-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 92-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 113-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 2-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 28-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 9-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 60-A | 202 | NAP | C2B-O2B-P2B-O3X |

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å²) | Q<0.9 | |
|-----|-------|---------------|--------|---------|----|----------|---------------|------------|
| 1 | 1-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 2-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 3-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 4-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 5-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 6-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 7-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 8-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 9-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 10-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 11-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 12-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 13-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 14-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 15-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 16-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 17-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 18-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 19-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 20-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 21-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 22-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 23-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 24-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------|----|----|-----------------------|------------|
| 1 | 25-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 26-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 27-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 28-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 29-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 30-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 31-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 32-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 33-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 34-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 35-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 36-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 37-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 38-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 39-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 40-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 41-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 42-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 43-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 44-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 45-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 46-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 47-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 48-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 49-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 50-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 51-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 52-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 53-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 54-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 55-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------|----|----|-----------------------|------------|
| 1 | 56-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 57-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 58-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 59-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 60-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 61-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 62-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 63-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 64-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 65-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 66-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 67-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 68-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 69-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 70-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 71-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 72-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 73-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 74-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 75-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 76-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 77-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 78-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 79-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 80-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 81-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 82-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 83-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 84-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 85-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 86-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------|----|----|-----------------------|------------|
| 1 | 87-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 88-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 89-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 90-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 91-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 92-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 93-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 94-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 95-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 96-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 97-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 98-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 99-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 100-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 101-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 102-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 103-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 104-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 105-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 106-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 107-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 108-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 109-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 110-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 111-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 112-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 113-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 114-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 115-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 116-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 117-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------|----|----|-----------------------|--------------|
| 1 | 118-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 119-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 120-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 121-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 122-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 123-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 124-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| 1 | 125-A | 158/159 (99%) | 0.58 | 10 (6%) | 20 | 19 | 9, 12, 15, 17 | 158 (100%) |
| All | All | 19750/19875 (99%) | 0.58 | 1250 (6%) | 18 | 19 | 9, 12, 15, 17 | 19750 (100%) |

All (1250) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 1-A | 22 | TRP | 13.0 |
| 1 | 2-A | 22 | TRP | 13.0 |
| 1 | 3-A | 22 | TRP | 13.0 |
| 1 | 4-A | 22 | TRP | 13.0 |
| 1 | 5-A | 22 | TRP | 13.0 |
| 1 | 6-A | 22 | TRP | 13.0 |
| 1 | 7-A | 22 | TRP | 13.0 |
| 1 | 8-A | 22 | TRP | 13.0 |
| 1 | 9-A | 22 | TRP | 13.0 |
| 1 | 10-A | 22 | TRP | 13.0 |
| 1 | 11-A | 22 | TRP | 13.0 |
| 1 | 12-A | 22 | TRP | 13.0 |
| 1 | 13-A | 22 | TRP | 13.0 |
| 1 | 14-A | 22 | TRP | 13.0 |
| 1 | 15-A | 22 | TRP | 13.0 |
| 1 | 16-A | 22 | TRP | 13.0 |
| 1 | 17-A | 22 | TRP | 13.0 |
| 1 | 18-A | 22 | TRP | 13.0 |
| 1 | 19-A | 22 | TRP | 13.0 |
| 1 | 20-A | 22 | TRP | 13.0 |
| 1 | 21-A | 22 | TRP | 13.0 |
| 1 | 22-A | 22 | TRP | 13.0 |
| 1 | 23-A | 22 | TRP | 13.0 |
| 1 | 24-A | 22 | TRP | 13.0 |
| 1 | 25-A | 22 | TRP | 13.0 |
| 1 | 26-A | 22 | TRP | 13.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 27-A | 22 | TRP | 13.0 |
| 1 | 28-A | 22 | TRP | 13.0 |
| 1 | 29-A | 22 | TRP | 13.0 |
| 1 | 30-A | 22 | TRP | 13.0 |
| 1 | 31-A | 22 | TRP | 13.0 |
| 1 | 32-A | 22 | TRP | 13.0 |
| 1 | 33-A | 22 | TRP | 13.0 |
| 1 | 34-A | 22 | TRP | 13.0 |
| 1 | 35-A | 22 | TRP | 13.0 |
| 1 | 36-A | 22 | TRP | 13.0 |
| 1 | 37-A | 22 | TRP | 13.0 |
| 1 | 38-A | 22 | TRP | 13.0 |
| 1 | 39-A | 22 | TRP | 13.0 |
| 1 | 40-A | 22 | TRP | 13.0 |
| 1 | 41-A | 22 | TRP | 13.0 |
| 1 | 42-A | 22 | TRP | 13.0 |
| 1 | 43-A | 22 | TRP | 13.0 |
| 1 | 44-A | 22 | TRP | 13.0 |
| 1 | 45-A | 22 | TRP | 13.0 |
| 1 | 46-A | 22 | TRP | 13.0 |
| 1 | 47-A | 22 | TRP | 13.0 |
| 1 | 48-A | 22 | TRP | 13.0 |
| 1 | 49-A | 22 | TRP | 13.0 |
| 1 | 50-A | 22 | TRP | 13.0 |
| 1 | 51-A | 22 | TRP | 13.0 |
| 1 | 52-A | 22 | TRP | 13.0 |
| 1 | 53-A | 22 | TRP | 13.0 |
| 1 | 54-A | 22 | TRP | 13.0 |
| 1 | 55-A | 22 | TRP | 13.0 |
| 1 | 56-A | 22 | TRP | 13.0 |
| 1 | 57-A | 22 | TRP | 13.0 |
| 1 | 58-A | 22 | TRP | 13.0 |
| 1 | 59-A | 22 | TRP | 13.0 |
| 1 | 60-A | 22 | TRP | 13.0 |
| 1 | 61-A | 22 | TRP | 13.0 |
| 1 | 62-A | 22 | TRP | 13.0 |
| 1 | 63-A | 22 | TRP | 13.0 |
| 1 | 64-A | 22 | TRP | 13.0 |
| 1 | 65-A | 22 | TRP | 13.0 |
| 1 | 66-A | 22 | TRP | 13.0 |
| 1 | 67-A | 22 | TRP | 13.0 |
| 1 | 68-A | 22 | TRP | 13.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 69-A | 22 | TRP | 13.0 |
| 1 | 70-A | 22 | TRP | 13.0 |
| 1 | 71-A | 22 | TRP | 13.0 |
| 1 | 72-A | 22 | TRP | 13.0 |
| 1 | 73-A | 22 | TRP | 13.0 |
| 1 | 74-A | 22 | TRP | 13.0 |
| 1 | 75-A | 22 | TRP | 13.0 |
| 1 | 76-A | 22 | TRP | 13.0 |
| 1 | 77-A | 22 | TRP | 13.0 |
| 1 | 78-A | 22 | TRP | 13.0 |
| 1 | 79-A | 22 | TRP | 13.0 |
| 1 | 80-A | 22 | TRP | 13.0 |
| 1 | 81-A | 22 | TRP | 13.0 |
| 1 | 82-A | 22 | TRP | 13.0 |
| 1 | 83-A | 22 | TRP | 13.0 |
| 1 | 84-A | 22 | TRP | 13.0 |
| 1 | 85-A | 22 | TRP | 13.0 |
| 1 | 86-A | 22 | TRP | 13.0 |
| 1 | 87-A | 22 | TRP | 13.0 |
| 1 | 88-A | 22 | TRP | 13.0 |
| 1 | 89-A | 22 | TRP | 13.0 |
| 1 | 90-A | 22 | TRP | 13.0 |
| 1 | 91-A | 22 | TRP | 13.0 |
| 1 | 92-A | 22 | TRP | 13.0 |
| 1 | 93-A | 22 | TRP | 13.0 |
| 1 | 94-A | 22 | TRP | 13.0 |
| 1 | 95-A | 22 | TRP | 13.0 |
| 1 | 96-A | 22 | TRP | 13.0 |
| 1 | 97-A | 22 | TRP | 13.0 |
| 1 | 98-A | 22 | TRP | 13.0 |
| 1 | 99-A | 22 | TRP | 13.0 |
| 1 | 100-A | 22 | TRP | 13.0 |
| 1 | 101-A | 22 | TRP | 13.0 |
| 1 | 102-A | 22 | TRP | 13.0 |
| 1 | 103-A | 22 | TRP | 13.0 |
| 1 | 104-A | 22 | TRP | 13.0 |
| 1 | 105-A | 22 | TRP | 13.0 |
| 1 | 106-A | 22 | TRP | 13.0 |
| 1 | 107-A | 22 | TRP | 13.0 |
| 1 | 108-A | 22 | TRP | 13.0 |
| 1 | 109-A | 22 | TRP | 13.0 |
| 1 | 110-A | 22 | TRP | 13.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 111-A | 22 | TRP | 13.0 |
| 1 | 112-A | 22 | TRP | 13.0 |
| 1 | 113-A | 22 | TRP | 13.0 |
| 1 | 114-A | 22 | TRP | 13.0 |
| 1 | 115-A | 22 | TRP | 13.0 |
| 1 | 116-A | 22 | TRP | 13.0 |
| 1 | 117-A | 22 | TRP | 13.0 |
| 1 | 118-A | 22 | TRP | 13.0 |
| 1 | 119-A | 22 | TRP | 13.0 |
| 1 | 120-A | 22 | TRP | 13.0 |
| 1 | 121-A | 22 | TRP | 13.0 |
| 1 | 122-A | 22 | TRP | 13.0 |
| 1 | 123-A | 22 | TRP | 13.0 |
| 1 | 124-A | 22 | TRP | 13.0 |
| 1 | 125-A | 22 | TRP | 13.0 |
| 1 | 1-A | 21 | PRO | 9.1 |
| 1 | 2-A | 21 | PRO | 9.1 |
| 1 | 3-A | 21 | PRO | 9.1 |
| 1 | 4-A | 21 | PRO | 9.1 |
| 1 | 5-A | 21 | PRO | 9.1 |
| 1 | 6-A | 21 | PRO | 9.1 |
| 1 | 7-A | 21 | PRO | 9.1 |
| 1 | 8-A | 21 | PRO | 9.1 |
| 1 | 9-A | 21 | PRO | 9.1 |
| 1 | 10-A | 21 | PRO | 9.1 |
| 1 | 11-A | 21 | PRO | 9.1 |
| 1 | 12-A | 21 | PRO | 9.1 |
| 1 | 13-A | 21 | PRO | 9.1 |
| 1 | 14-A | 21 | PRO | 9.1 |
| 1 | 15-A | 21 | PRO | 9.1 |
| 1 | 16-A | 21 | PRO | 9.1 |
| 1 | 17-A | 21 | PRO | 9.1 |
| 1 | 18-A | 21 | PRO | 9.1 |
| 1 | 19-A | 21 | PRO | 9.1 |
| 1 | 20-A | 21 | PRO | 9.1 |
| 1 | 21-A | 21 | PRO | 9.1 |
| 1 | 22-A | 21 | PRO | 9.1 |
| 1 | 23-A | 21 | PRO | 9.1 |
| 1 | 24-A | 21 | PRO | 9.1 |
| 1 | 25-A | 21 | PRO | 9.1 |
| 1 | 26-A | 21 | PRO | 9.1 |
| 1 | 27-A | 21 | PRO | 9.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 28-A | 21 | PRO | 9.1 |
| 1 | 29-A | 21 | PRO | 9.1 |
| 1 | 30-A | 21 | PRO | 9.1 |
| 1 | 31-A | 21 | PRO | 9.1 |
| 1 | 32-A | 21 | PRO | 9.1 |
| 1 | 33-A | 21 | PRO | 9.1 |
| 1 | 34-A | 21 | PRO | 9.1 |
| 1 | 35-A | 21 | PRO | 9.1 |
| 1 | 36-A | 21 | PRO | 9.1 |
| 1 | 37-A | 21 | PRO | 9.1 |
| 1 | 38-A | 21 | PRO | 9.1 |
| 1 | 39-A | 21 | PRO | 9.1 |
| 1 | 40-A | 21 | PRO | 9.1 |
| 1 | 41-A | 21 | PRO | 9.1 |
| 1 | 42-A | 21 | PRO | 9.1 |
| 1 | 43-A | 21 | PRO | 9.1 |
| 1 | 44-A | 21 | PRO | 9.1 |
| 1 | 45-A | 21 | PRO | 9.1 |
| 1 | 46-A | 21 | PRO | 9.1 |
| 1 | 47-A | 21 | PRO | 9.1 |
| 1 | 48-A | 21 | PRO | 9.1 |
| 1 | 49-A | 21 | PRO | 9.1 |
| 1 | 50-A | 21 | PRO | 9.1 |
| 1 | 51-A | 21 | PRO | 9.1 |
| 1 | 52-A | 21 | PRO | 9.1 |
| 1 | 53-A | 21 | PRO | 9.1 |
| 1 | 54-A | 21 | PRO | 9.1 |
| 1 | 55-A | 21 | PRO | 9.1 |
| 1 | 56-A | 21 | PRO | 9.1 |
| 1 | 57-A | 21 | PRO | 9.1 |
| 1 | 58-A | 21 | PRO | 9.1 |
| 1 | 59-A | 21 | PRO | 9.1 |
| 1 | 60-A | 21 | PRO | 9.1 |
| 1 | 61-A | 21 | PRO | 9.1 |
| 1 | 62-A | 21 | PRO | 9.1 |
| 1 | 63-A | 21 | PRO | 9.1 |
| 1 | 64-A | 21 | PRO | 9.1 |
| 1 | 65-A | 21 | PRO | 9.1 |
| 1 | 66-A | 21 | PRO | 9.1 |
| 1 | 67-A | 21 | PRO | 9.1 |
| 1 | 68-A | 21 | PRO | 9.1 |
| 1 | 69-A | 21 | PRO | 9.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 70-A | 21 | PRO | 9.1 |
| 1 | 71-A | 21 | PRO | 9.1 |
| 1 | 72-A | 21 | PRO | 9.1 |
| 1 | 73-A | 21 | PRO | 9.1 |
| 1 | 74-A | 21 | PRO | 9.1 |
| 1 | 75-A | 21 | PRO | 9.1 |
| 1 | 76-A | 21 | PRO | 9.1 |
| 1 | 77-A | 21 | PRO | 9.1 |
| 1 | 78-A | 21 | PRO | 9.1 |
| 1 | 79-A | 21 | PRO | 9.1 |
| 1 | 80-A | 21 | PRO | 9.1 |
| 1 | 81-A | 21 | PRO | 9.1 |
| 1 | 82-A | 21 | PRO | 9.1 |
| 1 | 83-A | 21 | PRO | 9.1 |
| 1 | 84-A | 21 | PRO | 9.1 |
| 1 | 85-A | 21 | PRO | 9.1 |
| 1 | 86-A | 21 | PRO | 9.1 |
| 1 | 87-A | 21 | PRO | 9.1 |
| 1 | 88-A | 21 | PRO | 9.1 |
| 1 | 89-A | 21 | PRO | 9.1 |
| 1 | 90-A | 21 | PRO | 9.1 |
| 1 | 91-A | 21 | PRO | 9.1 |
| 1 | 92-A | 21 | PRO | 9.1 |
| 1 | 93-A | 21 | PRO | 9.1 |
| 1 | 94-A | 21 | PRO | 9.1 |
| 1 | 95-A | 21 | PRO | 9.1 |
| 1 | 96-A | 21 | PRO | 9.1 |
| 1 | 97-A | 21 | PRO | 9.1 |
| 1 | 98-A | 21 | PRO | 9.1 |
| 1 | 99-A | 21 | PRO | 9.1 |
| 1 | 100-A | 21 | PRO | 9.1 |
| 1 | 101-A | 21 | PRO | 9.1 |
| 1 | 102-A | 21 | PRO | 9.1 |
| 1 | 103-A | 21 | PRO | 9.1 |
| 1 | 104-A | 21 | PRO | 9.1 |
| 1 | 105-A | 21 | PRO | 9.1 |
| 1 | 106-A | 21 | PRO | 9.1 |
| 1 | 107-A | 21 | PRO | 9.1 |
| 1 | 108-A | 21 | PRO | 9.1 |
| 1 | 109-A | 21 | PRO | 9.1 |
| 1 | 110-A | 21 | PRO | 9.1 |
| 1 | 111-A | 21 | PRO | 9.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 112-A | 21 | PRO | 9.1 |
| 1 | 113-A | 21 | PRO | 9.1 |
| 1 | 114-A | 21 | PRO | 9.1 |
| 1 | 115-A | 21 | PRO | 9.1 |
| 1 | 116-A | 21 | PRO | 9.1 |
| 1 | 117-A | 21 | PRO | 9.1 |
| 1 | 118-A | 21 | PRO | 9.1 |
| 1 | 119-A | 21 | PRO | 9.1 |
| 1 | 120-A | 21 | PRO | 9.1 |
| 1 | 121-A | 21 | PRO | 9.1 |
| 1 | 122-A | 21 | PRO | 9.1 |
| 1 | 123-A | 21 | PRO | 9.1 |
| 1 | 124-A | 21 | PRO | 9.1 |
| 1 | 125-A | 21 | PRO | 9.1 |
| 1 | 1-A | 20 | MET | 8.1 |
| 1 | 2-A | 20 | MET | 8.1 |
| 1 | 3-A | 20 | MET | 8.1 |
| 1 | 4-A | 20 | MET | 8.1 |
| 1 | 5-A | 20 | MET | 8.1 |
| 1 | 6-A | 20 | MET | 8.1 |
| 1 | 7-A | 20 | MET | 8.1 |
| 1 | 8-A | 20 | MET | 8.1 |
| 1 | 9-A | 20 | MET | 8.1 |
| 1 | 10-A | 20 | MET | 8.1 |
| 1 | 11-A | 20 | MET | 8.1 |
| 1 | 12-A | 20 | MET | 8.1 |
| 1 | 13-A | 20 | MET | 8.1 |
| 1 | 14-A | 20 | MET | 8.1 |
| 1 | 15-A | 20 | MET | 8.1 |
| 1 | 16-A | 20 | MET | 8.1 |
| 1 | 17-A | 20 | MET | 8.1 |
| 1 | 18-A | 20 | MET | 8.1 |
| 1 | 19-A | 20 | MET | 8.1 |
| 1 | 20-A | 20 | MET | 8.1 |
| 1 | 21-A | 20 | MET | 8.1 |
| 1 | 22-A | 20 | MET | 8.1 |
| 1 | 23-A | 20 | MET | 8.1 |
| 1 | 24-A | 20 | MET | 8.1 |
| 1 | 25-A | 20 | MET | 8.1 |
| 1 | 26-A | 20 | MET | 8.1 |
| 1 | 27-A | 20 | MET | 8.1 |
| 1 | 28-A | 20 | MET | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 29-A | 20 | MET | 8.1 |
| 1 | 30-A | 20 | MET | 8.1 |
| 1 | 31-A | 20 | MET | 8.1 |
| 1 | 32-A | 20 | MET | 8.1 |
| 1 | 33-A | 20 | MET | 8.1 |
| 1 | 34-A | 20 | MET | 8.1 |
| 1 | 35-A | 20 | MET | 8.1 |
| 1 | 36-A | 20 | MET | 8.1 |
| 1 | 37-A | 20 | MET | 8.1 |
| 1 | 38-A | 20 | MET | 8.1 |
| 1 | 39-A | 20 | MET | 8.1 |
| 1 | 40-A | 20 | MET | 8.1 |
| 1 | 41-A | 20 | MET | 8.1 |
| 1 | 42-A | 20 | MET | 8.1 |
| 1 | 43-A | 20 | MET | 8.1 |
| 1 | 44-A | 20 | MET | 8.1 |
| 1 | 45-A | 20 | MET | 8.1 |
| 1 | 46-A | 20 | MET | 8.1 |
| 1 | 47-A | 20 | MET | 8.1 |
| 1 | 48-A | 20 | MET | 8.1 |
| 1 | 49-A | 20 | MET | 8.1 |
| 1 | 50-A | 20 | MET | 8.1 |
| 1 | 51-A | 20 | MET | 8.1 |
| 1 | 52-A | 20 | MET | 8.1 |
| 1 | 53-A | 20 | MET | 8.1 |
| 1 | 54-A | 20 | MET | 8.1 |
| 1 | 55-A | 20 | MET | 8.1 |
| 1 | 56-A | 20 | MET | 8.1 |
| 1 | 57-A | 20 | MET | 8.1 |
| 1 | 58-A | 20 | MET | 8.1 |
| 1 | 59-A | 20 | MET | 8.1 |
| 1 | 60-A | 20 | MET | 8.1 |
| 1 | 61-A | 20 | MET | 8.1 |
| 1 | 62-A | 20 | MET | 8.1 |
| 1 | 63-A | 20 | MET | 8.1 |
| 1 | 64-A | 20 | MET | 8.1 |
| 1 | 65-A | 20 | MET | 8.1 |
| 1 | 66-A | 20 | MET | 8.1 |
| 1 | 67-A | 20 | MET | 8.1 |
| 1 | 68-A | 20 | MET | 8.1 |
| 1 | 69-A | 20 | MET | 8.1 |
| 1 | 70-A | 20 | MET | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 71-A | 20 | MET | 8.1 |
| 1 | 72-A | 20 | MET | 8.1 |
| 1 | 73-A | 20 | MET | 8.1 |
| 1 | 74-A | 20 | MET | 8.1 |
| 1 | 75-A | 20 | MET | 8.1 |
| 1 | 76-A | 20 | MET | 8.1 |
| 1 | 77-A | 20 | MET | 8.1 |
| 1 | 78-A | 20 | MET | 8.1 |
| 1 | 79-A | 20 | MET | 8.1 |
| 1 | 80-A | 20 | MET | 8.1 |
| 1 | 81-A | 20 | MET | 8.1 |
| 1 | 82-A | 20 | MET | 8.1 |
| 1 | 83-A | 20 | MET | 8.1 |
| 1 | 84-A | 20 | MET | 8.1 |
| 1 | 85-A | 20 | MET | 8.1 |
| 1 | 86-A | 20 | MET | 8.1 |
| 1 | 87-A | 20 | MET | 8.1 |
| 1 | 88-A | 20 | MET | 8.1 |
| 1 | 89-A | 20 | MET | 8.1 |
| 1 | 90-A | 20 | MET | 8.1 |
| 1 | 91-A | 20 | MET | 8.1 |
| 1 | 92-A | 20 | MET | 8.1 |
| 1 | 93-A | 20 | MET | 8.1 |
| 1 | 94-A | 20 | MET | 8.1 |
| 1 | 95-A | 20 | MET | 8.1 |
| 1 | 96-A | 20 | MET | 8.1 |
| 1 | 97-A | 20 | MET | 8.1 |
| 1 | 98-A | 20 | MET | 8.1 |
| 1 | 99-A | 20 | MET | 8.1 |
| 1 | 100-A | 20 | MET | 8.1 |
| 1 | 101-A | 20 | MET | 8.1 |
| 1 | 102-A | 20 | MET | 8.1 |
| 1 | 103-A | 20 | MET | 8.1 |
| 1 | 104-A | 20 | MET | 8.1 |
| 1 | 105-A | 20 | MET | 8.1 |
| 1 | 106-A | 20 | MET | 8.1 |
| 1 | 107-A | 20 | MET | 8.1 |
| 1 | 108-A | 20 | MET | 8.1 |
| 1 | 109-A | 20 | MET | 8.1 |
| 1 | 110-A | 20 | MET | 8.1 |
| 1 | 111-A | 20 | MET | 8.1 |
| 1 | 112-A | 20 | MET | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 113-A | 20 | MET | 8.1 |
| 1 | 114-A | 20 | MET | 8.1 |
| 1 | 115-A | 20 | MET | 8.1 |
| 1 | 116-A | 20 | MET | 8.1 |
| 1 | 117-A | 20 | MET | 8.1 |
| 1 | 118-A | 20 | MET | 8.1 |
| 1 | 119-A | 20 | MET | 8.1 |
| 1 | 120-A | 20 | MET | 8.1 |
| 1 | 121-A | 20 | MET | 8.1 |
| 1 | 122-A | 20 | MET | 8.1 |
| 1 | 123-A | 20 | MET | 8.1 |
| 1 | 124-A | 20 | MET | 8.1 |
| 1 | 125-A | 20 | MET | 8.1 |
| 1 | 1-A | 128 | TYR | 8.1 |
| 1 | 2-A | 128 | TYR | 8.1 |
| 1 | 3-A | 128 | TYR | 8.1 |
| 1 | 4-A | 128 | TYR | 8.1 |
| 1 | 5-A | 128 | TYR | 8.1 |
| 1 | 6-A | 128 | TYR | 8.1 |
| 1 | 7-A | 128 | TYR | 8.1 |
| 1 | 8-A | 128 | TYR | 8.1 |
| 1 | 9-A | 128 | TYR | 8.1 |
| 1 | 10-A | 128 | TYR | 8.1 |
| 1 | 11-A | 128 | TYR | 8.1 |
| 1 | 12-A | 128 | TYR | 8.1 |
| 1 | 13-A | 128 | TYR | 8.1 |
| 1 | 14-A | 128 | TYR | 8.1 |
| 1 | 15-A | 128 | TYR | 8.1 |
| 1 | 16-A | 128 | TYR | 8.1 |
| 1 | 17-A | 128 | TYR | 8.1 |
| 1 | 18-A | 128 | TYR | 8.1 |
| 1 | 19-A | 128 | TYR | 8.1 |
| 1 | 20-A | 128 | TYR | 8.1 |
| 1 | 21-A | 128 | TYR | 8.1 |
| 1 | 22-A | 128 | TYR | 8.1 |
| 1 | 23-A | 128 | TYR | 8.1 |
| 1 | 24-A | 128 | TYR | 8.1 |
| 1 | 25-A | 128 | TYR | 8.1 |
| 1 | 26-A | 128 | TYR | 8.1 |
| 1 | 27-A | 128 | TYR | 8.1 |
| 1 | 28-A | 128 | TYR | 8.1 |
| 1 | 29-A | 128 | TYR | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 30-A | 128 | TYR | 8.1 |
| 1 | 31-A | 128 | TYR | 8.1 |
| 1 | 32-A | 128 | TYR | 8.1 |
| 1 | 33-A | 128 | TYR | 8.1 |
| 1 | 34-A | 128 | TYR | 8.1 |
| 1 | 35-A | 128 | TYR | 8.1 |
| 1 | 36-A | 128 | TYR | 8.1 |
| 1 | 37-A | 128 | TYR | 8.1 |
| 1 | 38-A | 128 | TYR | 8.1 |
| 1 | 39-A | 128 | TYR | 8.1 |
| 1 | 40-A | 128 | TYR | 8.1 |
| 1 | 41-A | 128 | TYR | 8.1 |
| 1 | 42-A | 128 | TYR | 8.1 |
| 1 | 43-A | 128 | TYR | 8.1 |
| 1 | 44-A | 128 | TYR | 8.1 |
| 1 | 45-A | 128 | TYR | 8.1 |
| 1 | 46-A | 128 | TYR | 8.1 |
| 1 | 47-A | 128 | TYR | 8.1 |
| 1 | 48-A | 128 | TYR | 8.1 |
| 1 | 49-A | 128 | TYR | 8.1 |
| 1 | 50-A | 128 | TYR | 8.1 |
| 1 | 51-A | 128 | TYR | 8.1 |
| 1 | 52-A | 128 | TYR | 8.1 |
| 1 | 53-A | 128 | TYR | 8.1 |
| 1 | 54-A | 128 | TYR | 8.1 |
| 1 | 55-A | 128 | TYR | 8.1 |
| 1 | 56-A | 128 | TYR | 8.1 |
| 1 | 57-A | 128 | TYR | 8.1 |
| 1 | 58-A | 128 | TYR | 8.1 |
| 1 | 59-A | 128 | TYR | 8.1 |
| 1 | 60-A | 128 | TYR | 8.1 |
| 1 | 61-A | 128 | TYR | 8.1 |
| 1 | 62-A | 128 | TYR | 8.1 |
| 1 | 63-A | 128 | TYR | 8.1 |
| 1 | 64-A | 128 | TYR | 8.1 |
| 1 | 65-A | 128 | TYR | 8.1 |
| 1 | 66-A | 128 | TYR | 8.1 |
| 1 | 67-A | 128 | TYR | 8.1 |
| 1 | 68-A | 128 | TYR | 8.1 |
| 1 | 69-A | 128 | TYR | 8.1 |
| 1 | 70-A | 128 | TYR | 8.1 |
| 1 | 71-A | 128 | TYR | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 72-A | 128 | TYR | 8.1 |
| 1 | 73-A | 128 | TYR | 8.1 |
| 1 | 74-A | 128 | TYR | 8.1 |
| 1 | 75-A | 128 | TYR | 8.1 |
| 1 | 76-A | 128 | TYR | 8.1 |
| 1 | 77-A | 128 | TYR | 8.1 |
| 1 | 78-A | 128 | TYR | 8.1 |
| 1 | 79-A | 128 | TYR | 8.1 |
| 1 | 80-A | 128 | TYR | 8.1 |
| 1 | 81-A | 128 | TYR | 8.1 |
| 1 | 82-A | 128 | TYR | 8.1 |
| 1 | 83-A | 128 | TYR | 8.1 |
| 1 | 84-A | 128 | TYR | 8.1 |
| 1 | 85-A | 128 | TYR | 8.1 |
| 1 | 86-A | 128 | TYR | 8.1 |
| 1 | 87-A | 128 | TYR | 8.1 |
| 1 | 88-A | 128 | TYR | 8.1 |
| 1 | 89-A | 128 | TYR | 8.1 |
| 1 | 90-A | 128 | TYR | 8.1 |
| 1 | 91-A | 128 | TYR | 8.1 |
| 1 | 92-A | 128 | TYR | 8.1 |
| 1 | 93-A | 128 | TYR | 8.1 |
| 1 | 94-A | 128 | TYR | 8.1 |
| 1 | 95-A | 128 | TYR | 8.1 |
| 1 | 96-A | 128 | TYR | 8.1 |
| 1 | 97-A | 128 | TYR | 8.1 |
| 1 | 98-A | 128 | TYR | 8.1 |
| 1 | 99-A | 128 | TYR | 8.1 |
| 1 | 100-A | 128 | TYR | 8.1 |
| 1 | 101-A | 128 | TYR | 8.1 |
| 1 | 102-A | 128 | TYR | 8.1 |
| 1 | 103-A | 128 | TYR | 8.1 |
| 1 | 104-A | 128 | TYR | 8.1 |
| 1 | 105-A | 128 | TYR | 8.1 |
| 1 | 106-A | 128 | TYR | 8.1 |
| 1 | 107-A | 128 | TYR | 8.1 |
| 1 | 108-A | 128 | TYR | 8.1 |
| 1 | 109-A | 128 | TYR | 8.1 |
| 1 | 110-A | 128 | TYR | 8.1 |
| 1 | 111-A | 128 | TYR | 8.1 |
| 1 | 112-A | 128 | TYR | 8.1 |
| 1 | 113-A | 128 | TYR | 8.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 114-A | 128 | TYR | 8.1 |
| 1 | 115-A | 128 | TYR | 8.1 |
| 1 | 116-A | 128 | TYR | 8.1 |
| 1 | 117-A | 128 | TYR | 8.1 |
| 1 | 118-A | 128 | TYR | 8.1 |
| 1 | 119-A | 128 | TYR | 8.1 |
| 1 | 120-A | 128 | TYR | 8.1 |
| 1 | 121-A | 128 | TYR | 8.1 |
| 1 | 122-A | 128 | TYR | 8.1 |
| 1 | 123-A | 128 | TYR | 8.1 |
| 1 | 124-A | 128 | TYR | 8.1 |
| 1 | 125-A | 128 | TYR | 8.1 |
| 1 | 1-A | 23 | ASN | 5.9 |
| 1 | 2-A | 23 | ASN | 5.9 |
| 1 | 3-A | 23 | ASN | 5.9 |
| 1 | 4-A | 23 | ASN | 5.9 |
| 1 | 5-A | 23 | ASN | 5.9 |
| 1 | 6-A | 23 | ASN | 5.9 |
| 1 | 7-A | 23 | ASN | 5.9 |
| 1 | 8-A | 23 | ASN | 5.9 |
| 1 | 9-A | 23 | ASN | 5.9 |
| 1 | 10-A | 23 | ASN | 5.9 |
| 1 | 11-A | 23 | ASN | 5.9 |
| 1 | 12-A | 23 | ASN | 5.9 |
| 1 | 13-A | 23 | ASN | 5.9 |
| 1 | 14-A | 23 | ASN | 5.9 |
| 1 | 15-A | 23 | ASN | 5.9 |
| 1 | 16-A | 23 | ASN | 5.9 |
| 1 | 17-A | 23 | ASN | 5.9 |
| 1 | 18-A | 23 | ASN | 5.9 |
| 1 | 19-A | 23 | ASN | 5.9 |
| 1 | 20-A | 23 | ASN | 5.9 |
| 1 | 21-A | 23 | ASN | 5.9 |
| 1 | 22-A | 23 | ASN | 5.9 |
| 1 | 23-A | 23 | ASN | 5.9 |
| 1 | 24-A | 23 | ASN | 5.9 |
| 1 | 25-A | 23 | ASN | 5.9 |
| 1 | 26-A | 23 | ASN | 5.9 |
| 1 | 27-A | 23 | ASN | 5.9 |
| 1 | 28-A | 23 | ASN | 5.9 |
| 1 | 29-A | 23 | ASN | 5.9 |
| 1 | 30-A | 23 | ASN | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 31-A | 23 | ASN | 5.9 |
| 1 | 32-A | 23 | ASN | 5.9 |
| 1 | 33-A | 23 | ASN | 5.9 |
| 1 | 34-A | 23 | ASN | 5.9 |
| 1 | 35-A | 23 | ASN | 5.9 |
| 1 | 36-A | 23 | ASN | 5.9 |
| 1 | 37-A | 23 | ASN | 5.9 |
| 1 | 38-A | 23 | ASN | 5.9 |
| 1 | 39-A | 23 | ASN | 5.9 |
| 1 | 40-A | 23 | ASN | 5.9 |
| 1 | 41-A | 23 | ASN | 5.9 |
| 1 | 42-A | 23 | ASN | 5.9 |
| 1 | 43-A | 23 | ASN | 5.9 |
| 1 | 44-A | 23 | ASN | 5.9 |
| 1 | 45-A | 23 | ASN | 5.9 |
| 1 | 46-A | 23 | ASN | 5.9 |
| 1 | 47-A | 23 | ASN | 5.9 |
| 1 | 48-A | 23 | ASN | 5.9 |
| 1 | 49-A | 23 | ASN | 5.9 |
| 1 | 50-A | 23 | ASN | 5.9 |
| 1 | 51-A | 23 | ASN | 5.9 |
| 1 | 52-A | 23 | ASN | 5.9 |
| 1 | 53-A | 23 | ASN | 5.9 |
| 1 | 54-A | 23 | ASN | 5.9 |
| 1 | 55-A | 23 | ASN | 5.9 |
| 1 | 56-A | 23 | ASN | 5.9 |
| 1 | 57-A | 23 | ASN | 5.9 |
| 1 | 58-A | 23 | ASN | 5.9 |
| 1 | 59-A | 23 | ASN | 5.9 |
| 1 | 60-A | 23 | ASN | 5.9 |
| 1 | 61-A | 23 | ASN | 5.9 |
| 1 | 62-A | 23 | ASN | 5.9 |
| 1 | 63-A | 23 | ASN | 5.9 |
| 1 | 64-A | 23 | ASN | 5.9 |
| 1 | 65-A | 23 | ASN | 5.9 |
| 1 | 66-A | 23 | ASN | 5.9 |
| 1 | 67-A | 23 | ASN | 5.9 |
| 1 | 68-A | 23 | ASN | 5.9 |
| 1 | 69-A | 23 | ASN | 5.9 |
| 1 | 70-A | 23 | ASN | 5.9 |
| 1 | 71-A | 23 | ASN | 5.9 |
| 1 | 72-A | 23 | ASN | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 73-A | 23 | ASN | 5.9 |
| 1 | 74-A | 23 | ASN | 5.9 |
| 1 | 75-A | 23 | ASN | 5.9 |
| 1 | 76-A | 23 | ASN | 5.9 |
| 1 | 77-A | 23 | ASN | 5.9 |
| 1 | 78-A | 23 | ASN | 5.9 |
| 1 | 79-A | 23 | ASN | 5.9 |
| 1 | 80-A | 23 | ASN | 5.9 |
| 1 | 81-A | 23 | ASN | 5.9 |
| 1 | 82-A | 23 | ASN | 5.9 |
| 1 | 83-A | 23 | ASN | 5.9 |
| 1 | 84-A | 23 | ASN | 5.9 |
| 1 | 85-A | 23 | ASN | 5.9 |
| 1 | 86-A | 23 | ASN | 5.9 |
| 1 | 87-A | 23 | ASN | 5.9 |
| 1 | 88-A | 23 | ASN | 5.9 |
| 1 | 89-A | 23 | ASN | 5.9 |
| 1 | 90-A | 23 | ASN | 5.9 |
| 1 | 91-A | 23 | ASN | 5.9 |
| 1 | 92-A | 23 | ASN | 5.9 |
| 1 | 93-A | 23 | ASN | 5.9 |
| 1 | 94-A | 23 | ASN | 5.9 |
| 1 | 95-A | 23 | ASN | 5.9 |
| 1 | 96-A | 23 | ASN | 5.9 |
| 1 | 97-A | 23 | ASN | 5.9 |
| 1 | 98-A | 23 | ASN | 5.9 |
| 1 | 99-A | 23 | ASN | 5.9 |
| 1 | 100-A | 23 | ASN | 5.9 |
| 1 | 101-A | 23 | ASN | 5.9 |
| 1 | 102-A | 23 | ASN | 5.9 |
| 1 | 103-A | 23 | ASN | 5.9 |
| 1 | 104-A | 23 | ASN | 5.9 |
| 1 | 105-A | 23 | ASN | 5.9 |
| 1 | 106-A | 23 | ASN | 5.9 |
| 1 | 107-A | 23 | ASN | 5.9 |
| 1 | 108-A | 23 | ASN | 5.9 |
| 1 | 109-A | 23 | ASN | 5.9 |
| 1 | 110-A | 23 | ASN | 5.9 |
| 1 | 111-A | 23 | ASN | 5.9 |
| 1 | 112-A | 23 | ASN | 5.9 |
| 1 | 113-A | 23 | ASN | 5.9 |
| 1 | 114-A | 23 | ASN | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 115-A | 23 | ASN | 5.9 |
| 1 | 116-A | 23 | ASN | 5.9 |
| 1 | 117-A | 23 | ASN | 5.9 |
| 1 | 118-A | 23 | ASN | 5.9 |
| 1 | 119-A | 23 | ASN | 5.9 |
| 1 | 120-A | 23 | ASN | 5.9 |
| 1 | 121-A | 23 | ASN | 5.9 |
| 1 | 122-A | 23 | ASN | 5.9 |
| 1 | 123-A | 23 | ASN | 5.9 |
| 1 | 124-A | 23 | ASN | 5.9 |
| 1 | 125-A | 23 | ASN | 5.9 |
| 1 | 1-A | 50 | ILE | 3.0 |
| 1 | 2-A | 50 | ILE | 3.0 |
| 1 | 3-A | 50 | ILE | 3.0 |
| 1 | 4-A | 50 | ILE | 3.0 |
| 1 | 5-A | 50 | ILE | 3.0 |
| 1 | 6-A | 50 | ILE | 3.0 |
| 1 | 7-A | 50 | ILE | 3.0 |
| 1 | 8-A | 50 | ILE | 3.0 |
| 1 | 9-A | 50 | ILE | 3.0 |
| 1 | 10-A | 50 | ILE | 3.0 |
| 1 | 11-A | 50 | ILE | 3.0 |
| 1 | 12-A | 50 | ILE | 3.0 |
| 1 | 13-A | 50 | ILE | 3.0 |
| 1 | 14-A | 50 | ILE | 3.0 |
| 1 | 15-A | 50 | ILE | 3.0 |
| 1 | 16-A | 50 | ILE | 3.0 |
| 1 | 17-A | 50 | ILE | 3.0 |
| 1 | 18-A | 50 | ILE | 3.0 |
| 1 | 19-A | 50 | ILE | 3.0 |
| 1 | 20-A | 50 | ILE | 3.0 |
| 1 | 21-A | 50 | ILE | 3.0 |
| 1 | 22-A | 50 | ILE | 3.0 |
| 1 | 23-A | 50 | ILE | 3.0 |
| 1 | 24-A | 50 | ILE | 3.0 |
| 1 | 25-A | 50 | ILE | 3.0 |
| 1 | 26-A | 50 | ILE | 3.0 |
| 1 | 27-A | 50 | ILE | 3.0 |
| 1 | 28-A | 50 | ILE | 3.0 |
| 1 | 29-A | 50 | ILE | 3.0 |
| 1 | 30-A | 50 | ILE | 3.0 |
| 1 | 31-A | 50 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 32-A | 50 | ILE | 3.0 |
| 1 | 33-A | 50 | ILE | 3.0 |
| 1 | 34-A | 50 | ILE | 3.0 |
| 1 | 35-A | 50 | ILE | 3.0 |
| 1 | 36-A | 50 | ILE | 3.0 |
| 1 | 37-A | 50 | ILE | 3.0 |
| 1 | 38-A | 50 | ILE | 3.0 |
| 1 | 39-A | 50 | ILE | 3.0 |
| 1 | 40-A | 50 | ILE | 3.0 |
| 1 | 41-A | 50 | ILE | 3.0 |
| 1 | 42-A | 50 | ILE | 3.0 |
| 1 | 43-A | 50 | ILE | 3.0 |
| 1 | 44-A | 50 | ILE | 3.0 |
| 1 | 45-A | 50 | ILE | 3.0 |
| 1 | 46-A | 50 | ILE | 3.0 |
| 1 | 47-A | 50 | ILE | 3.0 |
| 1 | 48-A | 50 | ILE | 3.0 |
| 1 | 49-A | 50 | ILE | 3.0 |
| 1 | 50-A | 50 | ILE | 3.0 |
| 1 | 51-A | 50 | ILE | 3.0 |
| 1 | 52-A | 50 | ILE | 3.0 |
| 1 | 53-A | 50 | ILE | 3.0 |
| 1 | 54-A | 50 | ILE | 3.0 |
| 1 | 55-A | 50 | ILE | 3.0 |
| 1 | 56-A | 50 | ILE | 3.0 |
| 1 | 57-A | 50 | ILE | 3.0 |
| 1 | 58-A | 50 | ILE | 3.0 |
| 1 | 59-A | 50 | ILE | 3.0 |
| 1 | 60-A | 50 | ILE | 3.0 |
| 1 | 61-A | 50 | ILE | 3.0 |
| 1 | 62-A | 50 | ILE | 3.0 |
| 1 | 63-A | 50 | ILE | 3.0 |
| 1 | 64-A | 50 | ILE | 3.0 |
| 1 | 65-A | 50 | ILE | 3.0 |
| 1 | 66-A | 50 | ILE | 3.0 |
| 1 | 67-A | 50 | ILE | 3.0 |
| 1 | 68-A | 50 | ILE | 3.0 |
| 1 | 69-A | 50 | ILE | 3.0 |
| 1 | 70-A | 50 | ILE | 3.0 |
| 1 | 71-A | 50 | ILE | 3.0 |
| 1 | 72-A | 50 | ILE | 3.0 |
| 1 | 73-A | 50 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 74-A | 50 | ILE | 3.0 |
| 1 | 75-A | 50 | ILE | 3.0 |
| 1 | 76-A | 50 | ILE | 3.0 |
| 1 | 77-A | 50 | ILE | 3.0 |
| 1 | 78-A | 50 | ILE | 3.0 |
| 1 | 79-A | 50 | ILE | 3.0 |
| 1 | 80-A | 50 | ILE | 3.0 |
| 1 | 81-A | 50 | ILE | 3.0 |
| 1 | 82-A | 50 | ILE | 3.0 |
| 1 | 83-A | 50 | ILE | 3.0 |
| 1 | 84-A | 50 | ILE | 3.0 |
| 1 | 85-A | 50 | ILE | 3.0 |
| 1 | 86-A | 50 | ILE | 3.0 |
| 1 | 87-A | 50 | ILE | 3.0 |
| 1 | 88-A | 50 | ILE | 3.0 |
| 1 | 89-A | 50 | ILE | 3.0 |
| 1 | 90-A | 50 | ILE | 3.0 |
| 1 | 91-A | 50 | ILE | 3.0 |
| 1 | 92-A | 50 | ILE | 3.0 |
| 1 | 93-A | 50 | ILE | 3.0 |
| 1 | 94-A | 50 | ILE | 3.0 |
| 1 | 95-A | 50 | ILE | 3.0 |
| 1 | 96-A | 50 | ILE | 3.0 |
| 1 | 97-A | 50 | ILE | 3.0 |
| 1 | 98-A | 50 | ILE | 3.0 |
| 1 | 99-A | 50 | ILE | 3.0 |
| 1 | 100-A | 50 | ILE | 3.0 |
| 1 | 101-A | 50 | ILE | 3.0 |
| 1 | 102-A | 50 | ILE | 3.0 |
| 1 | 103-A | 50 | ILE | 3.0 |
| 1 | 104-A | 50 | ILE | 3.0 |
| 1 | 105-A | 50 | ILE | 3.0 |
| 1 | 106-A | 50 | ILE | 3.0 |
| 1 | 107-A | 50 | ILE | 3.0 |
| 1 | 108-A | 50 | ILE | 3.0 |
| 1 | 109-A | 50 | ILE | 3.0 |
| 1 | 110-A | 50 | ILE | 3.0 |
| 1 | 111-A | 50 | ILE | 3.0 |
| 1 | 112-A | 50 | ILE | 3.0 |
| 1 | 113-A | 50 | ILE | 3.0 |
| 1 | 114-A | 50 | ILE | 3.0 |
| 1 | 115-A | 50 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 116-A | 50 | ILE | 3.0 |
| 1 | 117-A | 50 | ILE | 3.0 |
| 1 | 118-A | 50 | ILE | 3.0 |
| 1 | 119-A | 50 | ILE | 3.0 |
| 1 | 120-A | 50 | ILE | 3.0 |
| 1 | 121-A | 50 | ILE | 3.0 |
| 1 | 122-A | 50 | ILE | 3.0 |
| 1 | 123-A | 50 | ILE | 3.0 |
| 1 | 124-A | 50 | ILE | 3.0 |
| 1 | 125-A | 50 | ILE | 3.0 |
| 1 | 1-A | 127 | ASP | 2.8 |
| 1 | 2-A | 127 | ASP | 2.8 |
| 1 | 3-A | 127 | ASP | 2.8 |
| 1 | 4-A | 127 | ASP | 2.8 |
| 1 | 5-A | 127 | ASP | 2.8 |
| 1 | 6-A | 127 | ASP | 2.8 |
| 1 | 7-A | 127 | ASP | 2.8 |
| 1 | 8-A | 127 | ASP | 2.8 |
| 1 | 9-A | 127 | ASP | 2.8 |
| 1 | 10-A | 127 | ASP | 2.8 |
| 1 | 11-A | 127 | ASP | 2.8 |
| 1 | 12-A | 127 | ASP | 2.8 |
| 1 | 13-A | 127 | ASP | 2.8 |
| 1 | 14-A | 127 | ASP | 2.8 |
| 1 | 15-A | 127 | ASP | 2.8 |
| 1 | 16-A | 127 | ASP | 2.8 |
| 1 | 17-A | 127 | ASP | 2.8 |
| 1 | 18-A | 127 | ASP | 2.8 |
| 1 | 19-A | 127 | ASP | 2.8 |
| 1 | 20-A | 127 | ASP | 2.8 |
| 1 | 21-A | 127 | ASP | 2.8 |
| 1 | 22-A | 127 | ASP | 2.8 |
| 1 | 23-A | 127 | ASP | 2.8 |
| 1 | 24-A | 127 | ASP | 2.8 |
| 1 | 25-A | 127 | ASP | 2.8 |
| 1 | 26-A | 127 | ASP | 2.8 |
| 1 | 27-A | 127 | ASP | 2.8 |
| 1 | 28-A | 127 | ASP | 2.8 |
| 1 | 29-A | 127 | ASP | 2.8 |
| 1 | 30-A | 127 | ASP | 2.8 |
| 1 | 31-A | 127 | ASP | 2.8 |
| 1 | 32-A | 127 | ASP | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 33-A | 127 | ASP | 2.8 |
| 1 | 34-A | 127 | ASP | 2.8 |
| 1 | 35-A | 127 | ASP | 2.8 |
| 1 | 36-A | 127 | ASP | 2.8 |
| 1 | 37-A | 127 | ASP | 2.8 |
| 1 | 38-A | 127 | ASP | 2.8 |
| 1 | 39-A | 127 | ASP | 2.8 |
| 1 | 40-A | 127 | ASP | 2.8 |
| 1 | 41-A | 127 | ASP | 2.8 |
| 1 | 42-A | 127 | ASP | 2.8 |
| 1 | 43-A | 127 | ASP | 2.8 |
| 1 | 44-A | 127 | ASP | 2.8 |
| 1 | 45-A | 127 | ASP | 2.8 |
| 1 | 46-A | 127 | ASP | 2.8 |
| 1 | 47-A | 127 | ASP | 2.8 |
| 1 | 48-A | 127 | ASP | 2.8 |
| 1 | 49-A | 127 | ASP | 2.8 |
| 1 | 50-A | 127 | ASP | 2.8 |
| 1 | 51-A | 127 | ASP | 2.8 |
| 1 | 52-A | 127 | ASP | 2.8 |
| 1 | 53-A | 127 | ASP | 2.8 |
| 1 | 54-A | 127 | ASP | 2.8 |
| 1 | 55-A | 127 | ASP | 2.8 |
| 1 | 56-A | 127 | ASP | 2.8 |
| 1 | 57-A | 127 | ASP | 2.8 |
| 1 | 58-A | 127 | ASP | 2.8 |
| 1 | 59-A | 127 | ASP | 2.8 |
| 1 | 60-A | 127 | ASP | 2.8 |
| 1 | 61-A | 127 | ASP | 2.8 |
| 1 | 62-A | 127 | ASP | 2.8 |
| 1 | 63-A | 127 | ASP | 2.8 |
| 1 | 64-A | 127 | ASP | 2.8 |
| 1 | 65-A | 127 | ASP | 2.8 |
| 1 | 66-A | 127 | ASP | 2.8 |
| 1 | 67-A | 127 | ASP | 2.8 |
| 1 | 68-A | 127 | ASP | 2.8 |
| 1 | 69-A | 127 | ASP | 2.8 |
| 1 | 70-A | 127 | ASP | 2.8 |
| 1 | 71-A | 127 | ASP | 2.8 |
| 1 | 72-A | 127 | ASP | 2.8 |
| 1 | 73-A | 127 | ASP | 2.8 |
| 1 | 74-A | 127 | ASP | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 75-A | 127 | ASP | 2.8 |
| 1 | 76-A | 127 | ASP | 2.8 |
| 1 | 77-A | 127 | ASP | 2.8 |
| 1 | 78-A | 127 | ASP | 2.8 |
| 1 | 79-A | 127 | ASP | 2.8 |
| 1 | 80-A | 127 | ASP | 2.8 |
| 1 | 81-A | 127 | ASP | 2.8 |
| 1 | 82-A | 127 | ASP | 2.8 |
| 1 | 83-A | 127 | ASP | 2.8 |
| 1 | 84-A | 127 | ASP | 2.8 |
| 1 | 85-A | 127 | ASP | 2.8 |
| 1 | 86-A | 127 | ASP | 2.8 |
| 1 | 87-A | 127 | ASP | 2.8 |
| 1 | 88-A | 127 | ASP | 2.8 |
| 1 | 89-A | 127 | ASP | 2.8 |
| 1 | 90-A | 127 | ASP | 2.8 |
| 1 | 91-A | 127 | ASP | 2.8 |
| 1 | 92-A | 127 | ASP | 2.8 |
| 1 | 93-A | 127 | ASP | 2.8 |
| 1 | 94-A | 127 | ASP | 2.8 |
| 1 | 95-A | 127 | ASP | 2.8 |
| 1 | 96-A | 127 | ASP | 2.8 |
| 1 | 97-A | 127 | ASP | 2.8 |
| 1 | 98-A | 127 | ASP | 2.8 |
| 1 | 99-A | 127 | ASP | 2.8 |
| 1 | 100-A | 127 | ASP | 2.8 |
| 1 | 101-A | 127 | ASP | 2.8 |
| 1 | 102-A | 127 | ASP | 2.8 |
| 1 | 103-A | 127 | ASP | 2.8 |
| 1 | 104-A | 127 | ASP | 2.8 |
| 1 | 105-A | 127 | ASP | 2.8 |
| 1 | 106-A | 127 | ASP | 2.8 |
| 1 | 107-A | 127 | ASP | 2.8 |
| 1 | 108-A | 127 | ASP | 2.8 |
| 1 | 109-A | 127 | ASP | 2.8 |
| 1 | 110-A | 127 | ASP | 2.8 |
| 1 | 111-A | 127 | ASP | 2.8 |
| 1 | 112-A | 127 | ASP | 2.8 |
| 1 | 113-A | 127 | ASP | 2.8 |
| 1 | 114-A | 127 | ASP | 2.8 |
| 1 | 115-A | 127 | ASP | 2.8 |
| 1 | 116-A | 127 | ASP | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 117-A | 127 | ASP | 2.8 |
| 1 | 118-A | 127 | ASP | 2.8 |
| 1 | 119-A | 127 | ASP | 2.8 |
| 1 | 120-A | 127 | ASP | 2.8 |
| 1 | 121-A | 127 | ASP | 2.8 |
| 1 | 122-A | 127 | ASP | 2.8 |
| 1 | 123-A | 127 | ASP | 2.8 |
| 1 | 124-A | 127 | ASP | 2.8 |
| 1 | 125-A | 127 | ASP | 2.8 |
| 1 | 1-A | 18 | ASN | 2.5 |
| 1 | 2-A | 18 | ASN | 2.5 |
| 1 | 3-A | 18 | ASN | 2.5 |
| 1 | 4-A | 18 | ASN | 2.5 |
| 1 | 5-A | 18 | ASN | 2.5 |
| 1 | 6-A | 18 | ASN | 2.5 |
| 1 | 7-A | 18 | ASN | 2.5 |
| 1 | 8-A | 18 | ASN | 2.5 |
| 1 | 9-A | 18 | ASN | 2.5 |
| 1 | 10-A | 18 | ASN | 2.5 |
| 1 | 11-A | 18 | ASN | 2.5 |
| 1 | 12-A | 18 | ASN | 2.5 |
| 1 | 13-A | 18 | ASN | 2.5 |
| 1 | 14-A | 18 | ASN | 2.5 |
| 1 | 15-A | 18 | ASN | 2.5 |
| 1 | 16-A | 18 | ASN | 2.5 |
| 1 | 17-A | 18 | ASN | 2.5 |
| 1 | 18-A | 18 | ASN | 2.5 |
| 1 | 19-A | 18 | ASN | 2.5 |
| 1 | 20-A | 18 | ASN | 2.5 |
| 1 | 21-A | 18 | ASN | 2.5 |
| 1 | 22-A | 18 | ASN | 2.5 |
| 1 | 23-A | 18 | ASN | 2.5 |
| 1 | 24-A | 18 | ASN | 2.5 |
| 1 | 25-A | 18 | ASN | 2.5 |
| 1 | 26-A | 18 | ASN | 2.5 |
| 1 | 27-A | 18 | ASN | 2.5 |
| 1 | 28-A | 18 | ASN | 2.5 |
| 1 | 29-A | 18 | ASN | 2.5 |
| 1 | 30-A | 18 | ASN | 2.5 |
| 1 | 31-A | 18 | ASN | 2.5 |
| 1 | 32-A | 18 | ASN | 2.5 |
| 1 | 33-A | 18 | ASN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 34-A | 18 | ASN | 2.5 |
| 1 | 35-A | 18 | ASN | 2.5 |
| 1 | 36-A | 18 | ASN | 2.5 |
| 1 | 37-A | 18 | ASN | 2.5 |
| 1 | 38-A | 18 | ASN | 2.5 |
| 1 | 39-A | 18 | ASN | 2.5 |
| 1 | 40-A | 18 | ASN | 2.5 |
| 1 | 41-A | 18 | ASN | 2.5 |
| 1 | 42-A | 18 | ASN | 2.5 |
| 1 | 43-A | 18 | ASN | 2.5 |
| 1 | 44-A | 18 | ASN | 2.5 |
| 1 | 45-A | 18 | ASN | 2.5 |
| 1 | 46-A | 18 | ASN | 2.5 |
| 1 | 47-A | 18 | ASN | 2.5 |
| 1 | 48-A | 18 | ASN | 2.5 |
| 1 | 49-A | 18 | ASN | 2.5 |
| 1 | 50-A | 18 | ASN | 2.5 |
| 1 | 51-A | 18 | ASN | 2.5 |
| 1 | 52-A | 18 | ASN | 2.5 |
| 1 | 53-A | 18 | ASN | 2.5 |
| 1 | 54-A | 18 | ASN | 2.5 |
| 1 | 55-A | 18 | ASN | 2.5 |
| 1 | 56-A | 18 | ASN | 2.5 |
| 1 | 57-A | 18 | ASN | 2.5 |
| 1 | 58-A | 18 | ASN | 2.5 |
| 1 | 59-A | 18 | ASN | 2.5 |
| 1 | 60-A | 18 | ASN | 2.5 |
| 1 | 61-A | 18 | ASN | 2.5 |
| 1 | 62-A | 18 | ASN | 2.5 |
| 1 | 63-A | 18 | ASN | 2.5 |
| 1 | 64-A | 18 | ASN | 2.5 |
| 1 | 65-A | 18 | ASN | 2.5 |
| 1 | 66-A | 18 | ASN | 2.5 |
| 1 | 67-A | 18 | ASN | 2.5 |
| 1 | 68-A | 18 | ASN | 2.5 |
| 1 | 69-A | 18 | ASN | 2.5 |
| 1 | 70-A | 18 | ASN | 2.5 |
| 1 | 71-A | 18 | ASN | 2.5 |
| 1 | 72-A | 18 | ASN | 2.5 |
| 1 | 73-A | 18 | ASN | 2.5 |
| 1 | 74-A | 18 | ASN | 2.5 |
| 1 | 75-A | 18 | ASN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 76-A | 18 | ASN | 2.5 |
| 1 | 77-A | 18 | ASN | 2.5 |
| 1 | 78-A | 18 | ASN | 2.5 |
| 1 | 79-A | 18 | ASN | 2.5 |
| 1 | 80-A | 18 | ASN | 2.5 |
| 1 | 81-A | 18 | ASN | 2.5 |
| 1 | 82-A | 18 | ASN | 2.5 |
| 1 | 83-A | 18 | ASN | 2.5 |
| 1 | 84-A | 18 | ASN | 2.5 |
| 1 | 85-A | 18 | ASN | 2.5 |
| 1 | 86-A | 18 | ASN | 2.5 |
| 1 | 87-A | 18 | ASN | 2.5 |
| 1 | 88-A | 18 | ASN | 2.5 |
| 1 | 89-A | 18 | ASN | 2.5 |
| 1 | 90-A | 18 | ASN | 2.5 |
| 1 | 91-A | 18 | ASN | 2.5 |
| 1 | 92-A | 18 | ASN | 2.5 |
| 1 | 93-A | 18 | ASN | 2.5 |
| 1 | 94-A | 18 | ASN | 2.5 |
| 1 | 95-A | 18 | ASN | 2.5 |
| 1 | 96-A | 18 | ASN | 2.5 |
| 1 | 97-A | 18 | ASN | 2.5 |
| 1 | 98-A | 18 | ASN | 2.5 |
| 1 | 99-A | 18 | ASN | 2.5 |
| 1 | 100-A | 18 | ASN | 2.5 |
| 1 | 101-A | 18 | ASN | 2.5 |
| 1 | 102-A | 18 | ASN | 2.5 |
| 1 | 103-A | 18 | ASN | 2.5 |
| 1 | 104-A | 18 | ASN | 2.5 |
| 1 | 105-A | 18 | ASN | 2.5 |
| 1 | 106-A | 18 | ASN | 2.5 |
| 1 | 107-A | 18 | ASN | 2.5 |
| 1 | 108-A | 18 | ASN | 2.5 |
| 1 | 109-A | 18 | ASN | 2.5 |
| 1 | 110-A | 18 | ASN | 2.5 |
| 1 | 111-A | 18 | ASN | 2.5 |
| 1 | 112-A | 18 | ASN | 2.5 |
| 1 | 113-A | 18 | ASN | 2.5 |
| 1 | 114-A | 18 | ASN | 2.5 |
| 1 | 115-A | 18 | ASN | 2.5 |
| 1 | 116-A | 18 | ASN | 2.5 |
| 1 | 117-A | 18 | ASN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 118-A | 18 | ASN | 2.5 |
| 1 | 119-A | 18 | ASN | 2.5 |
| 1 | 120-A | 18 | ASN | 2.5 |
| 1 | 121-A | 18 | ASN | 2.5 |
| 1 | 122-A | 18 | ASN | 2.5 |
| 1 | 123-A | 18 | ASN | 2.5 |
| 1 | 124-A | 18 | ASN | 2.5 |
| 1 | 125-A | 18 | ASN | 2.5 |
| 1 | 1-A | 51 | GLY | 2.5 |
| 1 | 2-A | 51 | GLY | 2.5 |
| 1 | 3-A | 51 | GLY | 2.5 |
| 1 | 4-A | 51 | GLY | 2.5 |
| 1 | 5-A | 51 | GLY | 2.5 |
| 1 | 6-A | 51 | GLY | 2.5 |
| 1 | 7-A | 51 | GLY | 2.5 |
| 1 | 8-A | 51 | GLY | 2.5 |
| 1 | 9-A | 51 | GLY | 2.5 |
| 1 | 10-A | 51 | GLY | 2.5 |
| 1 | 11-A | 51 | GLY | 2.5 |
| 1 | 12-A | 51 | GLY | 2.5 |
| 1 | 13-A | 51 | GLY | 2.5 |
| 1 | 14-A | 51 | GLY | 2.5 |
| 1 | 15-A | 51 | GLY | 2.5 |
| 1 | 16-A | 51 | GLY | 2.5 |
| 1 | 17-A | 51 | GLY | 2.5 |
| 1 | 18-A | 51 | GLY | 2.5 |
| 1 | 19-A | 51 | GLY | 2.5 |
| 1 | 20-A | 51 | GLY | 2.5 |
| 1 | 21-A | 51 | GLY | 2.5 |
| 1 | 22-A | 51 | GLY | 2.5 |
| 1 | 23-A | 51 | GLY | 2.5 |
| 1 | 24-A | 51 | GLY | 2.5 |
| 1 | 25-A | 51 | GLY | 2.5 |
| 1 | 26-A | 51 | GLY | 2.5 |
| 1 | 27-A | 51 | GLY | 2.5 |
| 1 | 28-A | 51 | GLY | 2.5 |
| 1 | 29-A | 51 | GLY | 2.5 |
| 1 | 30-A | 51 | GLY | 2.5 |
| 1 | 31-A | 51 | GLY | 2.5 |
| 1 | 32-A | 51 | GLY | 2.5 |
| 1 | 33-A | 51 | GLY | 2.5 |
| 1 | 34-A | 51 | GLY | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 35-A | 51 | GLY | 2.5 |
| 1 | 36-A | 51 | GLY | 2.5 |
| 1 | 37-A | 51 | GLY | 2.5 |
| 1 | 38-A | 51 | GLY | 2.5 |
| 1 | 39-A | 51 | GLY | 2.5 |
| 1 | 40-A | 51 | GLY | 2.5 |
| 1 | 41-A | 51 | GLY | 2.5 |
| 1 | 42-A | 51 | GLY | 2.5 |
| 1 | 43-A | 51 | GLY | 2.5 |
| 1 | 44-A | 51 | GLY | 2.5 |
| 1 | 45-A | 51 | GLY | 2.5 |
| 1 | 46-A | 51 | GLY | 2.5 |
| 1 | 47-A | 51 | GLY | 2.5 |
| 1 | 48-A | 51 | GLY | 2.5 |
| 1 | 49-A | 51 | GLY | 2.5 |
| 1 | 50-A | 51 | GLY | 2.5 |
| 1 | 51-A | 51 | GLY | 2.5 |
| 1 | 52-A | 51 | GLY | 2.5 |
| 1 | 53-A | 51 | GLY | 2.5 |
| 1 | 54-A | 51 | GLY | 2.5 |
| 1 | 55-A | 51 | GLY | 2.5 |
| 1 | 56-A | 51 | GLY | 2.5 |
| 1 | 57-A | 51 | GLY | 2.5 |
| 1 | 58-A | 51 | GLY | 2.5 |
| 1 | 59-A | 51 | GLY | 2.5 |
| 1 | 60-A | 51 | GLY | 2.5 |
| 1 | 61-A | 51 | GLY | 2.5 |
| 1 | 62-A | 51 | GLY | 2.5 |
| 1 | 63-A | 51 | GLY | 2.5 |
| 1 | 64-A | 51 | GLY | 2.5 |
| 1 | 65-A | 51 | GLY | 2.5 |
| 1 | 66-A | 51 | GLY | 2.5 |
| 1 | 67-A | 51 | GLY | 2.5 |
| 1 | 68-A | 51 | GLY | 2.5 |
| 1 | 69-A | 51 | GLY | 2.5 |
| 1 | 70-A | 51 | GLY | 2.5 |
| 1 | 71-A | 51 | GLY | 2.5 |
| 1 | 72-A | 51 | GLY | 2.5 |
| 1 | 73-A | 51 | GLY | 2.5 |
| 1 | 74-A | 51 | GLY | 2.5 |
| 1 | 75-A | 51 | GLY | 2.5 |
| 1 | 76-A | 51 | GLY | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 77-A | 51 | GLY | 2.5 |
| 1 | 78-A | 51 | GLY | 2.5 |
| 1 | 79-A | 51 | GLY | 2.5 |
| 1 | 80-A | 51 | GLY | 2.5 |
| 1 | 81-A | 51 | GLY | 2.5 |
| 1 | 82-A | 51 | GLY | 2.5 |
| 1 | 83-A | 51 | GLY | 2.5 |
| 1 | 84-A | 51 | GLY | 2.5 |
| 1 | 85-A | 51 | GLY | 2.5 |
| 1 | 86-A | 51 | GLY | 2.5 |
| 1 | 87-A | 51 | GLY | 2.5 |
| 1 | 88-A | 51 | GLY | 2.5 |
| 1 | 89-A | 51 | GLY | 2.5 |
| 1 | 90-A | 51 | GLY | 2.5 |
| 1 | 91-A | 51 | GLY | 2.5 |
| 1 | 92-A | 51 | GLY | 2.5 |
| 1 | 93-A | 51 | GLY | 2.5 |
| 1 | 94-A | 51 | GLY | 2.5 |
| 1 | 95-A | 51 | GLY | 2.5 |
| 1 | 96-A | 51 | GLY | 2.5 |
| 1 | 97-A | 51 | GLY | 2.5 |
| 1 | 98-A | 51 | GLY | 2.5 |
| 1 | 99-A | 51 | GLY | 2.5 |
| 1 | 100-A | 51 | GLY | 2.5 |
| 1 | 101-A | 51 | GLY | 2.5 |
| 1 | 102-A | 51 | GLY | 2.5 |
| 1 | 103-A | 51 | GLY | 2.5 |
| 1 | 104-A | 51 | GLY | 2.5 |
| 1 | 105-A | 51 | GLY | 2.5 |
| 1 | 106-A | 51 | GLY | 2.5 |
| 1 | 107-A | 51 | GLY | 2.5 |
| 1 | 108-A | 51 | GLY | 2.5 |
| 1 | 109-A | 51 | GLY | 2.5 |
| 1 | 110-A | 51 | GLY | 2.5 |
| 1 | 111-A | 51 | GLY | 2.5 |
| 1 | 112-A | 51 | GLY | 2.5 |
| 1 | 113-A | 51 | GLY | 2.5 |
| 1 | 114-A | 51 | GLY | 2.5 |
| 1 | 115-A | 51 | GLY | 2.5 |
| 1 | 116-A | 51 | GLY | 2.5 |
| 1 | 117-A | 51 | GLY | 2.5 |
| 1 | 118-A | 51 | GLY | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 119-A | 51 | GLY | 2.5 |
| 1 | 120-A | 51 | GLY | 2.5 |
| 1 | 121-A | 51 | GLY | 2.5 |
| 1 | 122-A | 51 | GLY | 2.5 |
| 1 | 123-A | 51 | GLY | 2.5 |
| 1 | 124-A | 51 | GLY | 2.5 |
| 1 | 125-A | 51 | GLY | 2.5 |
| 1 | 1-A | 65 | GLN | 2.2 |
| 1 | 2-A | 65 | GLN | 2.2 |
| 1 | 3-A | 65 | GLN | 2.2 |
| 1 | 4-A | 65 | GLN | 2.2 |
| 1 | 5-A | 65 | GLN | 2.2 |
| 1 | 6-A | 65 | GLN | 2.2 |
| 1 | 7-A | 65 | GLN | 2.2 |
| 1 | 8-A | 65 | GLN | 2.2 |
| 1 | 9-A | 65 | GLN | 2.2 |
| 1 | 10-A | 65 | GLN | 2.2 |
| 1 | 11-A | 65 | GLN | 2.2 |
| 1 | 12-A | 65 | GLN | 2.2 |
| 1 | 13-A | 65 | GLN | 2.2 |
| 1 | 14-A | 65 | GLN | 2.2 |
| 1 | 15-A | 65 | GLN | 2.2 |
| 1 | 16-A | 65 | GLN | 2.2 |
| 1 | 17-A | 65 | GLN | 2.2 |
| 1 | 18-A | 65 | GLN | 2.2 |
| 1 | 19-A | 65 | GLN | 2.2 |
| 1 | 20-A | 65 | GLN | 2.2 |
| 1 | 21-A | 65 | GLN | 2.2 |
| 1 | 22-A | 65 | GLN | 2.2 |
| 1 | 23-A | 65 | GLN | 2.2 |
| 1 | 24-A | 65 | GLN | 2.2 |
| 1 | 25-A | 65 | GLN | 2.2 |
| 1 | 26-A | 65 | GLN | 2.2 |
| 1 | 27-A | 65 | GLN | 2.2 |
| 1 | 28-A | 65 | GLN | 2.2 |
| 1 | 29-A | 65 | GLN | 2.2 |
| 1 | 30-A | 65 | GLN | 2.2 |
| 1 | 31-A | 65 | GLN | 2.2 |
| 1 | 32-A | 65 | GLN | 2.2 |
| 1 | 33-A | 65 | GLN | 2.2 |
| 1 | 34-A | 65 | GLN | 2.2 |
| 1 | 35-A | 65 | GLN | 2.2 |

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Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 36-A | 65 | GLN | 2.2 |
| 1 | 37-A | 65 | GLN | 2.2 |
| 1 | 38-A | 65 | GLN | 2.2 |
| 1 | 39-A | 65 | GLN | 2.2 |
| 1 | 40-A | 65 | GLN | 2.2 |
| 1 | 41-A | 65 | GLN | 2.2 |
| 1 | 42-A | 65 | GLN | 2.2 |
| 1 | 43-A | 65 | GLN | 2.2 |
| 1 | 44-A | 65 | GLN | 2.2 |
| 1 | 45-A | 65 | GLN | 2.2 |
| 1 | 46-A | 65 | GLN | 2.2 |
| 1 | 47-A | 65 | GLN | 2.2 |
| 1 | 48-A | 65 | GLN | 2.2 |
| 1 | 49-A | 65 | GLN | 2.2 |
| 1 | 50-A | 65 | GLN | 2.2 |
| 1 | 51-A | 65 | GLN | 2.2 |
| 1 | 52-A | 65 | GLN | 2.2 |
| 1 | 53-A | 65 | GLN | 2.2 |
| 1 | 54-A | 65 | GLN | 2.2 |
| 1 | 55-A | 65 | GLN | 2.2 |
| 1 | 56-A | 65 | GLN | 2.2 |
| 1 | 57-A | 65 | GLN | 2.2 |
| 1 | 58-A | 65 | GLN | 2.2 |
| 1 | 59-A | 65 | GLN | 2.2 |
| 1 | 60-A | 65 | GLN | 2.2 |
| 1 | 61-A | 65 | GLN | 2.2 |
| 1 | 62-A | 65 | GLN | 2.2 |
| 1 | 63-A | 65 | GLN | 2.2 |
| 1 | 64-A | 65 | GLN | 2.2 |
| 1 | 65-A | 65 | GLN | 2.2 |
| 1 | 66-A | 65 | GLN | 2.2 |
| 1 | 67-A | 65 | GLN | 2.2 |
| 1 | 68-A | 65 | GLN | 2.2 |
| 1 | 69-A | 65 | GLN | 2.2 |
| 1 | 70-A | 65 | GLN | 2.2 |
| 1 | 71-A | 65 | GLN | 2.2 |
| 1 | 72-A | 65 | GLN | 2.2 |
| 1 | 73-A | 65 | GLN | 2.2 |
| 1 | 74-A | 65 | GLN | 2.2 |
| 1 | 75-A | 65 | GLN | 2.2 |
| 1 | 76-A | 65 | GLN | 2.2 |
| 1 | 77-A | 65 | GLN | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 78-A | 65 | GLN | 2.2 |
| 1 | 79-A | 65 | GLN | 2.2 |
| 1 | 80-A | 65 | GLN | 2.2 |
| 1 | 81-A | 65 | GLN | 2.2 |
| 1 | 82-A | 65 | GLN | 2.2 |
| 1 | 83-A | 65 | GLN | 2.2 |
| 1 | 84-A | 65 | GLN | 2.2 |
| 1 | 85-A | 65 | GLN | 2.2 |
| 1 | 86-A | 65 | GLN | 2.2 |
| 1 | 87-A | 65 | GLN | 2.2 |
| 1 | 88-A | 65 | GLN | 2.2 |
| 1 | 89-A | 65 | GLN | 2.2 |
| 1 | 90-A | 65 | GLN | 2.2 |
| 1 | 91-A | 65 | GLN | 2.2 |
| 1 | 92-A | 65 | GLN | 2.2 |
| 1 | 93-A | 65 | GLN | 2.2 |
| 1 | 94-A | 65 | GLN | 2.2 |
| 1 | 95-A | 65 | GLN | 2.2 |
| 1 | 96-A | 65 | GLN | 2.2 |
| 1 | 97-A | 65 | GLN | 2.2 |
| 1 | 98-A | 65 | GLN | 2.2 |
| 1 | 99-A | 65 | GLN | 2.2 |
| 1 | 100-A | 65 | GLN | 2.2 |
| 1 | 101-A | 65 | GLN | 2.2 |
| 1 | 102-A | 65 | GLN | 2.2 |
| 1 | 103-A | 65 | GLN | 2.2 |
| 1 | 104-A | 65 | GLN | 2.2 |
| 1 | 105-A | 65 | GLN | 2.2 |
| 1 | 106-A | 65 | GLN | 2.2 |
| 1 | 107-A | 65 | GLN | 2.2 |
| 1 | 108-A | 65 | GLN | 2.2 |
| 1 | 109-A | 65 | GLN | 2.2 |
| 1 | 110-A | 65 | GLN | 2.2 |
| 1 | 111-A | 65 | GLN | 2.2 |
| 1 | 112-A | 65 | GLN | 2.2 |
| 1 | 113-A | 65 | GLN | 2.2 |
| 1 | 114-A | 65 | GLN | 2.2 |
| 1 | 115-A | 65 | GLN | 2.2 |
| 1 | 116-A | 65 | GLN | 2.2 |
| 1 | 117-A | 65 | GLN | 2.2 |
| 1 | 118-A | 65 | GLN | 2.2 |
| 1 | 119-A | 65 | GLN | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 120-A | 65 | GLN | 2.2 |
| 1 | 121-A | 65 | GLN | 2.2 |
| 1 | 122-A | 65 | GLN | 2.2 |
| 1 | 123-A | 65 | GLN | 2.2 |
| 1 | 124-A | 65 | GLN | 2.2 |
| 1 | 125-A | 65 | GLN | 2.2 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1 | CSD | 52-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 48-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 70-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 58-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 63-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,11,12 | 11 |
| 1 | CSD | 121-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 85-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 37-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 8-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 19-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 65-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 5-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 107-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 30-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 88-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 40-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 2-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,11,12 | 11 |
| 1 | CSD | 103-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 16-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 38-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 41-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 114-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 105-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 50-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 28-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 125-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 106-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1 | CSD | 75-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 6-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 35-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 20-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 92-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 49-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 97-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 64-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 31-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 89-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 76-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 24-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 51-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 33-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 110-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 60-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 56-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 15-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 4-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 124-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 10-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 109-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 11-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 42-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 72-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 120-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 45-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 18-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 68-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 53-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 117-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 101-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 104-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 111-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 57-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 14-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 98-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 93-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 29-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 71-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 26-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 55-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1 | CSD | 115-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 86-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 47-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 91-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 73-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 44-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 1-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 119-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 3-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 67-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 123-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 116-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 80-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 78-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 87-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 66-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 13-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 46-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 77-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 32-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 108-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 82-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 7-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 69-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 27-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 25-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 34-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 22-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 9-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 100-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 43-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 94-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 62-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 102-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 59-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 81-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 90-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 84-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 12-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 17-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 112-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 21-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1 | CSD | 74-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 61-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 96-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 36-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 113-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 39-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 99-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 118-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 95-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 54-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 122-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 83-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 23-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |
| 1 | CSD | 79-A | 152 | 8/9 | 0.98 | 0.11 | 10,11,12,12 | 11 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | FOL | 31-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 99-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 51-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 82-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 21-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 55-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 76-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 18-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 60-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 80-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 23-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 57-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 62-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,13,14 | 49 |
| 2 | FOL | 111-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | FOL | 39-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 61-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,13,13 | 49 |
| 2 | FOL | 48-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 120-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 104-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 30-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 117-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 41-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,11 | 49 |
| 2 | FOL | 54-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 45-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 116-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 113-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 103-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 77-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 123-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 26-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 46-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,11 | 49 |
| 2 | FOL | 36-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 20-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 72-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 79-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 67-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,13,13 | 49 |
| 2 | FOL | 87-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 64-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,13,14 | 49 |
| 2 | FOL | 110-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 91-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 5-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,11 | 49 |
| 2 | FOL | 81-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 50-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 112-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 93-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 98-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 6-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 95-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 25-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 29-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 13-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 19-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 100-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 16-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 38-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 69-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | FOL | 43-A | 201 | 32/32 | 0.97 | 0.10 | 9,9,11,11 | 49 |
| 2 | FOL | 92-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 84-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 85-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 119-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 10-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 125-A | 201 | 32/32 | 0.97 | 0.10 | 9,9,12,13 | 49 |
| 2 | FOL | 121-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 9-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 14-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 75-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 107-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 124-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 40-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 7-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 74-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 78-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 35-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 73-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 2-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 97-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,13 | 49 |
| 2 | FOL | 12-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 59-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 32-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 115-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 102-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 58-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 53-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 63-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,13,14 | 49 |
| 2 | FOL | 49-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 42-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 88-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 17-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 106-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 24-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 122-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 89-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 4-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 114-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 94-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 56-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 33-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | FOL | 101-A | 201 | 32/32 | 0.97 | 0.10 | 9,9,11,12 | 49 |
| 2 | FOL | 65-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,13,14 | 49 |
| 2 | FOL | 27-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 34-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 11-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 118-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 44-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,11 | 49 |
| 2 | FOL | 3-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 28-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 70-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 52-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 22-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 83-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 2 | FOL | 96-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 8-A | 201 | 32/32 | 0.97 | 0.10 | 9,9,12,12 | 49 |
| 2 | FOL | 108-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 66-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 90-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 47-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,11 | 49 |
| 2 | FOL | 109-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 105-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 71-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 86-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 37-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 68-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,13 | 49 |
| 2 | FOL | 15-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,12,12 | 49 |
| 2 | FOL | 1-A | 201 | 32/32 | 0.97 | 0.10 | 9,10,11,12 | 49 |
| 3 | NAP | 88-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 75-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 81-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 43-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 71-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 10-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 74-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 17-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 3-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 56-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 94-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 80-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 61-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 62-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 41-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MN | 96-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 58-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 107-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 110-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 6-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 25-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 35-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 4-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 76-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 101-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 29-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 7-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 35-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 119-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 113-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 12-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 4 | MN | 120-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 62-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 4 | MN | 15-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 23-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 70-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 103-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 61-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 59-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 31-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 63-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 30-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 46-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 1-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 11-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 44-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 120-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 89-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 118-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 37-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 104-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 51-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 50-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 124-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 7-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 45-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 117-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MN | 69-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 5-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 4 | MN | 2-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 66-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 109-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 71-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 48-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 100-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 65-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 80-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 6-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 4 | MN | 68-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 54-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 105-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 122-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 4 | MN | 63-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 39-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 97-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 99-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 59-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 79-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 36-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 99-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 83-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 125-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 70-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 68-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 52-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 111-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 84-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 100-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 48-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 16-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 115-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 31-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 103-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 55-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 32-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 86-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 106-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 108-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 34-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | NAP | 91-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 98-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 89-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 74-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 39-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 41-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 87-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 34-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 8-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 37-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 104-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 84-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 38-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 114-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 121-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 110-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 44-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 24-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 90-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 66-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 4 | MN | 94-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 82-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 51-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 85-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 30-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 3 | NAP | 72-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 38-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 82-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 47-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 36-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 60-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 112-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 53-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 123-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 72-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 116-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 29-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 105-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 28-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 64-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 4 | MN | 107-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 81-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | NAP | 96-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 90-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 20-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 77-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 12-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 108-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 21-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 95-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 77-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 115-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 57-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 14-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 116-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 57-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 23-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 55-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 69-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 111-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 56-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 14-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 124-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 67-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 4 | MN | 119-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 3 | NAP | 25-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 33-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 13-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 83-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 40-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 91-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 123-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 26-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 45-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 27-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 9-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 3 | NAP | 16-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 18-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 22-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 78-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 78-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 85-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 121-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 117-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MN | 118-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 3 | NAP | 13-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 79-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 112-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 40-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 75-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 106-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 86-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 8-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 52-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 46-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 93-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 101-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 102-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 32-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 11-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 92-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 15-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 18-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 58-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 102-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 24-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 64-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 98-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 97-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 47-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 33-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 20-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 21-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 3-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 3 | NAP | 67-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 26-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 10-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 125-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 122-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 95-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 42-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 50-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 54-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 5-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 93-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 49-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | NAP | 27-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 53-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 43-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 4 | MN | 76-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 73-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 87-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 1-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 19-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 42-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 17-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 92-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 3 | NAP | 113-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 109-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 4 | MN | 19-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 73-A | 204 | 1/1 | 0.99 | 0.30 | 11,11,11,11 | 1 |
| 3 | NAP | 2-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 88-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 49-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 4 | MN | 65-A | 204 | 1/1 | 0.99 | 0.30 | 13,13,13,13 | 1 |
| 3 | NAP | 28-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,13 | 73 |
| 4 | MN | 4-A | 204 | 1/1 | 0.99 | 0.30 | 9,9,9,9 | 1 |
| 4 | MN | 22-A | 204 | 1/1 | 0.99 | 0.30 | 10,10,10,10 | 1 |
| 3 | NAP | 9-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 3 | NAP | 60-A | 202 | 48/48 | 0.99 | 0.09 | 9,10,12,12 | 73 |
| 4 | MN | 114-A | 204 | 1/1 | 0.99 | 0.30 | 12,12,12,12 | 1 |
| 4 | MN | 89-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 5-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 50-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 93-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 121-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 55-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 51-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 98-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 87-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 83-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 88-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 3-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 58-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 86-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 82-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 44-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 92-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MN | 13-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 29-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 117-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 104-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 111-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 108-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 61-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 106-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 91-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 32-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 20-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 30-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 60-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 114-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 107-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 53-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 80-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 77-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 37-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 34-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 21-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 84-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 47-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 105-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 18-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 118-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 90-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 4-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 94-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 76-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 102-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 69-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 115-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 8-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 124-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 100-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 25-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 31-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 36-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 17-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 63-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 65-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MN | 110-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 42-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 54-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 120-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 7-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 35-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 109-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 40-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 43-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 39-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 125-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 99-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 49-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 12-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 67-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 73-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 122-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 85-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 24-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 15-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 81-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 33-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 103-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 22-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 28-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 66-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 45-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 14-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 116-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 113-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 59-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 52-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 10-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 57-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 71-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 123-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 78-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 119-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 56-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 19-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 6-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 16-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |

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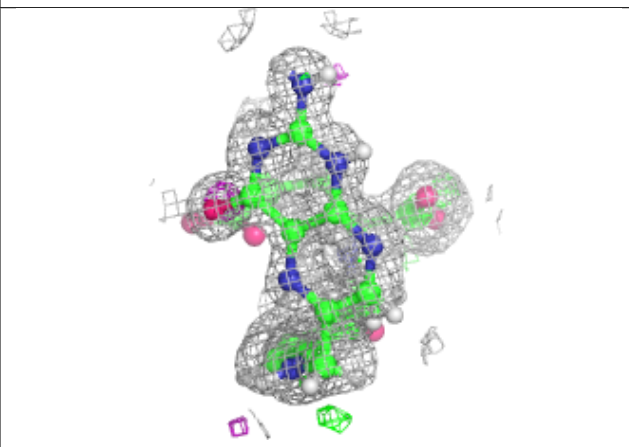
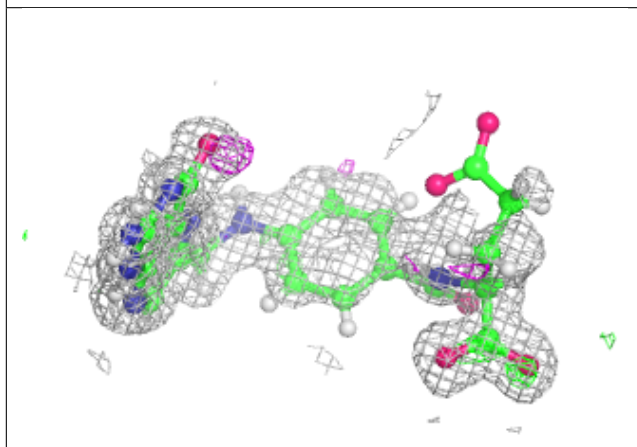
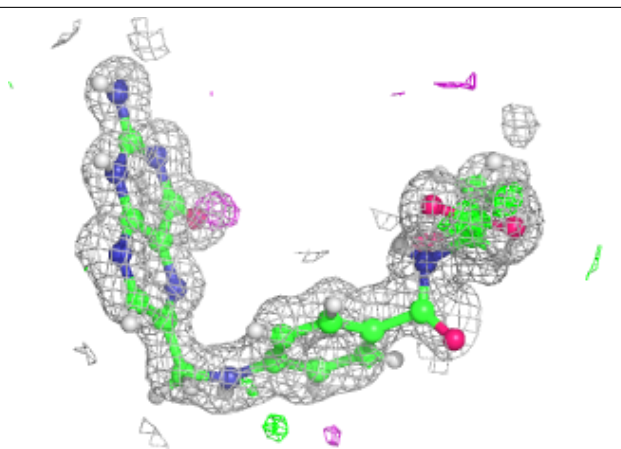
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | MN | 2-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 64-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 96-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 70-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 72-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 62-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 79-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 48-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 97-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 1-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 11-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 74-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 112-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 68-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 27-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 26-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 23-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 9-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 95-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 41-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 101-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 38-A | 203 | 1/1 | 1.00 | 0.20 | 14,14,14,14 | 1 |
| 4 | MN | 75-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |
| 4 | MN | 46-A | 203 | 1/1 | 1.00 | 0.20 | 13,13,13,13 | 1 |

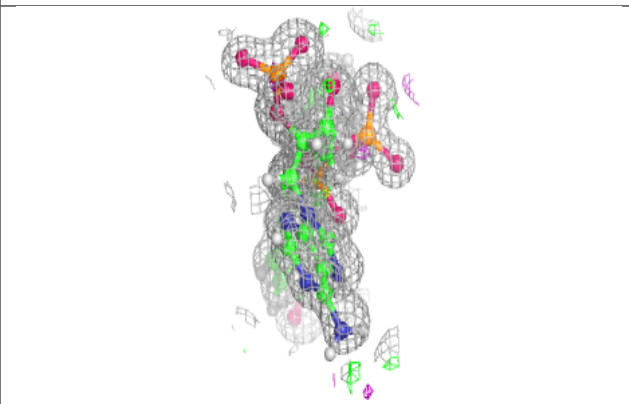
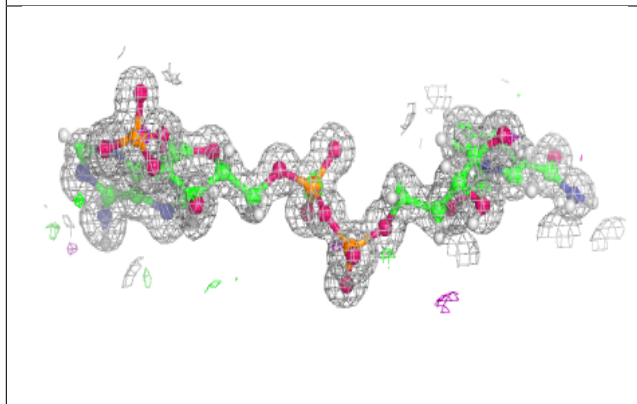
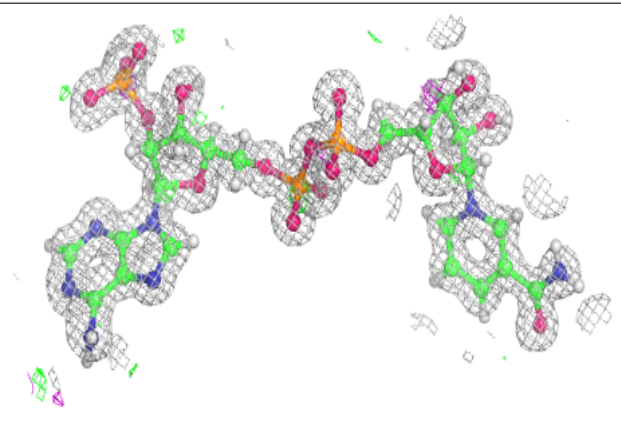
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FOL A 201:

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

**Electron density around NAP A 202:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.